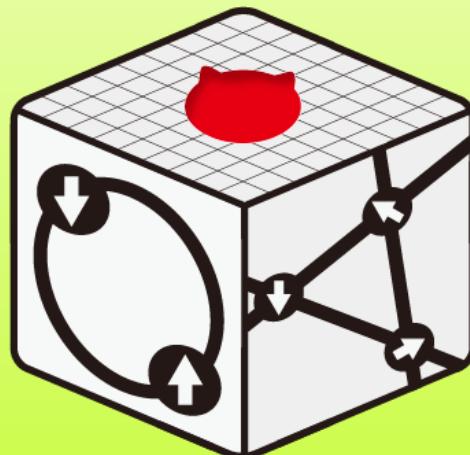


# Introduction to mVMC

Takahiro Misawa

Beijing Academy of Quantum Information Sciences (BAQIS)



**mVMC**

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

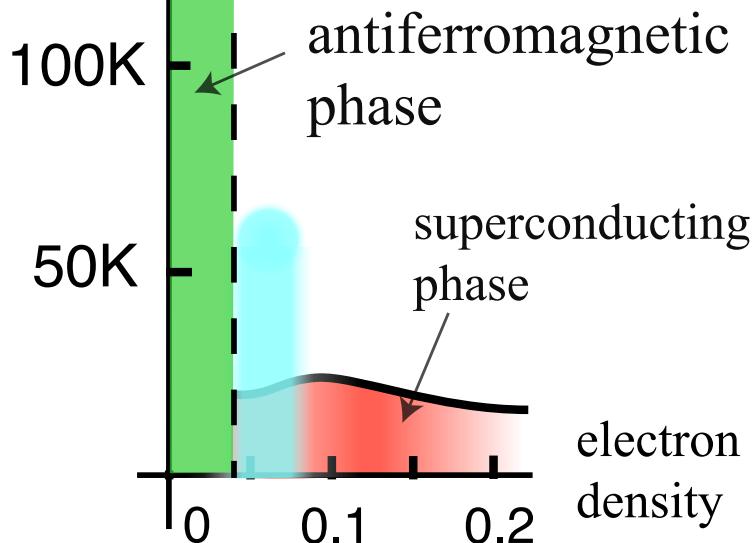
# Outline

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

temperature



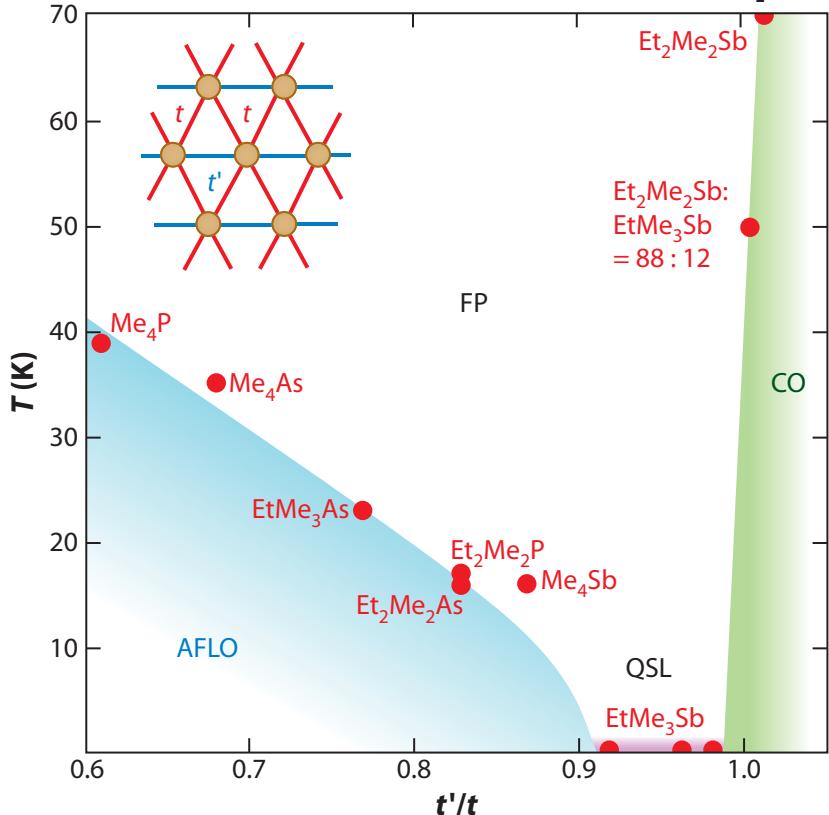
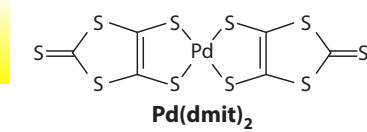
Y. Kamihara *et al*, JACS (2008)

High-Tc SC in iron-based compound

To clarify and predict exotic phenomena in SCES

→ Accurate numerical methods for solving low-energy effective models are necessary

$\beta'$ -X[Pd(dmit)<sub>2</sub>]<sub>2</sub>



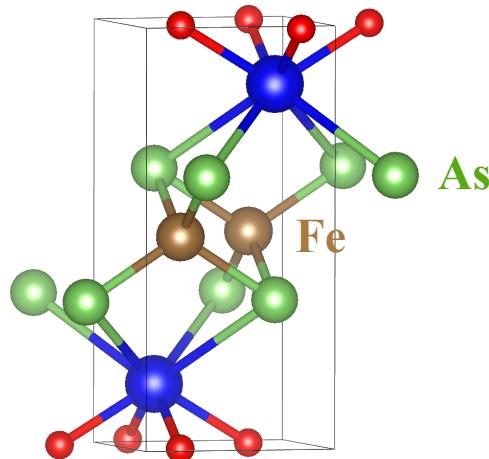
K. Kanoda and R. Kato,  
Annu. Rev. Condens. Phys. 2011  
QSL in organic solids

# Low-energy effective models

LaFeAsO

5-orbital Hubbard Hamiltonians  
obtained by ab initio calculations

$$\begin{aligned} \mathcal{H} = & \sum_{\sigma} \sum_{RR'} \sum_{nm} t_{mRnR'} a_{nR}^{\sigma\dagger} a_{mR'}^{\sigma} \rightarrow \text{Hopping Term} \\ & + \frac{1}{2} \sum_{\sigma\rho} \sum_{RR'} \sum_{nm} \left\{ U_{mRnR'} a_{nR}^{\sigma\dagger} a_{mR'}^{\rho\dagger} a_{mR'}^{\rho} a_{nR}^{\sigma} \right. \rightarrow \text{Coulomb Term} \\ & \left. + J_{mRnR'} (a_{nR}^{\sigma\dagger} a_{mR'}^{\rho\dagger} a_{nR}^{\rho} a_{mR'}^{\sigma} + a_{nR}^{\sigma\dagger} a_{nR'}^{\rho\dagger} a_{mR'}^{\rho} a_{mR'}^{\sigma}) \right\} \rightarrow \text{Exchange Term} \end{aligned}$$

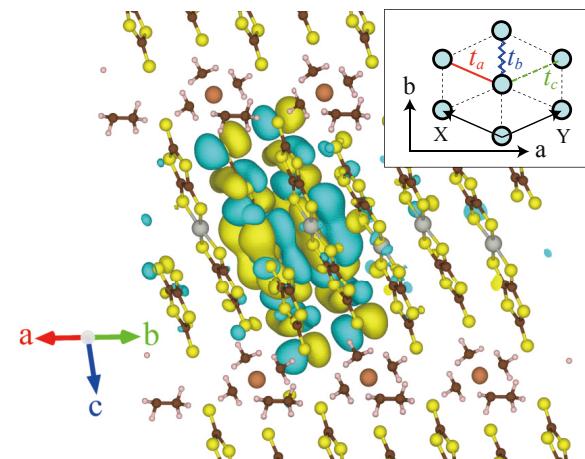


T. Misawa *et al.*, Nat. Com. 5, 5738 (2014)

EtMe<sub>3</sub>Pb[Pd(dmit)<sub>2</sub>]<sub>2</sub>

Single-band Hubbard Hamiltonians  
obtained by ab initio calculations

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



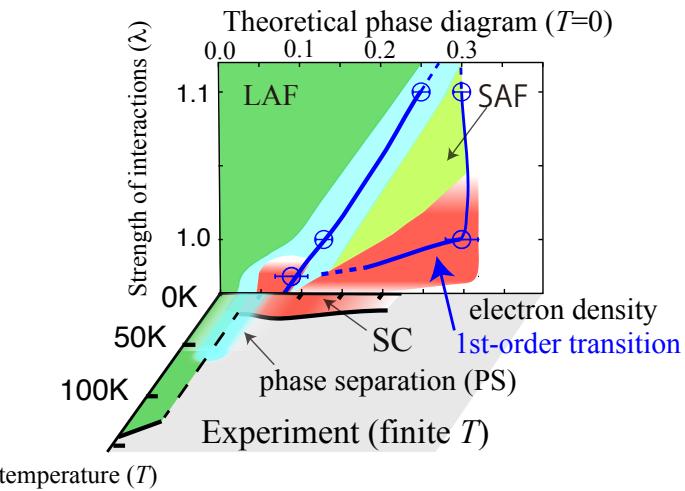
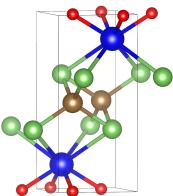
T. Misawa *et al.*, PRR 2, 032072(R) (2020)  
K. Yoshimi *et al.*, PRR 3, 043224 (2021)  
K. Ido *et al.*, npj Quantum mat. 7, 48 (2022)

# Low-energy effective models

**LaFeAsO**

**5-orbital Hubbard Hamiltonians  
obtained by ab initio calculations**

$$\begin{aligned} \mathcal{H} = & \sum_{\sigma} \sum_{RR'} \sum_{nm} t_{mRnR'} a_{nR}^{\sigma\dagger} a_{mR'}^{\sigma} \rightarrow \text{Hopping Term} \\ & + \frac{1}{2} \sum_{\sigma\rho} \sum_{RR'} \sum_{nm} \left\{ U_{mRnR'} a_{nR}^{\sigma\dagger} a_{mR'}^{\rho\dagger} a_{mR'}^{\rho} a_{nR}^{\sigma} \right. \rightarrow \text{Coulomb Term} \\ & \left. + J_{mRnR'} (a_{nR}^{\sigma\dagger} a_{mR'}^{\rho\dagger} a_{nR}^{\rho} a_{mR'}^{\sigma} + a_{nR}^{\sigma\dagger} a_{nR'}^{\rho\dagger} a_{mR'}^{\rho} a_{mR'}^{\sigma}) \right\} \rightarrow \text{Exchange Term} \end{aligned}$$

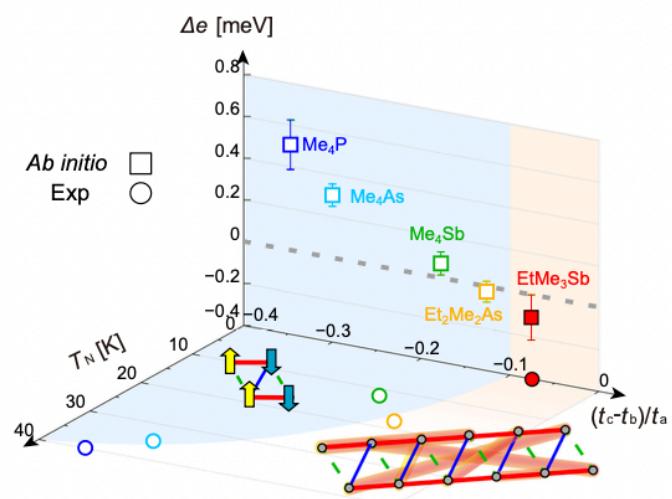
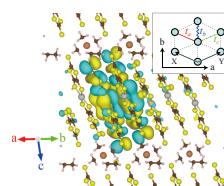


T. Misawa *et al.*, Nat. Com. 5, 5738 (2014)

**$\beta'$ -X[Pd(dmit)<sub>2</sub>]<sub>2</sub>**

**Single-band Hubbard Hamiltonians  
obtained by ab initio calculations**

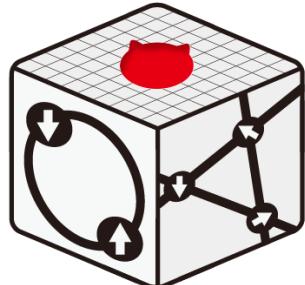
$$H = \sum_{i,j} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i,j} V_{i,j} n_i n_j$$



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)

# 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 ( $H\Phi$ )



Exact calculations for

- Ground state (Lanczos, LOBCG)
- Low-energy excited state (LOBCG)
- Finite-temperature calculations (TPQ)
- Dynamical structure factors (Lanczos, 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

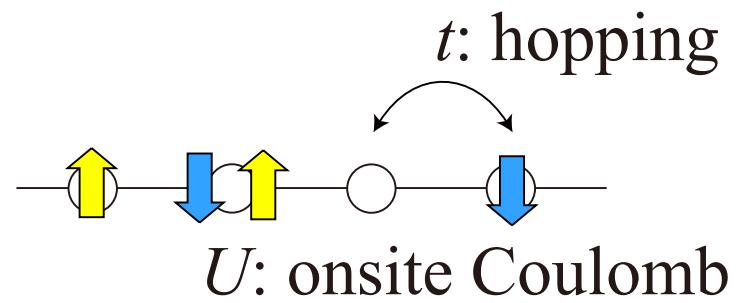
$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_t + \hat{\mathcal{H}}_U$$

Electrons as waves

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

Electrons as particles

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



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

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

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

Pauli's principle

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

# Wave function = eigenvectors of Hamiltonian

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

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

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

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

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

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

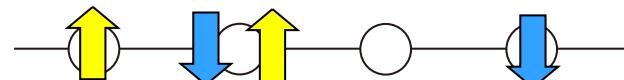
Diagonalization → eigenvalues, eigenvectors  
→ Problem is completely solved ( $H\Phi$ )

# One-body approximation

## Slater determinant

$$|\phi_{\text{one}}\rangle = \prod_{\sigma, n=1}^{N_e} \psi_{n\sigma}^\dagger |0\rangle \quad \psi_{n\sigma}^\dagger = \sum_{i=1}^{N_s} \Phi_{i\sigma n} c_{i\sigma}^\dagger$$

Real-space configuration ( $t=0$ )



$$\Phi_{i\sigma n} = \delta_{i,n} \rightarrow \psi_{n\sigma}^\dagger = c_{n\sigma}^\dagger \rightarrow |\phi_{\text{one}}\rangle = \prod_{\sigma, n}^{N_e} c_{n\sigma}^\dagger |0\rangle$$

Plane wave ( $U=0$ )

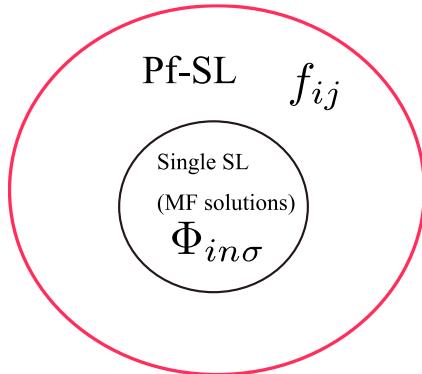
$$\Phi_{i\sigma n} = \frac{1}{N_s^{1/2}} e^{i \vec{k}_n \cdot \vec{r}_i} \rightarrow c_{k_n \sigma}^\dagger \equiv \sum_i \Phi_{i\sigma n} c_{i\sigma}^\dagger$$

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

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



Pfaffian wave function

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

Introducing many-body correlations

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

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)

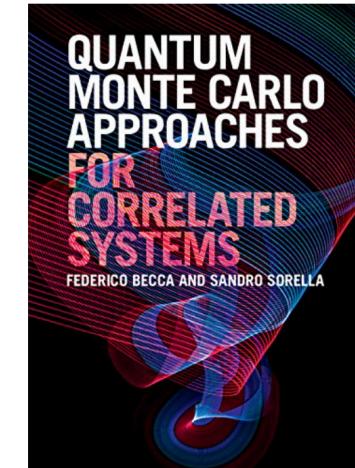
## Variational principle

$\alpha$ : variational parameters

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

Physical properties [MC sampling]

$x$  : real space configuration



F. Becca & S. Sorella

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

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

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

Inner product

positive weight

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

# Variational Monte Carlo (VMC) II

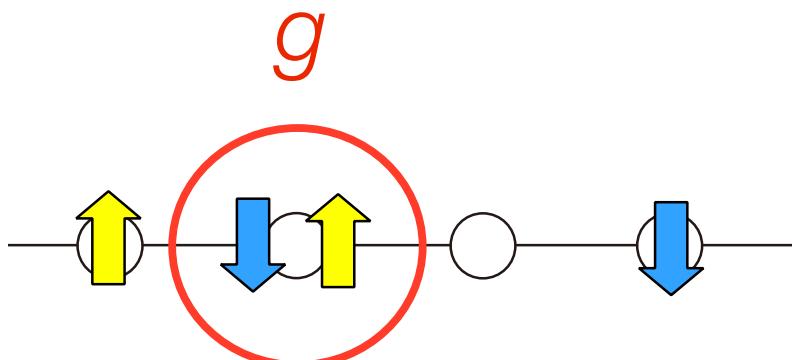
$$|\psi\rangle = \mathcal{P}_{\text{cor}} |\phi_0\rangle \rightarrow \langle\psi|x\rangle = \langle\phi_0|x\rangle \mathcal{P}_{\text{cor}}(x)$$

One-body part  
correlation factor

determinant or Pfaffian

Ex. Gutzwiller factor

$$\mathcal{P}_G = e^{-g \sum_i n_{i\uparrow} n_{i\downarrow}}$$



$$\mathcal{P}_G |x\rangle = |x\rangle e^{-g D(x)}$$

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)

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

## One-body part

$$|\phi_{\text{pair}}\rangle = \left[ \sum_{i,j=1}^{N_s} f_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \right]^{N/2} |0\rangle$$

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

## Correlation factors

Gutzwiller-Jastrow  $\mathcal{P}_G$   $\mathcal{P}_J$   
doublon-holon  $\mathcal{P}_{d-h}^{(2)}$   $\mathcal{P}_{d-h}^{(4)}$

## Projections

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

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

## Update (SR method)

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

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

$$g_k = \frac{\partial E_{\vec{\alpha}}}{\partial \alpha_k} \quad \begin{array}{l} \text{gradient of energy} \\ \text{(MC Sampling)} \end{array}$$

**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

$$|\phi_{\text{AF}}\rangle = \prod_{|\mathbf{k}| < k_F, \sigma} a_{\mathbf{k}\sigma}^\dagger |0\rangle$$

$$a_{\mathbf{k}\sigma}^\dagger = u_{\mathbf{k}} c_{\mathbf{k},\sigma}^\dagger + \sigma v_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q},\sigma}^\dagger$$

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left( 1 - \frac{E_{\mathbf{k}}}{\sqrt{E_{\mathbf{k}}^2 + \Delta_{\text{AF}}^2}} \right)$$

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)

$$\begin{aligned} \mathcal{H} = & \sum_{\sigma} \sum_{\mathbf{R}\mathbf{R}'} \sum_{nm} t_{m\mathbf{R}n\mathbf{R}'} a_{n\mathbf{R}}^{\sigma\dagger} a_{m\mathbf{R}'}^{\sigma} \rightarrow \text{Hopping Term} \\ & + \frac{1}{2} \sum_{\sigma\rho} \sum_{\mathbf{R}\mathbf{R}'} \sum_{nm} \left\{ U_{m\mathbf{R}n\mathbf{R}'} a_{n\mathbf{R}}^{\sigma\dagger} a_{m\mathbf{R}'}^{\rho\dagger} a_{m\mathbf{R}'}^{\rho} a_{n\mathbf{R}}^{\sigma} \right\} \rightarrow \text{Coulomb Term} \\ & + J_{m\mathbf{R}n\mathbf{R}'} (a_{n\mathbf{R}}^{\sigma\dagger} a_{m\mathbf{R}}^{\rho\dagger} a_{n\mathbf{R}}^{\rho} a_{m\mathbf{R}'}^{\sigma} + a_{n\mathbf{R}}^{\sigma\dagger} a_{n\mathbf{R}'}^{\rho\dagger} a_{m\mathbf{R}'}^{\rho} a_{m\mathbf{R}}^{\sigma}) \} \rightarrow \text{Exchange Term} \end{aligned}$$

# Conventional VMC v.s. mVMC

Conventional VMC:

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

ex. antiferromagnetic phase

$$|\phi_{\text{AF}}\rangle = \prod_{|\mathbf{k}| < k_F, \sigma} a_{\mathbf{k}\sigma}^\dagger |0\rangle$$

$$\begin{aligned} a_{\mathbf{k}\sigma}^\dagger &= u_{\mathbf{k}} c_{\mathbf{k},\sigma}^\dagger + \sigma v_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q},\sigma}^\dagger \\ u_{\mathbf{k}}^2 &= \frac{1}{2} \left( 1 - \frac{E_{\mathbf{k}}}{\sqrt{E_{\mathbf{k}}^2 + \Delta_{\text{AF}}^2}} \right) \end{aligned}$$

Variational parameters = AF order parameter + etc.

many-variable VMC (mVMC):

flexibility of one-body part [**# of parameters > 10000**]

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

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

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

$f_{ij}$  [  $i, j$  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

$\alpha$ :variational parameters

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

# Optimization method

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

## (General) Gradient method

$\alpha$ :variational parameters

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

Steepest decent method [slow due to *redundancy*]

$X = I$  (identity matrix)

Newton method [second derivatives are expensive]

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

# Optimization method

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

## (General) Gradient method

$\alpha$ :variational parameters

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

Steepest decent method [slow due to *redundancy*]

$X = I$  (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]

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

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

# Time-dependent variational principle

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

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

(imaginary) time-dependent *variational principle*

A. D. McLachlan, Mol. Phys. 8, 39 (1964)

SR method

= imaginary-time evolution in restricted Hilbert space

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

$$\rightarrow \Delta\alpha = -\frac{\Delta\tau}{2} S^{-1} g \quad S: \text{overlap matrix}$$

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

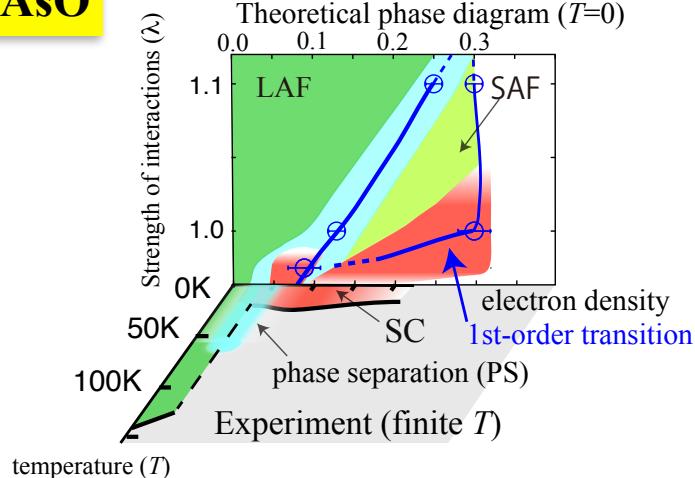


- **No negative-sign problem  
positive weight  $\rho(x) > 0$**
- **Wide applicable range [strong correlations, geometrical frustration, multi orbital system, any dimensions ... ]**
- **Natural extensions of mean-field calculations**
- **Easy to include many-body correlations through correlation factors (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

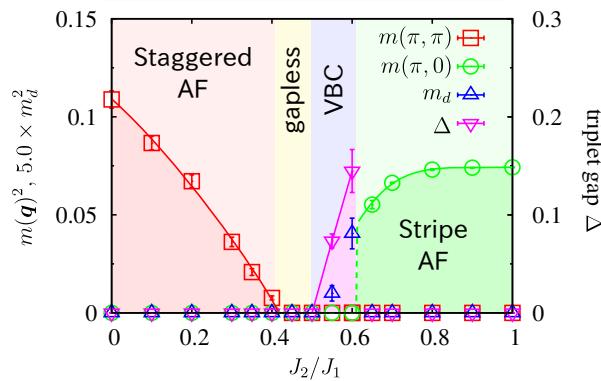
### LaFeAsO



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

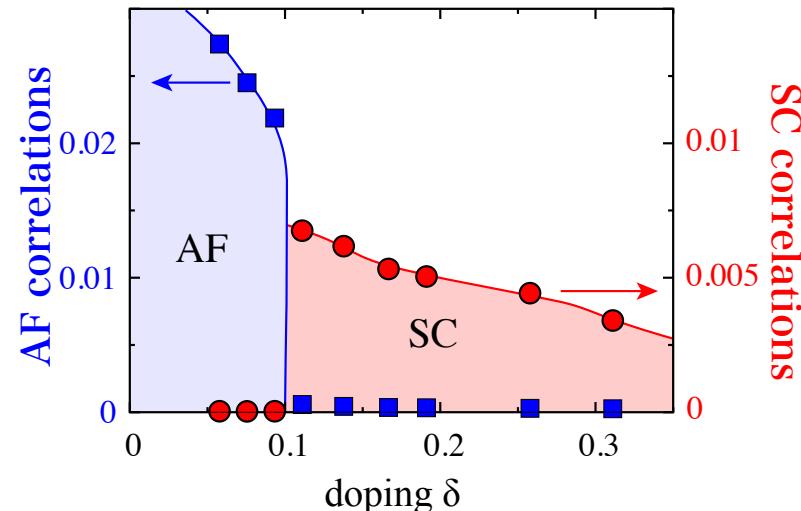
## Quantum spin liquid

### $J_1$ - $J_2$ Heisenberg



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

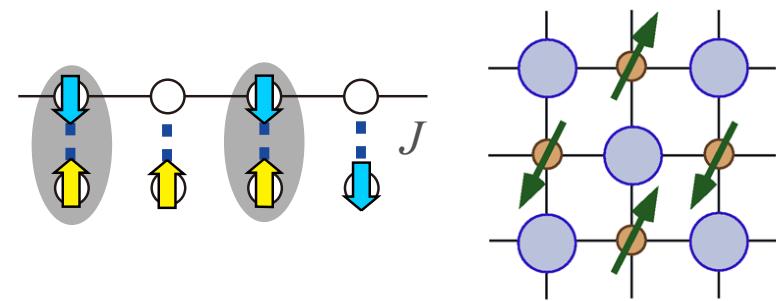
### HgBa<sub>2</sub>CuO<sub>4+δ</sub>



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

## Heavy fermion systems

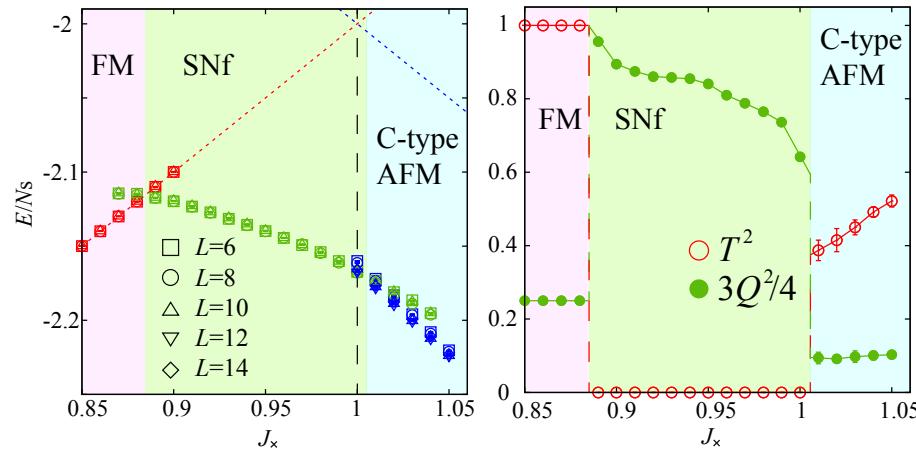
### CO in Kondo lattice model



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

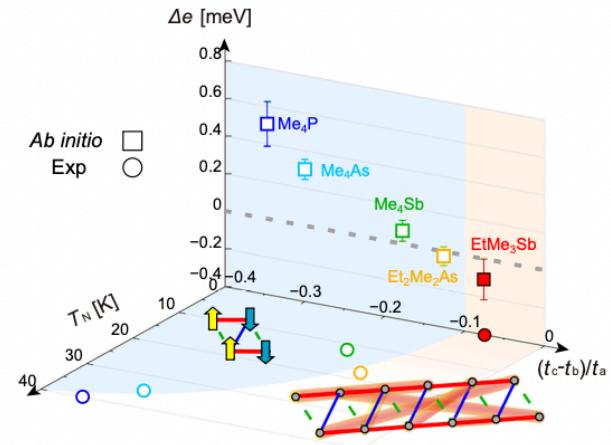
# Applications of mVMC II

## Spin nematic phase



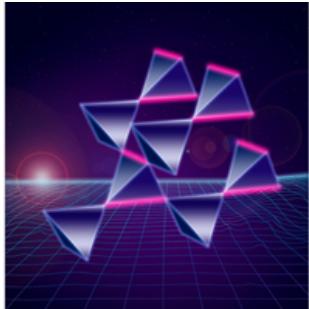
T. Hikihara et al., PRB(2019)

## Quantum spin liquid in dmit salts



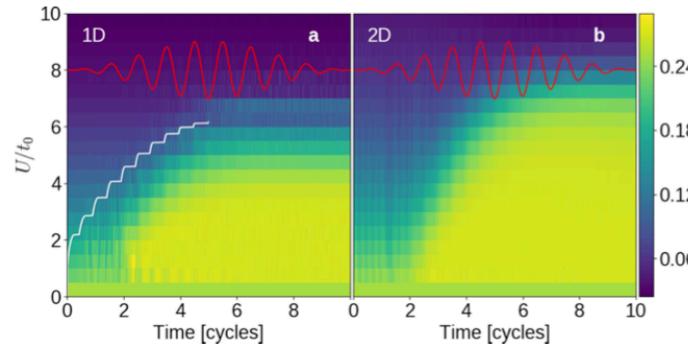
K. Ido *et al.*, npj QM (2022)

## Heisenberg model on pyrochlore lattice



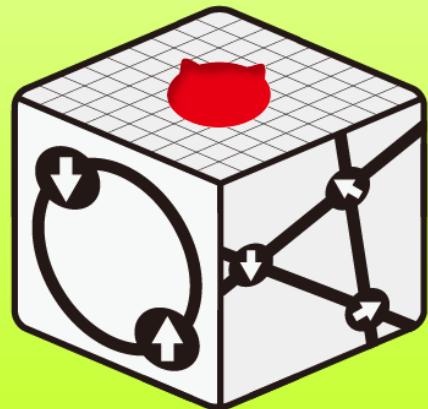
N. Astrakhantsev et al., PRX (2021)

## HHG in 2D Mott ins.



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

# Open-source software of mVMC

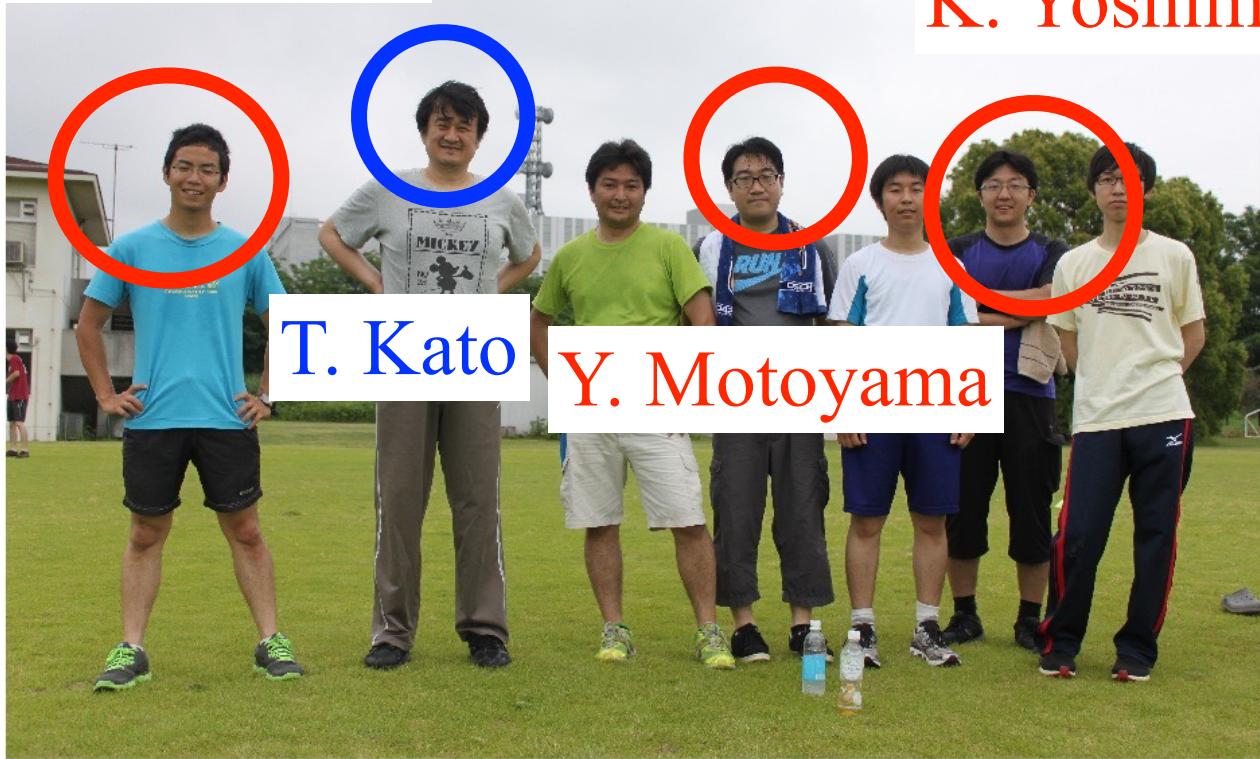


mVMC

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

# Developers of mVMC

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

K. Ido



RuQing Xu



M. Imada



# 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](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)

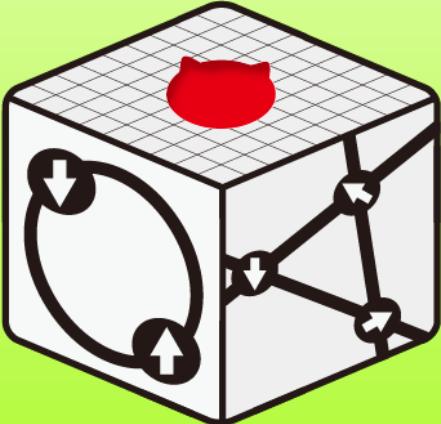
東工大 学術国際情報センター (TUBAME3.0)

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

Standard mode

ex.1D Hubbard model

L= 16

model = "Hubbard"

lattice = "chain"

U = 4

t = 1

nelec=16

2Sz=0

automatically generated

Expert mode

general Hamiltonians

$$\mathcal{H} = \mathcal{H}_T + \mathcal{H}_I,$$

$$\mathcal{H}_T = - \sum_{i,j} \sum_{\sigma_1, \sigma_2} t_{ij\sigma_1\sigma_2} c_{i\sigma_1}^\dagger c_{j\sigma_2},$$

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

users prepare  
all necessary input files

Input files

- Files for Hamiltonian
- Files for wave functions

optimization by SR method

[NVMCCalMode=0]

output

- optimization process
- optimized wave function

calculating correlation  
[NVMCCalMode=1]

output: one/two-body Green functions

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

fourier tool:  
calculating structure factors/visualization)

output: momentum distribution,  
charge/spin structure factors

$$n(\mathbf{k}), N(\mathbf{k}), S(\mathbf{k})$$

## 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

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

**W = 4**

**L = 4**

**Wsub = 2**

**Lsub = 2**

**model = "FermionHubbard"**

**lattice = "Tetragonal"**

**t = 1.0**

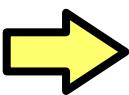
**U = 4.0**

**nelec = 16**

**Simple input files for conventional models**

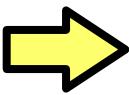
# How to use mVMC: Standard mode II

vmcdry stan\_opt.in

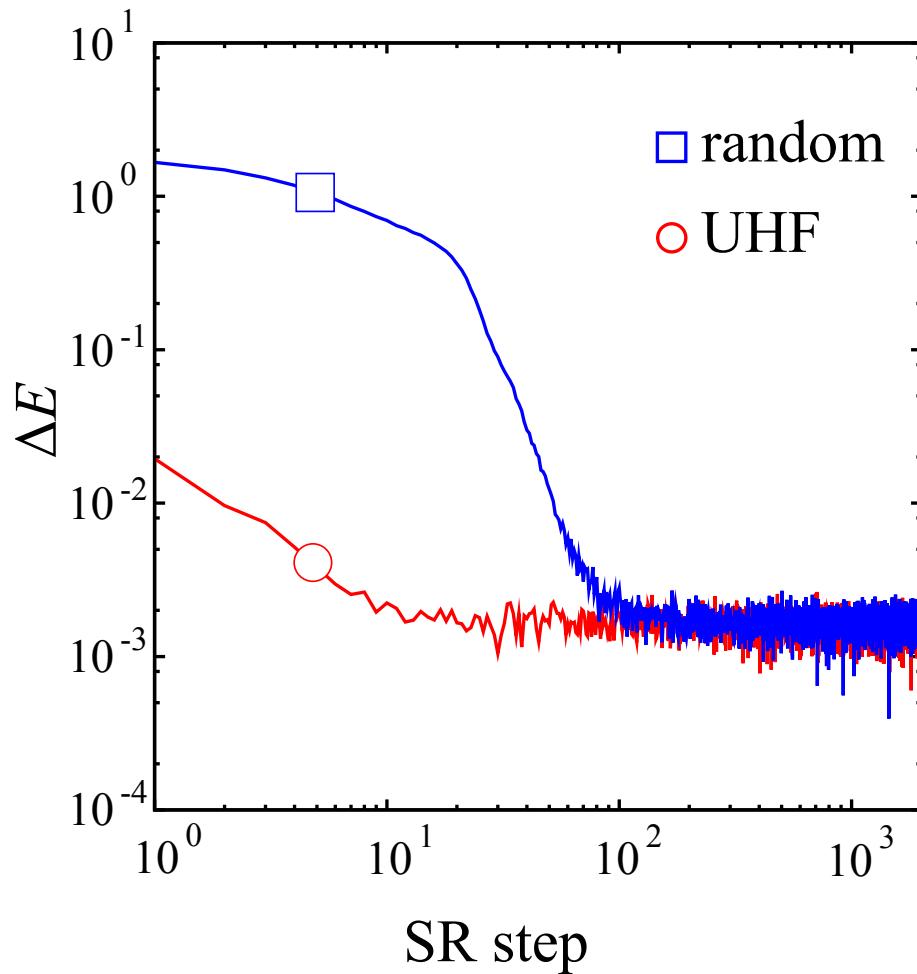


Generating input files

vmc namelist.def



Optimization



2D Hubbard model,  
 $4 \times 4, U/t=4, n=1$

on laptop  
 $\sim 2\text{-}3$  minutes

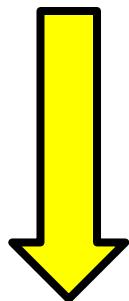
# Generating initial states

Slater determinant [mean-field wave func.]

$$|\phi_{\text{SL}}\rangle = \prod_{n=1,\sigma}^{N_e/2} \psi_{n\sigma}^\dagger |0\rangle$$

unitary trans.  
of one-body  
states

$$\psi_{n\sigma}^\dagger = \sum_{i=1}^{N_s} \Phi_{in\sigma} c_{i\sigma}^\dagger$$



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

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

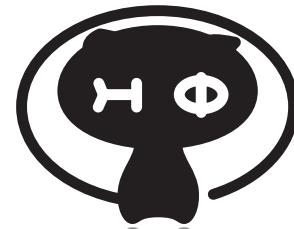
Pfaffian Slater determinant  
(Pairing wave function)

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

Initial states from Unrestricted Hartree-Fock (UHF) calc.  
Preparing the codes for performing UHF calc. (`usr/share/mvmc/tool`)

# Hubbard model

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

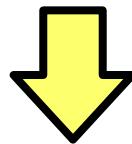


Physical Properties	mVMC( $2 \times 2$ )	ED
$4 \times 4$ (PP), $n = 1$		
Energy per site	-0.8500(1)	-0.8513
$S(\mathbf{q}_{\text{peak}})/N_s$	0.0575(2)	0.0569
$\mathbf{q}_{\text{peak}}$	$(\pi, \pi)$	$(\pi, \pi)$
$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$	-0.2063(14)	-0.2063
$4 \times 4$ (PP), $n = 0.625$		
Energy per site	-1.2196(1)	-1.22380
$S(\mathbf{q}_{\text{peak}})/N_s$	0.0130(1)	0.01300
$\mathbf{q}_{\text{peak}}$	$(\pi/2, \pi)$	$(\pi/2, \pi)$
$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$	-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

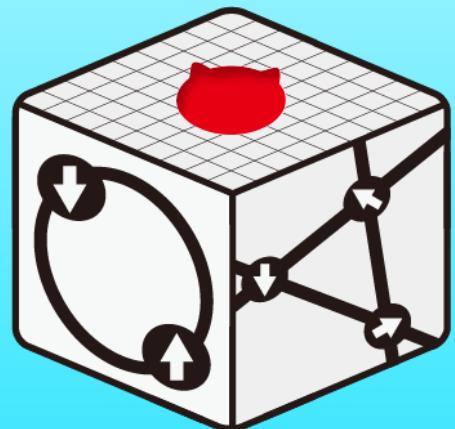
[mVMC]

**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

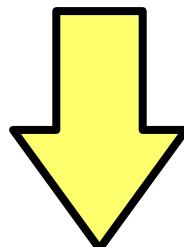
modpara.def

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

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

NInterAll	96	# of interactions parameters								
zInterAll								real part	imaginary part	
...	i	$\sigma_1$	j	$\sigma_2$	k	$\sigma_3$	l	$\sigma_4$		
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	

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

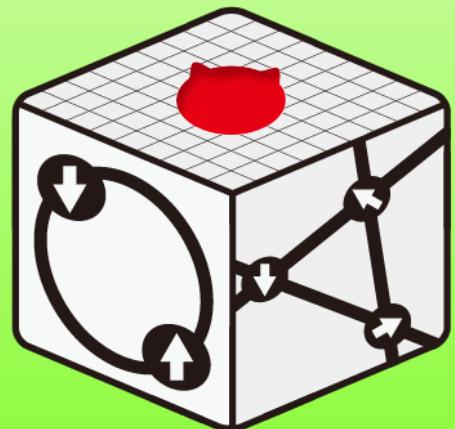
- **Exchange**  $\mathcal{H}_E = \sum_{i,j} J_{ij}^{\text{Ex}} (c_{i\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow}^\dagger c_{i\uparrow})$

=====  
NExchange 2  
=====

=====Exchange=====  
=====

0 1 0.5  
1 2 0.5

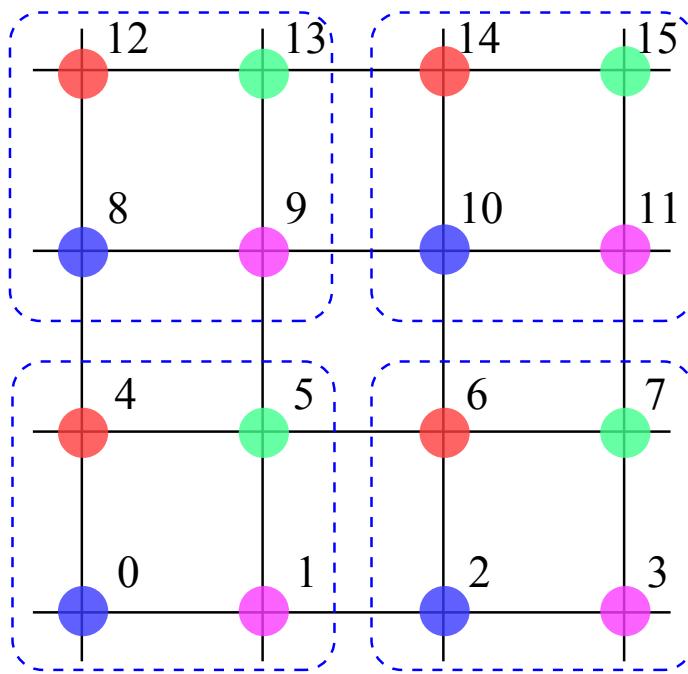
For details, see  
manuals



mVMC

Tips on 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

$$|\psi\rangle = \mathcal{PL}|\phi_{\text{pair}}\rangle$$

- 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 Hamiltonians ?

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  $f_{ij}$ )**
- Compare with the results by exact diagonalization for small system sizes !
- Energy is lower than the mean-filed calculations ?
- Sub lattice structure is proper ?

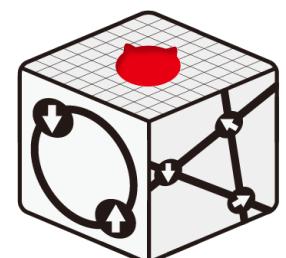
# Summary

## 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**