多体問題の計算科学

Computational Science for Many-Body Problems

#13 Modern algorithms for quantum many-body problems

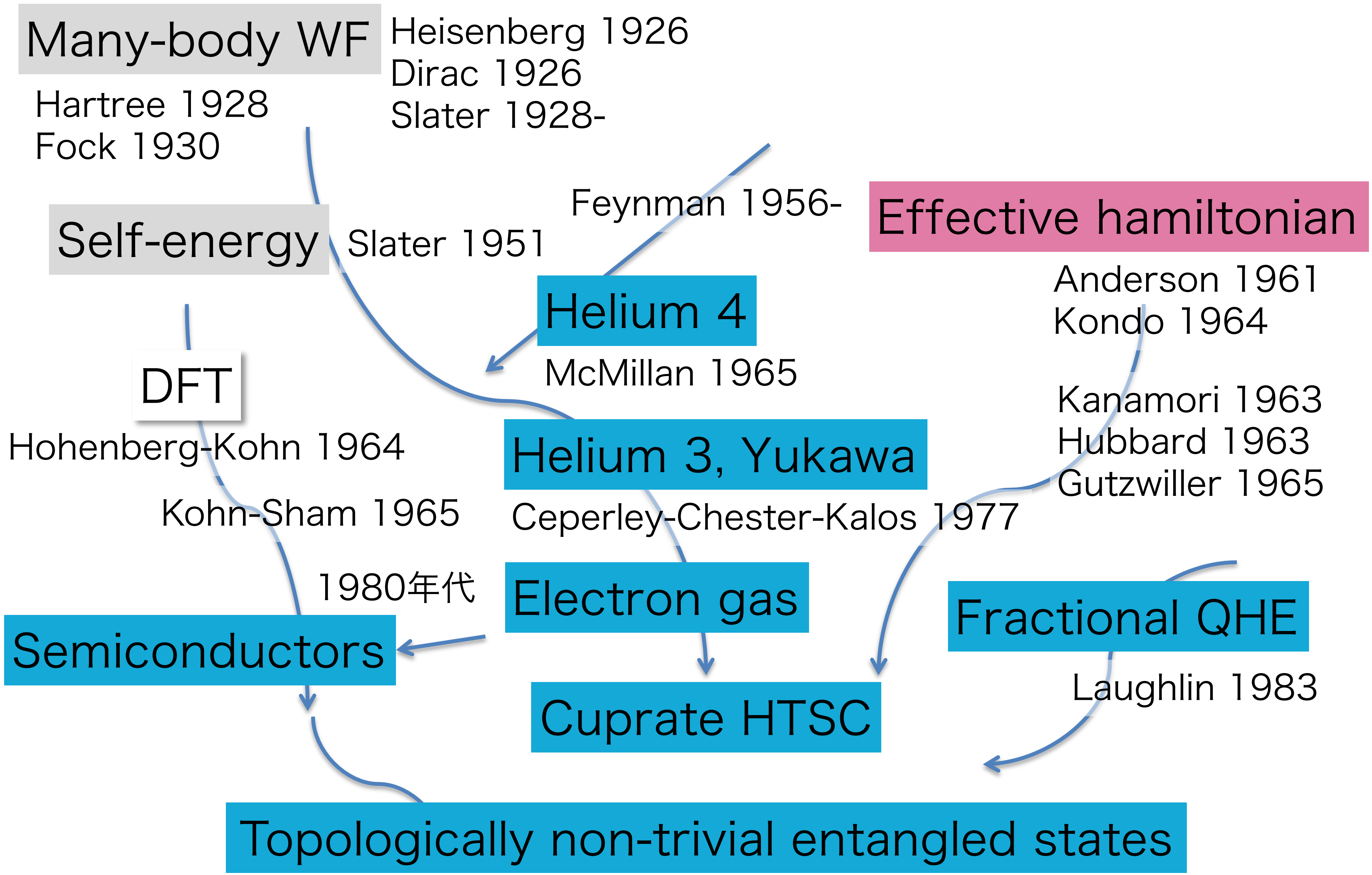
14:55-16:40 July 11, 2023

1. Representation of many-body quantum systems
2. Research history of many-body electrons
3. Combination of *ab initio* and many-body methods
4. WFs to Green's functions
5. Appendix

1. Representation of Many-Body Quantum Systems

		Equilibrium	Non-equilibrium
Wave function	pure state	Variational Typicality	Stochastic Schrödinger eq.
Density matrix	mixed state	Variational (DMRG)	Gorini-Kossakowski-Sudarshan-Lindblad master eq.
Partition function			
Green's function			Keldysh: Starting from an equilibrium state

2. Research History of Many-Body Electron WF



2. Research History of Many-Body Electron WF

Krylov subspace method

1926

Krylov 1931

Lanczos 1950

Slater 1928-

Markov chain MC

Variational WF (Machines for ML)

Effective hamiltonian

Anderson 1961

Kondo 1964

Helium 4

Density Functional Thoery

Millan 1965

Numerical RG

Hohenberg-Kohn 1964

Helium 3, Yukawa

Wilson 1965

Gutzwiller 1965

Kohn-Sham 1965

Ceperley-Chester-Kalos 1977

1980年代

Electron gas

Fractional QHE

Semiconductors

Laughlin 1983

Matrix・tensor product state

Topologically non

Singular value decomposition

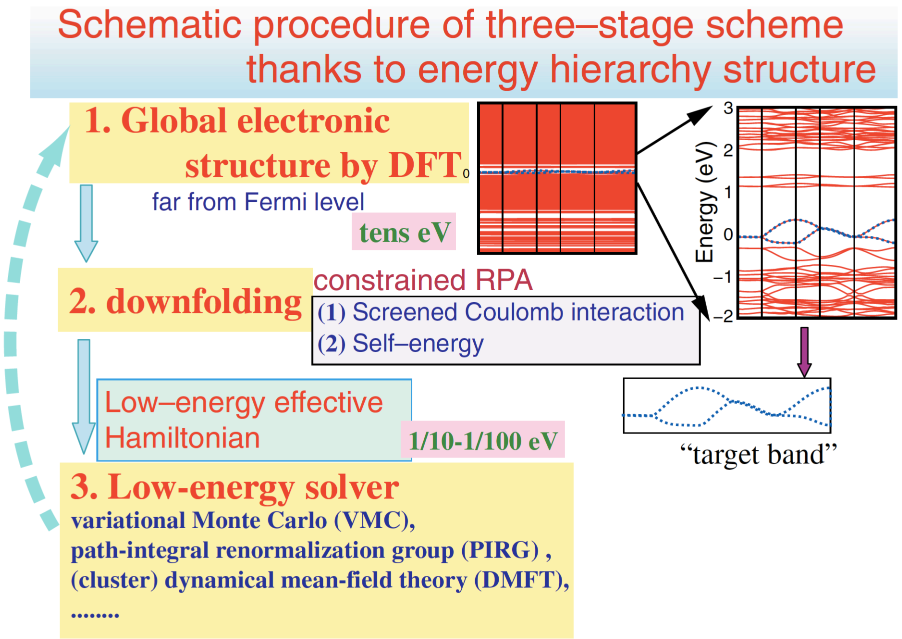
3. Combination of *Ab Initio* and Many-Body Methods

3-1. Effective Hamiltonians of Many-Body Electrons in 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 inpurities in alloys
  -Rare earth alloys

Derivation of *Ab Initio* Low-Energy Effective Hamiltonians



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

High-energy Hilbert space $O(10^2)$ eV

-Density functional theory

Hohenberg-Kohn 1964, Kohn-Sham 1965

→Low-energy Hilbert space $O(1)$ eV

Maximally localized Wannier function

Souza-Marzari-Vanderbilt

Effective dielectric function by cRPA

F. Aryasetiawan, M. Imada, A. Georges,
G. Kotliar, S. Biermann, & A. I. Lichtenstein,
Phys. Rev. B 70, 195104 (2004)

-Low-energy effective hamiltonian

$$\hat{H} = \hat{H}_K + \hat{H}_I$$

$$\hat{H}_K = -\sum_{\ell_1,\ell_2}\sum_{\sigma_1,\sigma_2} t^{\sigma_1\sigma_2}_{\ell_1\ell_2}\hat{c}^\dagger_{\ell_1\sigma_1}\hat{c}_{\ell_2\sigma_2}$$

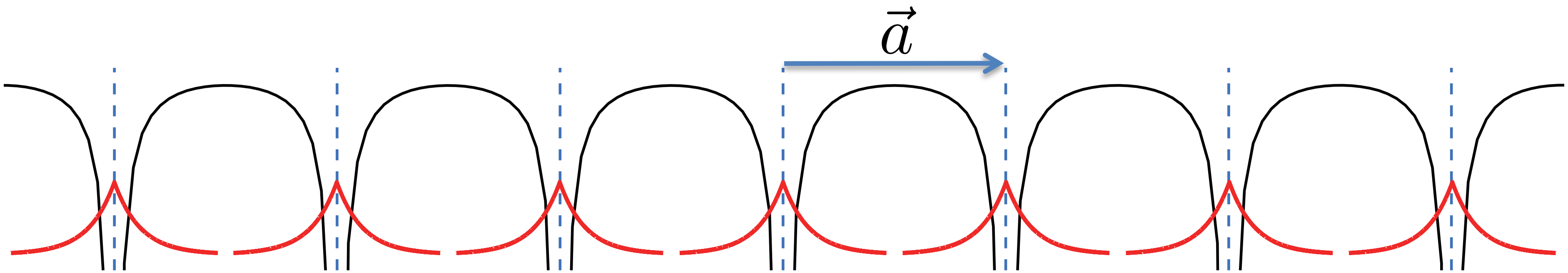
$$\hat{H}_I = \sum_{\ell_1,\ell_2,\ell_3,\ell_4}\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I^{\sigma_1\sigma_2\sigma_3\sigma_4}_{\ell_1\ell_2\ell_3\ell_4}\hat{c}^\dagger_{\ell_1\sigma_1}\hat{c}_{\ell_2\sigma_2}\hat{c}^\dagger_{\ell_3\sigma_3}\hat{c}_{\ell_4\sigma_4}$$

Pros: Long-range correlation & quantum entanglement

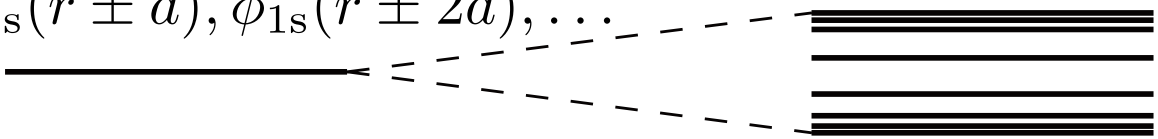
Cons: Crystal structure optimization

Model of Many-Body Electrons

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

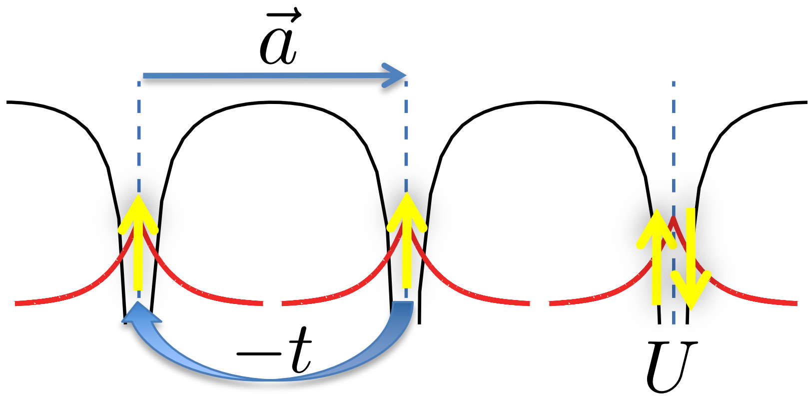


$$\phi_{1\mathrm{s}}(\vec{r}), \phi_{1\mathrm{s}}(\vec{r} \pm \vec{a}), \phi_{1\mathrm{s}}(\vec{r} \pm 2\vec{a}), \ldots$$



Gedankenexperiment of F. N. Mott

One of the Simplest Model: 1D Hubbard Model



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

-Tunnelling among neighboring 1s orbitals

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

-Intra-atomic Coulomb in 1s orbitals

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

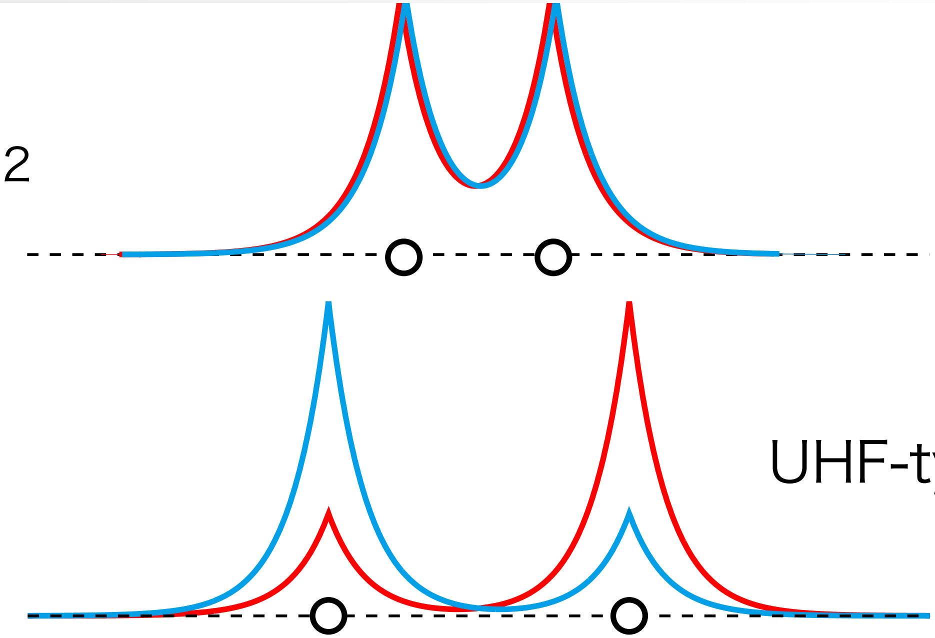
1D Hubbard model (periodic boundary condition, *L* site)

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

cf.) Bethe ansatz, Tomonaga-Luttinger liquid

Hydrogen Molecule

H_2

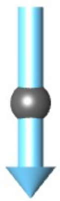


UHF-type wave function

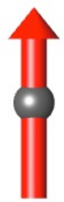
Hubbard model   cf.) Chiappe *et al.*, Phys. Rev. B 75, 195104 (2007)

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

Heisenberg model or *J*-coupling $\hat{H} = J\left(\hat{S}^x_0\hat{S}^x_1 + \hat{S}^y_0\hat{S}^y_1 + \hat{S}^z_0\hat{S}^z_1\right)$



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

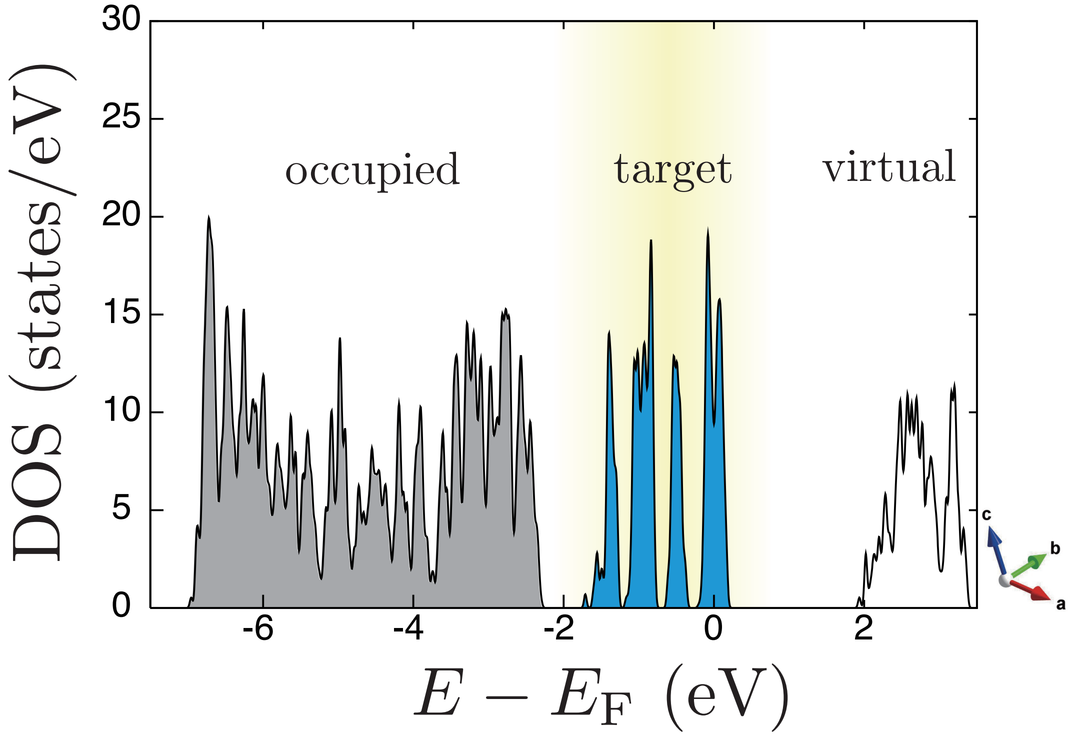


Singlet ground state

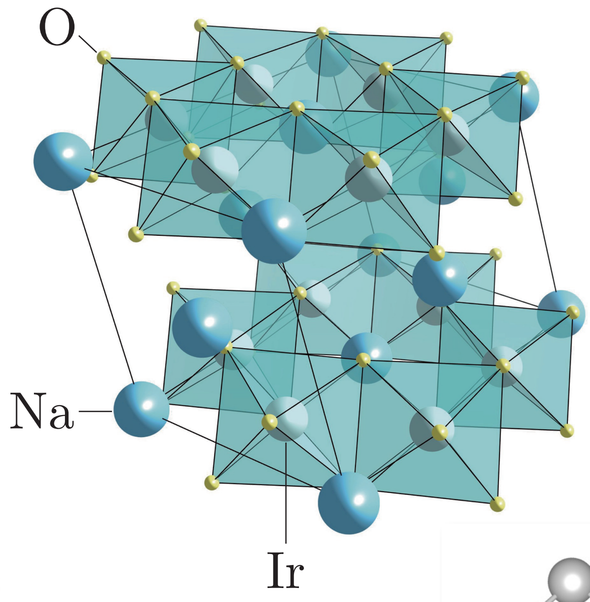
Construction of Effective Hamiltonians: An Example

- Target Hilbert space expanded by localized Wannier orbitals

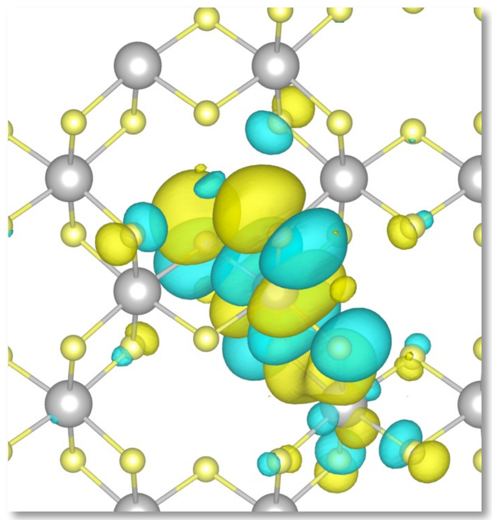
DFT result for energy spectrum



Souza-Marzari-Vanderbilt



Na_2IrO_3



- Effective Coulomb interactions in target space
  Renormalization due to
  infinite virtual particle-hole excitations
  ← Constrained random phase approximation

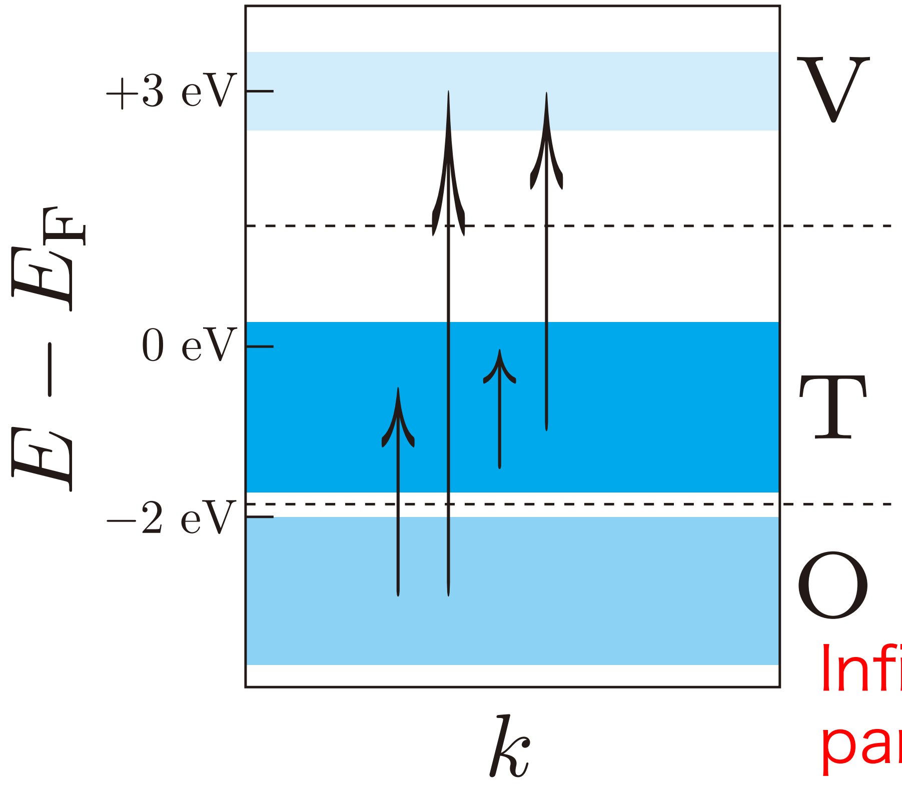
Imada & Miyake, J. Phys. Soc. Jpn. **79**, 112001 (2010)

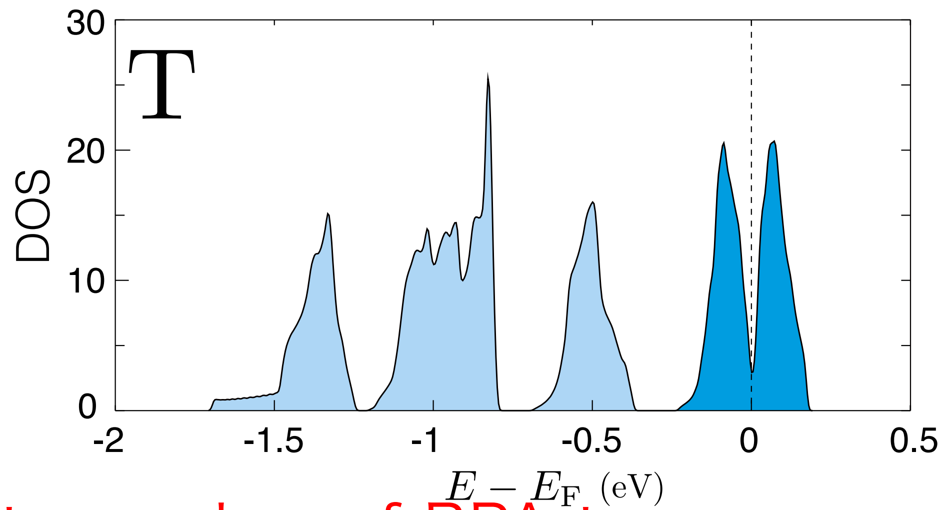
Constrained RPA Estimate on Coulomb Interaction of t_{2g}-Hubbard

$$W^{\mathrm{cRPA}} = \frac{V}{1 + V\chi^{\mathrm{cRPA}}}$$ ←Dielectric constant

$$\chi^{\mathrm{RPA}} = \chi_{\mathrm{O}\to\mathrm{T}} + \chi_{\mathrm{O}\to\mathrm{V}} + \chi_{\mathrm{T}\to\mathrm{T}} + \chi_{\mathrm{T}\to\mathrm{V}}$$

$$\chi^{\mathrm{cRPA}} = \chi_{\mathrm{O}\to\mathrm{T}} + \chi_{\mathrm{O}\to\mathrm{V}} + \cancel{\chi_{\mathrm{T}\to\mathrm{T}}} + \chi_{\mathrm{T}\to\mathrm{V}}$$





Infinite number of RPA-type particle-hole excitations

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

Hopping

$$\hat{H}_0 = \sum_{\ell\neq m}\sum_{a,b=xy,yz,zx}\sum_{\sigma,\sigma'} t^{\sigma\sigma'}_{\ell,m;a,b}\left[\hat{c}^\dagger_{\ell a\sigma}\hat{c}_{mb\sigma'} + \text{h.c.}\right]$$

Trigonal+orbital-dependent μ

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

SOC

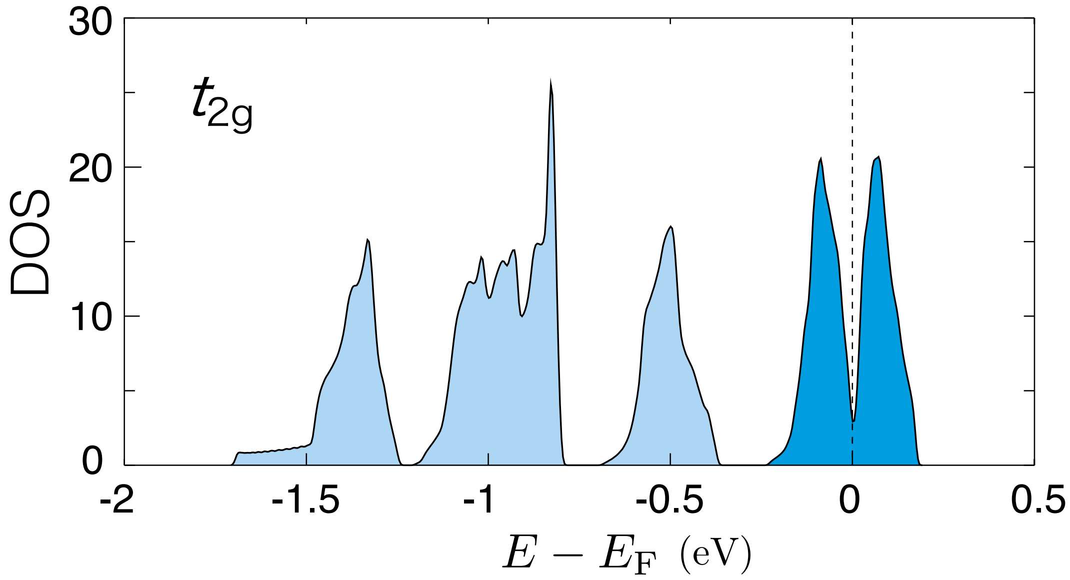
$$\hat{H}_{\text{SOC}} = \frac{\zeta_{\text{so}}}{2}\sum_{\ell}\vec{\hat{c}}^\dagger_\ell \begin{bmatrix} 0 & +i\hat{\sigma}_z & -i\hat{\sigma}_y \\ -i\hat{\sigma}_z & 0 & +i\hat{\sigma}_x \\ +i\hat{\sigma}_y & -i\hat{\sigma}_x & 0\end{bmatrix}\vec{\hat{c}}_\ell$$

$$\vec{\hat{c}}^\dagger_\ell = \left(\hat{c}^\dagger_{\ell yz\uparrow}, \hat{c}^\dagger_{\ell yz\downarrow}, \hat{c}^\dagger_{\ell zx\uparrow}, \hat{c}^\dagger_{\ell zx\downarrow}, \hat{c}^\dagger_{\ell xy\uparrow}, \hat{c}^\dagger_{\ell xy\downarrow}\right)$$

Coulomb

$$\hat{H}_U = U\sum_{\ell}\sum_{a=yz,zx,xy}\hat{n}_{\ell a\uparrow}\hat{n}_{\ell a\downarrow}$$
$$+\sum_{\ell\neq m}\sum_{a,b}\frac{V_{\ell,m}}{2}(\hat{n}_{\ell a\uparrow}+\hat{n}_{\ell a\downarrow})(\hat{n}_{mb\uparrow}+\hat{n}_{mb\downarrow})$$
$$+\sum_{\ell}\sum_{a<b}\sum_{\sigma}\left[U'\hat{n}_{\ell a\sigma}\hat{n}_{\ell b\overline{\sigma}} + (U'-J_{\text{H}})\hat{n}_{\ell a\sigma}\hat{n}_{\ell b\sigma}\right]$$
$$+J_{\text{H}}\sum_{\ell}\sum_{a\neq b}\left[\hat{c}^\dagger_{\ell a\uparrow}\hat{c}^\dagger_{\ell b\downarrow}\hat{c}_{\ell a\downarrow}\hat{c}_{\ell b\uparrow} + \hat{c}^\dagger_{\ell a\uparrow}\hat{c}^\dagger_{\ell a\downarrow}\hat{c}_{\ell b\downarrow}\hat{c}_{\ell b\uparrow}\right]$$

F. Aryasetiawan, *et al.*,
Phys. Rev. B 70, 195104 (2004)
M. Imada & T. Miyake, JPSJ 79, 112001 (2010)



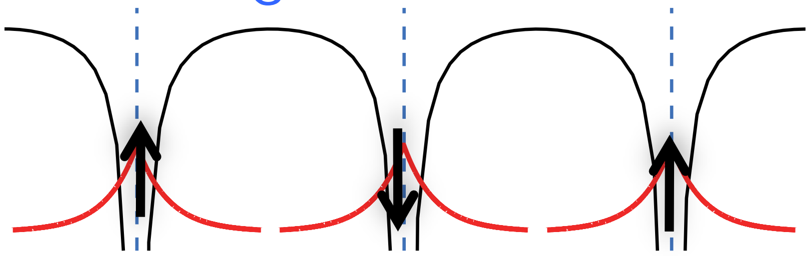
DFT: Elk (FLAPW) http://elk.sourceforge.net
Vxc: Perdew-Wang 1992

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

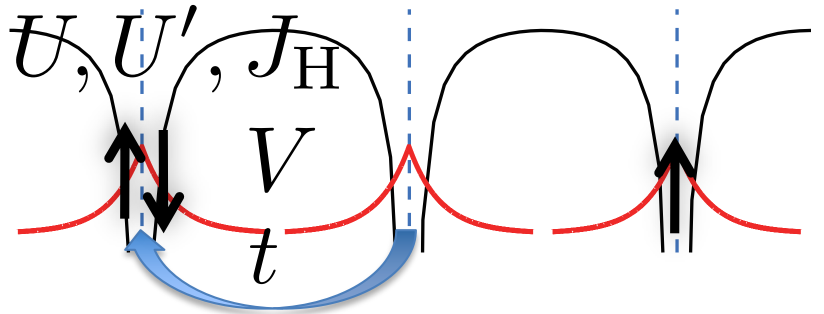
Unperturbed atomic Hamiltonian

2^N degenerated states



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).

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

$$\mathcal{J}_X = \begin{bmatrix} \boxed{\mathbf{-23.9}} & -3.1 & -8.4 \\ -3.1 & 3.2 & 1.8 \\ -8.4 & 1.8 & 2.0 \end{bmatrix} \text{(meV)} \qquad \mathcal{J}_{Z_{2\mathrm{nd}}} = \begin{bmatrix} -0.8 & 1.0 & -1.4 \\ 1.0 & -0.8 & -1.4 \\ -1.4 & -1.4 & -1.2 \end{bmatrix} \text{(meV)}$$

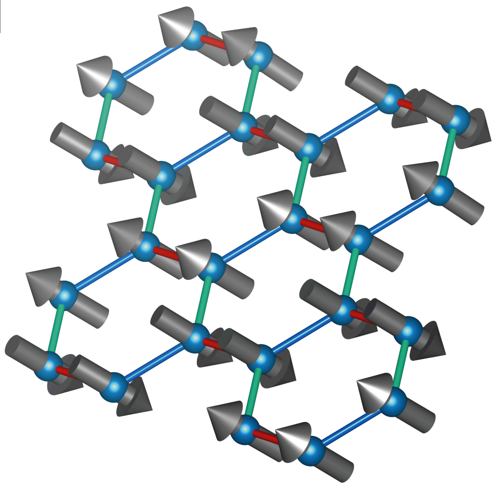
$$\mathcal{J}_Y = \begin{bmatrix} 3.2 & -3.1 & 1.8 \\ -3.1 & \boxed{\mathbf{-23.9}} & -8.4 \\ 1.8 & -8.4 & 2.0 \end{bmatrix} \text{(meV)} \qquad \mathcal{J}_3 = \begin{bmatrix} 1.7 & 0.0 & 0.0 \\ 0.0 & 1.7 & 0.0 \\ 0.0 & 0.0 & 1.7 \end{bmatrix} \text{(meV)}$$

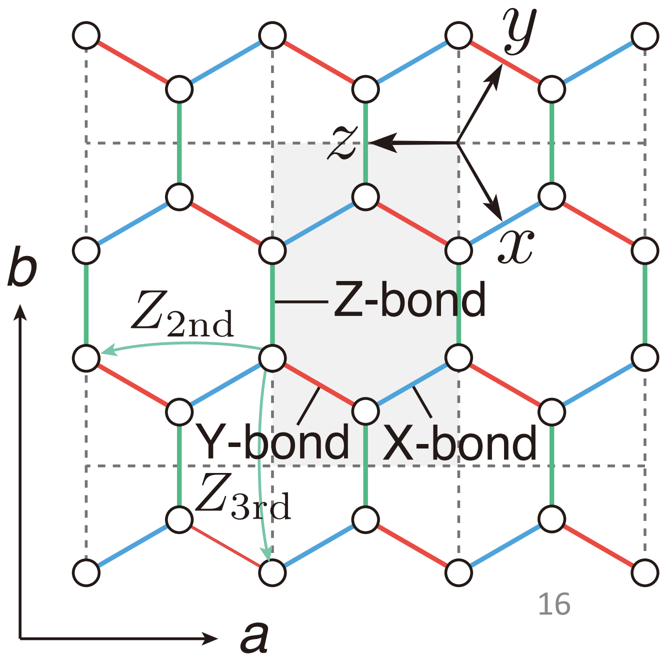
$$\mathcal{J}_Z = \begin{bmatrix} 4.4 & -0.4 & 1.1 \\ -0.4 & 4.4 & 1.1 \\ 1.1 & 1.1 & \boxed{\mathbf{-30.7}} \end{bmatrix} \text{(meV)}$$

Ground state:
Zigzag order

agrees with experiments

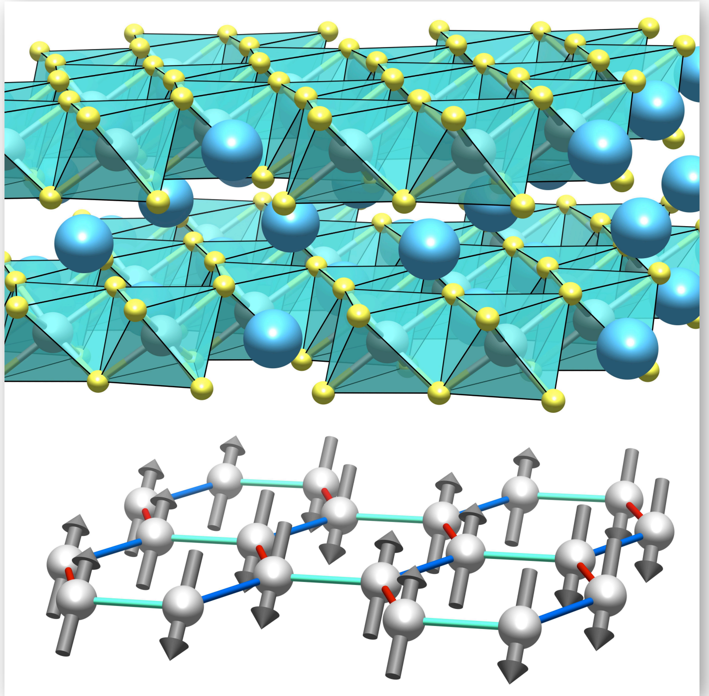
iPEPS, 2D DMRG, & ED:
T. Okubo, K. Shinjo, Y. Yamaji, *et al.*,

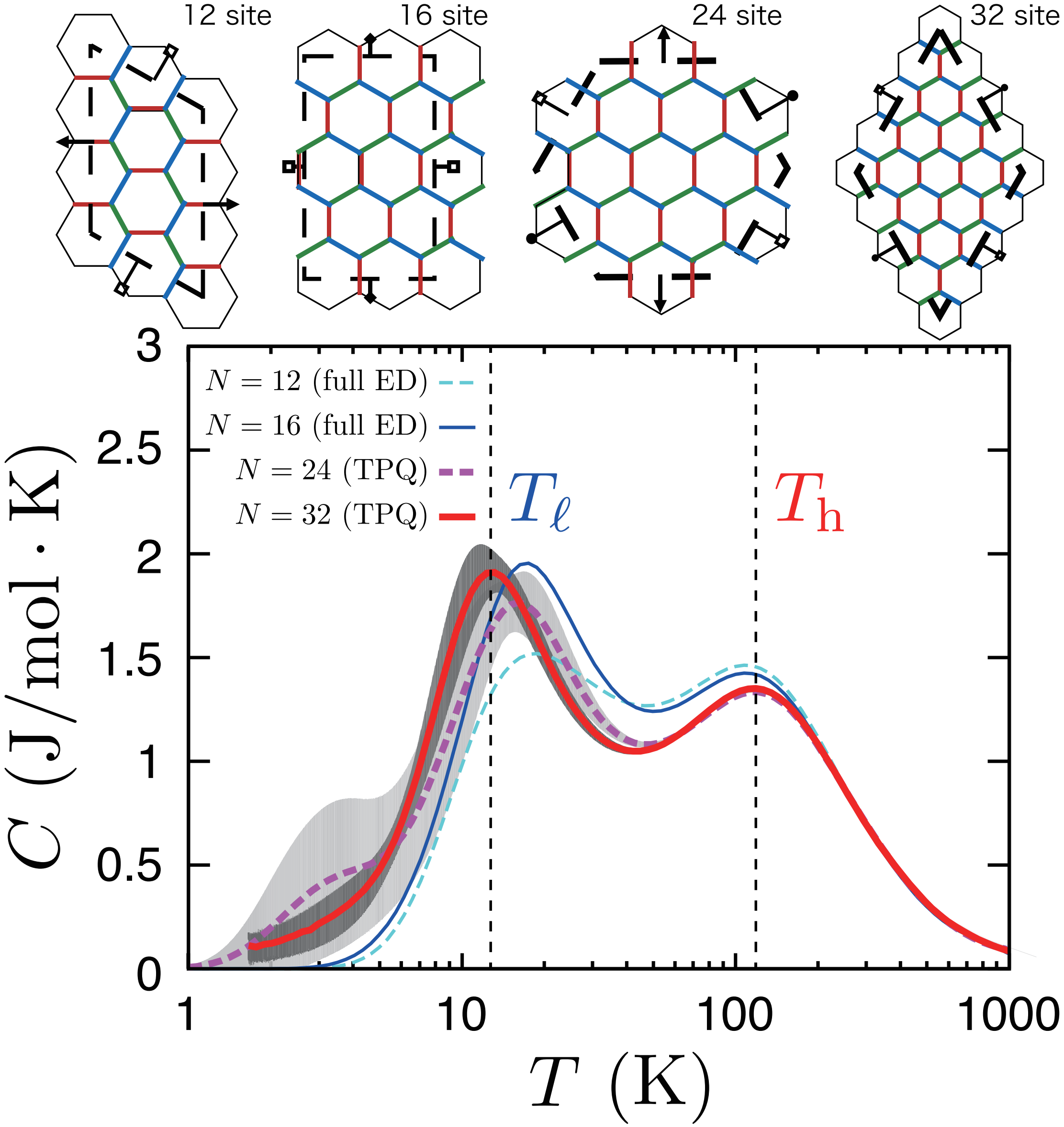




Example: Simulation of Heat Capacity

Frustrated magnet Na_2IrO_3





3-2. Numerical Solvers for Effective Hamiltonians

A Low-Energy Solver: Variational WF Method

Imaginary-time Schrödinger eq. $$-\frac{\partial}{\partial \tau}|\Phi(\tau)\rangle = \hat{H}|\Phi(\tau)\rangle$$

Time-dependent variational principle

J. Frenkel (1934)

A. D. McLachlan and M. A. Ball, Rev. Mod. Phys. 36, 844 (1964)

cf.) variational principle

$$\frac{\langle \psi_{\boldsymbol{\alpha}}|H|\psi_{\boldsymbol{\alpha}}\rangle}{\langle \psi_{\boldsymbol{\alpha}}|\psi_{\boldsymbol{\alpha}}\rangle} \geq E_0$$

-Optimization of variational WF $\left|\psi_{\boldsymbol{\alpha}(\tau)}\right\rangle$

$$\frac{d\alpha_\ell}{d\tau} = -\sum_m (\mathcal{S}^{-1})_{\ell m} g_m$$

Fisher information matrix:

$$\mathcal{S}_{k\ell} = \partial_{\overline{\alpha}_k}\partial_{\alpha_\ell} \ln \langle \psi_{\overline{\boldsymbol{\alpha}}}|\psi_{\boldsymbol{\alpha}}\rangle$$

gradient: $g_m = \dfrac{\partial}{\partial \overline{\alpha}_m} \dfrac{\langle \psi_{\overline{\boldsymbol{\alpha}}}|\,\hat{H}\,|\psi_{\boldsymbol{\alpha}}\rangle}{\langle \psi_{\overline{\boldsymbol{\alpha}}}|\psi_{\boldsymbol{\alpha}}\rangle}$

Natural gradient: S.-I. Amari, Neural Comput. 10, 251 (1998).
SR method: S. Sorella, Phys. Rev. B 64, 024512 (2001).

Variational Ansatz

Typical variational WF

$$|\psi_{\boldsymbol{\alpha}}\rangle = \mathcal{L}^S \mathcal{L}^K \exp\left[\sum_{\ell,m}\sum_{\sigma',\tau'} v_{\ell m}^{\sigma'\tau'} \hat{n}_{\ell\sigma'}\hat{n}_{m\tau'}\right] \left(\sum_{i,j}\sum_{\sigma,\tau} f_{ij}^{\sigma\tau} \hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\tau}^{\dagger}\right)^{N_{\mathrm{e}}/2} |0\rangle$$

S =1/2 lattice fermions

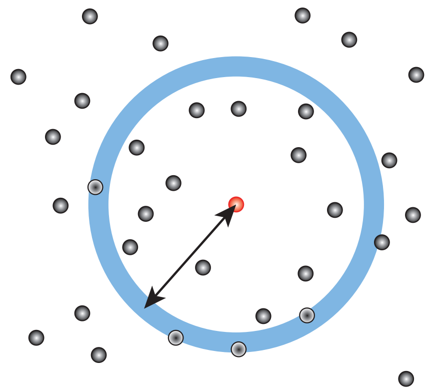
-Two-particle correlation

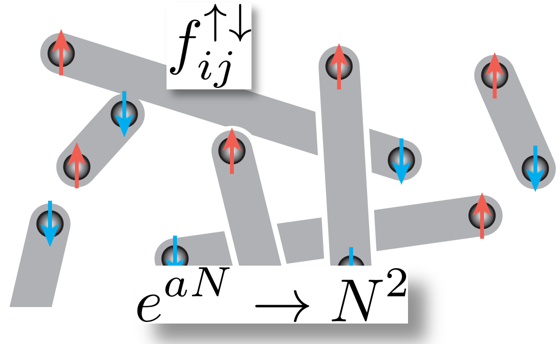
R. Jastrow. Phys. Rev. 98, 1479 (1955).
M. C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963).

-Geminal/Pair product (PP) state

P. W. Anderson, Mater. Res. Bull. 8, 153 (1973).
P. Fazekas & P. W. Anderson, Philos. Mag. 30, 423 (1974).

-Quantum number projection





*Flexibility to represent, SDW, CDW, stripes, SCs, and quantum spin liquids
**Quantum entanglement beyond the area law

Monte Carlo sampling

W. L. McMillan, Phys. Rev. 138, A442 (1965).
D. Ceperley, G. V. Chester, & M. H. Kalos, Phys. Rev. B 16, 3081 (1977).

$$\frac{\langle\psi_{\boldsymbol{\alpha}}|\hat{O}|\psi_{\boldsymbol{\alpha}}\rangle}{\langle\psi_{\boldsymbol{\alpha}}|\psi_{\boldsymbol{\alpha}}\rangle} = \sum_x \rho(x)\frac{\langle x|\hat{O}|\psi_{\boldsymbol{\alpha}}\rangle}{\langle x|\psi_{\boldsymbol{\alpha}}\rangle} \simeq \frac{1}{N_{\mathrm{MC}}}\sum_{x\in\Gamma_{\mathrm{MC}}}\frac{\langle x|\hat{O}|\psi_{\boldsymbol{\alpha}}\rangle}{\langle x|\psi_{\boldsymbol{\alpha}}\rangle}$$

$$\rho(x) = \frac{|\langle x|\psi_{\boldsymbol{\alpha}}\rangle|^2}{\langle\psi_{\boldsymbol{\alpha}}|\psi_{\boldsymbol{\alpha}}\rangle}$$

$$|x\rangle = |i_1\sigma_1, i_2\sigma_2, \ldots, i_{N_{\mathrm{e}}}\sigma_{N_{\mathrm{e}}}\rangle \quad \left(i_\ell \in [0,1,\ldots,L-1]^d, \sigma_\ell = \uparrow,\downarrow\right)$$

Exponentially large complex vector represented by
variational parameters of polynomial of number of orbitals N

OSS mVMC T. Misawa *et al.*, CPC 235, 447 (2019)

Improved by Tensor Network/Neural Network

$\mathcal{N}$-body correlation

$$|\psi_{\boldsymbol{\alpha}}\rangle = \mathcal{N}\left(\hat{n}_{1\uparrow}, \hat{n}_{1\downarrow}, \hat{n}_{2\uparrow}, \hat{n}_{2\downarrow}, \ldots, \hat{n}_{N\uparrow}, \hat{n}_{N\downarrow}\right) \left(\sum_{i,j} \sum_{\sigma,\tau} f_{ij}^{\sigma\tau} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\tau}^{\dagger} \right)^{N_{\mathrm{e}}/2} |0\rangle \quad (N = L^d)$$

$$\mathcal{N}\left(\hat{n}_{1\uparrow}, \hat{n}_{1\downarrow}, \hat{n}_{2\uparrow}, \hat{n}_{2\downarrow}, \ldots, \hat{n}_{N\uparrow}, \hat{n}_{N\downarrow}\right)|x\rangle = \mathcal{N}\left(n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow}, \ldots, n_{N\uparrow}, n_{N\downarrow}\right)|x\rangle$$

-Tree tensor network (TTN)

H.-H. Zhao, K. Ido, S. Morita. & M. Imada, Phys. Rev. B 96, 085103 (2017).

-Restricted Boltzmann machine

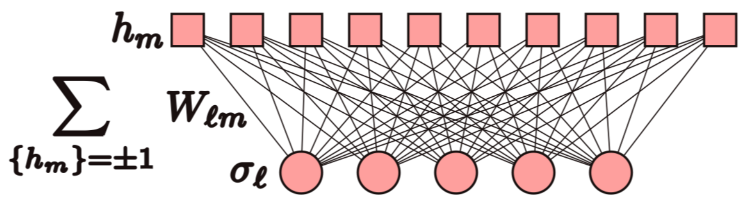
P. Smolensky 1986

$$\mathcal{N}\left(n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow}, \ldots, n_{N\uparrow}, n_{N\downarrow}\right) = \sum_{\{h_\ell\}} \exp\left(\sum_{\ell} a_\ell \sigma_\ell + \sum_{\ell,m} W_{\ell,m} \sigma_\ell h_m + \sum_m b_m h_m \right)$$

$$(\sigma_{2i}, \sigma_{2i+1}) = (2n_{i\uparrow} - 1, 2n_{i\downarrow} - 1) \quad (n_{i\sigma} = 0, 1)$$

cf.) G. Carleo & M. Troyer, Science 355, 602 (2017).

Y. Nomura, A. S. Darmawan, Y. Yamaji, & M. Imada,
Phys. Rev. B 83, 205152 (2017).



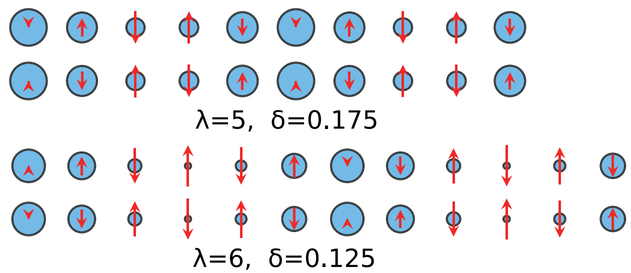
Example of Applications: Superconductivity in Hubbard Model

B.-X. Zheng, *et al.*, Science358,1155(2017).
D. Wu, *et al.*, arXiv:2302.04919

Hubbard model

$$H = -t \sum_{\langle i,j \rangle,\sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

-Stripe order (SO) correlation

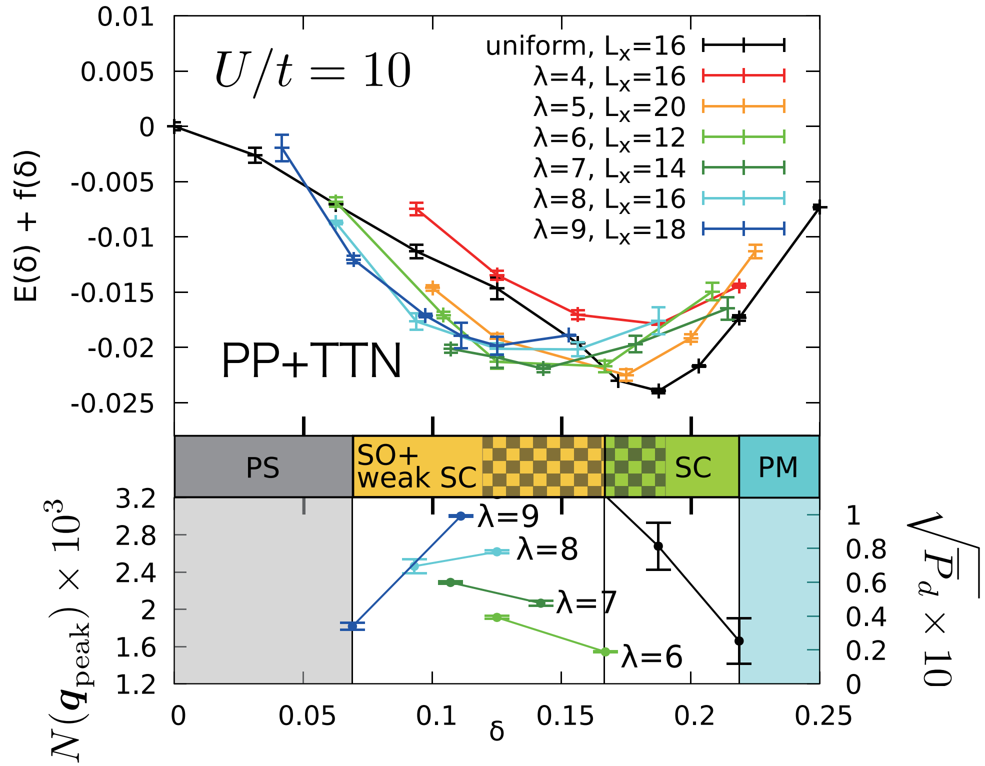


-Superconducting correlation

$$P_d(\boldsymbol{r}) = \frac{1}{2N_s}\sum_{i=1}^{N_s}\left(\frac{\langle\psi|\Delta_d{}^{\dagger}(\boldsymbol{r}_i)\Delta_d(\boldsymbol{r}_i+\boldsymbol{r})|\psi\rangle}{\langle\psi|\,\psi\rangle} + \mathrm{h.c.}\right)$$

$$\Delta_d(\boldsymbol{r}_i) = \frac{1}{\sqrt{2}}\sum_{\boldsymbol{r}} f_d(\boldsymbol{r})(\hat{c}_{\boldsymbol{r}_i\uparrow}\hat{c}_{\boldsymbol{r}_i+\boldsymbol{r}\downarrow} - \hat{c}_{\boldsymbol{r}_i\downarrow}\hat{c}_{\boldsymbol{r}_i+\boldsymbol{r}\uparrow})$$

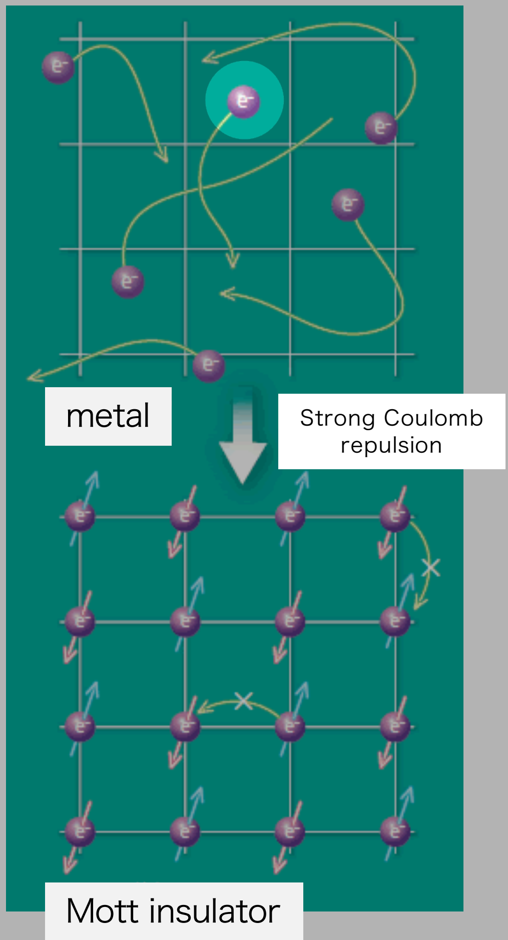
An example: A. S. Darmawan, Y. Nomura, Y. Yamaji, & M. Imada, Phys. Rev. B 98, 205132 (2018)



4. WFs to Green's Functions

Many-Body Schrödinger Equation to Green's Function

from CMSI torrent No.5



$$i\frac{\partial}{\partial t}\Phi(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N)=\hat{H}\Phi(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N)$$

$$\hat{H}=\sum_{j=1}^{N}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\vec{x}_j^2}+V_{\rm ext}(\vec{x}_j)\right]+\frac{e^2}{4\pi\varepsilon}\sum_{j<\ell}\frac{1}{|\vec{x}_j-\vec{x}_\ell|}$$

EOM for Green's function

$$\left(i\frac{\partial}{\partial t}-\hat{H}_0\right)G(\vec{x},t)-(G*\mathbf{\Sigma})(\vec{x},t)=\delta(\vec{x})\delta(t)$$

Self-energy/memory func.: $\Sigma=\Sigma^{\rm nor}+W$

${\rm Im}\Sigma^{\rm nor}$ e-e scattering

${\rm Im}W$ formation of Cooper pairs

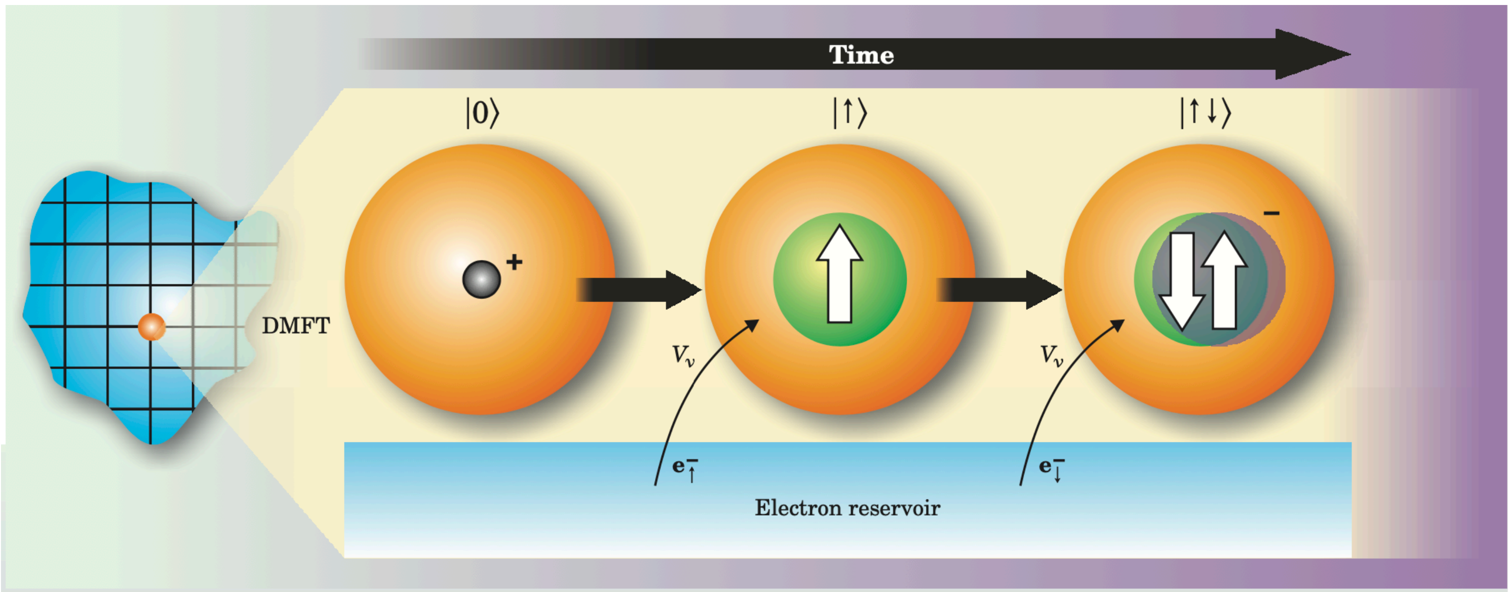
$$A(\vec{k},\omega)=-\frac{1}{\pi}{\rm Im}G(\vec{k},\omega)$$

Combination of *Ab Initio* and Many-Body Methods

Dynamical Mean-Field Theory (DMFT)

W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).
E. Müller-Hartmann, Z. Phys. B 74, 507 (1989).
A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996) .

G. Kotliar, and D. Vollhardt, Physics Today 57, 3, 53 (2004).

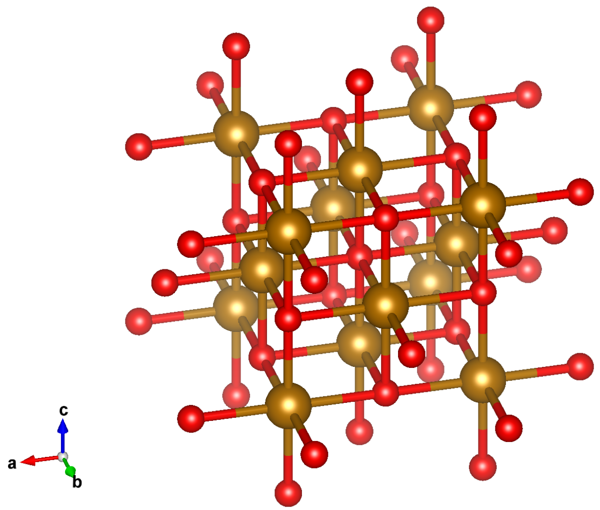


Self-energy effects

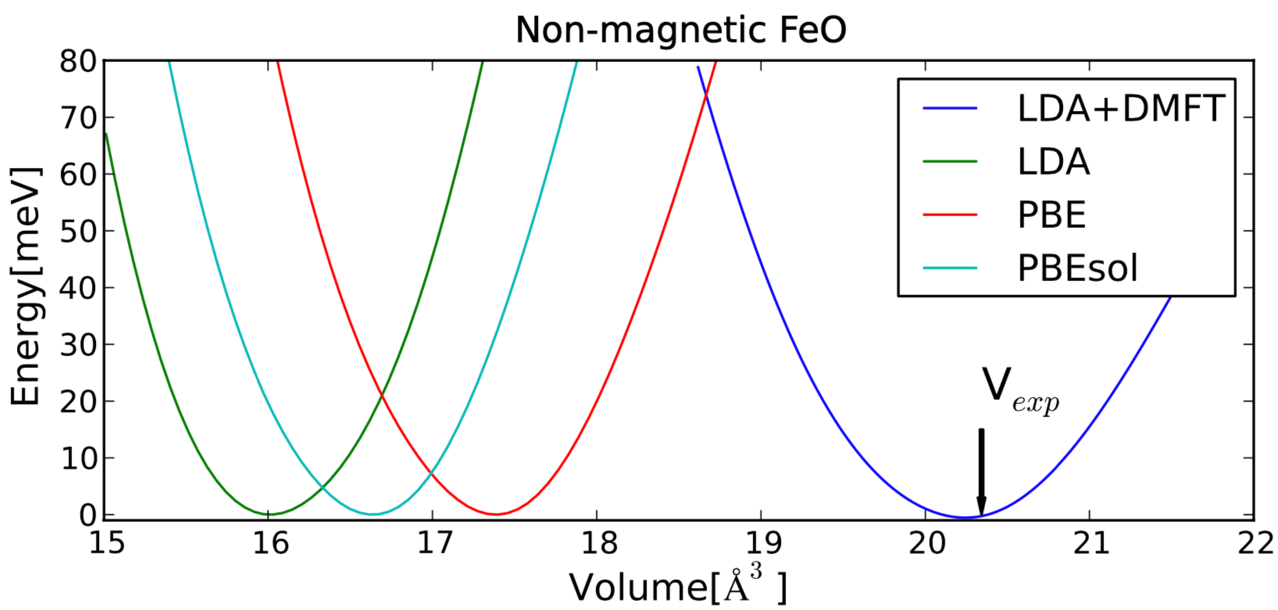
→DFT+DMFT G. Kotliar, *et al.*, Rev. Mod. Phys. 78, 865 (2006)

Combination of *Ab Initio* and Many-Body Methods

DFT+DMFT



Optimization of crystal structure



K. Haule and T. Birol, Phys. Rev. Lett. 115, 256402 (2015)

A. Paul and T. Birol, Annu. Rev. Mater. Res. 49, 31 (2019)

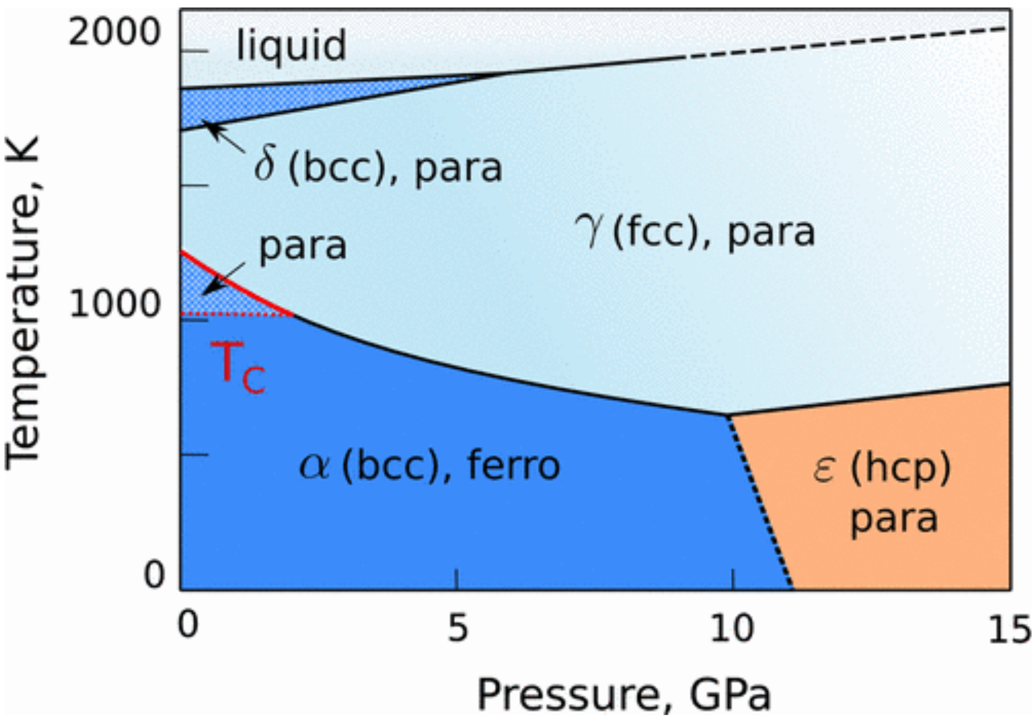
Combination of *Ab Initio* and Many-Body Methods

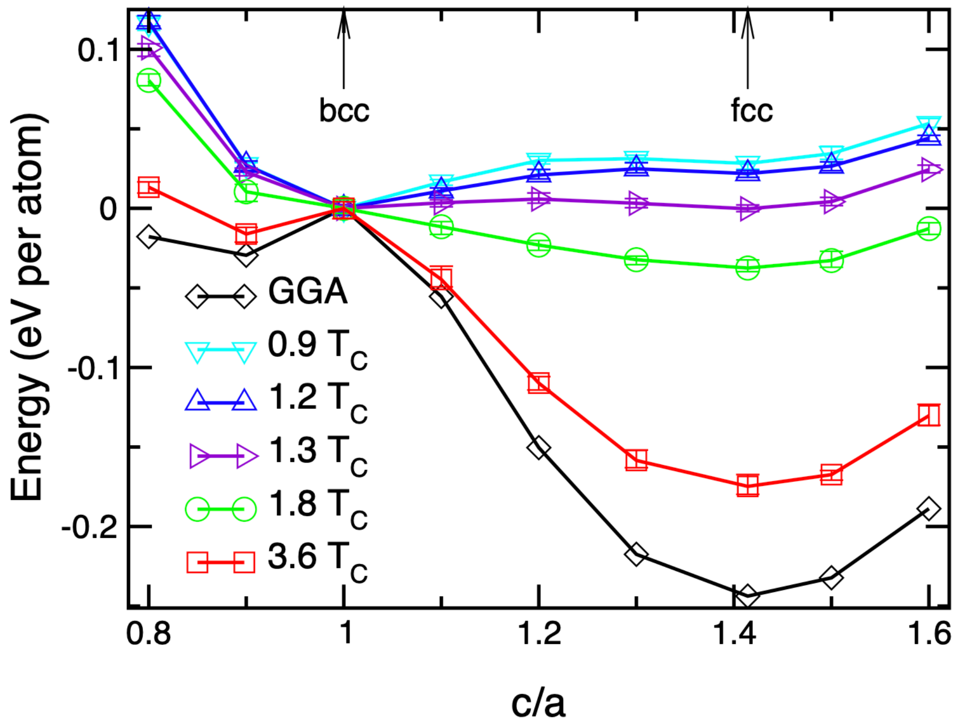
DFT+DMFT

Optimization of crystal structure
\+ *finite temperatures*

Electronic Correlations at
the α(bcc)–γ(fcc) Structural Phase Transition
in Paramagnetic Iron

I. Leonov, A. Poteryaev, V. Anisimov, and D. Vollhardt, Phys. Rev. Lett 106, 106405 (2011).





Bain transformation path

Appendix.

Let’s Solve 2-Site Hubbard Model by HΦ

HΦ

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. Cumput. 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

HΦ https://www.pasums.issp.u-tokyo.ac.jp/hphi/en/
MatriApps LIVE! http://cmsi.github.io/MateriAppsLive/

HΦ Developers

Dr. Takahiro Misawa
ISSP, UTokyo

Dr. Kota Ido
ISSP, UTokyo

Prof. Synge Todo
UTokyo

Dr. Mitsuaki Kawamura
UTokyo

Dr. Yuichi Motoyama
ISSP, UTokyo

Prof. Naoki Kawashima
ISSP, UTokyo

Dr. Kazuyoshi Yoshimi
ISSP, UTokyo

Dr. Youhei Yamaji
MANA, NIMS

Acknowledgment:
Prof. Yoshinori Nakanishi-Ohno (Doshisha U.)
Prof. Takeo Hoshi (Tottori U.)
Prof. Tomohiro Sogabe (Nagoya U.)

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

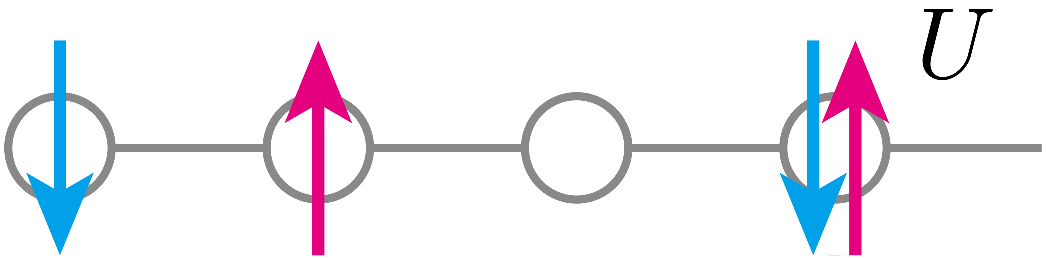
Target Hamiltonian

- Standard Hamiltonian 1

Itinerant electrons: Hubbard-type model

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

N



Fermion Hubbard: Particle # & total S_z conserved

HubbardNConserved: Particle # conserved & total S_z not

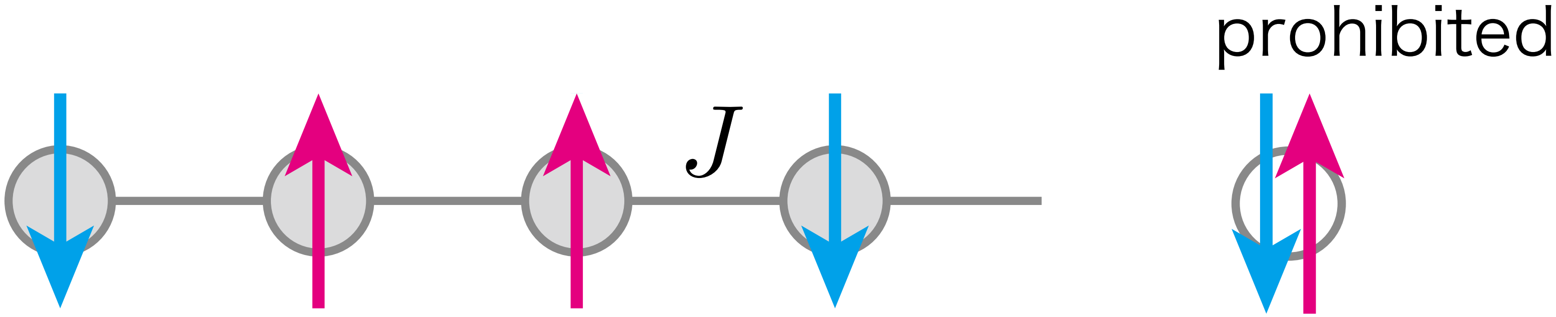
Fermion HubbardGC: Particle # & total S_z not conserved

Target Hamiltonian

- Standard Hamiltonian 2

Localized spin: Heisenberg-type model

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



`Spin:` total S_z conserved

`SpinGC:` total S_z not conserved

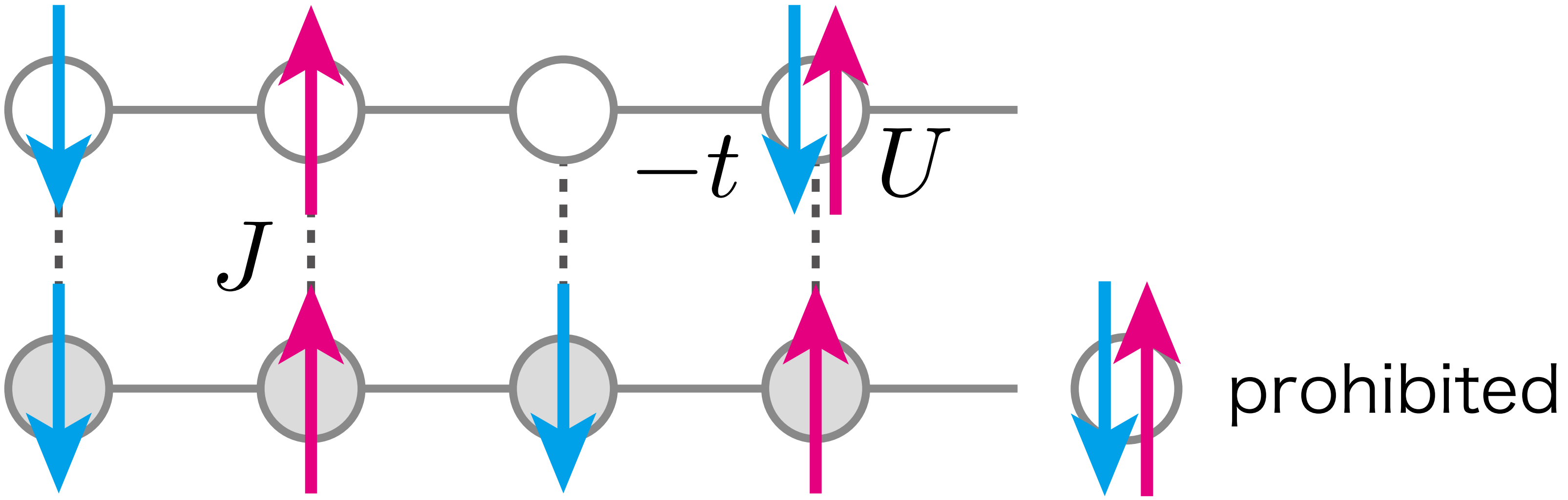
$S > 1/2$ can be simulated
if your memory is enough large

Target Hamiltonian

- Standard Hamiltonian 3

Mixture: Kondo-lattice-type model

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



`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

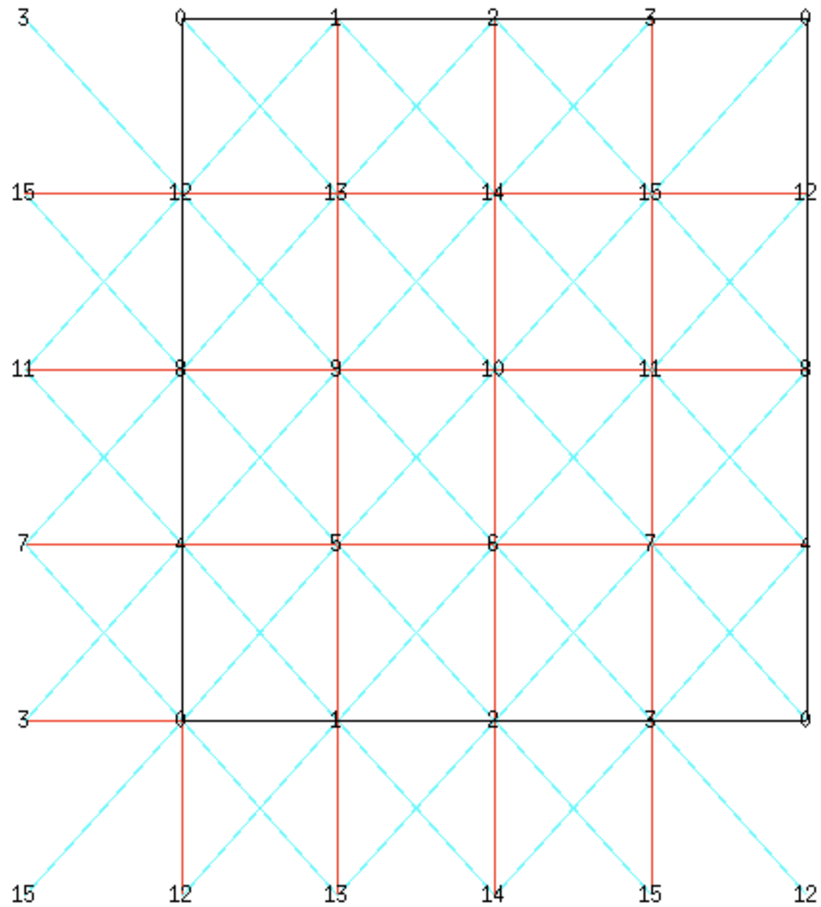
$$H = -\mu \sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{i\sigma} - t \sum_{\langle i,j\rangle} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{J}{2} \sum_{i=1}^{N} \left\{ S_i^{+} c_{i\downarrow}^{\dagger} c_{i\uparrow} + S_i^{-} c_{i\uparrow}^{\dagger}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

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

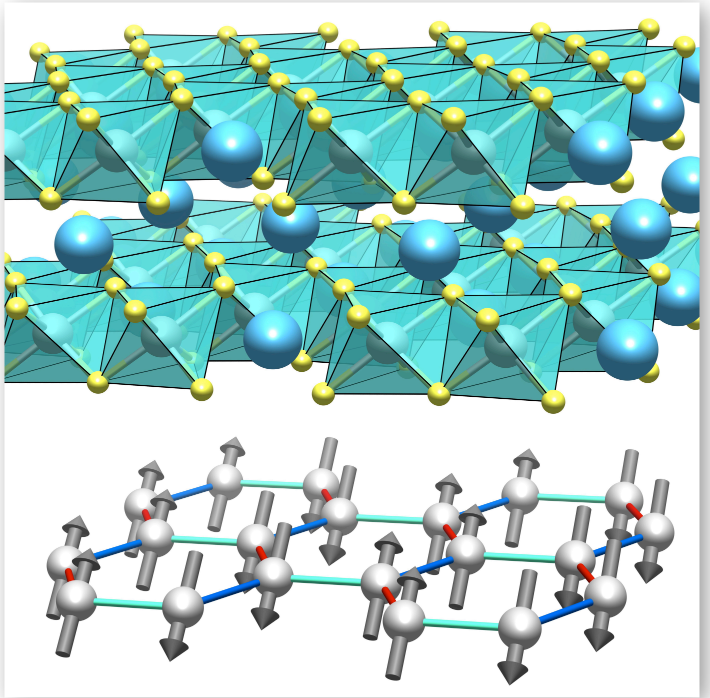
$$\langle H \rangle,\ \langle H^2 \rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} \rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} c^\dagger_{k\sigma_3} c_{\ell\sigma_4} \rangle$$

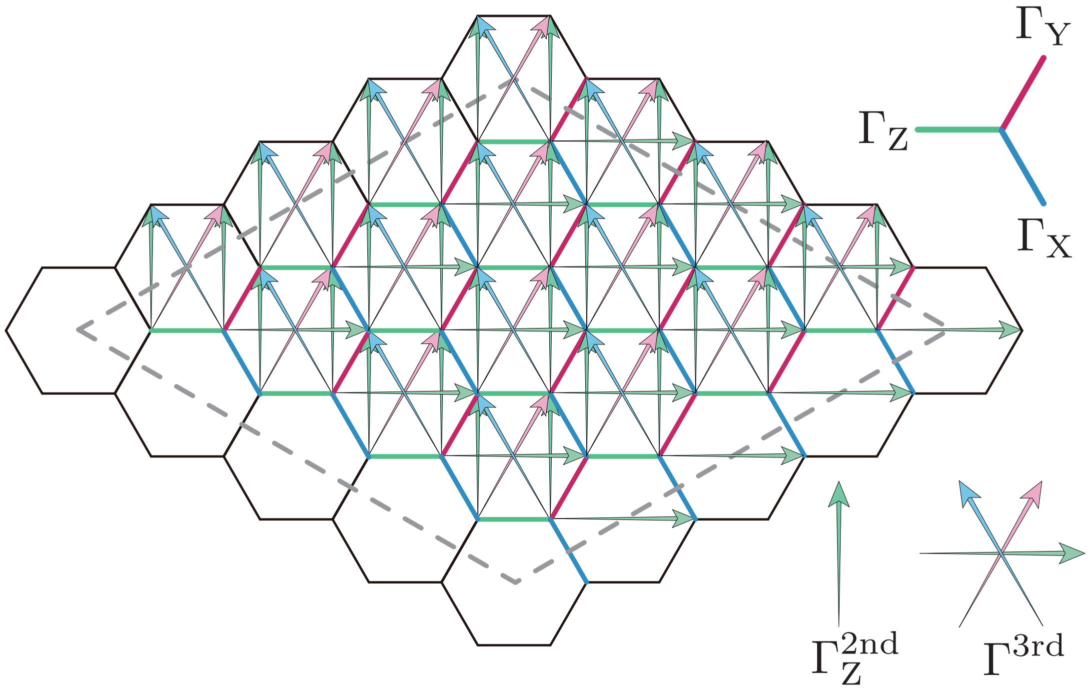
-Dynamical Green's function is also available

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



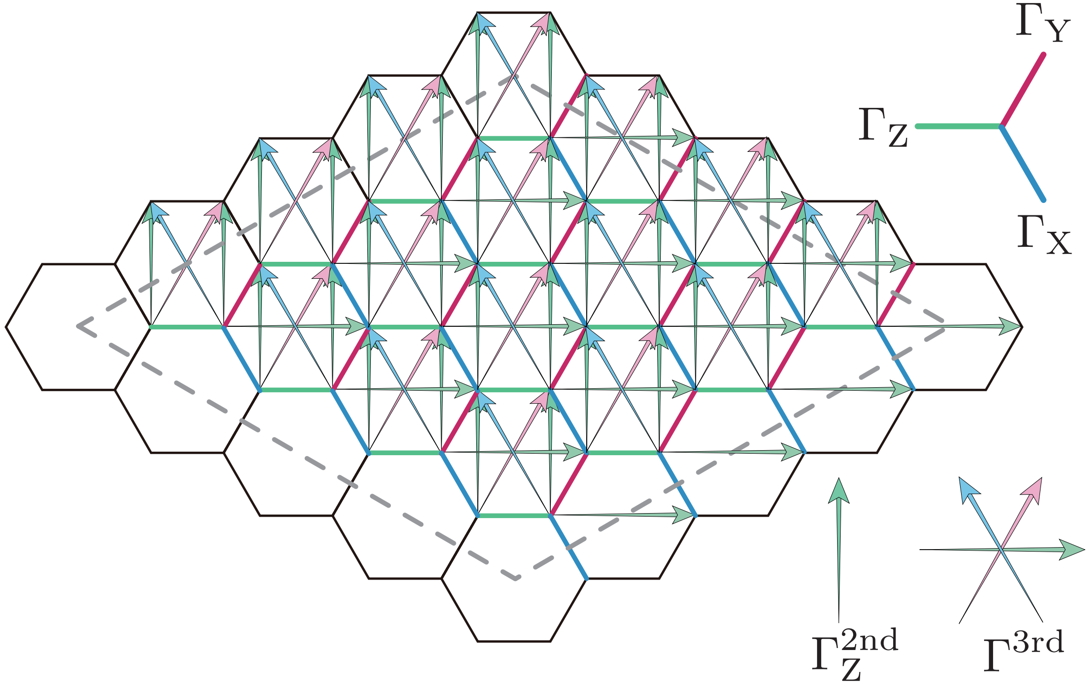


An Example of Expert Input: *Ab Initio* Spin Hamiltonian

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

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

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



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

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

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

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

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

cf.) RESPACK

Overview of Software HΦ

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

For installation, cmake is required

Flow of Simulation

Standard input

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

Standard interface

Making input files from scratch

Expert input

Def. files for Hamiltonian

Def. files for controlling simulation

Expert interface

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

Standard output
Output files

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

$E = 0$

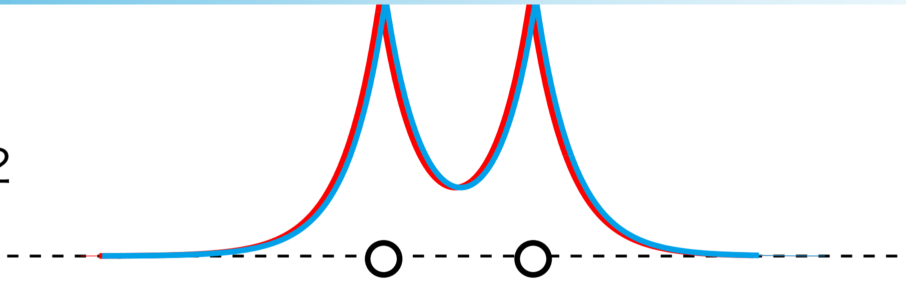
$$\frac{1}{\sqrt{2}} \hat{c}^\dagger_{0\uparrow} \hat{c}^\dagger_{1\downarrow} |0\rangle + \frac{1}{\sqrt{2}} \hat{c}^\dagger_{0\downarrow} \hat{c}^\dagger_{1\uparrow} |0\rangle$$

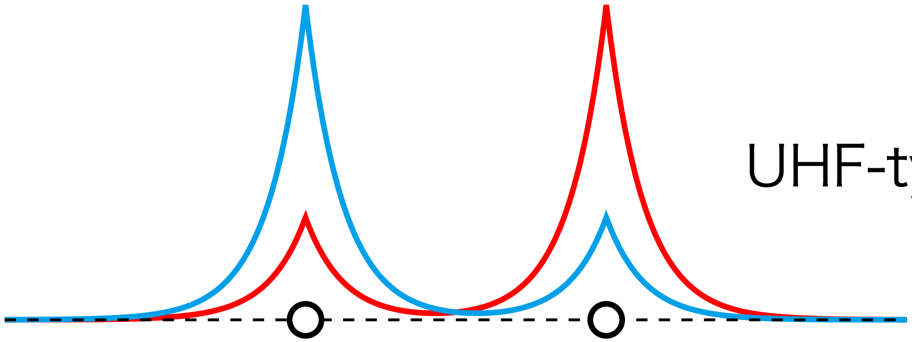
$$E = -\frac{4t^2}{U} + \mathcal{O}(\frac{t^3}{U^2})$$

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

Hydrogen Molecule

H_2





UHF-type wave function

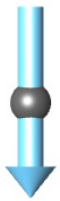
Hubbard model

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

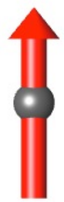
$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} \left(\hat{c}^{\dagger}_{0\sigma} \hat{c}_{1\sigma} + \hat{c}^{\dagger}_{1\sigma} \hat{c}_{0\sigma} \right) + U \sum_{j=0,1} \hat{c}^{\dagger}_{j\uparrow} \hat{c}_{j\uparrow} \hat{c}^{\dagger}_{j\downarrow} \hat{c}_{j\downarrow}$$

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

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 $1/N_{\mathrm{MC}}^{1/2}$, 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

<u>2-1-1 (compulsory).</u>

-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.

<u>2-1-2 (compulsory).</u>

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

<u>2-2 (Optional).</u>

-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 ($L \to \infty$). 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 Feedback Survey for Students from Faculty of Science

2023年度　Sセメスター　授業評価アンケート

AY2023　S semester　Lecture Feedback Survey

締切：9月15日

Deadline: Sep. 15

学部生/学部科目
https://forms.office.com/r/p60VVjF875

学部生/物理学実験I
https://forms.office.com/r/canvcNmZZH

大学院生/大学院科目
https://forms.office.com/r/XG0kFqkiQ6

○　このアンケートは、理学部で開講されている全ての授業に対して実施します。
○　授業の方法や内容、設備などの改善に役立てることを目的として、受講学生全員に、無記名で、授業に対する評価や要望をお聞きします。
○　複数の教員が担当した科目については、平均的な評価で構いません。
○　選択式の回答方法は、該当する選択肢にチェックしてください。
●This survey applies to all courses delivered in the School of Science.
●The survey gives you the opportunity to provide feedback and express your opinions ANONYMOUSLY to further improve various aspects of the lecture such as contents, method of delivering etc.
●Provide overall feedback if there are more than one instructor for the course.
●Please check the appropriate option to answer the choice type.

■科目番号検索サイト/Please find the code below：
https://catalog.he.u-tokyo.ac.jp/result?type=ug&faculty_id

ご協力をよろしくお願いします。
Thank you for your cooperation.

Lecture Schedule

Quantum

#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

7/18 No lecture!!
7/31 will be the deadline for Report 2