

多体問題の計算科学

Computational Science for Many-Body Problems

#12 Large sparse matrices and quantum statistical mechanics

15:10-16:40 July 6, 2021

Lecture slide:

<https://github.com/compsci-alliance/many-body-problems>

1. Typicality and Application of ED
2. Numerical implementation
3. Lattice Model of Solids
4. Report problems

Typicality Approach

Finite Temperature: Heat Capacity

Spread of energy distribution

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

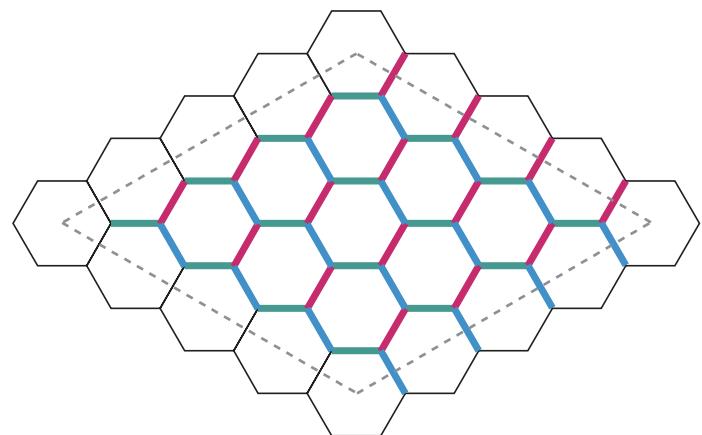
-Average with Boltzmann distribution

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

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

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

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

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).

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

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

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

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

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

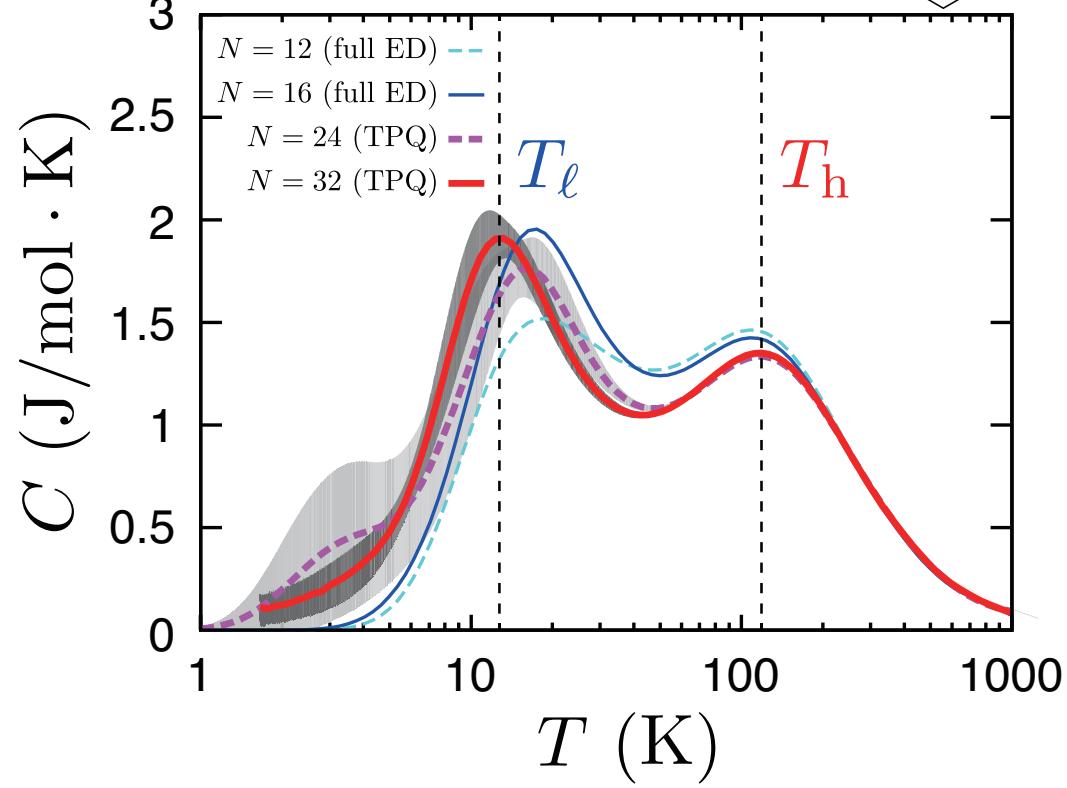
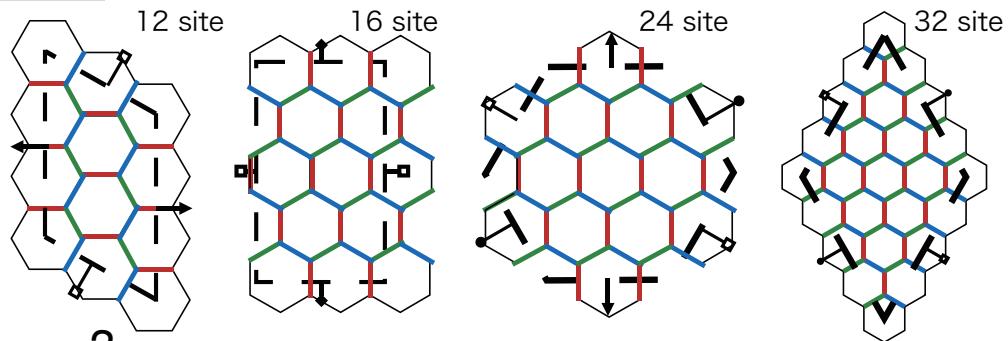
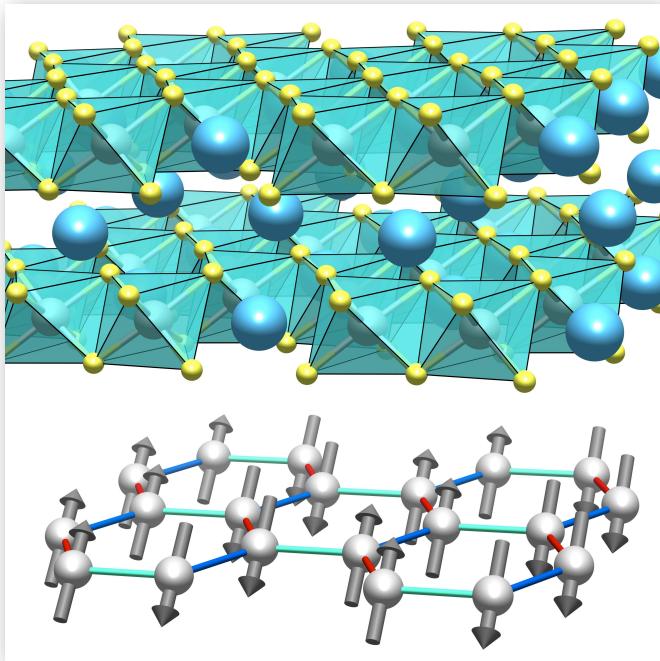
Every eigenstate contained
in a random vector with
equal probability

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

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

Example: Simulation of Heat Capacity

Frustrated magnet Na_2IrO_3



Combination of Shifted Krylov Method and Typicality Approach

An Alternative to Spectral Projection

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

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

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

Discretized by Riemann sum

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).

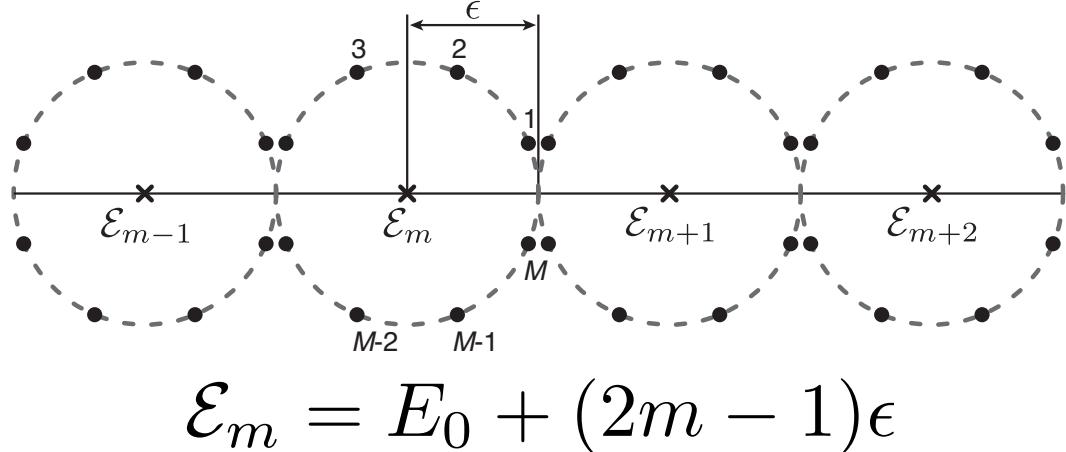
$$\hat{P}_{\gamma,\rho,M} = \frac{1}{M} \sum_{j=1}^M \frac{\rho e^{i\theta_j}}{\rho e^{i\theta_j} + \gamma - \hat{H}}$$

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

Probability Distribution by Typical Pure States

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

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



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

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

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

Probability distribution

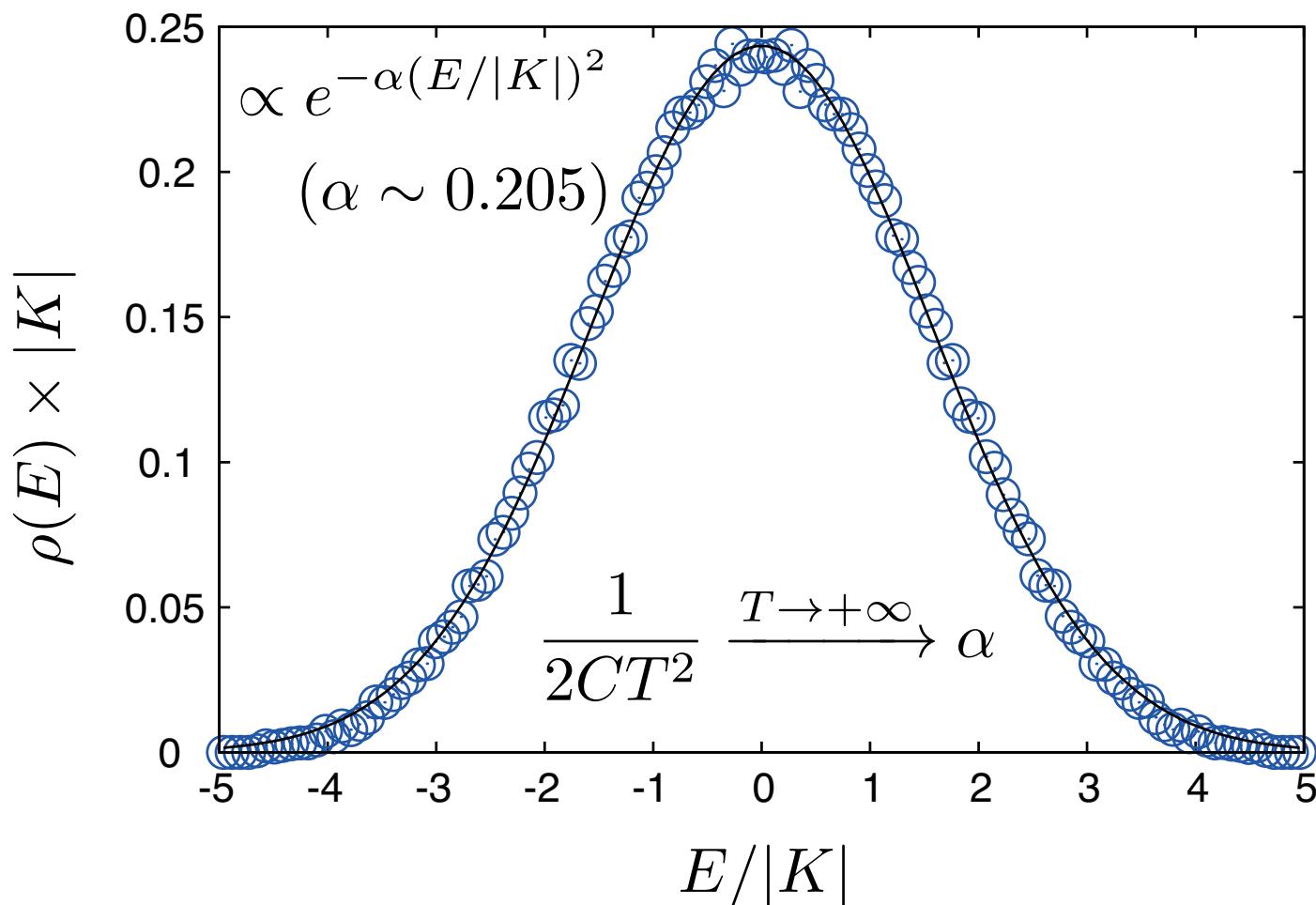
$$\tilde{P}_\delta(\mathcal{E}_m) = \langle \phi_{\beta,\delta}^m | \phi_{\beta,\delta}^m \rangle$$

An Example of Density of State

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

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

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

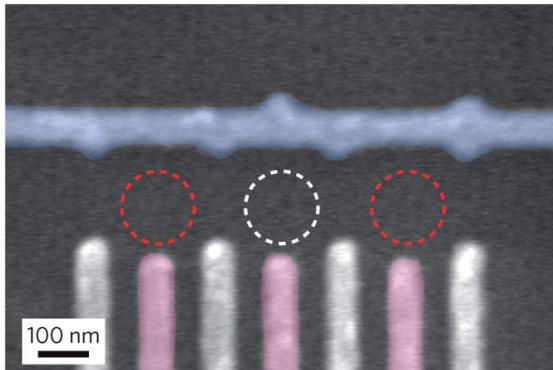


Numerical Implementation

Quantum Many-Body Problems

An example: 3 Quantum dots

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

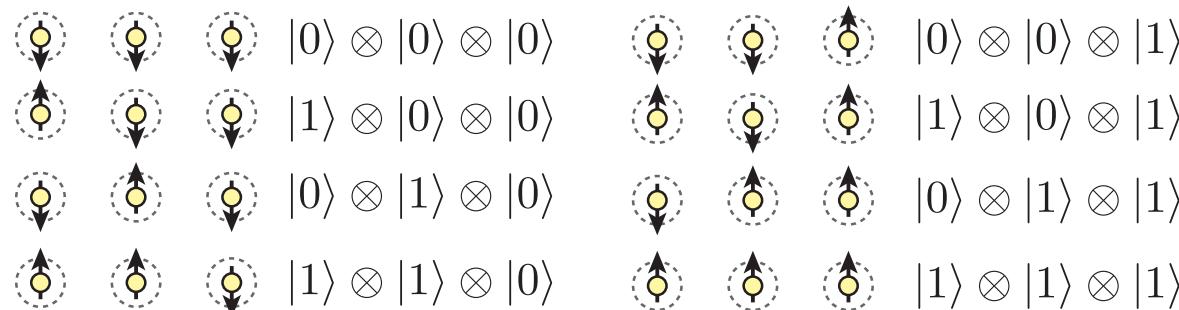


Quantum dot:

- 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 = $2^N = 4096$

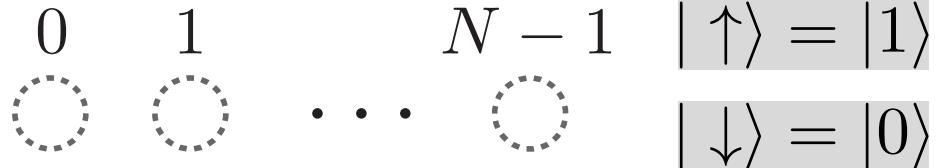
Extreme example: N=36

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

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

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

2^N -dimensional Fock space:

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

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

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

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

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

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

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

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
$ 1\rangle_d$	$=$	$ \downarrow\rangle$	\otimes
$ 2\rangle_d$	$=$	$ \uparrow\rangle$	\otimes
$ 3\rangle_d$	$=$	$ \uparrow\rangle$	\otimes

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

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

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

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

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

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

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

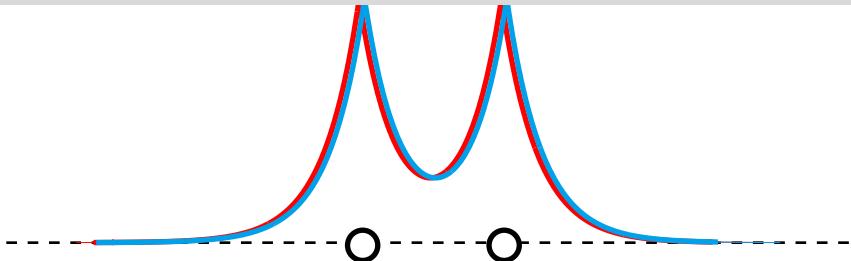
Bit rep. is not enough: Fermionic sign is necessary

Example: Tunneling

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

2-Site Hubbard Model

2-Site Hubbard Model



Hubbard model

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

Problem 3:

Create 4 by 4 Hamiltonian matrix with following 4 bases

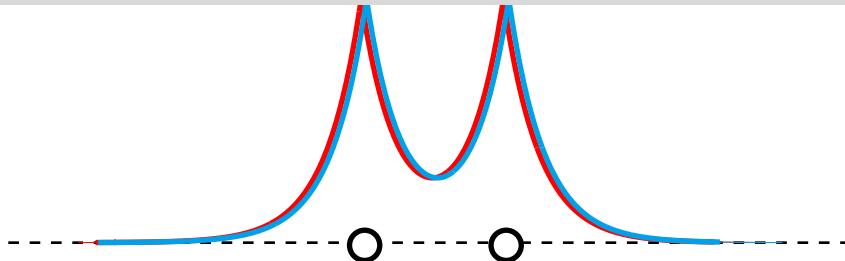
$$\hat{c}_{0\uparrow}^\dagger \hat{c}_{0\downarrow}^\dagger |0\rangle$$

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

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

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

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 Problem 3:

4 by 4 Hamiltonian matrix with the following 4 bases

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

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

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

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

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

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

$\text{H}\Phi$

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 [2]: Finite temperatures

-Real-time evolution

-Parallelization with MPI and OpenMP

[1] E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).

[2] A. V. Knyazev, SIAM J. Sci. Comput. 23, 517 (2001).

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

Open source program package (latest release: ver.3.4.1)

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/>

HΦ Developers



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UTokyo



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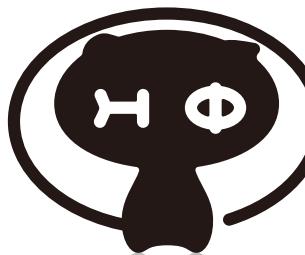
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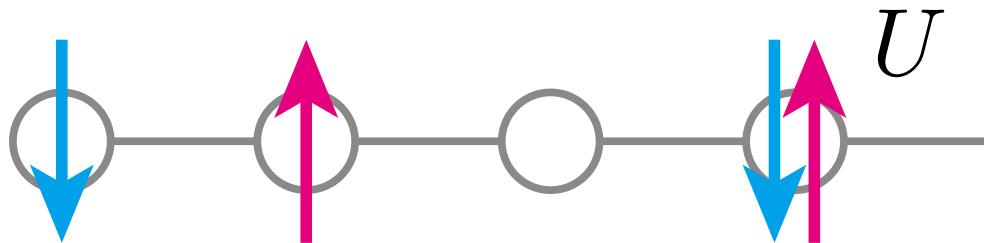
“Project for advancement of software usability in materials science” by ISSP

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

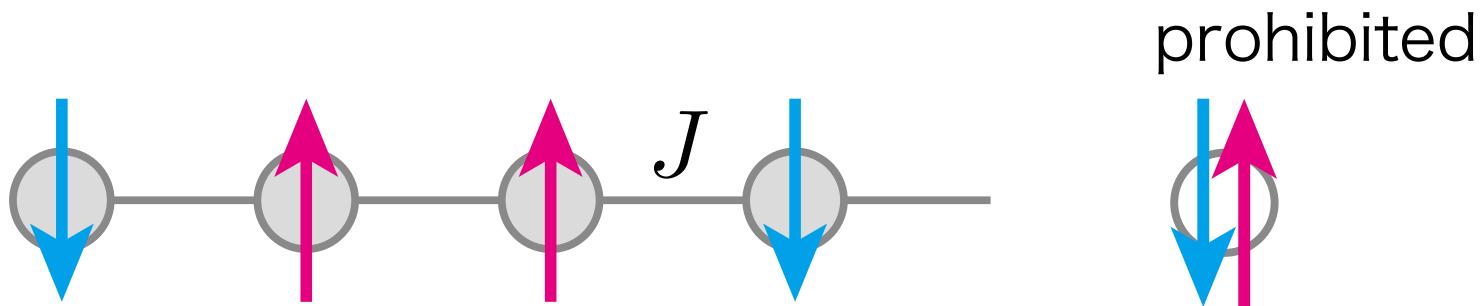
Fermion HubbardGC: Particle # & total S_z not conserved

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

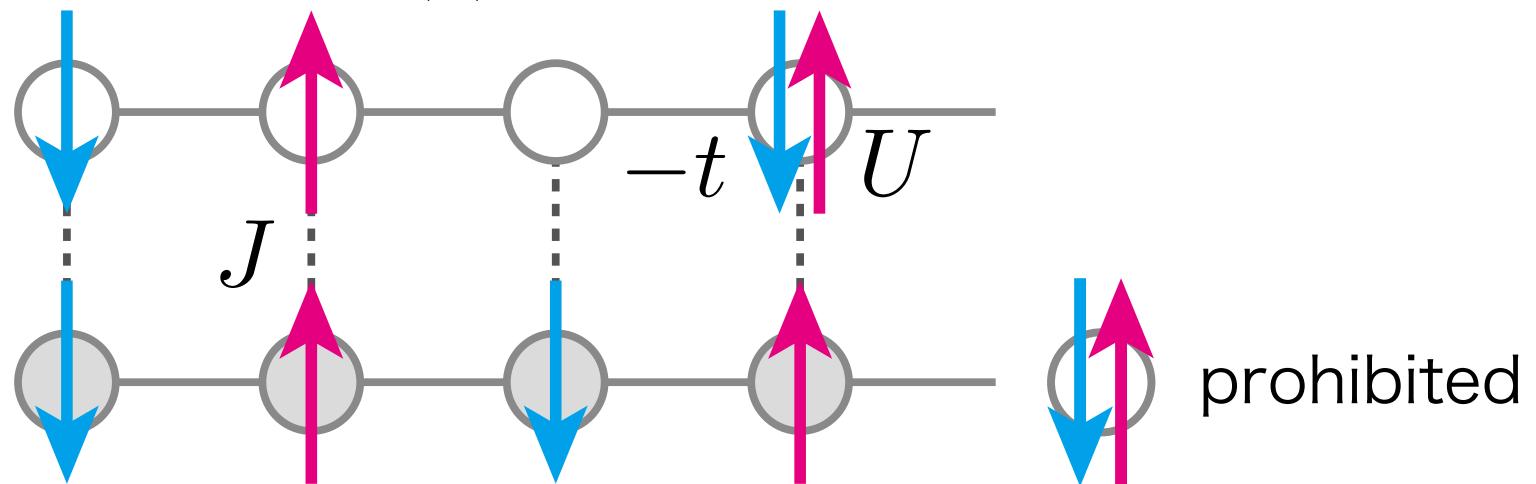
$S > 1/2$ can be simulated
if your memory is enough large

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

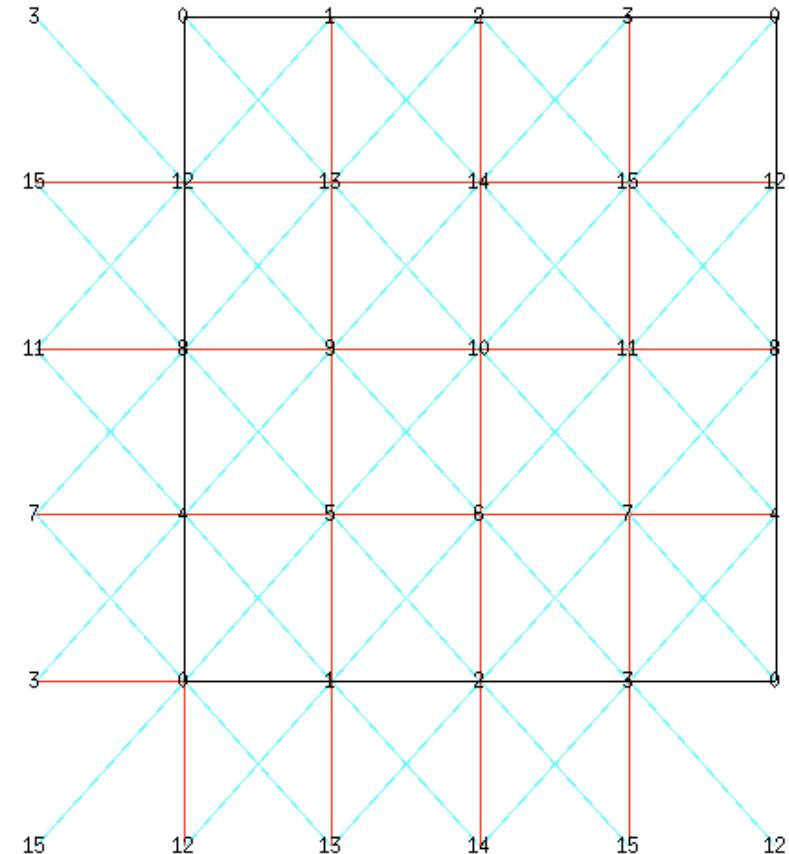
Hubbard	$H = -\mu \sum_{i=1}^N \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^\dagger c_{i\sigma} - \sum_{i \neq j} \sum_{\sigma=\uparrow,\downarrow} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow} + \sum_{i \neq j} V_{ij} n_i n_j$
Quantum spins	$H = -h \sum_{i=1}^N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

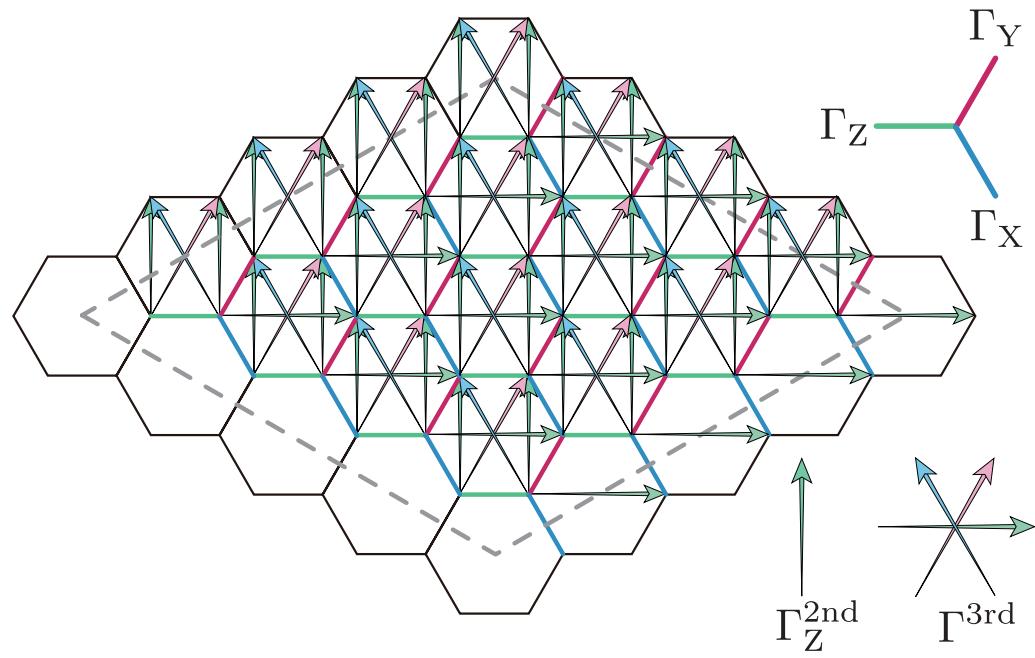
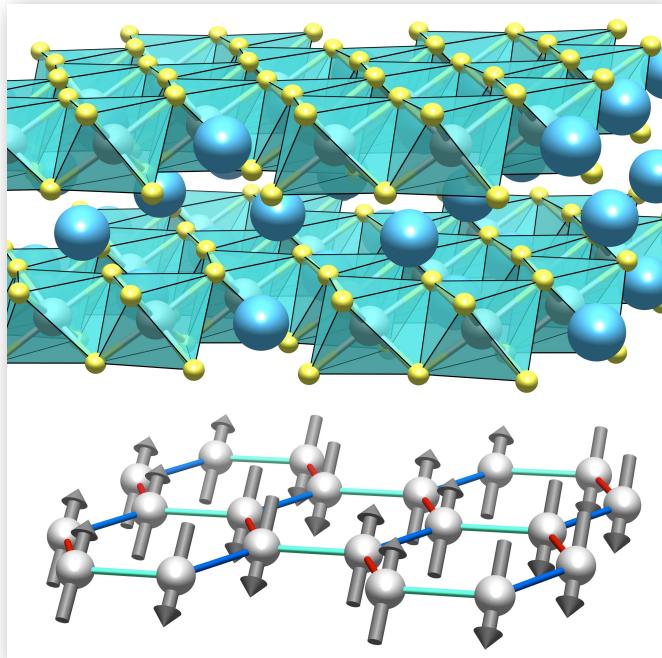
$$\langle H \rangle, \langle H^2 \rangle, \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle, \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{\ell\sigma_4} \rangle$$

-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

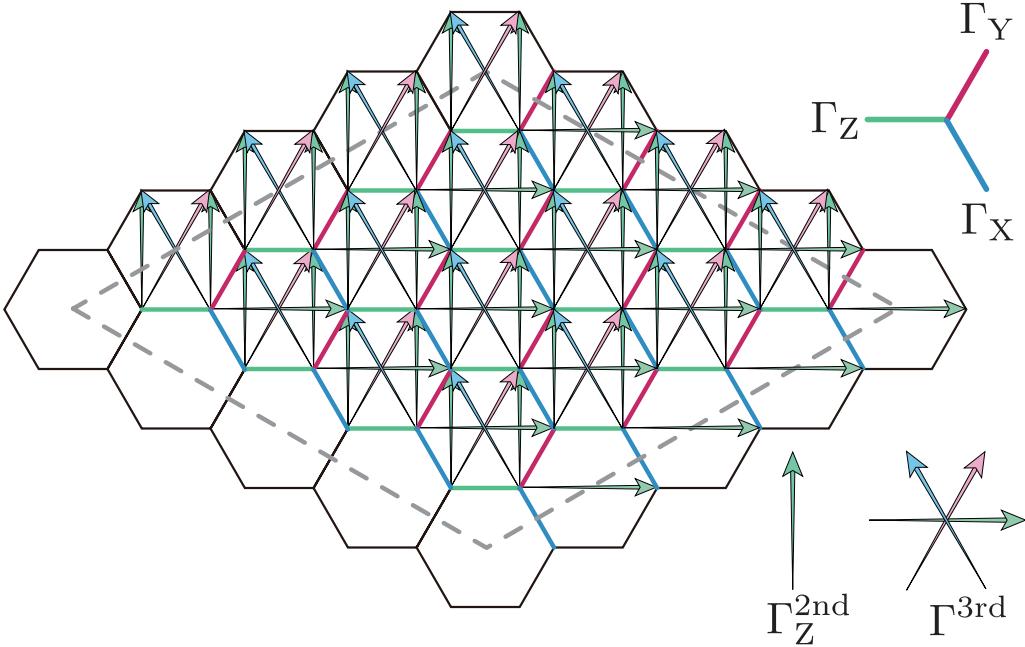


An Example of Expert Input: *Ab Initio* Spin Hamiltonian

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

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

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



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

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

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

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

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

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

```
graph TD; A[Standard input] --> B[Standard interface]; A --> C[Expert input]; B --> D[Def. files for Hamiltonian]; B --> E[Def. files for controlling simulation]; C --> F[Expert interface]; F --> G[Subroutines: -Lanczos, -CG, -TPQ, -TimeEvolution, -Full diag. (LAPACK, Scalapack, MAGMA)]; G --> H[Standard output Output files]
```

Def. files for Hamiltonian

Def. files for controlling simulation

```
graph TD; A[Standard input] --> B[Standard interface]; A --> C[Expert input]; B --> D[Def. files for Hamiltonian]; B --> E[Def. files for controlling simulation]; C --> F[Expert interface]; F --> G[Subroutines: -Lanczos, -CG, -TPQ, -TimeEvolution, -Full diag. (LAPACK, Scalapack, MAGMA)]; G --> H[Standard output Output files]
```

Expert interface



Subroutines:

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

```
graph TD; A[Standard input] --> B[Standard interface]; A --> C[Expert input]; B --> D[Def. files for Hamiltonian]; B --> E[Def. files for controlling simulation]; C --> F[Expert interface]; F --> G[Subroutines: -Lanczos, -CG, -TPQ, -TimeEvolution, -Full diag. (LAPACK, Scalapack, MAGMA)]; G --> H[Standard output Output files]
```

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 Sz = 0)

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

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

Low energy state \rightarrow 2 spins

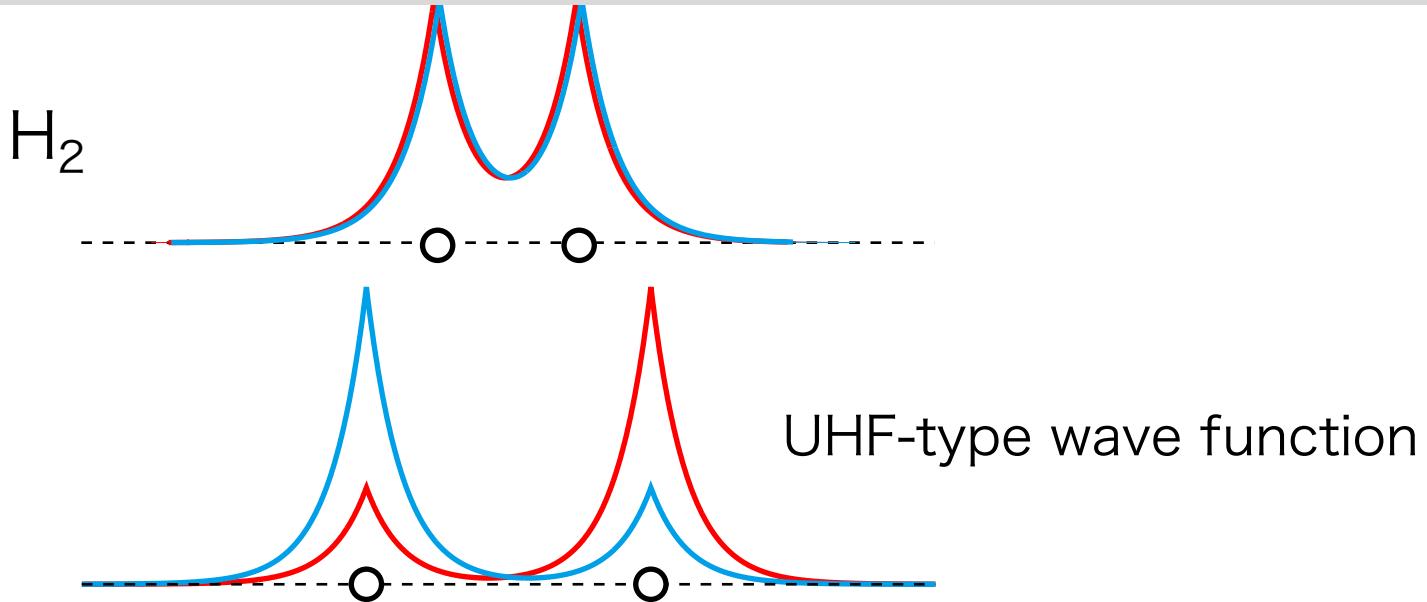
$$E = 0$$

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

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

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

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

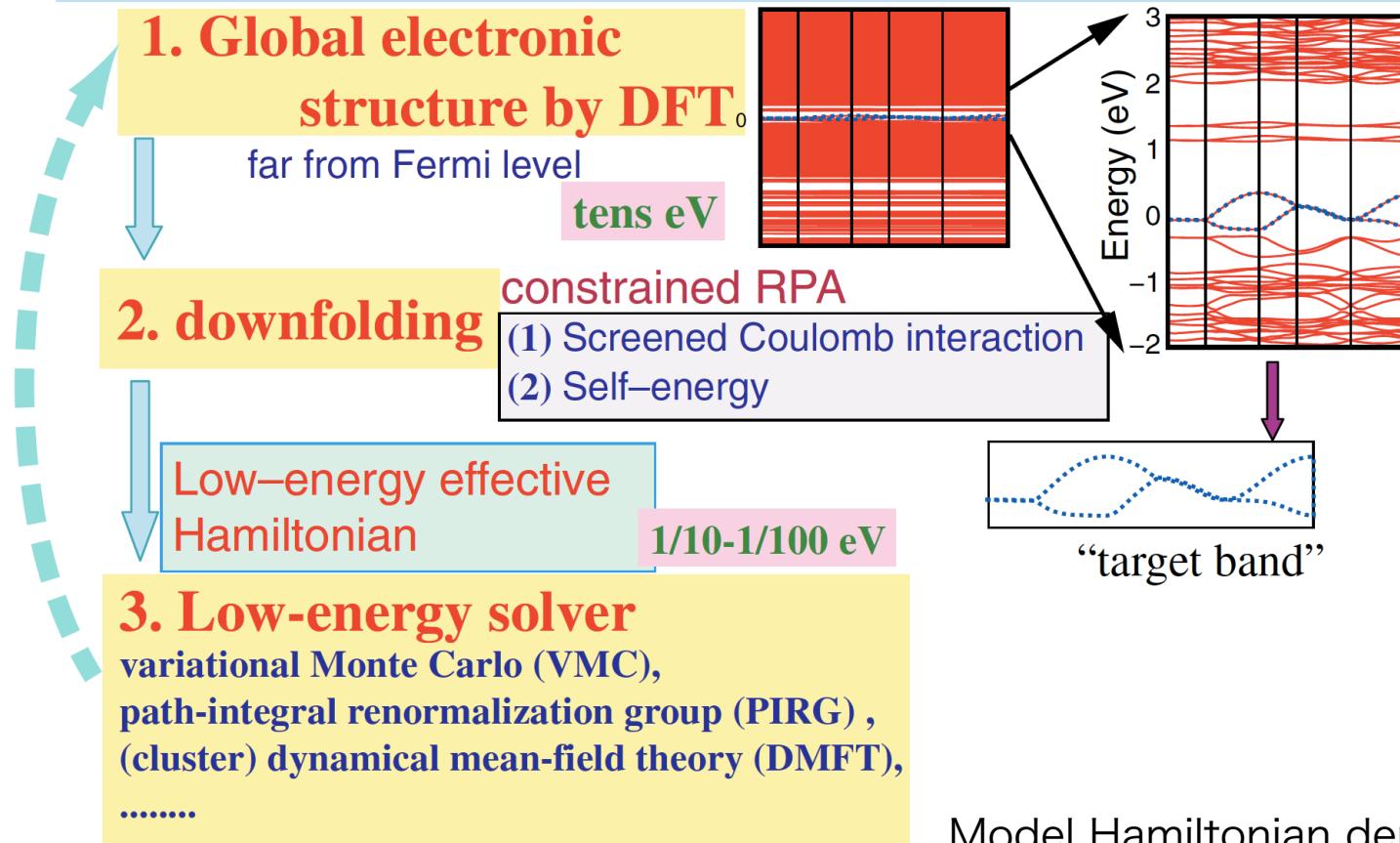
Lattice Model of Solids

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

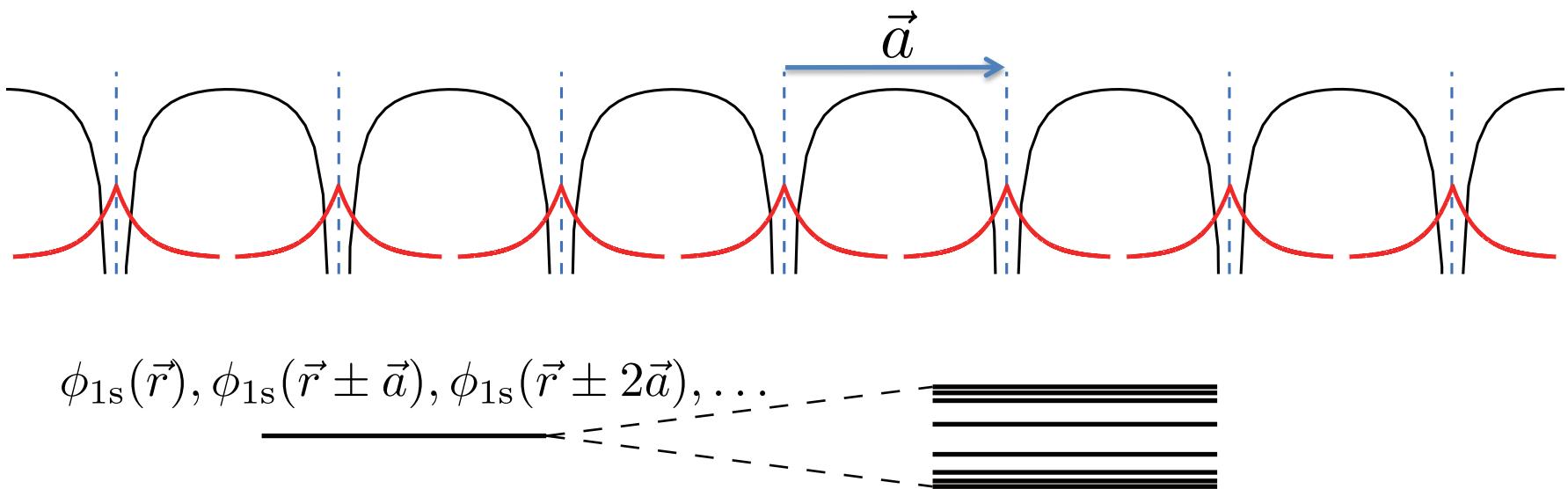
Schematic procedure of three-stage scheme
thanks to energy hierarchy structure



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

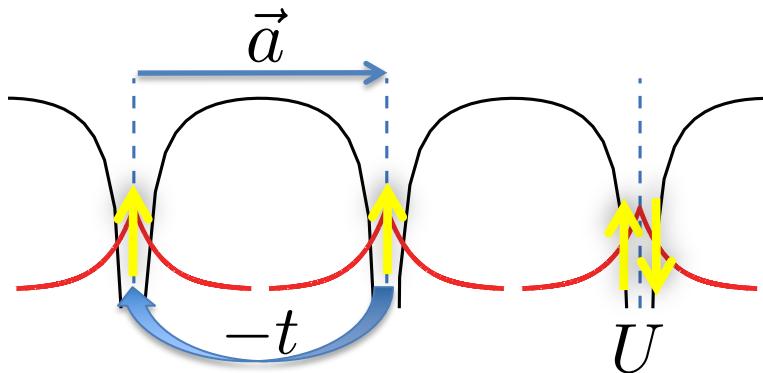
Model of Many-Body Electrons

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

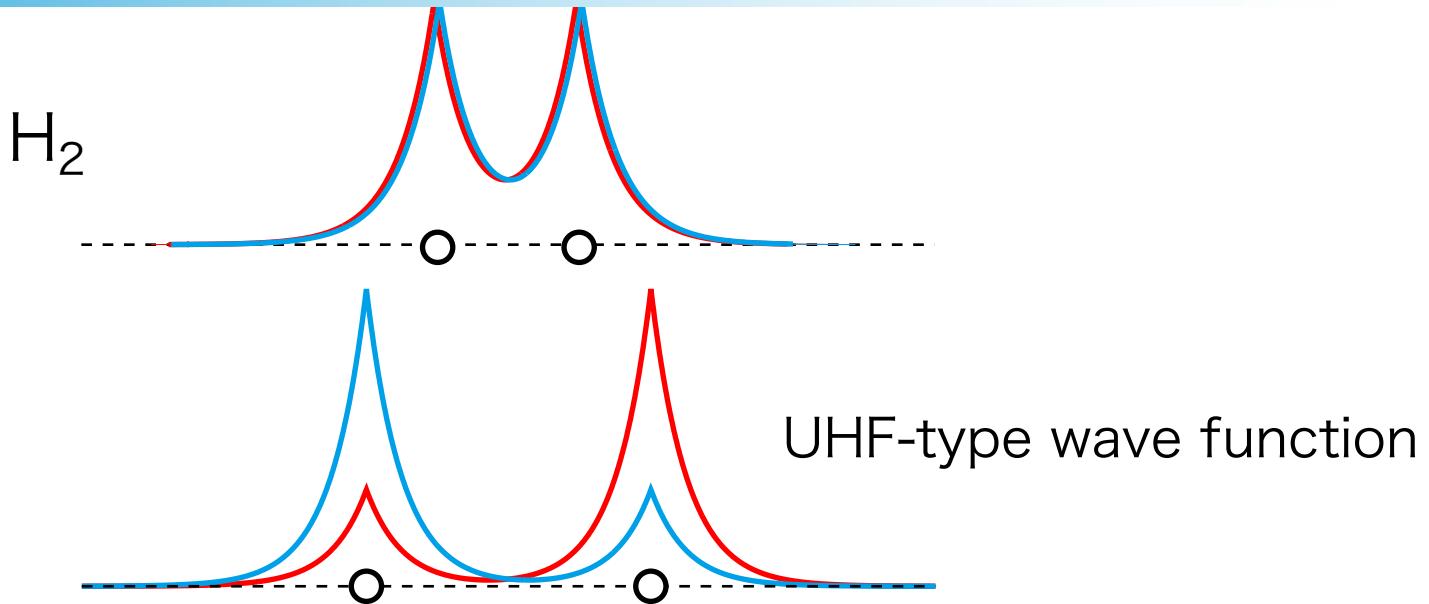
$$U = \int d^3r \int d^3r' \phi_{1s}^*(\vec{r}) \phi_{1s}^*(\vec{r}') \frac{e^2}{|\vec{r} - \vec{r}'|} \phi_{1s}(\vec{r}') \phi_{1s}(\vec{r})$$

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



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

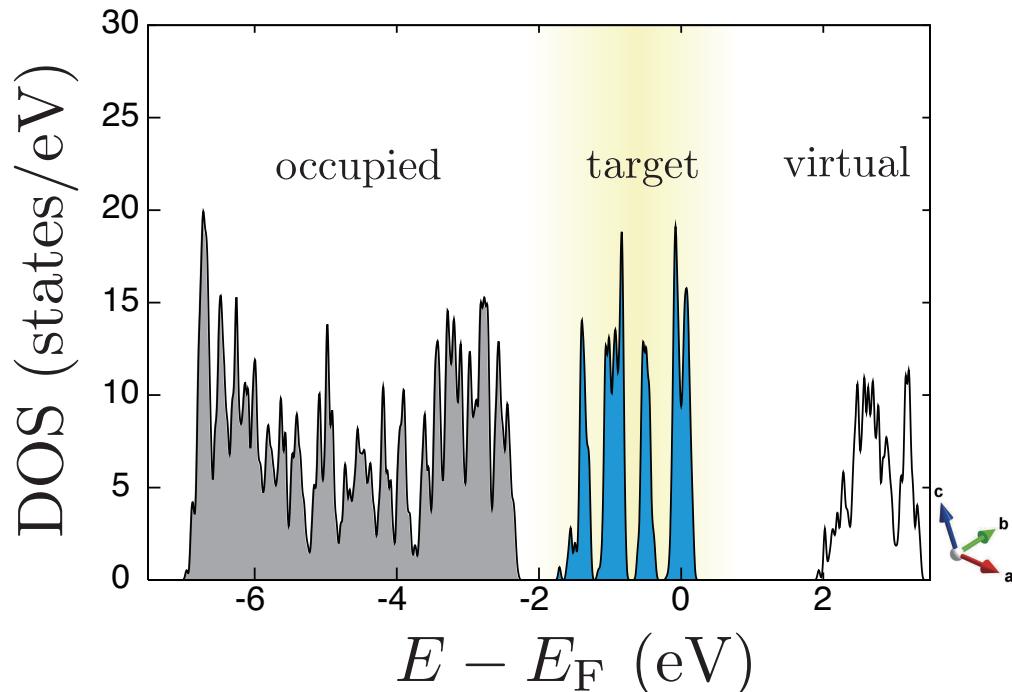


Singlet ground state

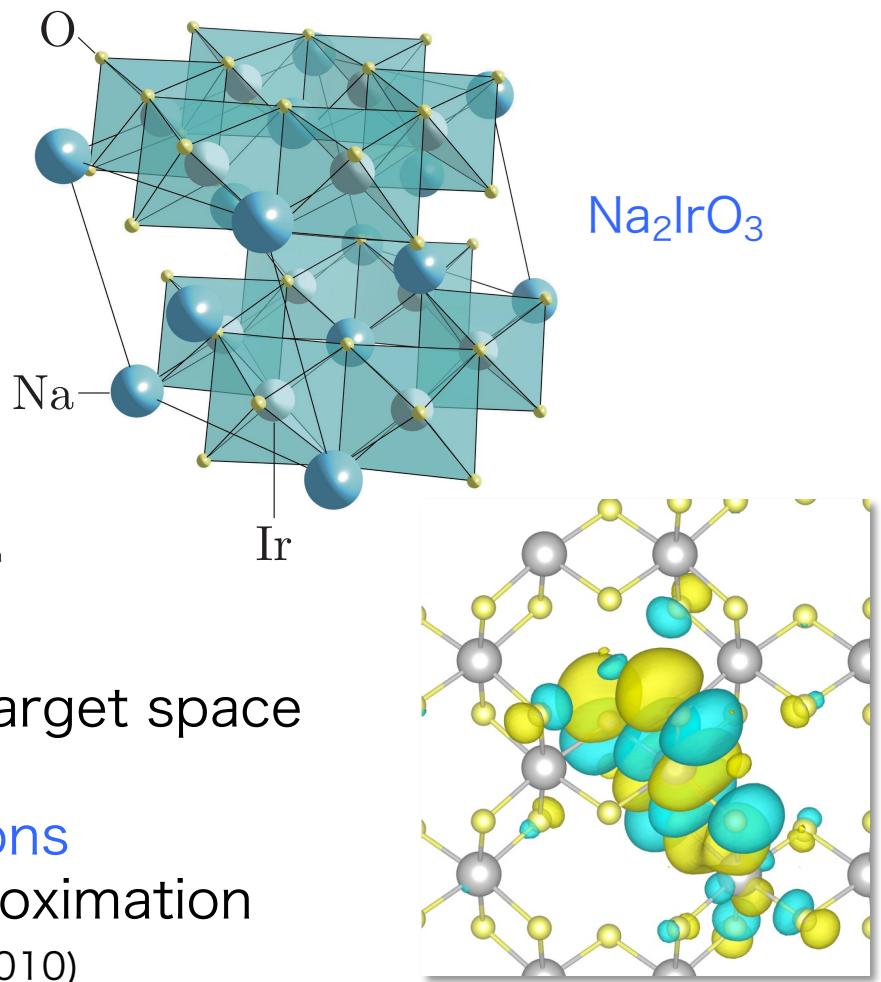
Construction of Effective Hamiltonians: An Example

- Target Hilbert space expanded by localized Wannier orbitals

DFT result for energy spectrum



Souza-Marzari-Vanderbilt



- Effective Coulomb interactions in target space

Renormalization due to
infinite virtual particle-hole excitations

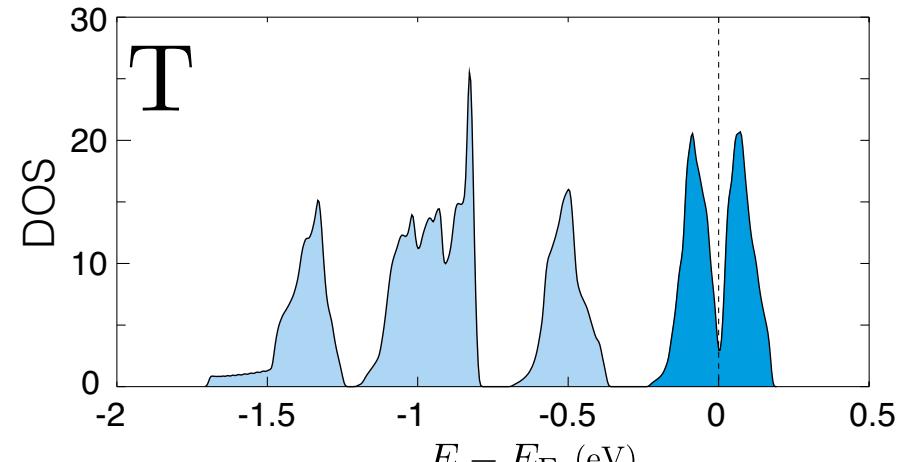
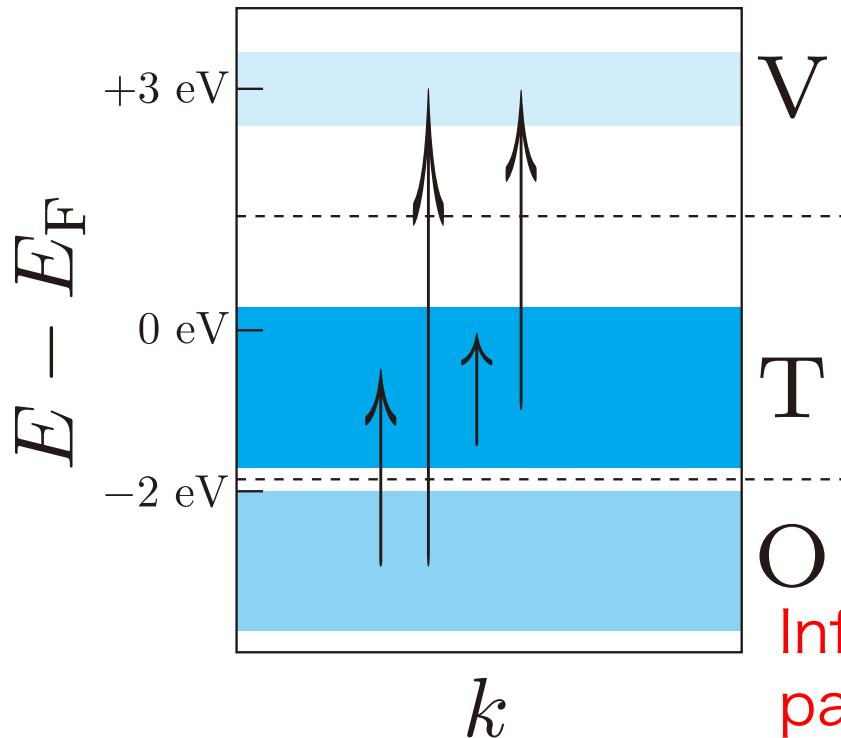
← Constrained random phase approximation

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

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

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

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



Infinite number of RPA-type
particle-hole excitations

Ab initio t_{2g} -Hubbard Model: cRPA+Wannier

Hopping

$$\hat{H}_0 = \sum_{\ell \neq m} \sum_{a,b=xy,yz,zx} \sum_{\sigma,\sigma'} t_{\ell,m;a,b}^{\sigma\sigma'} [\hat{c}_{\ell a\sigma}^\dagger \hat{c}_{mb\sigma'} + \text{h.c.}]$$

Trigonal+orbital-dependent μ

$$\hat{H}_{\text{tri}} = \sum_{\ell} \vec{\hat{c}}_{\ell}^\dagger \begin{bmatrix} -\mu_{yz} & \Delta & \Delta \\ \Delta & -\mu_{zx} & \Delta \\ \Delta & \Delta & -\mu_{xy} \end{bmatrix} \hat{\sigma}_0 \vec{\hat{c}}_{\ell}$$

SOC

$$\hat{H}_{\text{SOC}} = \frac{\zeta_{\text{so}}}{2} \sum_{\ell} \vec{\hat{c}}_{\ell}^\dagger \begin{bmatrix} 0 & +i\hat{\sigma}_z & -i\hat{\sigma}_y \\ -i\hat{\sigma}_z & 0 & +i\hat{\sigma}_x \\ +i\hat{\sigma}_y & -i\hat{\sigma}_x & 0 \end{bmatrix} \vec{\hat{c}}_{\ell}$$

$$\vec{\hat{c}}_{\ell}^\dagger = (\hat{c}_{\ell yz\uparrow}^\dagger, \hat{c}_{\ell yz\downarrow}^\dagger, \hat{c}_{\ell zx\uparrow}^\dagger, \hat{c}_{\ell zx\downarrow}^\dagger, \hat{c}_{\ell xy\uparrow}^\dagger, \hat{c}_{\ell xy\downarrow}^\dagger)$$

Coulomb

$$\hat{H}_U = U \sum_{\ell} \sum_{a=yz,zx,xy} \hat{n}_{\ell a\uparrow} \hat{n}_{\ell a\downarrow}$$

$$+ \sum_{\ell \neq m} \sum_{a,b} \frac{V_{\ell,m}}{2} (\hat{n}_{\ell a\uparrow} + \hat{n}_{\ell a\downarrow})(\hat{n}_{mb\uparrow} + \hat{n}_{mb\downarrow})$$

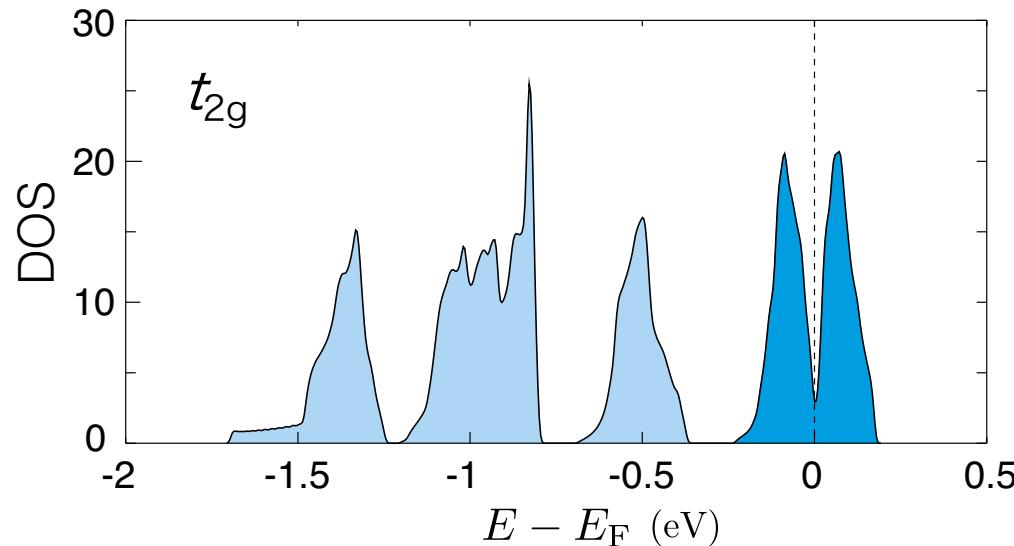
$$+ \sum_{\ell} \sum_{a < b} \sum_{\sigma} [U' \hat{n}_{\ell a\sigma} \hat{n}_{\ell b\bar{\sigma}} + (U' - J_H) \hat{n}_{\ell a\sigma} \hat{n}_{\ell b\sigma}]$$

$$+ J_H \sum_{\ell} \sum_{a \neq b} [\hat{c}_{\ell a\uparrow}^\dagger \hat{c}_{\ell b\downarrow}^\dagger \hat{c}_{\ell a\downarrow} \hat{c}_{\ell b\uparrow} + \hat{c}_{\ell a\uparrow}^\dagger \hat{c}_{\ell a\downarrow}^\dagger \hat{c}_{\ell b\downarrow} \hat{c}_{\ell b\uparrow}]$$

F. Aryasetiawan, *et al.*,

Phys. Rev. B 70, 195104 (2004)

M. Imada & T. Miyake, JPSJ 79, 112001 (2010)



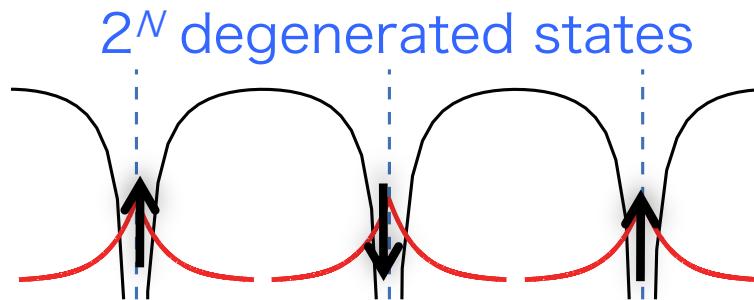
DFT: Elk (FLAPW)

<http://elk.sourceforge.net>
Vxc: Perdew-Wang 1992

One-body parameters (eV)	t	$\mu_{xy} - \mu_{yz,zx}$	ζ_{so}	Δ
	0.27	0.035	0.39	-0.028
Two-body parameters (eV)	U	U'	J_H	V
	2.72	2.09	0.23	1.1

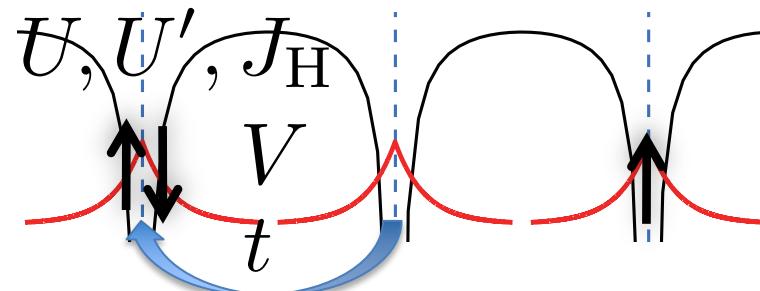
Heisenberg (Spin) Hamiltonian from Strong Coupling Expansion

Unperturbed atomic Hamiltonian



Perturbation: Tunneling

virtual states lift the degeneracy



Spin Hamiltonian

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

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

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

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

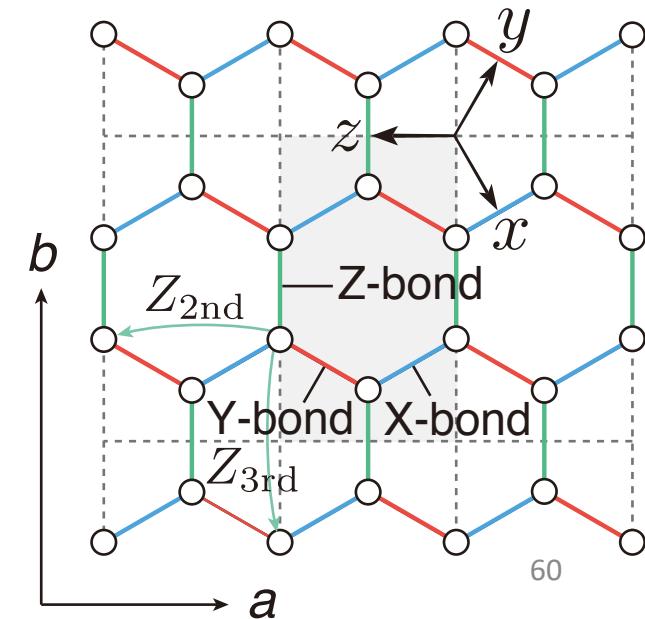
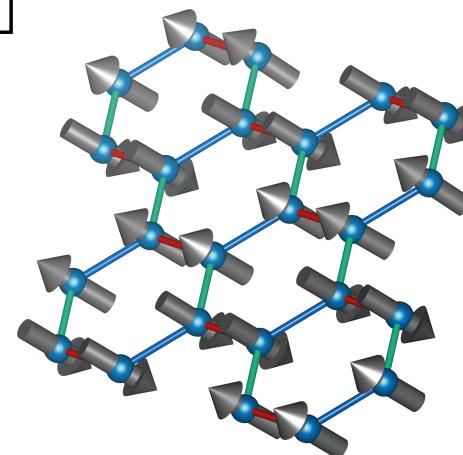
$$\mathcal{J}_Z = \begin{bmatrix} 4.4 & -0.4 & 1.1 \\ -0.4 & 4.4 & 1.1 \\ 1.1 & 1.1 & -30.7 \end{bmatrix} \text{ (meV)}$$

Ground state:
Zigzag order

agrees with experiments

iPEPS, 2D DMRG, & ED:

T. Okubo, K. Shinjo, Y. Yamaji, *et al.*,



2nd Report Problems
Please choose one of three

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 .

You may use McMillan's variational Jastrow wave function and variational parameters given in `vmc_helium4_2021.ipynb`.

-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).

1-2 (optional).

-Obtain 2-point distribution functions $g(r)$ of liquid helium 3 for likewise (not likewise) spin pairs at ambient pressure.

You may use variational Jastrow-Slater wave functions and variational parameters obtained in D. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B 16, 3081 (1977).

Report 2

Problem 2: Krylov subspace method

2-1 (compulsory).

-Implement CG and solve a linear question.

Please select a symmetric positive-definite matrix A with non-zero offdiagonal element.

The vector b should not be the zero vector.

Please choose A and b with N_H (linear dimension of A) = 5.

-Illustrate convergence of the solution obtained at each CG step.

You may plot step dependence of 2-norm of residual vectors r_k .

-Obtain the solution of $Ax=b$ by Lapack and compare with the solution by CG.

2-2 (Optional). Implement LOBCG method.

-Confirm that the code can calculate eigenvalues and eigenvectors for a real symmetric matrix.

-Solve an eigenvalue problem with $N_H > 5$

-Obtain the solution by Lapack and compare with the solution by CG.

Report 2

Problem 3: Open source software

3-1 (compulsory).

-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.

3-2 (optional). Reproduce the figures in Sec. 2.2 of the tutorials of HΦ: [https://issp-center-dev.github.io/HPhi/
manual/develop/tutorial/en/html/finite_temperature/Kitaev.html](https://issp-center-dev.github.io/HPhi/manual/develop/tutorial/en/html/finite_temperature/Kitaev.html)

-Please choose one out of the three problems

-The code should be included (a jupyter notebook is recommended).

-Deadline: 8/6

Report 1 & 2

Deadline for Report 1:

-2020/7/13

Deadline for Report 2:

-2020/8/6

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.

Lecture Schedule

Classical

Quantum

- #1 Many-body problems in physics
- #2 Why many-body problem is hard to solve
- #3 Classical statistical model and numerical simulation
- #4 Classical Monte Carlo method and its applications
- #5 Molecular dynamics and its application
- #6 Extended ensemble method for Monte Carlo methods
- #7 Quantum lattice models and numerical approaches
- #8 Quantum Monte Carlo methods
- #9 Applications of quantum Monte Carlo methods
 - Path integral & applications
- #10 Linear algebra of large and sparse matrices for quantum many-body problems
- #11 Krylov subspace methods and their applications to quantum many-body problems
- #12 Large sparse matrices and quantum statistical mechanics
- #13 Parallelization for many-body problems