Introduction to mVMC

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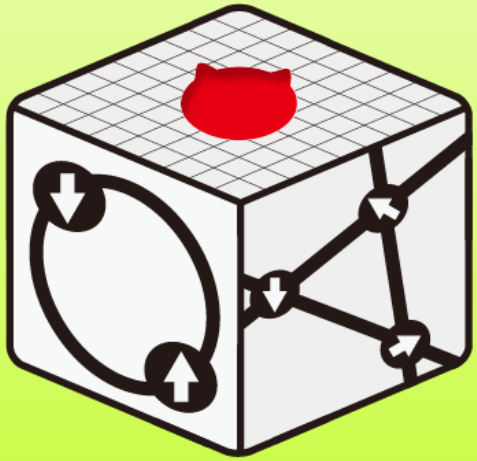


mVMC

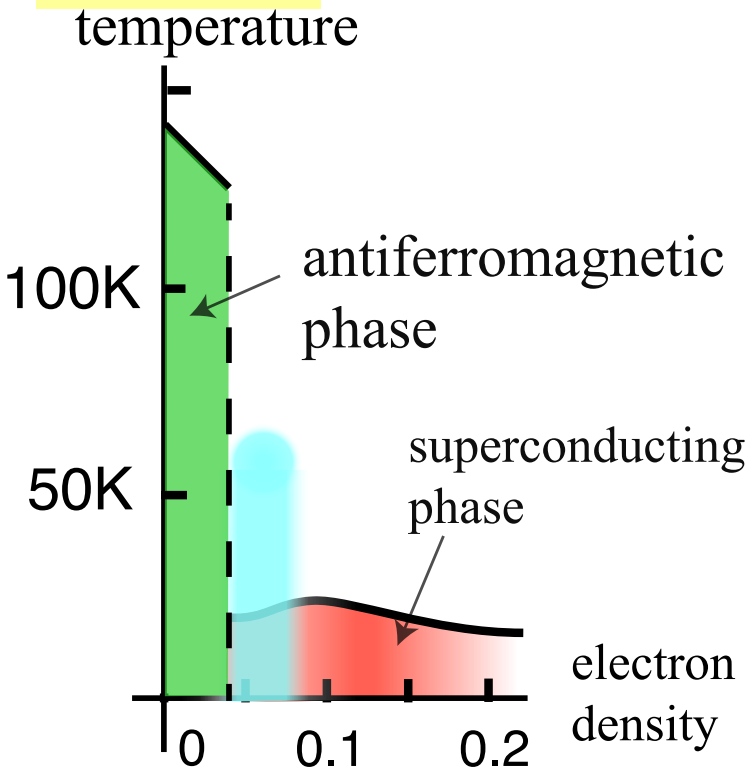
https://www.pasums.issp.u-tokyo.ac.jp/mvmc/

Outline

1. Introduction
 - Strongly correlated electron systems (SCES)
2. Basics of wavefunction methods
3. Basics of mVMC
 - What is variational Monte Carlo (VMC) ?
 - Conventional VMC vs mVMC
 - Optimization method (SR method) based on time-dependent variational principle
4. Open-source software of mVMC
 - How to get mVMC
 - How to use mVMC [Standard & Expert mode]

Exotic phenomena in SCES

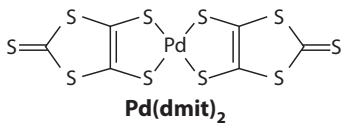
LaFeAsO

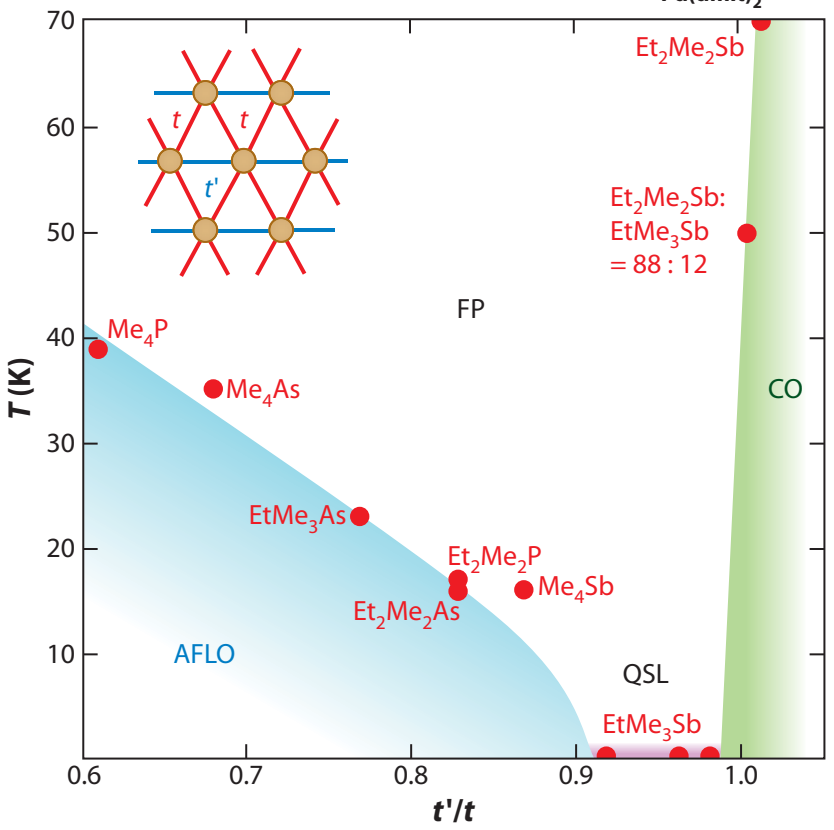


Y. Kamihara *et al*, JACS (2008)

High-Tc SC in iron-based compound

β'-X[Pd(dmit)$_2$]$_2$





K. Kanoda and R. Kato,
Annu. Rev. Condes. Phys. 2011

QSL in organic solids

To clarify and predict exotic phenomena in SCES
→ Accurate numerical methods for solving low-energy effective models are necessary

Low-energy effective models

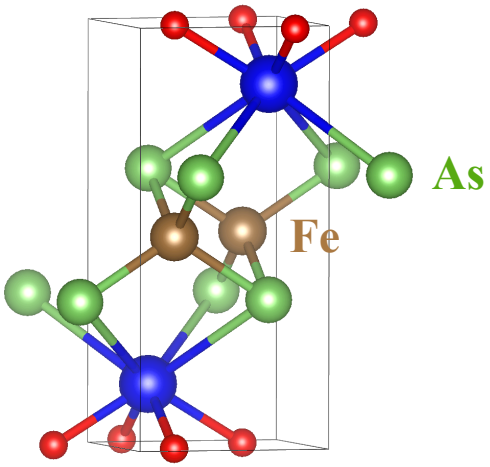
LaFeAsO

5-orbital Hubbard Hamiltonians obtained by ab initio calculations

$$\mathcal{H} = \sum_{\sigma}\sum_{\boldsymbol{R}\boldsymbol{R}'}\sum_{nm} t_{m\mathbf{R}n\mathbf{R}'} a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'} \quad \rightarrow \text{Hopping Term}$$

$$+\frac{1}{2}\sum_{\sigma\rho}\sum_{\boldsymbol{R}\boldsymbol{R}'}\sum_{nm}\Big\{U_{m\mathbf{R}n\mathbf{R}'} a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{m\boldsymbol{R}'} a^{\rho}_{m\boldsymbol{R}'} a^{\sigma}_{n\boldsymbol{R}} \rightarrow \text{Coulomb Term}$$

$$+J_{m\mathbf{R}n\mathbf{R}'}\left(a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{m\boldsymbol{R}} a^{\rho}_{n\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'} + a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{n\boldsymbol{R}} a^{\rho}_{m\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'}\right)\Big\} \rightarrow \text{Exchange Term}$$



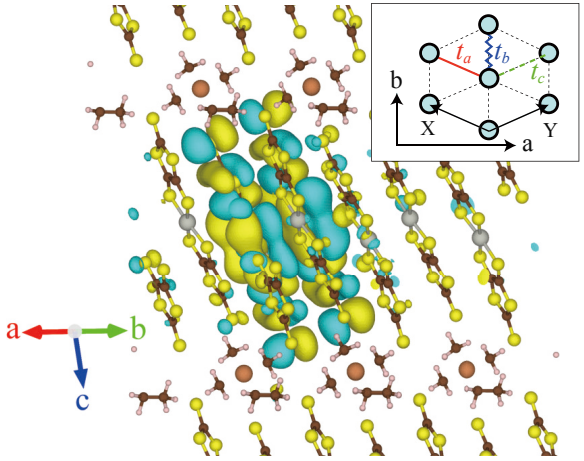
T. Misawa *et al.*, Nat. Com. 5, 5738 (2014)

$EtMe_3Pb[Pd(dmit)_2]_2$

Single-band Hubbard Hamiltonians obtained by ab initio calculations

$$H = \sum_{i,j} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{H.c.}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

$$+ \sum_{i,j} V_{i,j} n_i n_j$$



T. Misawa *et al.*, PRR 2, 032072(R) (2020)
K. Yoshimi *et al.*, PRR 3, 043224 (2021)
K. Ido *et al.*, npj Quantum mat. 7, 48 (2022)

Low-energy effective models

LaFeAsO

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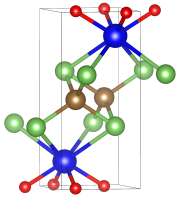

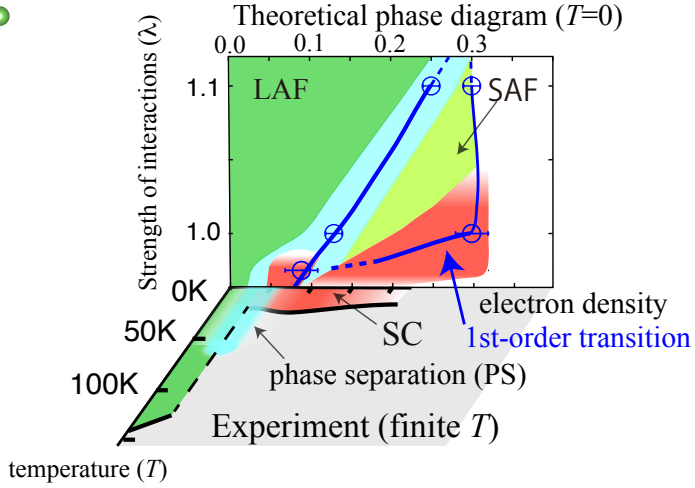

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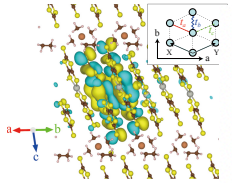

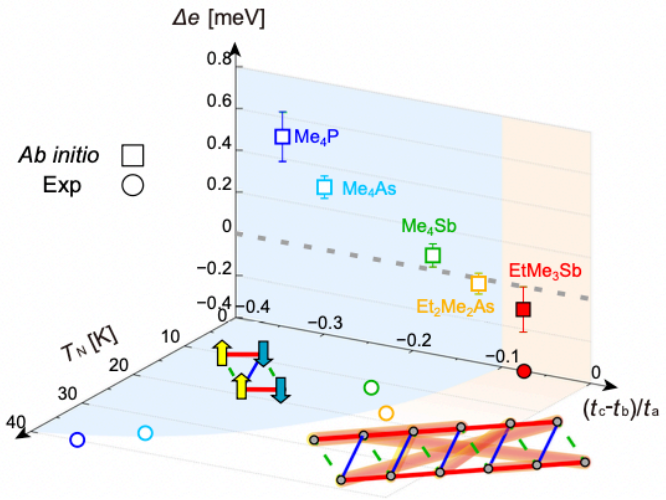

T. Misawa *et al.*, PRR 2, 032072(R) (2020)
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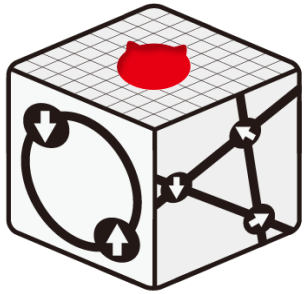
K. Ido *et al.*, npj Quantum mat. 7, 48 (2022)

Introduction: Our open-source software

✓many-variable variational Monte Carlo method (mVMC)



mVMC

-Accurate and flexible wave function method.

-Applicable to wide range of Hamiltonians including complicated low-energy Hamiltonians for real materials

Connection with ab initio derivation of low-energy effective Hamiltonians
cf. RESPACK by K. Nakamura *et al.*

✓Exact diagonalization (HΦ)

Exact calculations for
- Ground state (Lanczos, LOBCG)
- Low-energy excited state (LOBCG)
- Finite-temperature calculations (TPQ)
- Dynamical structure factors (Laczos, shifted Krylov)
- Real-time evolution

https://www.pasums.issp.u-tokyo.ac.jp/hphi/doc/presentation/

Basics of wave function methods

Model for strongly correlated electron systems

e.g. Hubbard model

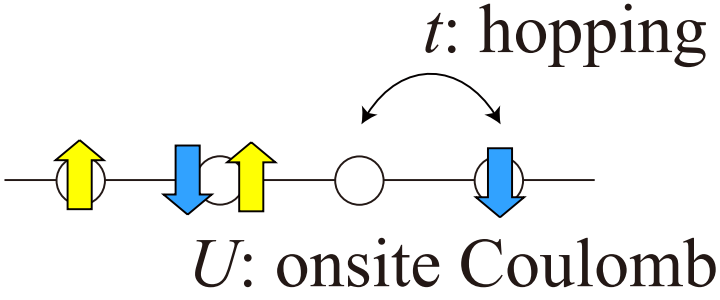
$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_t + \hat{\mathcal{H}}_U$$

Electrons as waves

$$\hat{H}_t = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma})$$

Electrons as particles

$$\hat{H}_U = \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad \hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma}$$



Relations of 2nd-quantized operators (these are all !)

$$\{\hat{c}^\dagger_{i\sigma}, \hat{c}_{j\sigma'}\} = \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma'} + \hat{c}_{j\sigma'} \hat{c}^\dagger_{i\sigma} = \delta_{i,j} \delta_{\sigma,\sigma'}$$

$$\{\hat{c}^\dagger_{i\sigma}, \hat{c}^\dagger_{j\sigma'}\} = 0 \rightarrow \hat{c}^\dagger_{i\sigma} \hat{c}^\dagger_{i\sigma} = 0$$

$$\{\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}\} = 0 \rightarrow \hat{c}_{i\sigma} \hat{c}_{i\sigma} = 0$$

Pauli's principle

Wave function = eigenvectors of Hamiltonian

Matrix representation of Hamiltonian (ex. 2 site Hubbard model)

Real-space configuration $|\uparrow,\downarrow\rangle = c^{\dagger}_{1\uparrow}c^{\dagger}_{2\uparrow}|0\rangle$

After some *tedious* calculations, $\langle\uparrow,\downarrow|\hat{H}_t|\uparrow\downarrow,0\rangle = \langle\uparrow,\downarrow|(t\sum_{\sigma} c^{\dagger}_{1\sigma}c_{2\sigma} + c^{\dagger}_{2\sigma}c_{1\sigma})|\uparrow\downarrow,0\rangle = -t$

$$\mathcal{H} = \begin{array}{c} \\ \langle\uparrow,\downarrow| \\ \langle\downarrow,\uparrow| \\ \langle\uparrow\downarrow,0| \\ \langle 0,\uparrow\downarrow| \end{array} \begin{array}{c} \begin{array}{cccc} |\uparrow,\downarrow\rangle & |\downarrow,\uparrow\rangle & |\uparrow\downarrow,0\rangle & |0,\uparrow\downarrow\rangle \end{array} \\ \begin{pmatrix} 0 & 0 & -t & -t \\ 0 & 0 & t & t \\ -t & t & U & 0 \\ -t & t & 0 & U \end{pmatrix} \end{array}$$

dimension of mat.
$d_H \sim 4^{Ns}$
[$N_s \sim 132$, $4^{132} \sim 10^{80}$]

$$|\phi\rangle = a_0|\uparrow,\downarrow\rangle + a_1|\downarrow,\uparrow\rangle + a_2|\uparrow\downarrow,0\rangle + a_3|0,\uparrow\downarrow\rangle$$

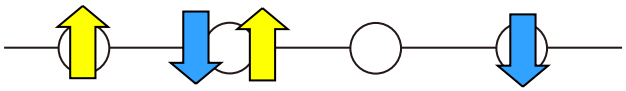
Diagonalization → eigenvalues, eigenvectors
→ Problem is completely solved (HΦ)

One-body approximation

Slater determinant

$$|\phi_{\rm one}\rangle = \prod_{\sigma,n=1}^{N_e} \psi^\dagger_{n\sigma}|0\rangle \qquad \psi^\dagger_{n\sigma} = \sum_{i=1}^{N_{\rm s}} \Phi_{i\sigma n} c^\dagger_{i\sigma}$$

Real-space configuration (t=0)



$$\Phi_{i\sigma n} = \delta_{i,n} \rightarrow \psi^\dagger_{n\sigma} = c^\dagger_{n\sigma} \rightarrow |\phi_{\rm one}\rangle = \prod_{\sigma,n}^{N_e} c^\dagger_{n\sigma}|0\rangle$$

Plane wave (U=0)

$$\Phi_{i\sigma n} = \frac{1}{N_{\rm s}^{1/2}} e^{i\vec{k}_n\cdot\vec{r}_i} \rightarrow c^\dagger_{k_n\sigma} \equiv \sum_i \Phi_{i\sigma n} c^\dagger_{i\sigma}$$

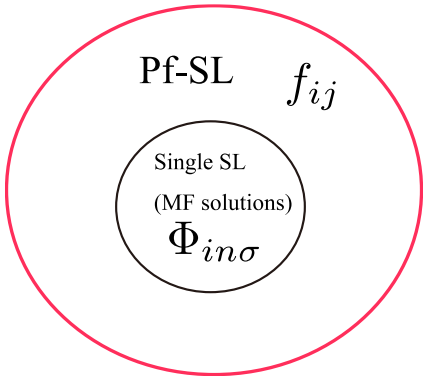
Slater determinant can describe conventional orders; antiferromagnetic order, charge orders, orbital orders …

[mVMC includes codes for UHF]

Beyond one-body approximation

Slater determinant → Pfaffian wave function

$$|\phi_{\rm one}\rangle = \prod_{\sigma,n=1}^{N_e} \left(\sum_{i=1}^{N_s} \Phi_{i\sigma n} c_{i\sigma}^\dagger\right)|0\rangle \rightarrow |\phi_{\rm Pf}\rangle = \left(\sum_{i,j}^{N_{\rm s}} f_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger\right)^{N_e}|0\rangle$$



Pfaffian wave function
- includes Slater wave function,
- can describe singlet correlations
→ superconductivity, quantum spin liquid

Introducing many-body correlations

$$|\Phi\rangle = \hat{\mathcal{P}}|\phi\rangle, \quad \hat{\mathcal{P}}_{\rm G} = e^{-g\sum_i n_{i\uparrow}n_{i\downarrow}}$$

Correlation factors → Many-body correlations can be included
→ Superconductivity by repulsive interactions can be described

Further improvement: power-Lanczos, backflow, multi-pfaffian …

Basics of variational Monte Carlo

- ***Optimization*** **of variational parameters**
  [time-dependent variational principle]

- ***Evaluation*** **of physical quantities [MC sampling]**

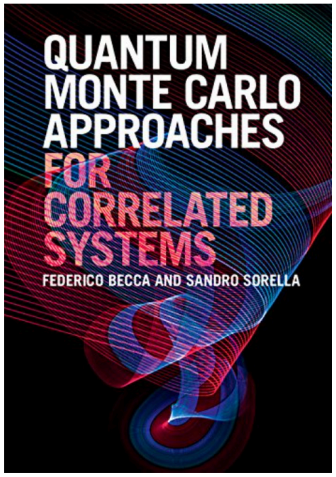
Variational Monte Carlo (VMC) I

review: C. Gros, Ann. Phys. 189, 53 (1989)

Variational principle

α:variational parameters

$$\min_{\boldsymbol{\alpha}} E(\boldsymbol{\alpha}) = \min_{\boldsymbol{\alpha}} \frac{\langle \psi(\boldsymbol{\alpha})|\hat{H}|\psi(\boldsymbol{\alpha})\rangle}{\langle \psi(\boldsymbol{\alpha})|\psi(\boldsymbol{\alpha})\rangle}$$



F. Becca & S. Sorella

Physical properties [MC sampling]

***x* :real space configuration**

$$\frac{\langle \psi|\hat{A}|\psi\rangle}{\langle \psi|\psi\rangle} = \sum_x \frac{\langle \psi|\hat{A}|x\rangle\langle x|\psi\rangle}{\langle \psi|\psi\rangle} = \sum_x \rho(x) \frac{\langle \psi|\hat{A}|x\rangle}{\langle \psi|x\rangle}$$

$$\sim \frac{1}{N_{\mathrm{MC}}} \sum_{\mathrm{MC\ sampling}} \frac{\langle \psi|\hat{A}|x\rangle}{\langle \psi|x\rangle}$$

$\langle \psi|\hat{A}|x\rangle = \langle \psi|x'\rangle$ Inner product

positive weight

$$\rho(x) = \frac{|\langle \psi|x\rangle|^2}{\langle \psi|\psi\rangle} > 0$$

Variational Monte Carlo (VMC) II

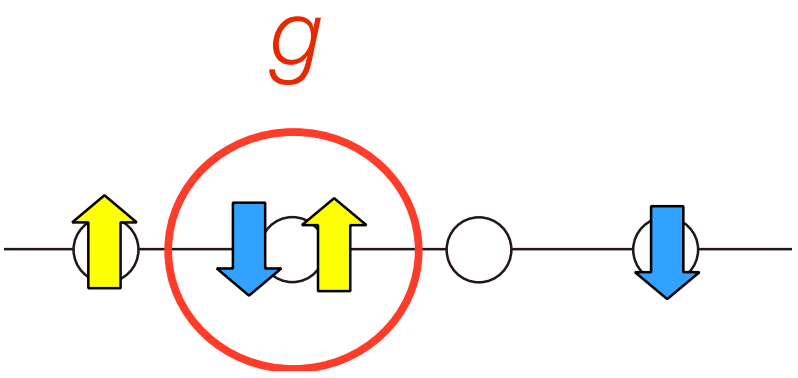
$$|\psi\rangle = \mathcal{P}_{\rm cor}|\phi_0\rangle \Rightarrow \langle\psi|x\rangle = \langle\phi_0|x\rangle\mathcal{P}_{\rm cor}(x)$$

One-body part

correlation factor

determinant or Pfaffian

Ex. Gutzwiller factor $\mathcal{P}_{\rm G} = e^{-g\sum_i n_{i\uparrow}n_{i\downarrow}}$



$$\mathcal{P}_{\rm G}|x\rangle = |x\rangle e^{-gD(x)}$$

Real-space diagonal correlation factor = easy to calculate inner product.

Wave function of mVMC

D. Tahara and M. Imada, JPSJ (2008)
T. Misawa *et al.*, CPC (2019)

$$|\psi\rangle = \mathcal{P}_{\mathrm{G}}\mathcal{P}_{\mathrm{J}}\mathcal{P}^{(2)}_{\mathrm{d-h}}\mathcal{P}^{(4)}_{\mathrm{d-h}}\mathcal{L}^{S}\mathcal{L}^{K}|\phi_{\mathrm{pair}}\rangle$$

One-body part

$$|\phi_{\mathrm{pair}}\rangle = \left[\sum_{i,j=1}^{N_{\mathrm{s}}} f_{ij}c^{\dagger}_{i\uparrow}c^{\dagger}_{j\downarrow}\right]^{N/2}|0\rangle$$

Generaized BCS wave func.
→ correlated metal,
AF, CO ordered states ,
superconducting state

Correlation factors

Gutzwiller-Jastrow $\mathcal{P}_{\mathrm{G}}$ $\mathcal{P}_{\mathrm{J}}$
doublon-holon $\mathcal{P}^{(2)}_{\mathrm{d-h}}$ $\mathcal{P}^{(4)}_{\mathrm{d-h}}$

Projections

$\mathcal{L}^{S}$: Total spin, S=0
$\mathcal{L}^{K}$: Total momentum, K=0

Update (SR method)

Mimimizing $E_{\vec{\alpha}} = \langle H \rangle_{\vec{\alpha}}$

$$\vec{\alpha}_{\mathrm{new}} - \vec{\alpha}_{\mathrm{old}} = -X^{-1}\vec{g}$$

$$g_k = \frac{\partial E_{\vec{\alpha}}}{\partial \alpha_k}$$ gradient of energy (MC Sampling)

Optimization of many variational parameters (>=10000)
→ High-accuracy wave functions for ground states

Conventional VMC v.s. mVMC

Conventional VMC:

Strong constraint on wave functions [# of parameters~10]

ex. antiferromagnetic phase

$$|\phi_{\mathrm{AF}}\rangle = \prod_{|\boldsymbol{k}|<k_F,\sigma} a^{\dagger}_{\boldsymbol{k}\sigma}|0\rangle$$

$$a^{\dagger}_{\boldsymbol{k}\sigma} = u_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} + \sigma v_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}+\boldsymbol{Q},\sigma}$$

$$u^2_{\boldsymbol{k}} = \frac{1}{2}\left(1 - \frac{E_{\boldsymbol{k}}}{\sqrt{E^2_{\boldsymbol{k}} + \Delta^2_{\mathrm{AF}}}}\right)$$

Variational parameters = AF order parameter + etc.

Disadvantages of conventional VMC

- Accuracy is *not enough* due to the strong constraint
- *Overestimating* the stability of ordered phases
- It is difficult to treat *realistic models* (*ab initio* models)

$$\mathcal{H} = \sum_{\sigma}\sum_{\boldsymbol{R}\boldsymbol{R}'}\sum_{nm} t_{m\mathbf{R}n\mathbf{R}'} a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'} \quad \rightarrow \text{Hopping Term}$$

$$+\frac{1}{2}\sum_{\sigma\rho}\sum_{\boldsymbol{R}\boldsymbol{R}'}\sum_{nm}\Big\{U_{m\mathbf{R}n\mathbf{R}'} a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{m\boldsymbol{R}'} a^{\rho}_{m\boldsymbol{R}'} a^{\sigma}_{n\boldsymbol{R}} \rightarrow \text{Coulomb Term}$$

$$+J_{m\mathbf{R}n\mathbf{R}'}\left(a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{m\boldsymbol{R}} a^{\rho}_{n\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'} + a^{\sigma\dagger}_{n\boldsymbol{R}} a^{\rho\dagger}_{n\boldsymbol{R}} a^{\rho}_{m\boldsymbol{R}} a^{\sigma}_{m\boldsymbol{R}'}\right)\Big\} \rightarrow \text{Exchange Term}$$

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Conventional VMC:

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Variational parameters = AF order parameter + etc.

many-variable VMC (mVMC):
flexibility of one-body part [# of parameters > 10000]

$$|\phi_{\mathrm{AP}}\rangle = \left(\sum_{i,j} f_{ij} c^\dagger_{i\uparrow} c^\dagger_{j\downarrow}\right)^{N_e/2}|0\rangle$$

$$|\phi_{\mathrm{AP+P}}\rangle = \left(\sum_{i\sigma,j\tau} F_{i\sigma,j\tau} c^\dagger_{i\sigma} c^\dagger_{j\tau}\right)^{N_e/2}|0\rangle$$

f_{ij} , F_{IJ}:variational parameters

f_{ij} [*i,j* real-space indices] → correlated paramagnetic state, symmetry breaking phase (AF etc.), SC states

Optimization method

SR method [S. Sorella, PRB 2001]
Natural gradient [S.-I. Amari, Neural Comp. 1998]

(General) Gradient method

α:variational parameters

$$\Delta\boldsymbol{\alpha} = \boldsymbol{\alpha}_{\mathrm{new}} - \boldsymbol{\alpha}_{\mathrm{old}} = -X^{-1}\boldsymbol{g} \quad \left(g_k = \frac{\partial E_{\boldsymbol{\alpha}}}{\partial \alpha_k}\right)$$

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Steepest decent method [slow due to *redundancy*]

$$X = I \ (\text{identity matrix})$$

Newton method [second derivatives are expensive]

$$X = h \ (\text{Hessian} : h_{\alpha\beta} = \frac{\partial^2 E}{\partial\alpha\partial\beta})$$

Optimization method

SR method [S. Sorella, PRB 2001]
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$$X = I \ (\text{identity matrix})$$

Newton method [second derivatives are expensive]

$$X = h \ (\text{Hessian} : h_{\alpha\beta} = \frac{\partial^2 E}{\partial\alpha\partial\beta})$$

Stochastic reconfiguration (SR) method [fast & stable]

$$X = S \ (\text{overlap matrix} : S_{\alpha\beta} = \langle\bar{\psi}_\alpha|\bar{\psi}_\beta\rangle)$$

$$|\bar{\psi}_\alpha\rangle = \frac{\partial|\bar{\psi}\rangle}{\partial\alpha}, \ |\bar{\psi}\rangle = \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}}$$

Time-dependent variational principle

Imaginary time evolution

$$\frac{\partial|\psi\rangle}{\partial\tau} = -\hat{H}|\psi\rangle$$

$$\left|\left|\frac{\partial|\psi\rangle}{\partial\tau} + \hat{H}|\psi\rangle\right|\right| = 0 \rightarrow \min_{\boldsymbol{\alpha}}\left|\left|\sum_k \frac{\partial\alpha_k}{\partial\tau}\frac{\partial|\psi\rangle}{\partial\alpha_k} + \hat{H}|\psi\rangle\right|\right|$$

(imaginary) time-dependent *variational principle*
A. D. McLachlan, Mol. Phys. 8, 39 (1964)

SR method
= imaginary-time evolution in restricted Hilbert space

$$\min_{\boldsymbol{\alpha}}\left|\left|\sum_k \frac{\partial\alpha_k}{\partial\tau}\frac{\partial|\bar{\psi}\rangle}{\partial\alpha_k} + (\hat{H} - \langle\hat{H}\rangle)|\bar{\psi}\rangle\right|\right|$$

$$\rightarrow \Delta\boldsymbol{\alpha} = -\frac{\Delta\tau}{2}S^{-1}\boldsymbol{g}$$

***S*: overlap matrix**

SR method can be used for real-time evolution (Ido et al., PRB 2015) & finite-temperature calculations (Takai et al., JPSJ 2016)

Advantages of mVMC

- **No negative-sign problem**
  positive weight $\rho(x) > 0$

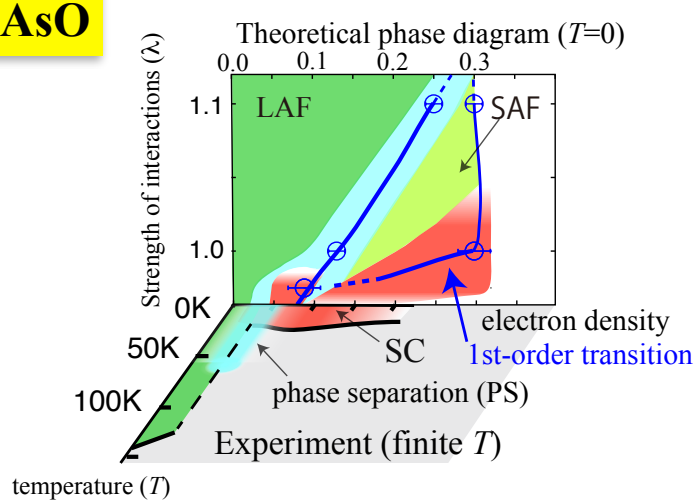
- **Wide applicable range [strong correlations, geometrical frustration, multi orbital system, any dimensions …]**
- **Natural extensions of mean-field calculations**
- **Easy to include many-body correlations through correlation factors (Gutzwiller, Jastrow, Doublon-Holon..)**
- **Systematic improvement is possible (power Lanczos, backflow, multi Pfaffian method …)**
- **Not only for ground-state calculations →**

finite-temperature calculations, real-time evolution !

Applications of mVMC I

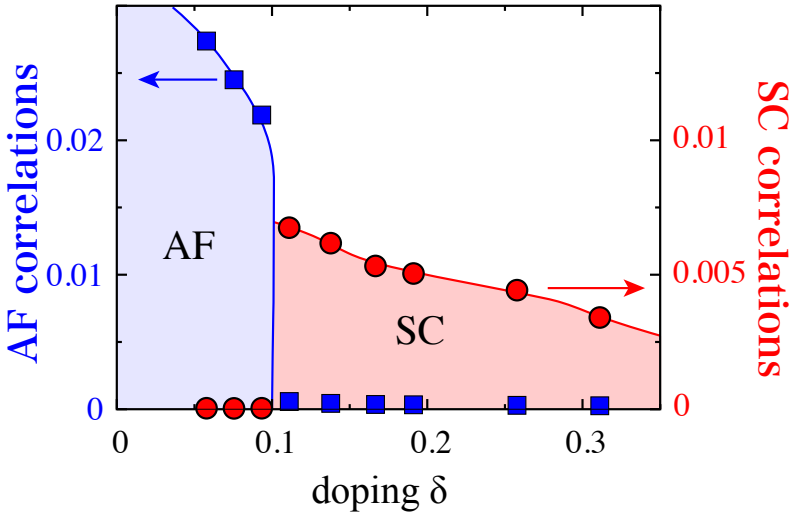
High-Tc SC

LaFeAsO



T. Misawa and M. Imada, Nat. Commun (2014).

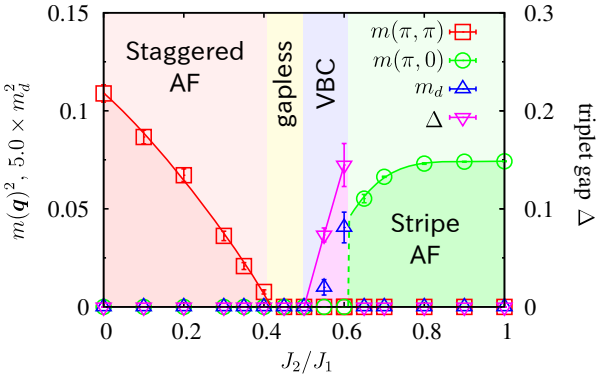
$HgBa_2CuO_{4+\delta}$



T. Ohgoe *at al*., PRB (2020).

Quantum spin liquid

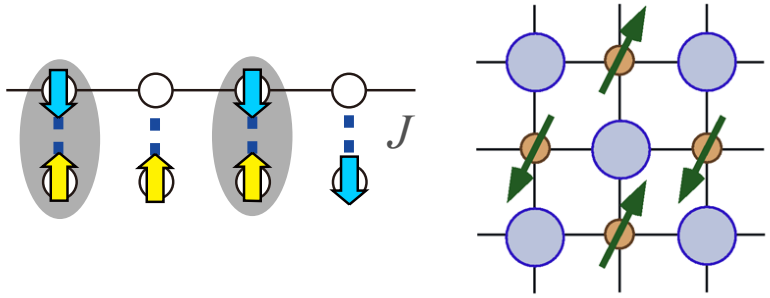
J_1-J_2 Heisenberg



S. Motira and M. Imada JPSJ (2014).
see also Y. Nomura and M. Imada PRX (2021).

Heavy fermion systems

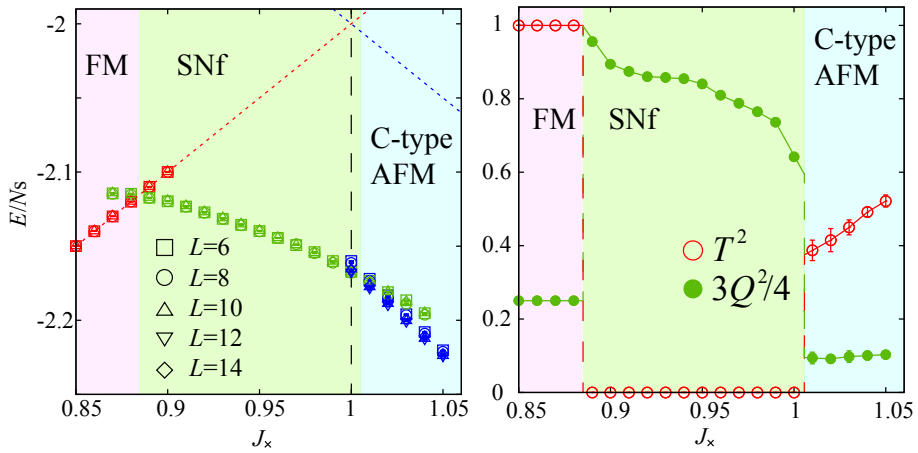
CO in Kondo larice model



T. Misawa *at al*., PRL (2013).

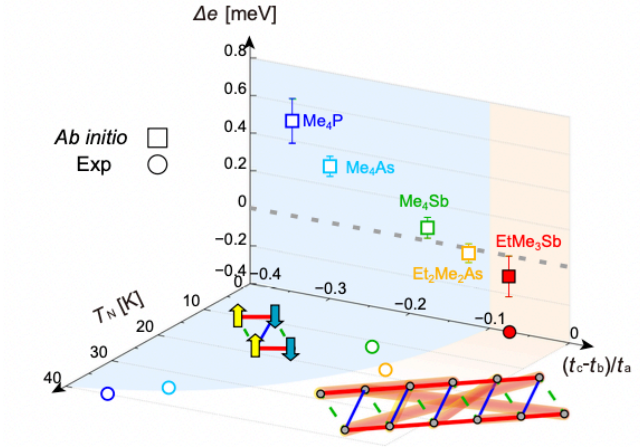
Applications of mVMC II

Spin nematic phase



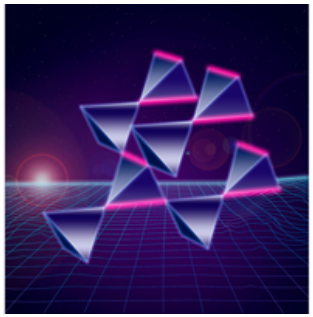
T. Hikihara et al., PRB(2019)

Quantum spin liquid in dmit salts



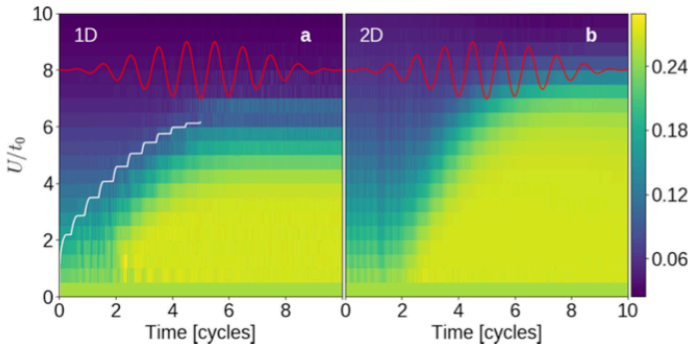
K. Ido *et al*., npj QM (2022)

Heisenberg model on pyrochlore lattice



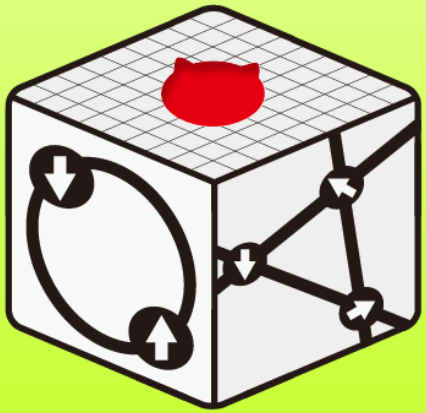
N. Astrakhantesev et al., PRX (2021)

HHG in 2D Mott ins.



C. Orthodoxou *et al*., npj QM (2021)

Open-source software of mVMC



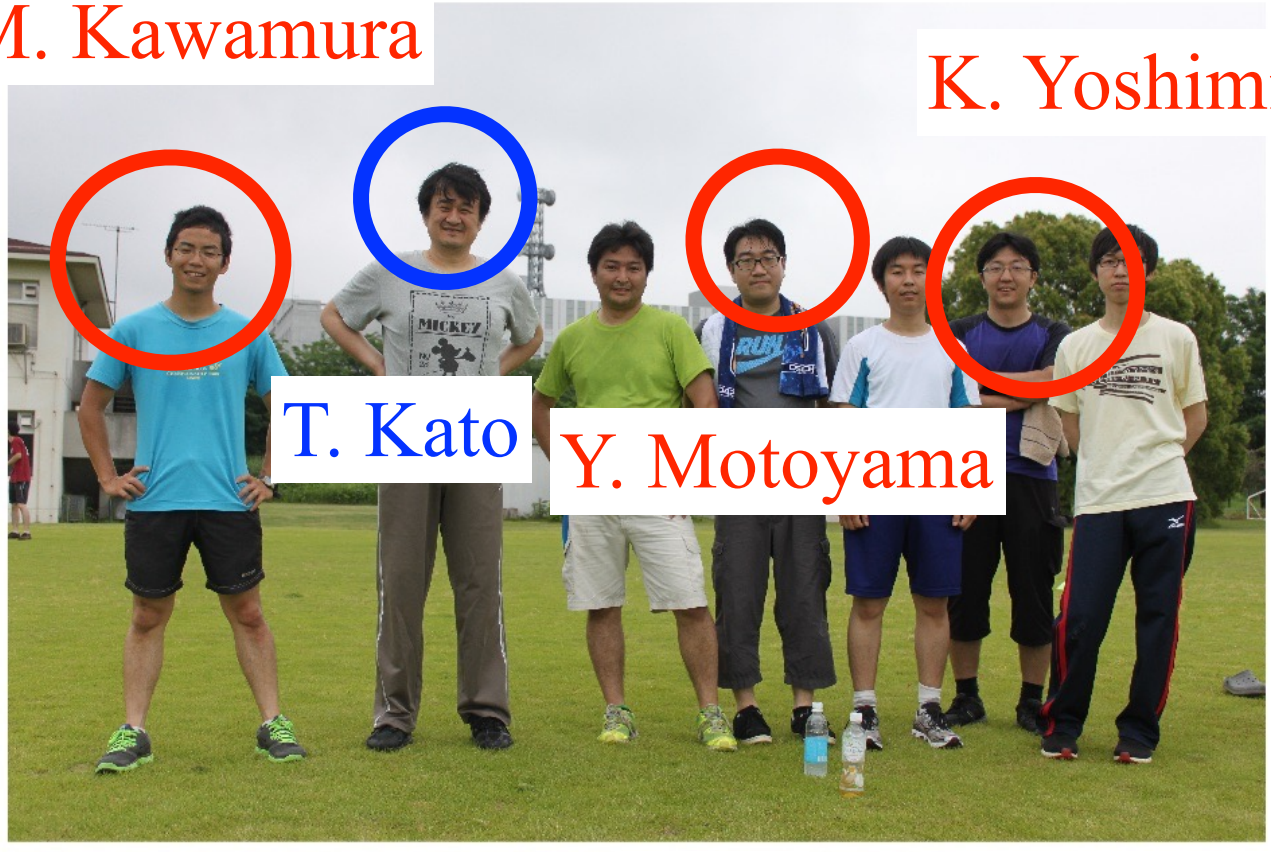
mVMC

https://www.pasums.issp.u-tokyo.ac.jp/mvmc/

Developers of mVMC

M. Kawamura

K. Yoshimi

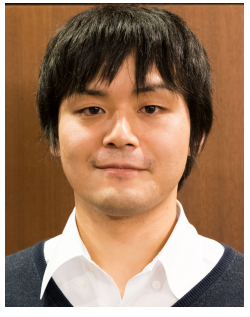


T. Kato

Y. Motoyama

S. Morita

T. Ohgoe



M. Imada

K. Ido

RuQing Xu

Development of mVMC is supported by "*Project for advancement of software usability in materials science*" by ISSP

How to get mVMC

GitHub → https://github.com/issp-center-dev/mVMC

HP → https://www.pasums.issp.u-tokyo.ac.jp/mvmc/

tutorial → https://github.com/issp-center-dev/mVMC-tutorial

- mVMC is pre-installed in supercomputer in ISSP (ohtaka, kugui)

/home/issp/materiapps/intel/mvmc/

全国のスパコンにもプレインストール [RIST]

https://www.hpci-office.jp/for_users/appli_software/appli_mvmc

北海道大学　情報基盤センター (Grand Chariot)

東北大学 サイバーサイエンスセンター (AOBA)

東京大 情報基盤センター(Wisteria, Oakbridge-CX)

東工大 学術国際情報センター (TUBAME3.0)

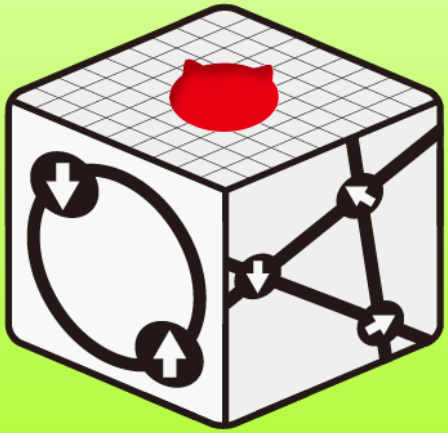
名古屋大工 情報基盤センター (不老 [Furou])

大阪大 サイバーメディアセンター (OCTOPUS)

理研　計算科学研究センター(富岳 [Fugaku])

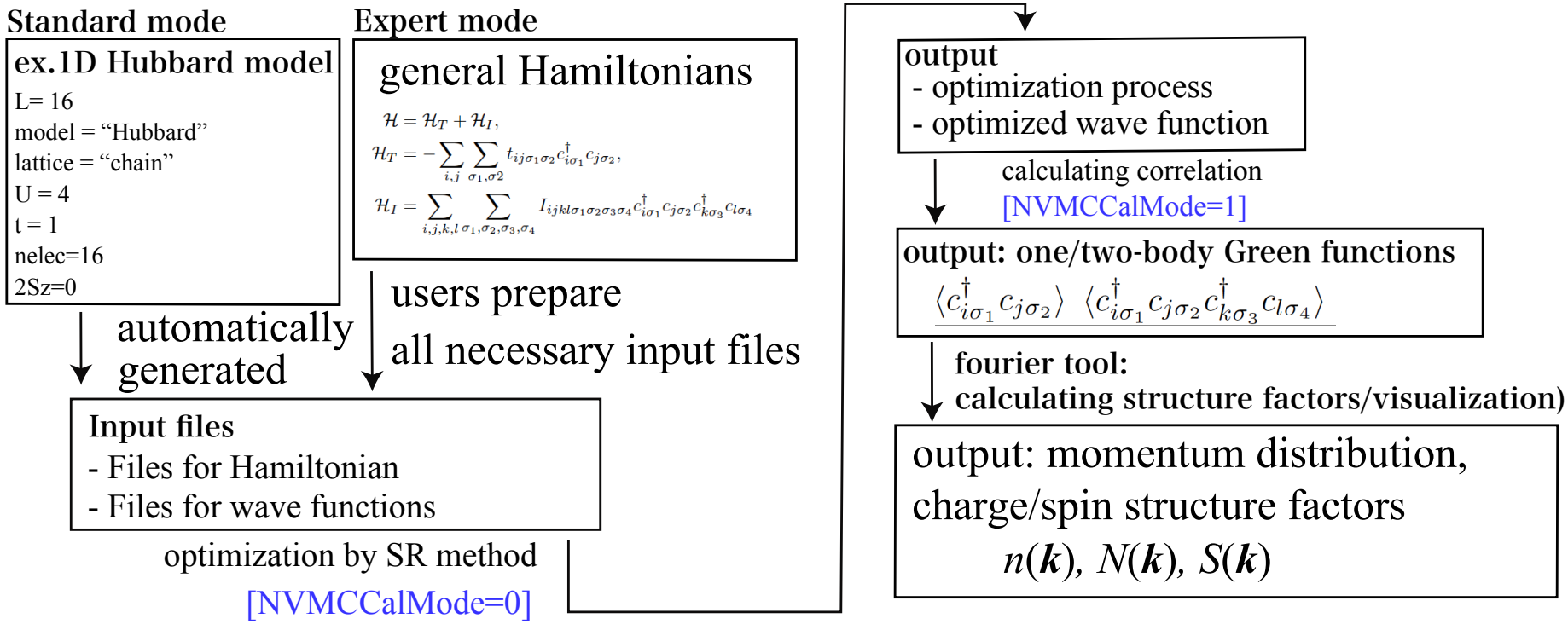
九州大学 情報基盤研究開発センター (ITO)

Let’s start mVMC !



mVMC

Flow of mVMC



Users

1.Preparing and/or modifying input files

2.Calculations structure factors from correlations functions

It is better to use *script languages* (python, perl, ruby ….) for preparing input files and calculation physical properties
In this tutorial, we use python3+bash scripts.

How to use mVMC: Standard model

$$H = -t \sum_{\langle i,j \rangle,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{H.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

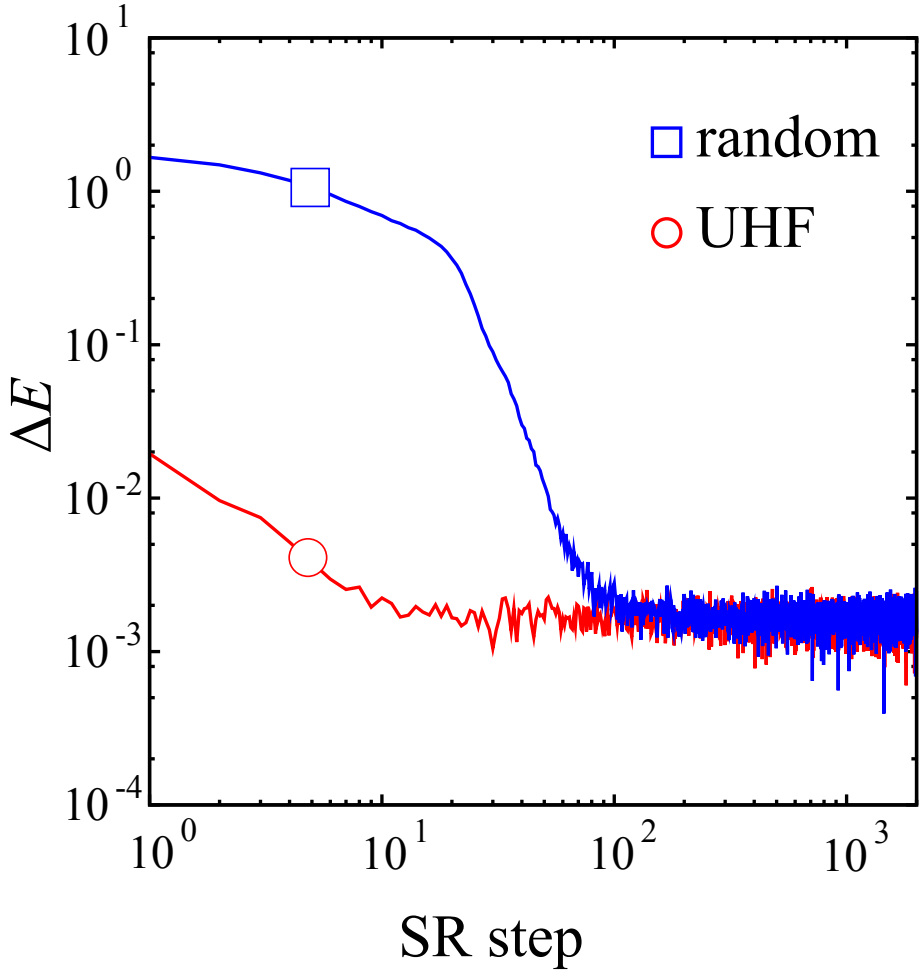
```
W = 4
L = 4
Wsub = 2
Lsub = 2
model = "FermionHubbard"
lattice = "Tetragonal"
t = 1.0
U = 4.0
nelec = 16
```

Simple input files for conventional models

How to use mVMC: Standard mode II

vmcdry stan_opt.in ⇨ Generating input files

vmc namelist.def ⇨ Optimization



2D Hubbard model,
4×4,U/t=4,n=1

on laptop
~ 2-3 minutes

Generating initial states

Slater determinant [mean-field wave func.]

$$|\phi_{\mathrm{SL}}\rangle = \prod_{n=1,\sigma}^{N_e/2} \psi^\dagger_{n\sigma}|0\rangle$$

unitary trans. of one-body states

$$\psi^\dagger_{n\sigma} = \sum_{i=1}^{N_s} \Phi_{in\sigma} c^\dagger_{i\sigma}$$

$$\sum_{i=1}^{N_s} \Phi_{in\sigma}\Phi_{im\sigma} = \delta_{nm}$$

$$f_{ij} = \sum_{n=1}^{\frac{N_e}{2}} \Phi_{in\uparrow}\Phi_{jn\downarrow}$$

Pfaffian Slater determinant
(Pairing wave function)

$$|\phi_{\mathrm{Pf}}\rangle = \left(\sum_{i,j=1}^{N_s} f_{ij} c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} \right)^{N_e/2} |0\rangle$$

Initial states from Unrestricted Hartree-Fock (UHF) calc.

Preparing the codes for performing UHF calc. (usr/share/mvmc/tool)

Hubbard model

$$S(\boldsymbol{q}) = \frac{1}{3N_{\mathrm{s}}} \sum_{i,j} \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}$$

Physical Properties	mVMC(2×2)	ED
4×4(PP),$n = 1$		
Energy per site	-0.8500(1)	-0.8513
$S(\boldsymbol{q}_{\mathrm{peak}})/N_{\mathrm{s}}$	0.0575(2)	0.0569
$\boldsymbol{q}_{\mathrm{peak}}$	(π,π)	(π,π)
$\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle$	-0.2063(14)	-0.2063
4×4(PP),$n = 0.625$		
Energy per site	-1.2196(1)	-1.22380
$S(\boldsymbol{q}_{\mathrm{peak}})/N_{\mathrm{s}}$	0.0130(1)	0.01300
$\boldsymbol{q}_{\mathrm{peak}}$	$(\pi/2,\pi)$	$(\pi/2,\pi)$
$\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle$	-0.0704(5)	-0.0683

mVMC well reproduces results of exact diagonalization!
It is possible to calculate larger system sizes (100-1000 sites)

How to use mVMC: What is Standard mode ?

vmcdry stan_opt.in

Standard mode:
Automatically generating input files

[Common in HΦ, mVMC]

Hamiltonians
coulombintra.def, trans.def, zlocspn.def …

Green functions
greenone.def, greentwo.def

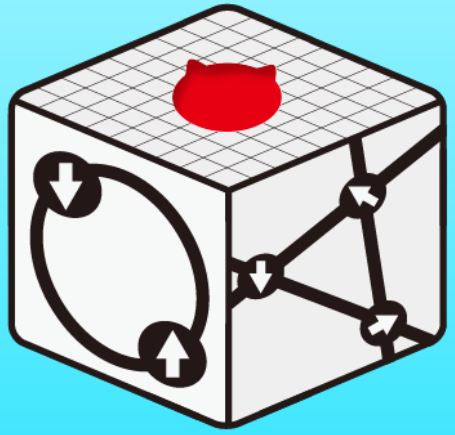
Specifying calculations conditions
modpara.def

[mVMC]

Specifying wave functions
orbitalidx.def, gutzwilleridx.def,jastrowidx.def…

+List of input files: namelist.def

Expert mode: preparing input files manually



mVMC

Expert mode !

How to use mVMC: What is Expert mode ?

Expert mode:preparing input files by yourself

[Common in HPhi,UHF] Specifying Hamiltonians

coulombintra.def, trans.def, zlocspn.def …

Specifying calculations conditions

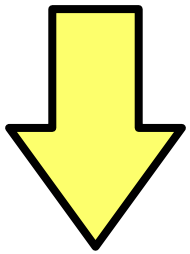
modpara.def

Specifying wave functions

orbitalidx.def, gutzwilleridx.def,jastrowidx.def…

[Common in HPhi,UHF] Specifying correlations factors

greenone.def, greentwo.def



vmc.out namelist.def

How to use mVMC: Interall.def

Example for general interactions

$$H+=\sum_{i,j,k,l}\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4} c^{\dagger}_{i\sigma_1} c_{j\sigma_2} c^{\dagger}_{k\sigma_3} c_{l\sigma_4}$$

```
======================
NInterAll      96
======================
========zInterAll=====
======================
```

# of interactions parameters

								real part	**imaginary part**
0	0	0	0	1	0	1	0	0.500000	0.000000
0	0	0	0	1	1	1	1	-0.500000	0.000000
0	1	0	1	1	0	1	0	-0.500000	0.000000
0	1	0	1	1	1	1	1	0.500000	0.000000
0	0	0	1	1	1	1	0	1.000000	0.000000
0	1	0	0	1	0	1	1	1.000000	0.000000
...									
i	σ_1	j	σ_2	k	σ_3	l	σ_4		

Arbitrary two-body interactions can be treated

How to use mVMC: Expert mode

For standards interactions

- CoulombIntra $H+ = \sum_i U_i n_{i\uparrow} n_{i\downarrow}$

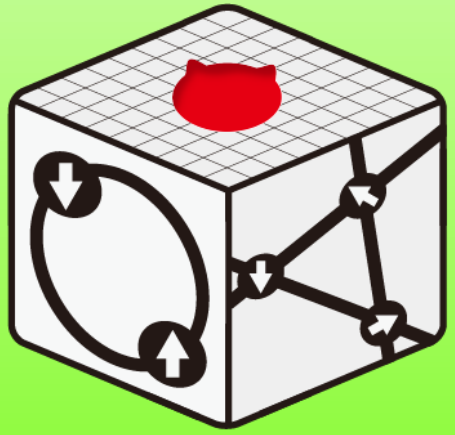
```
================================
NCoulombintra 2
================================
===========Exchange=============
================================
 0    4.0
 1    4.0
```

-Exchange $\mathcal{H}_E = \sum_{i,j} J_{ij}^{\mathrm{Ex}} (c_{i\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow}^\dagger c_{i\uparrow})$

```
================================
NExchange 2
================================
===========Exchange=============
================================
 0    1   0.5
 1    2   0.5
```

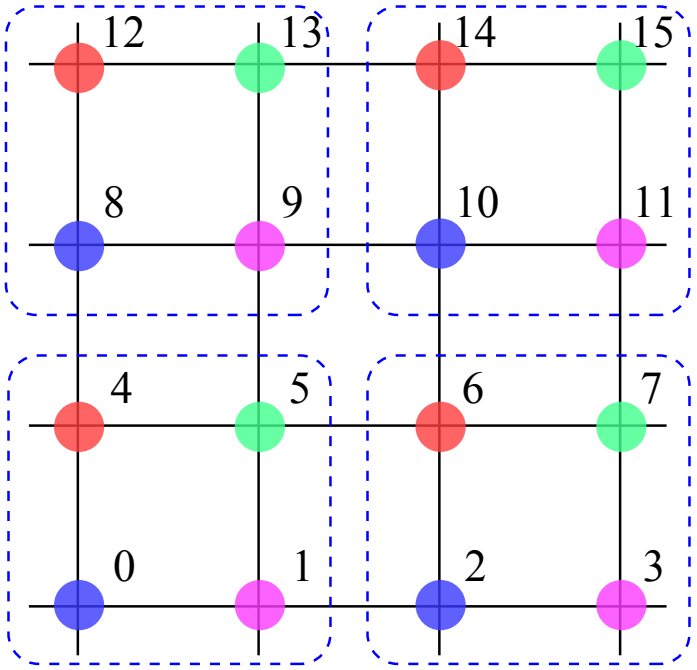
For details, see manuals

Tips on mVMC !



mVMC

sub lattice



ex.

$$f_{0,9} = f_{2,11}$$

To reduce numerical cost, we often assume the sub lattice structure in the wave functions

2×2 structure is standard one in the square lattice

[Lsub ,Wsub]

Tips:

- **Sub lattice structure is consistent with the ordered states?**
- **Sub lattice structure is consistent with the sym. of Hamiltonian?**
- **Sub lattice structure is consistent with the momentum projection?**

Quantum number projections

$$|\psi\rangle = \mathcal{P}\mathcal{L}|\phi_{\mathrm{pair}}\rangle$$

- Total spin projection is *only* applicable to the Hamiltonian with SU(2) symmetry and total Sz=0 [modpara.def]

-Momentum projection is only applicable to *only* for systems with translational symmetry [modpara.def, qptrans.def]

Tips:

- **Projection is consistent with the sym. of ground states ?**
- **Projection is consistent with the sym. of Hamiltonias ?**

Note that there is systems with total Sz=0 but SU(2) symmetry is not conserved [ex. Kane-Mele,BHZ model]

- **Projection is consistent with the sym. of correlations factors ?**

Check points

- For non-interactions case, exact energy is reproduced ?

(Check for fij)

- Compare with the results by exact diagonalization for small system sizes !

- Energy is lower than the mean-filed calculations ?

- Sub lattice structure is proper ?

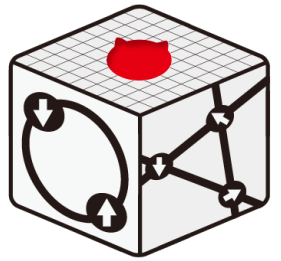
Summary

Basics of mVMC:

- **Flexible wave functions (# of parameter > 10^4)**
- ***Time-dependent variational principle*** **→ optimization of many variational parameters**
  finite-temperature calculations
  real-time evolutions

How to use mVMC:

- **Simple & Flexible user interfaces**
- ***Very easy*** **to study conventional models**
- ***Easy*** **to study general models**



mVMC