Introduction to HΦ –A numerical solver for quantum lattice models

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Outline

0. What can we do by HΦ ?
1. How to get HΦ
2. How to use Standard mode
3. How to use Expert mode
4. Applications of HΦ
5. Short introduction to mVMC

@東北大学

2016/12/01

http://ma.cms-initiative.jp/ja/listapps/hphi

Developers of HΦ

M. Kawamura

T. Misawa

K. Yoshimi

Y. Yamaji

S. Todo

N. Kawashima

Basic properties of HΦ

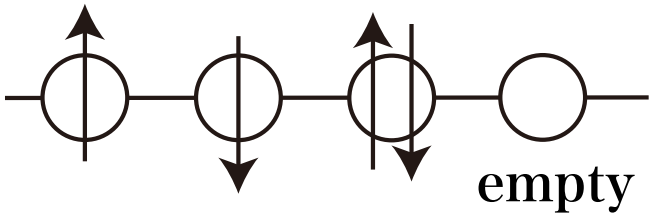
What can we do by HΦ?

For Hubbard model, spin-*S* Heisenberg model, Kondo-lattice model

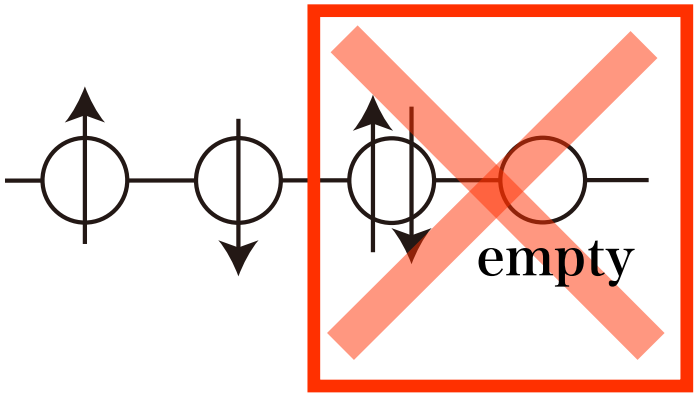
- Full diagonalization
- Ground state calculations by Lanczos method
- Finite-temperature calculations by thermal pure quantum (TPQ) states
- Dynamical properties (optical conductivity ..)

models

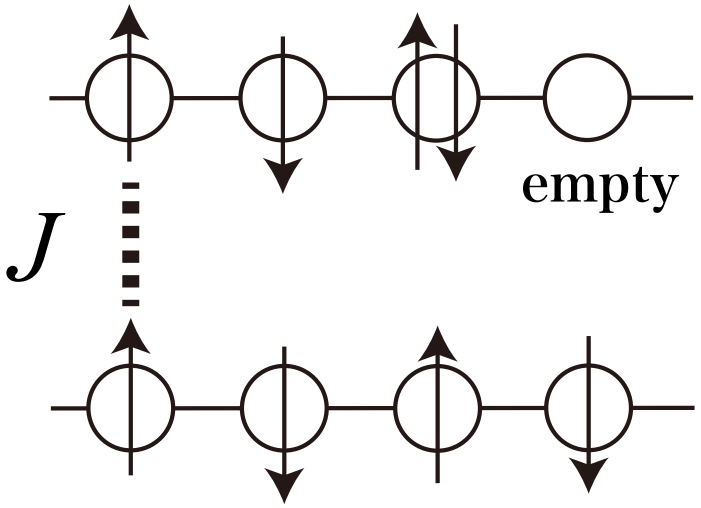
Hubbard (itinerant) $\sim 4^N$



Heisenberg (localized) $\sim 2^N$



Kondo=itinerant+localized



３つの異なる模型を扱えるように整備

(Heisenbergはspin-Sも対応)

Full diagonalization

Matrix representation of Hamiltonian

(real space basis) → Full diagonalization for the matrix

$$H_{ij} = \langle i|\hat{H}|j\rangle \qquad |i\rangle \text{ real-space basis}$$

dim. of matrix= # of real-space bases

=exponentially large

ex. spin1/2 system: $S_z=0$ $\quad {}_{N_s}C_{N_s/2}$

- Ns=16: dim.=12800, required memory (~dim.^{2}) ~ 1 GB
- Ns=32: dim.~6×10^8 , required memory (~dim.^{2}) ~ 3 EB!

Lanczos method

By multiplying the Hamiltonian to initial vector, we can obtain the ground state (power method)

$$\mathcal{H}^n \boldsymbol{x}_0 = E_0^n \left[a_0 \boldsymbol{e}_0 + \sum_{i \neq 0} \left(\frac{E_i}{E_0} \right)^n a_i \boldsymbol{e}_i \right]$$

A few (at least two) vectors are necessary→

We can treat larger system size than full diagonalization

ex. spin 1/2 system: S_z=0

- Ns=16: dim. =12800,required memory (~dim.) ~0.1 MB
- Ns=32: dim. ~6×10^8,required memory (~dim.) ~5 GB !
- Ns=36: dim. ~9×10^9,required memory (~dim.) ~72 GB !

Meaning of name & logo

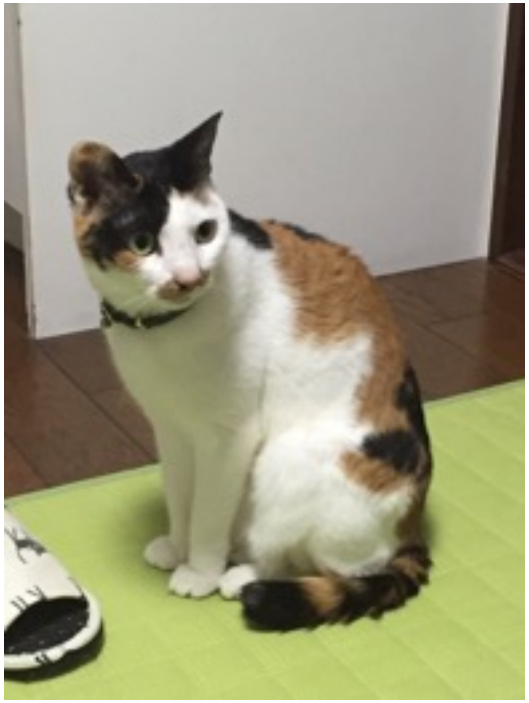
- Multiplying H to Φ (HΦ)
- This cat means wave function in two ways

cat is a symbol of superposition.. (Schrödinger's cat)

wake

sleep

Φ=



+

Finite-temperature calculations by TPQ

-Conventional finite-temperature cal.:

ensemble average is necessary

→ Full diag. is necessary

$$\langle E \rangle = \frac{\sum_n E_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}$$

It is shown that thermal pure quantum state (TPQ) states enable us to calculate the physical properties at finite temperatures w/o ensemble average [Sugiura-Shimizu, PRL 2012,2013]

→ Cost of finite-tempeature calculations ~ Lanczos method !

pioneering works :
Quantum-transfer MC method (Imada-Takahashi, 1986),
Finite-temperature Lanczos (Jaklic-Prelovsek,1994),
Hams-Raedt (2000)

Sugiura-Shimizu method [mTPQ state]

Procedure

S. Sugiura and A. Shimizu, PRL 2012 & 2013

$|\psi_0\rangle$: random vector

$$|\psi_k\rangle \equiv \frac{(l - \hat{H}/N_{\rm s})|\psi_{k-1}\rangle}{|(l - \hat{H}/N_{\rm s})|\psi_{k-1}\rangle|}$$

***l*:constant larger the maximum eigenvalues**

$$u_k \sim \langle\psi_k|\hat{H}|\psi_k\rangle/N_{\rm s}$$

$$\beta_k \sim \frac{2k/N_{\rm s}}{(l - u_k)}, \quad \langle\hat{A}\rangle_{\beta_k} \sim \langle\psi_k|\hat{A}|\psi_k\rangle$$

All the finite temperature properties can be calculated by using *one* thermal pure quantum [TPQ] state.

Drastic reduction of numerical cost

Heisenberg model, 32 sites, S_z=0

Full diagonalization:
Dimension of Hamiltonian ~ $10^8 \times 10^8$
Memory ~ 3E Byte → Almost impossible.

TPQ method:
Only two vectors are required:
dimension of vector ~ 10^8 ~~$\times 10^8$~~
Memory ~ 10 G Byte
→ Possible even in lab's cluster machine !

Basic properties of HΦ

What can we do by HΦ?

For Hubbard model, spin-*S* Heisenberg model, Kondo-lattice model

- Full diagonalization

- Ground state calculations by Lanczos method

- Finite-temperature calculations by thermal pure quantum (TPQ) states

- Dynamical properties (optical conductivity ..)

maximum system sizes@ ISSP system B (sekirei)

- spin 1/2: ~ 40 sites (Sz conserved)
- Hubbard model: ~ 20sites (# of particles & Sz conserved)

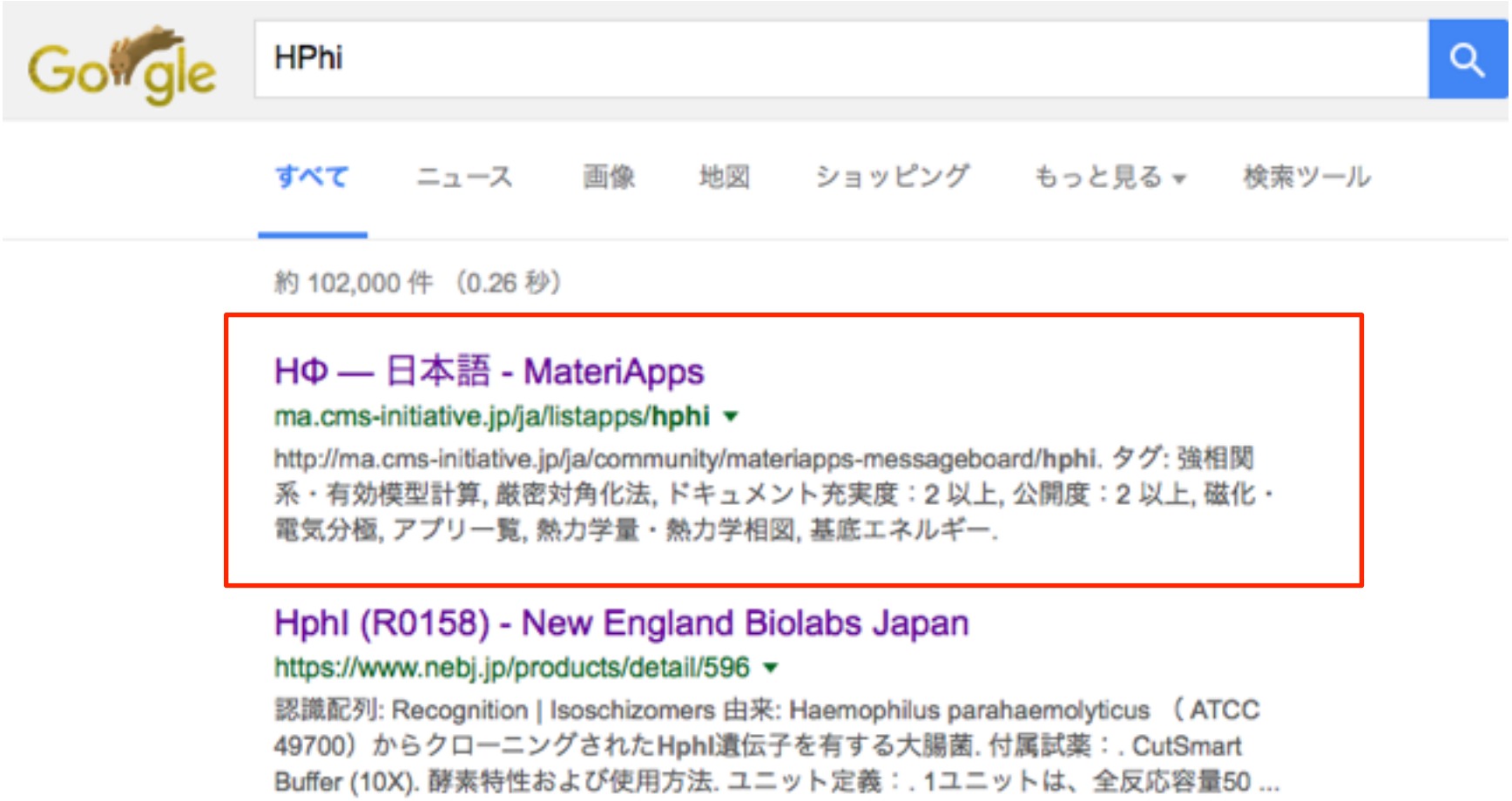

Let’s get НФ !
НФ

How to find HΦ

http://ma.cms-initiative.jp/en/application-list/hphi/hphi

search by “HPhi” → You can find our homepage in the first page (maybe, the first or second candidate)

GitHub → https://github.com/QLMS/HPhi



How to compile HΦ

ex. linux + gcc-mac

```
tar xzvf HPhi-release-1.2.tar.gz
cd HPhi-release-1.2
bash HPhiconfig.sh gcc-mac
make HPhi
```

For details,

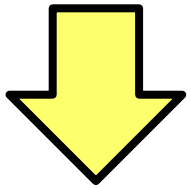
```
$ bash HPhiconfig.sh

Usage:
./HPhiconfig.sh system_name
 system_name should be chosen from below:
     sekirei : ISSP system-B
        maki : ISSP system-C
       intel : Intel compiler + Linux PC
 mpicc-intel : Intel compiler + Linux PC + mpicc
         gcc : GCC + Linux
     gcc-mac : GCC + Mac
```

Let's start HΦ !
(Standard mode)

How to use HΦ: Standard mode I (Lanczos)

Only StdFace.def is necessary (< 10 lines) !

```
L          = 4
model      = "Spin"
method     = "Lanczos"
lattice    = "square lattice"
J          = 1.0
2Sz        = 0
```



HPhi -s StdFace.def

ex. 4×4 2d Heisenberg model,
GS by Lanczos method

Method

Lanczos — ground state

TPQ — finite-temperature

FullDiag — full-diagonalization

./ouput : results are output

Important files

./output/zvo_energy.dat → energy

./output/zvo_Lanczos_Step.dat → convergence

./output/zvo_cisajs.dat → one-body Green func.

./output/zvo_cisajscktalt.dat → two-body Green func.

How to use HΦ: Standard mode II

./output/zvo_energy.dat

ex. 4by4, 2d Heisenberg model,
GS calculations by Lanczos

```
$ cat output/zvo_energy.dat
Energy  -11.2284832084288109
Doublon   0.0000000000000000
Sz        0.0000000000000000
```

GS energy

./output/zvo_Lanczos_Step.dat

```
$ tail output/zvo_Lanczos_Step.dat
stp=28 -11.2284832084 -9.5176841765 -8.7981539671 -8.5328120558
stp=30 -11.2284832084 -9.5176875029 -8.8254961060 -8.7872255591
stp=32 -11.2284832084 -9.5176879460 -8.8776934418 -8.7939798590
stp=34 -11.2284832084 -9.5176879812 -8.8852955092 -8.7943260103
stp=36 -11.2284832084 -9.5176879838 -8.8863380562 -8.7943736678
stp=38 -11.2284832084 -9.5176879839 -8.8864307327 -8.7943782609
stp=40 -11.2284832084 -9.5176879839 -8.8864405361 -8.7943787937
stp=42 -11.2284832084 -9.5176879839 -8.8864422628 -8.7943788984
stp=44 -11.2284832084 -9.5176879839 -8.8864424018 -8.7943789077
stp=46 -11.2284832084 -9.5176879839 -8.8864424075 -8.7943789081
```

convergence process by Lanczos method

How to use HΦ: Standard mode III

./output/zvo_cisajs.dat

$\langle c^\dagger_{i\sigma} c_{j\tau} \rangle$

```
$ head output/zvo_cisajs.dat
    0    0    0    0 0.5000000000 0.0000000000
    0    1    0    1 0.5000000000 0.0000000000
```

$\langle c^\dagger_{0\downarrow} c_{0\downarrow} \rangle$

$\langle c^\dagger_{0\uparrow} c_{0\uparrow} \rangle$

./output/zvo_cisajscktalt.dat

```
$ head output/zvo_cisajscktalt.dat
    0    0    0    0    0    0    0    0 0.5000000000 0.0000000000
    0    0    0    0    0    1    0    1 0.0000000000 0.0000000000
    0    0    0    0    1    0    1    0 0.1330366332 0.0000000000
    0    0    0    0    1    1    1    1 0.3669633668 0.0000000000
```

$\langle c^\dagger_{0\downarrow} c_{0\downarrow} c^\dagger_{0\downarrow} c_{0\downarrow} \rangle$

$\langle c^\dagger_{0\downarrow} c_{0\downarrow} c^\dagger_{0\uparrow} c_{0\uparrow} \rangle$

$\langle c^\dagger_{0\downarrow} c_{0\downarrow} c^\dagger_{1\downarrow} c_{1\downarrow} \rangle$

$\langle c^\dagger_{0\downarrow} c_{0\downarrow} c^\dagger_{1\uparrow} c_{1\uparrow} \rangle$

ex. onsite・nn-site correlation func.

How to use HΦ: Standard mode IV

HPhi/samples/Standard/
StdFace.def for
Hubbard model, Heisenberg model, Kitaev model,
Kondo-lattice model

By changing StdFace.def slightly, you can easily perform the calculations for different models.

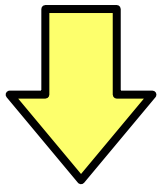
Cautions：

- Do not input too large system size
(upper limit@laptop: spin 1/2→24 sites, Hubbard model 12 sites)
- Lanczos method is unstable for too small size
(dim. > 1000)
-TPQ method does no work well for small size
(dim. > 1000)

Expert mode !

How to use HΦ: What is Expert mode ?

HPhi -s StdFace.def



Standard mode: Necessary input files are automatically generated

Files for Hamiltonian (three files)
zInterAll.def,zTrans.def, zlocspn.def

Files for basic parameters (two files)
modpara.def,calcmod.def

Files for correlations functions (two files)
greenone.def, greentwo.def

+ list of input files: namelist.def

Expert mode: preparing the following files by yourself

How to use HΦ: What is Expert mode ?

Expert mode: preparing the following files by yourself

Files for Hamiltonian (three files)
zInterAll.def,zTrans.def, zlocspn.def

Files for basic parameters (two files)
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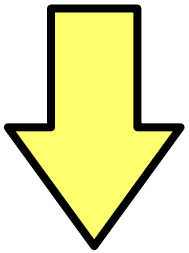
greenone.def, greentwo.def



execute following command

HPhi -e namelist.def

How to use HΦ: zInterall.def

Examples of input files for Hamiltonian

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

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

# of interactions

								real	imaginary
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		

You can specify *arbitrary* two-body interactions
→ You can treat *any* lattice structures

How to use HΦ: Expert mode

Simple version of zInterall.def

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

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

-Exchange $H+=\sum_{i,j} J_{ij}^{\mathrm{Ex}}(S_i^+ S_j^- + S_i^- S_j^+)$

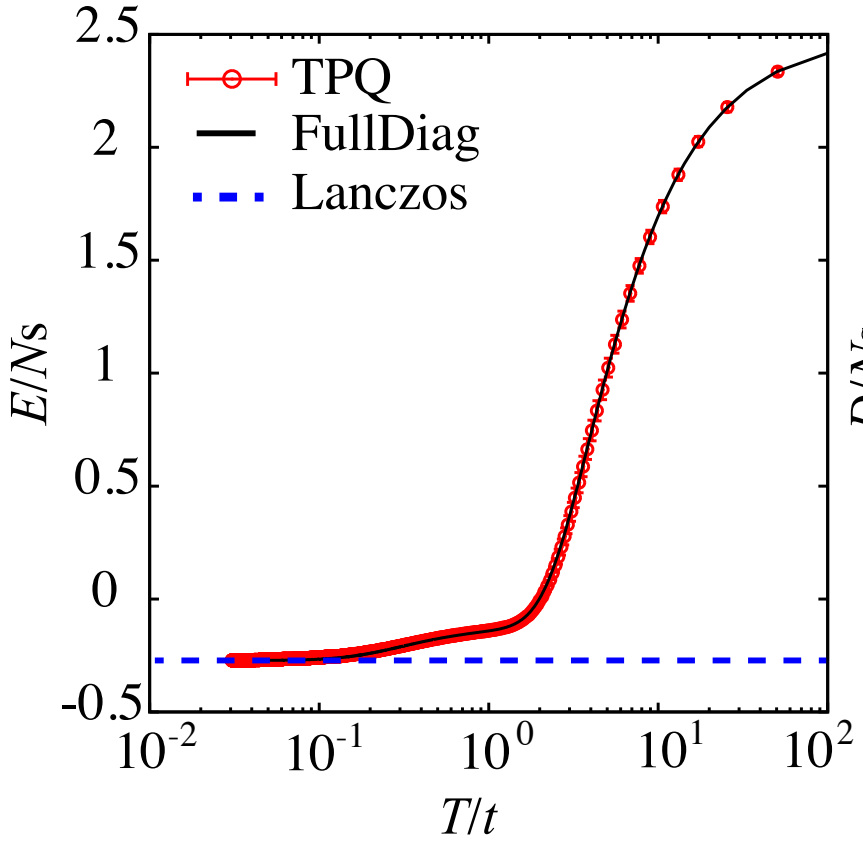
```
================================
NExchange 2
================================
==========Exchange=============
================================
 0   1  0.5
 1   2  0.5
```

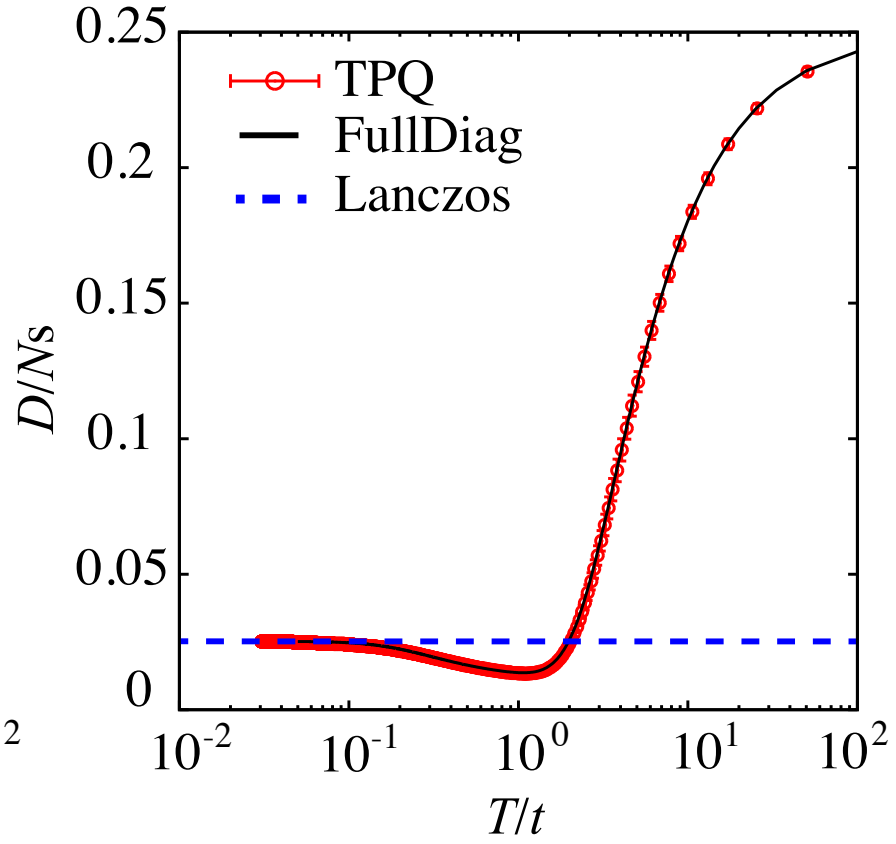
Easy to input interactions


Applications of НФ!

Comparison of three different methods

Comparison of FullDiag, TPQ, Lanczos method
Hubbard model, L=8, U/t=8, half filling, S_z=0





TPQ method works well !

Studies using HPhi

1. Finite-temperature crossover phenomenon in the S=1/2 antiferromagnetic Heisenberg model on the kagome lattice
Tokuro Shimokawa, Hikaru Kawamura (arXiv:1607.06205)

2. Finite-Temperature Signatures of Spin Liquids in Frustrated Hubbard Model
Takahiro Misawa, Youhei Yamaji (arXiv:1608.09006)

3. Four-body correlation embedded in antisymmetrized geminal power wave function
Airi Kawasaki, Osamu Sugino (arXiv:1609.01438)

4. Liquid-Liquid Transition in Kitaev Magnets Driven by Spin Fractionalization
Joji Nasu, Yasuyuki Kato, Junki Yoshitake, Yoshitomo Kamiya, Yukitoshi Motome (arXiv:1610.07343)

既に、4本の論文がHPhiを使用！

HPhiの使い方

0. 汎用性を優先して、速度・サイズなどは犠牲にしている部分がある→
対角化(Lanczos法)での世界最大の計算は（現段階では)無理

1. spin 1/2 36 sites, Hubbard 18 sites程度までの有限温度計算
は比較的すぐできる。とくに、エントロピーが低温まで残る
フラスレート系が得意 [論文 1(kagome),2(*t*-*t*' Hubbard)]。

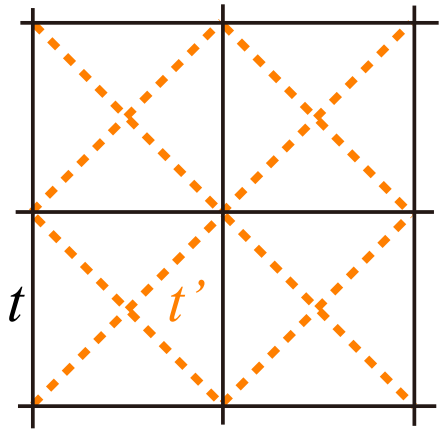
2. 平均場計算などで「面白い」ことがおきることを確認
→HPhiでその結果を確認する[論文4(extended Kitaev model)]

3. 新手法開発した際の精度確認[論文3(extended geminal wave functions)]
~20 site Hubbard model

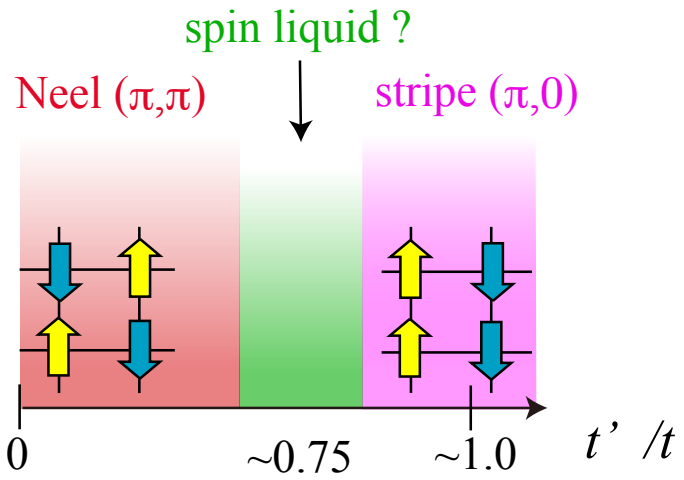
4. 新奇物質に対する現実的な有効模型の妥当性の確認,物性予測
(基底状態、有限温度、動的物理量)[Na_2IrO_3, Yamaji *et al.*]

Frustrated *t-t'* Hubbard model

Lattice geometry

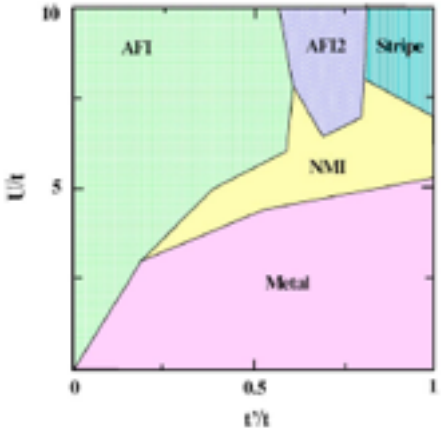


Schematic phase diagram

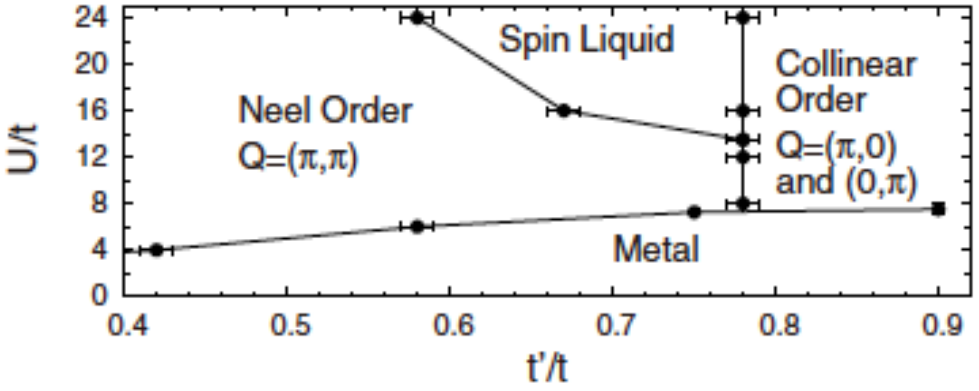


Previous studies

PIRG: Mizusaki and Imada, PRB 2004



VMC: L. Tocchio *et al.*, PRB(R) 2008



NB: Spin liquid is also reported in J_1-J_2 Heisenberg model

Spin liquid may appear at intermediate region

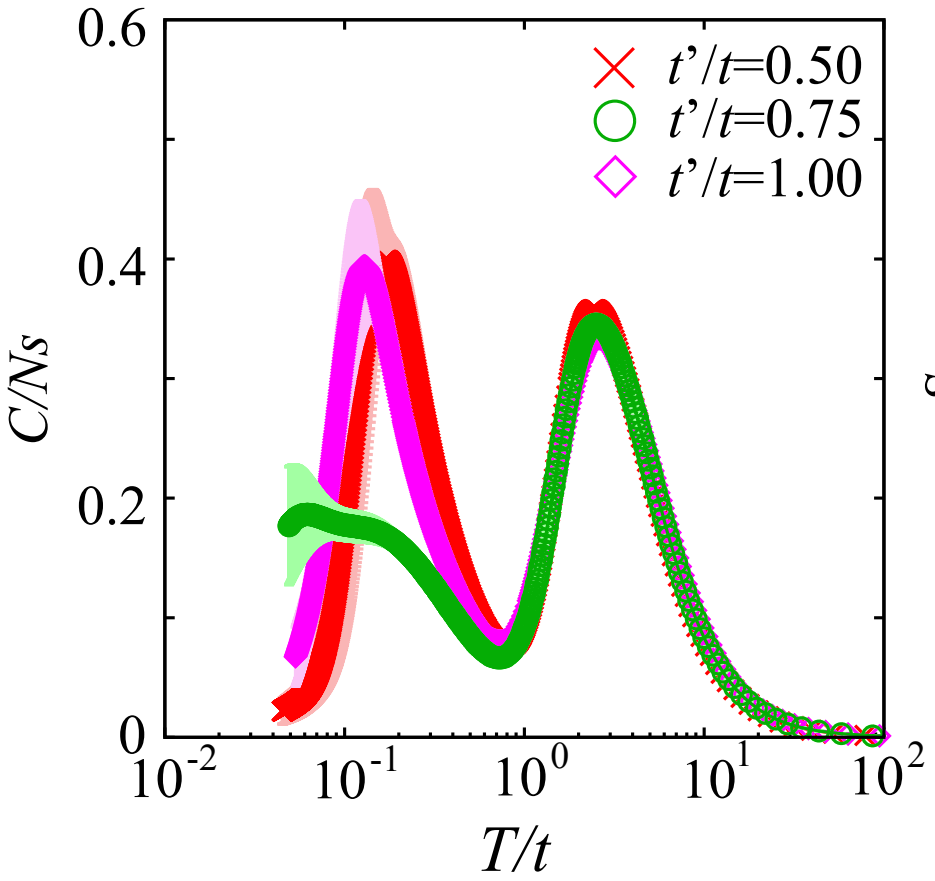
Input file

```
W = 4
L = 4
model = "FermionHubbard"
method = "TPQ"
lattice = "Tetragonal"
t  = 1.0
t' = 0.75
U  = 10.0
nelec = 16
2Sz = 0
```

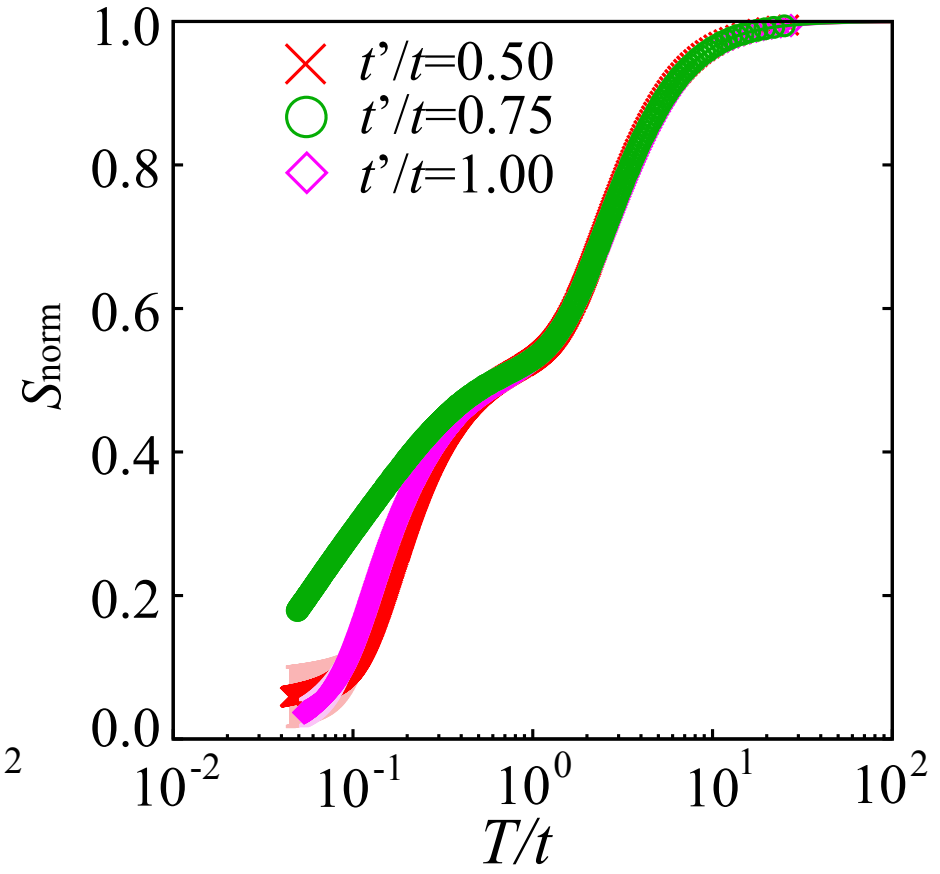
たった、これだけ！そのまま並列計算も可能

Signature of spin liquid [U/t=10]

specific heat



entropy



At t'/t~0.75 large entropy remains at low temperatures
→ Signature of spin liquid

Available system size in SC@ISSP

ISSP system B (sekirei)

✓fat node: 1node (40 cores) memory/node = 1TB、
up to 2nodes → ~2TB

✓cpu node: 1node (24cores) memory/node=120GB,
up to 144nodes→~17TB

SC@ISSP:

- It is *very easy (cheap)* to perform the calculations up to spin 1/2 = 32 sites, Hubbard = 16 sites

- It is possible (but expensive !) to perform the calculations up to spin 1/2 40 sites, Hubbard 20 sites
(state-of-the-art calculations 5-10 years ago)

Summary

- Explained basic properties of HΦ:
Full diagonalization, Lanzcos method, TPQ method
for Heisenberg, Hubbard, Kondo, Kitaev model ….

- Explained how to use HΦ:
Very easy to start calculations by using Standard mode
Easy to treat general Hamiltonians by using Expert mode

- Shown applications of HΦ:
Found the finite-temperature signature of QSL in
t-*t*' Hubbard model

If you have any questions,
please join HPhi ML and ask questions

More about HPhi

http://qlms.github.io/HPhi/

日本語 English

ホーム

ダウンロード(最新版)

フォーラム

リポジトリ

マニュアル

ソースブラウザ

開発者ノート

発表資料

HPhiを用いた計算事例

HPhi HomePage

News

2016/11/15 : バージョン1.2.0がリリースされました.

2016/9/15 : 日本物理学会秋季大会でポスター発表を行いました. 発表資料はこちらです.

2016/7/26 : HPhiの講習会を物性研で行いました. 講習会の資料はこちらです.

2016/6/27 : バージョン1.1.1がリリースされました.

2016/5/25 : バージョン1.1がリリースされました.

2016/4/5 : バージョン1.0がリリースされました.

2016/3/20 : 日本物理学会春季大会でポスター発表を行いました. 発表資料はこちらです.

2016/2/23 : バージョン0.3がリリースされました.

2016/1/22 : バージョン0.2.1がリリースされました.

2015/12/28 : バージョン0.2がリリースされました.

2015/12/7 : 「第 6 回 CMSI 研究会 (HPCI 戦略プログラム分野2最終報告会)」でポスター発表を行いました. 発表資料はこちらです.

More about HPhi

http://qlms.github.io/HPhi/

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開発者ノート

発表資料

HPhiを用いた計算事例

開発者ノート

HPhiにおけるいくつかの工夫(三澤)

cf.. ハッカーの楽しみ

bit演算周りの工夫を掲載

More about HPhi

http://qlms.github.io/HPhi/

cf.. ハッカーの楽しみ

同じ個数の1のbitを持つ、次に大きい数の生成方法

```
unsigned long int snoob(unsigned long int x){
  unsigned long int smallest, ripple, ones;
  smallest = x &(-x);
  ripple   = x  + smallest;
  ones     = x ^ ripple;
  ones     = (ones>>2)/smallest;
  return   ripple|ones;
}
```

他にも、

1のbitの総数を数えるアルゴリズム、

1のbitの総数の偶奇を数えるアルゴリズム, …

many-variable variational Monte Carlo method

Ver0.1を公開

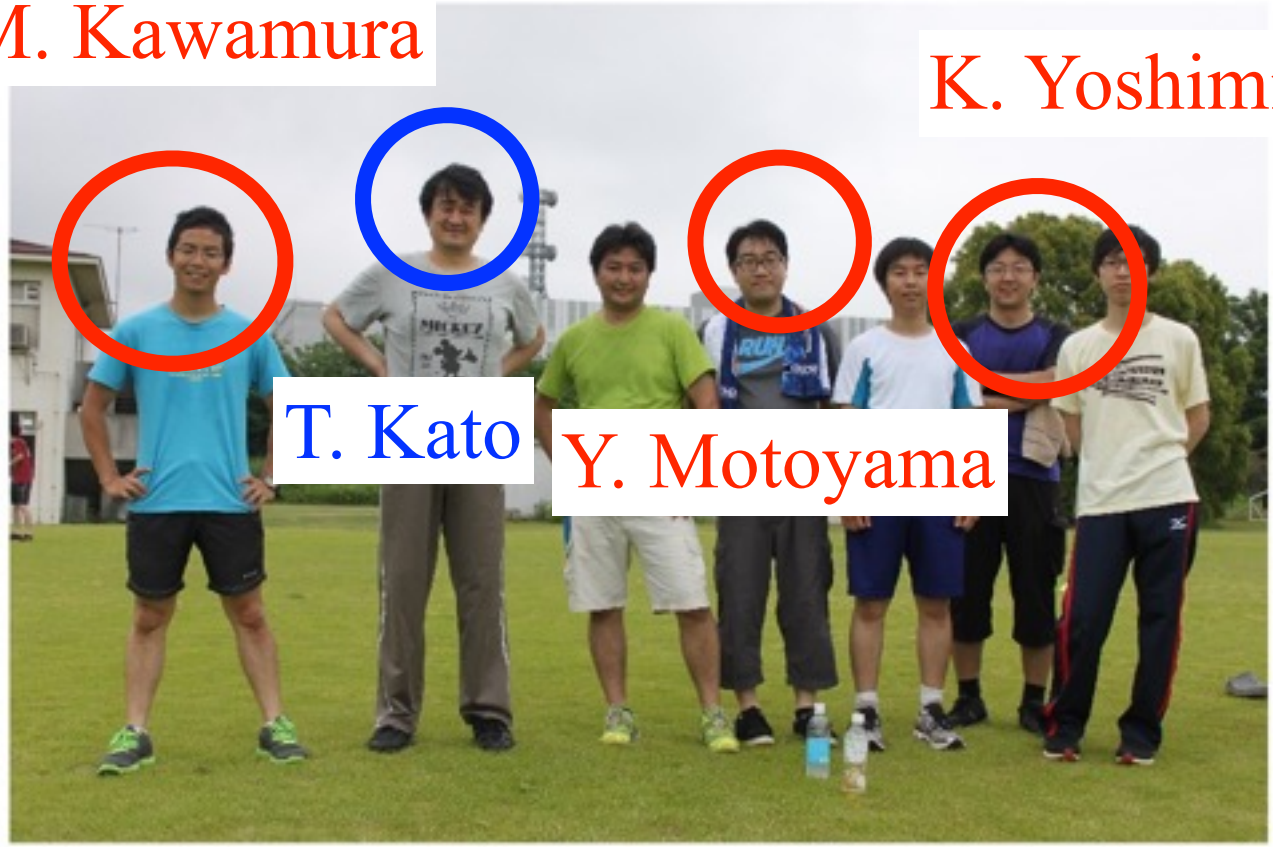
http://ma.cms-initiative.jp/ja/index/listapps/mvmc/mvmc

search by “mVMC materiapps”

→ You can find our homepage in the first page

Developers of mVMC

M. Kawamura



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多変数変分モンテカルロ法 (mVMC)

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

D. Tahara and M. Imada, JPSJ (2008)
T. Misawa and M. Imada, PRB (2014)

一体波動関数

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

拡張したBCS波動関数
→ 金属、反強磁性、
異方的超伝導を
統一的に記述

相関因子

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

量子数射影

$\mathcal{L}^{S}$: 全スピン射影, S=0
$\mathcal{L}^{K}$: 全運動量射影, K=0

変分パラメータ更新(SR法)

エネルギー $E_{\vec{\alpha}} = \langle H \rangle_{\vec{\alpha}}$ を最小化する

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

$$g_k = \frac{\partial E_{\vec{\alpha}}}{\partial \alpha_k}$$ エネルギー勾配 (MC Sampling)

多変数の変分パラメータ(~10000)を最適化
→基底状態の高精度な波動関数を数値的に生成

手法の特徴・独自性

1.多数の変分パラメータ:

✓空間・量子ゆらぎを取り込んだ高精度な計算

✓複雑な相互作用をもつ第一原理有効模型にも適用可能

2. 汎用性：

✓負符号問題なし。強相関系、多軌道系、フラストレーションのある系にも適用可能

✓「任意」の2体相互作用に対応 $H+=\sum_{i,j,k,l}\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4} c^{\dagger}_{i\sigma_1} c_{j\sigma_2} c^{\dagger}_{k\sigma_3} c_{l\sigma_4}$

3. 拡張性:

✓波動関数の系統的な改善→

-平均場近似の結果の系統的な改良

-厳密な数値計算手法に匹敵する精度に到達することも可能

(✓SR法を利用した実時間発展・有限温度計算)

多変数変分モンテカルロ法の適用例[2009-]

1. Iron-based SC： [misawa,nakamura,miyake,hirayama,imada]
   LaFeAsO,LaFePO,$BaFe_2As_2$,FeTe,FeSe
2. Doped Hubbard model： [misawa,imada]
   Origin of SC in doped Hubbard model
3. Organic conductors: [shinaoka,misawa,nakamura,imada]
   κ-$(BEDT\text{-}TTF)_2Cu(NCS)_2$
4. Kondo lattice model: [misawa,yoshitake,motome]
   CO around ¼ filling
5. Frustrated Kondo model:[nakamikawa,yamaji,udagawa,motome]
   Partial Kondo singlet phase in triangular lattice
6. Spin liquids： [morita, kaneko, imada]
   J_1-J_2 Heisenberg model, frustrated Hubbard model
7. Topological insulators: [yamaji, kurita, imada]
   Kane-Mele-Hubbard model,Topological Mott ins., Kitaev model
8. Electron-phonon coupling system [ohgoe, imada]
9. *real-time & imaginary-time evolution* [takai, ido, imada]

Ex. Hubbard 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
```

HPhiとほとんど同じインプットファイル！

Ex. 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

厳密対角化の結果をよく再現!→厳密対角化より大きなサイズの計算も可能 (100-1000 sites)


Enjoy HΦ & mVMC!
HΦ