[24aPS-16]多変数変分モンテカルロ法のオープンソフトウェア mVMC ver1.0の新機能・利用事例の紹介

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1. What is mVMC ?

A low-energy solver for a wide range of quantum lattice models such as the multi-orbital Hubbard model, Heisenberg model, and Kondo-lattice model by using variational Monte Carlo method. Users can obtain high-accuracy wave functions for ground states of the above models. Users flexibly choose the correlation factors in wavefunctions such as Gutzwiller, Jastrow, and doublon-holon binding factors and optimize more than ten thousand variational parameters. It also allows to obtain low-energy excited states by specifying quantum numbers by using the quantum-number projections.

Open-source software distributed through GitHub (latest version: ver.1.0.2)
Parallelization: Hybrid (MPI & OpenMP)
License: GNU GPL version3

2. What you can do with mVMC

2-1. Summary of features

Target :
- Hubbard model (particle # conserved system)
- Heisenberg model (spin 1/2)
- Kondo lattice system (spin 1/2+ itinerant electrons)

Method: Variational wave functions D. Tahara and M. Imada, JPSJ 77, 114701 (2008); T. Misawa and M. Imada, PRB, 90, 115137 (2014)

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

Pair-product part

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

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

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

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

Update (SR method)
Minimizing $E_{\vec{\alpha}} = \langle H\rangle_{\vec{\alpha}}$
$\vec{\alpha}_{\rm new} - \vec{\alpha}_{\rm old} = -X^{-1}\vec{g}$
$g_k = \dfrac{\partial E_{\vec{\alpha}}}{\partial \alpha_k}$ gradient of energy (MC Sampling)
$X_{\alpha\beta} = \langle\bar{\psi}_\alpha|\bar{\psi}_\beta\rangle, |\bar{\psi}_\alpha\rangle = \dfrac{\partial|\bar{\psi}\rangle}{\partial\alpha}, |\bar{\psi}\rangle = \dfrac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}}$

2-2. Flow of calculations

Standard mode

ex. 1D Hubbard model
Lx= 16
model = "Hubbard"
lattice = "chain"
U = 4
t = 1
nelec=16
2Sz=0

↓ automatically generated

input files
- Files for Hamiltonian
- Files for wave functions

↓ optimization by SR method [NVMCCalMode=0]

output
- optimization process
- optimized wave function

↓ calculating correlation functions [NVMCCalMode=1]

output: thermodynamic quantities, one/two-body Green's functions
$\langle c^{\dagger}_{i\sigma_1}c_{j\sigma_2}\rangle$ $\langle c^{\dagger}_{i\sigma_1}c_{j\sigma_2}c^{\dagger}_{k\sigma_3}c_{l\sigma_4}\rangle$

↓ fourier tool

output: momentum distribution, charge/spin structure factors
$n(k)$, $N(q)$, $S(q)$

Expert mode

Users can treat general Hamiltonians

$$\mathcal{H} = \mathcal{H}_T + \mathcal{H}_I,$$
$$\mathcal{H}_T = -\sum_{i,j}\sum_{\sigma_1,\sigma 2} t_{ij\sigma_1\sigma_2}c^{\dagger}_{i\sigma_1}c_{j\sigma_2},$$
$$\mathcal{H}_I = \sum_{i,j,k,l}\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4}c^{\dagger}_{i\sigma_1}c_{j\sigma_2}c^{\dagger}_{k\sigma_3}c_{l\sigma_4}$$

↓ users prepare all necessary files

✓ **Download**
Source codes & manuals @ GitHub
✓ **Prerequisite**
- C compiler (Intel, Fujitsu, GNU)
- LAPACK or Scalapack
- MPI library

power Lanczos [NLanczosMode=1,2]

1st-step power Lanczos
$|\psi_1\rangle = (1+\alpha_1 H)|\psi\rangle$

- mVMC is pre-installed in sekirei (ISSP system B)

3. Basics of mVMC

Variational principle

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

α: variational parameters

Physical properties [MC sampling] x: real-space configurations

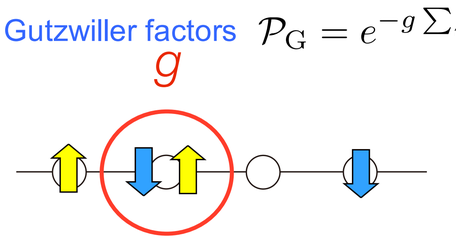
$$\frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle} = \sum_x \frac{\langle\psi|\hat{A}|x\rangle\langle x|\psi\rangle}{\langle\psi|\psi\rangle} = \sum_x \rho(x)\frac{\langle\psi|\hat{A}|x\rangle}{\langle\psi|x\rangle}$$

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

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

Correlation factors

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



$$\mathcal{P}_{\rm G}|x\rangle = |x\rangle e^{-gD(x)}$$
$$\langle\psi|x\rangle = \langle\phi_0|x\rangle\mathcal{P}_{\rm G}(x)$$

determinant or Pfaffian

Conventional VMC: [# of parameters~10]

Only AF order parameter is the variational parameter

Ex. Antiferromagnetic phase

$$|\phi_{\rm AF}\rangle = \prod_{|\boldsymbol{k}|<k_F,\sigma} a^{\dagger}_{\boldsymbol{k}\sigma}|0\rangle$$
$$a^{\dagger}_{\boldsymbol{k}\sigma} = u_{\boldsymbol{k}}c^{\dagger}_{\boldsymbol{k},\sigma} + \sigma v_{\boldsymbol{k}}c^{\dagger}_{\boldsymbol{k}+\boldsymbol{Q},\sigma}$$
$$u^2_{\boldsymbol{k}} = \frac{1}{2}\Big(1 - \frac{E_{\boldsymbol{k}}}{\sqrt{E^2_{\boldsymbol{k}} + \Delta^2_{\rm AF}}}\Big)$$

$\Delta_{\rm AF}$:variational parameters

many-variable VMC (mVMC): Large-degrees of freedom in pair-product part [# of parameters >=10000]

$$|\phi_{\rm Pf}\rangle = \sum_{i,j,\sigma,\tau}\Big(F_{i\sigma j\tau}c^{\dagger}_{i\sigma}c^{\dagger}_{j\tau}\Big)^{N_{\rm e}/2}|0\rangle$$

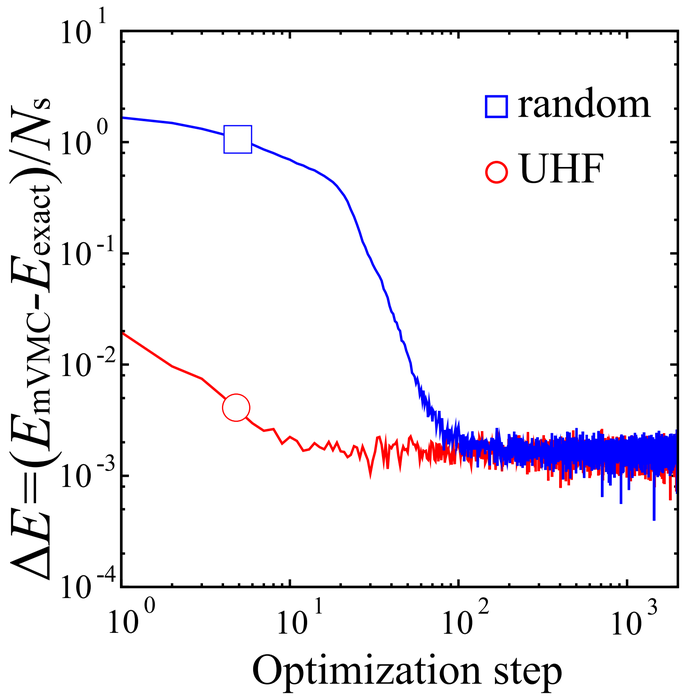
$F_{ij\sigma\tau}$:variational parameters

$F_{i\sigma j\tau}$ [i,j real-space indices]→ AF order, superconducting phases, spin-orbit couplings, non-collinear magnetism

4. Example Hubbard model on the square lattice

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

Optimization process (U/t=4, half filling)



Exact diagonalization by using HPhi

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

$S_{\rm nn} = \frac{1}{4N_{\rm s}}\sum_{i,\mu}\langle\boldsymbol{S}_{\boldsymbol{r}_i}\cdot\boldsymbol{S}_{\boldsymbol{r}_i+\boldsymbol{e}_\mu}\rangle$

Comparison with exact diagonalization

	$E/N_{\rm s}$	doublon	$S_{\rm nn}$	$S(\pi,\pi)$
ED	-0.85136	0.11512	-0.2063	0.05699
mVMC(2×2)	-0.84982(4)	0.11529(5)	-0.2062(1)	0.05773(4)
mVMC(4×4)	-0.85068(4)	0.1153(4)	-0.2062(5)	0.0573(2)

mVMC well reproduces exact results !

5. Summary

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

Examples and lecture notes of mVMC are available at mVMC-tutorial @ GitHub