Introduction to HΦ –A numerical solver for quantum lattice models

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Outline

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

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

Developers of HΦ

M. Kawamura T. Misawa K. Yoshimi

Y. Yamaji

S. Todo

N. Kawashima

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

What can we do by HΦ?

For Hubbard model, spin-*S* Heisenberg model, Kondo-lattice model *with arbitrary one-body and two-body interactions*

- Full diagonalization

- Ground state calculations by Lanczos method

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

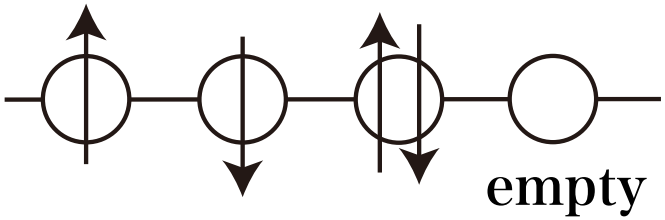
- Dynamical properties (optical conductivity ..)

maximum system sizes@ ISSP system B (sekirei)

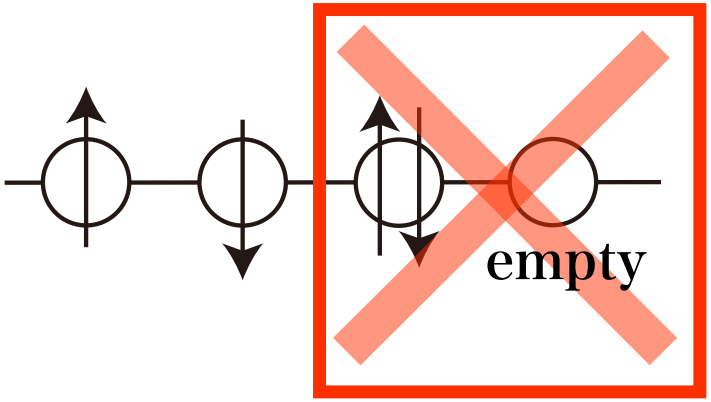
- spin 1/2: ~ 40 sites (Sz conserved)
- Hubbard model: ~ 20sites (# of particles & Sz conserved)

Available models in HΦ

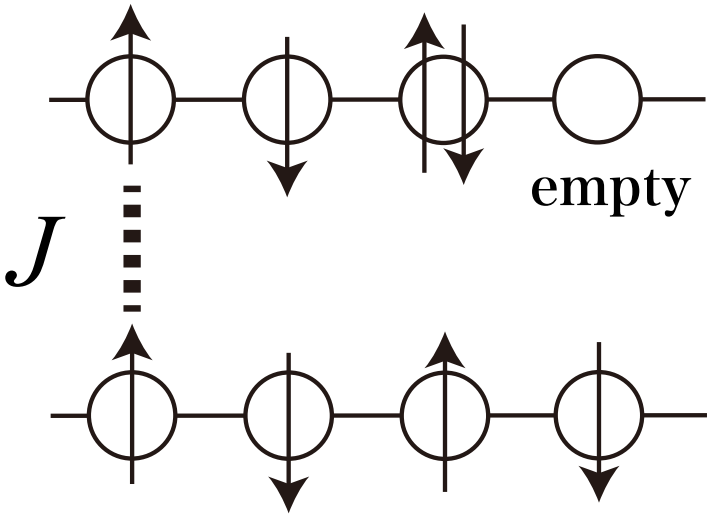
Hubbard (itinerant) ~ 4^N



Heisenberg (localized) ~ 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)

Descriptions of quantum models

e.g. Hubbard model

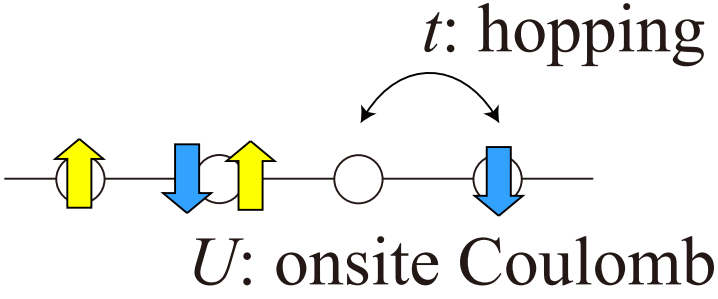
$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_t + \hat{\mathcal{H}}_U$$

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

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



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

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

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

Pauli's principle

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

Full diagonalization by *hand*

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

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

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

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

Full diagonalization by HΦ

Matrix representation of Hamiltonian

(real space basis) → Full diagonalization for the matrix

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

HΦ automatically generates matrix elements !

[2-digit binary number & bit operations]

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 !

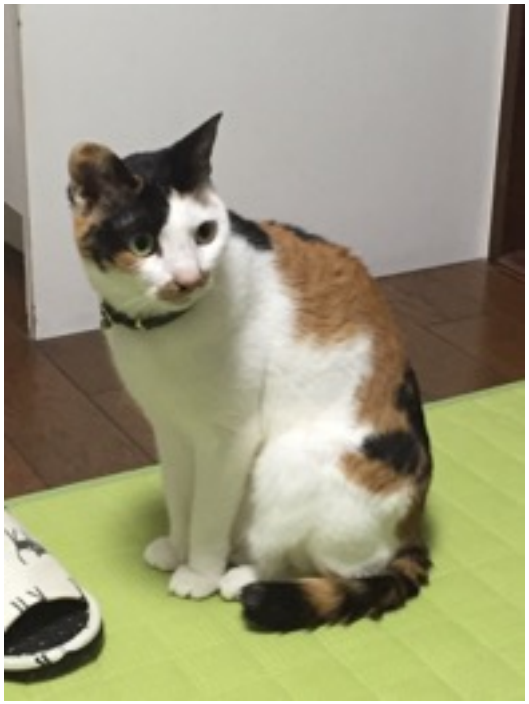
Meaning of name & logo

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

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

waking **sleeping**

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.

Essence of TPQ

cf. 二重ヒルベルト空間 (熱場ダイナミクス)
鈴木増雄, 統計力学(岩波書店); 高橋康, 物性研究 20, 97(1973)

1. Random vector (high-temperature limit) *equally* includes all eigenvectors

$$|\Phi_{\rm rand}\rangle = \sum_n a_n |n\rangle, |a_n|^2 \sim 1/N_{\rm H}$$

$$\langle \hat{H} \rangle = \frac{\langle \Phi_{\rm rand}|\hat{H}|\Phi_{\rm rand}\rangle}{\langle \Phi_{\rm rand}|\Phi_{\rm rand}\rangle} = \frac{\sum_n |a_n|^2 E_n}{\sum_n |a_n|^2} \sim \frac{1}{N_{\rm H}} \sum_n E_n$$

2. Commutative quantities can be calculated by *single wave function*

$$|\Phi(\beta)\rangle = e^{-\beta \hat{H}/2} |\Phi_{\rm rand}\rangle$$

$$\frac{\langle \Phi(\beta)|\hat{H}|\Phi(\beta)\rangle}{\langle \Phi(\beta)|\Phi(\beta)\rangle} = \frac{\sum_n |a_n|^2 E_n e^{-\beta E_n}}{\sum_n |a_n|^2 e^{-\beta E_n}} \sim \frac{\sum_n E_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}} = E(\beta)$$

3. Non-commutative quantities can be also calculated by *single wave function*

Proofs: Hams and De Raedt PRE 2000; Sugiura and Shimizu PRL 2012,2013

Thermal Pure Quantum state (熱的純粋量子状態) by Sugiura and Shimizu

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

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maximum system sizes@ ISSP system B (sekirei)

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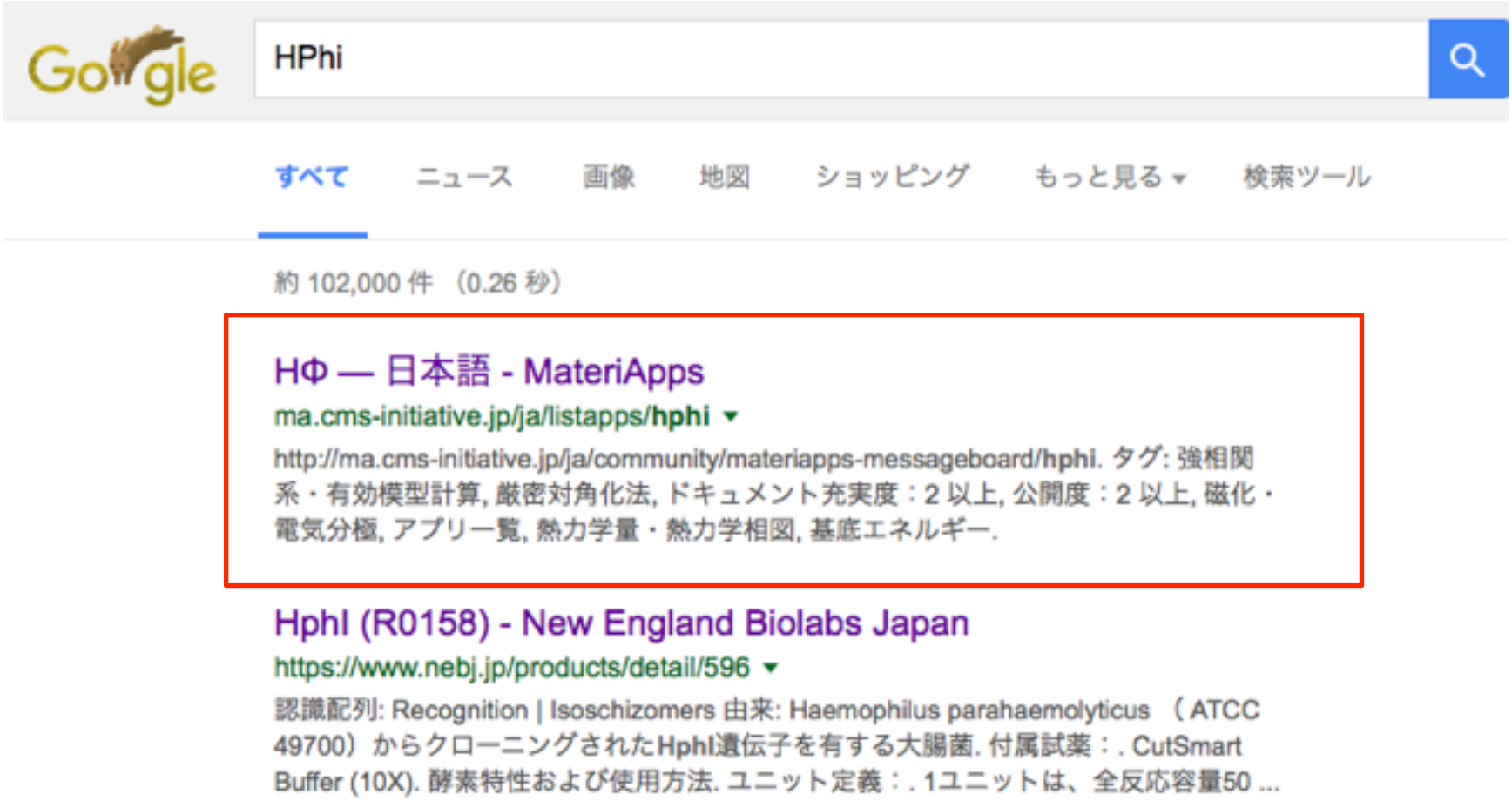
Let’s get НФ !
НФ

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,

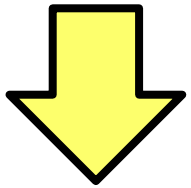
```
$ bash HPhiconfig.sh

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.

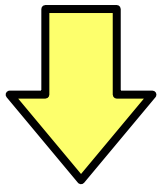
Cautions：

- 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 not 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

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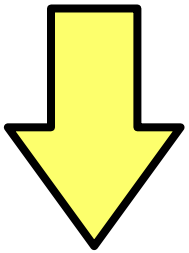


execute following command

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

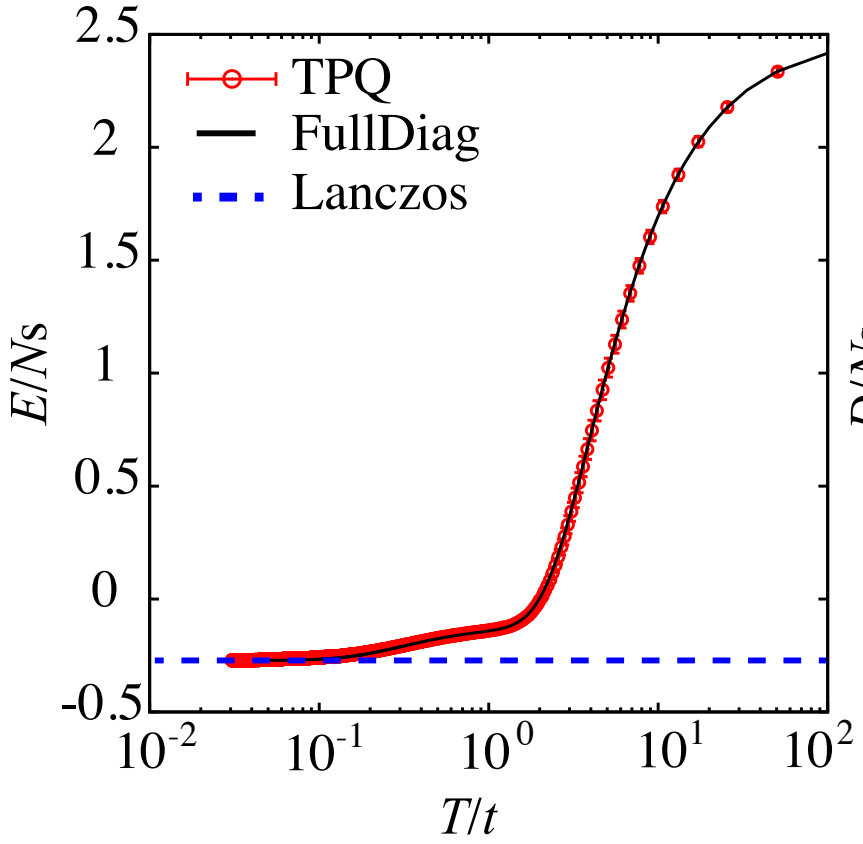
```
================================
NExchange 2
================================
==========Exchange=============
================================
 0   1  0.5
 1   2  0.5
```

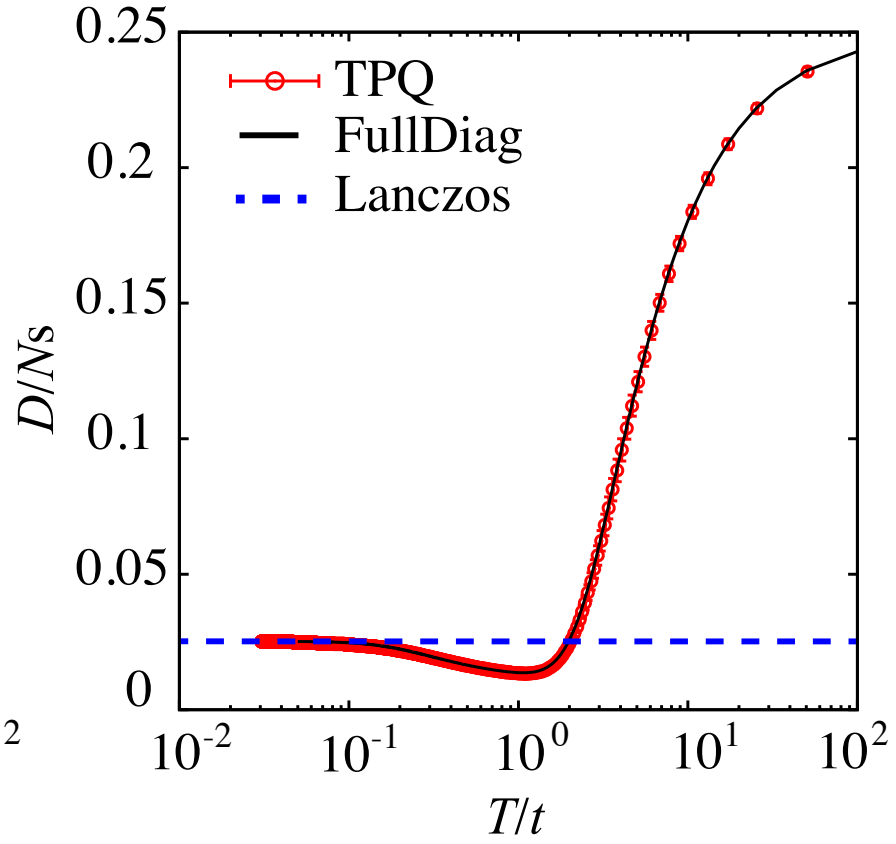
Easy to input interactions


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: J. Phys. Soc. Jpn. 85, 113702 (2016)

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, The Journal of Chemical Physics 145, 244110 (2016)

4. Liquid-Liquid Transition in Kitaev Magnets Driven by Spin Fractionalization
Joji Nasu, Yasuyuki Kato, Junki Yoshitake, Yoshitomo Kamiya, Yukitoshi Motome, Phys. Rev. Lett. 118,137203 (2017)

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・励起状態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トレート系が得意 [論文 1(kagome),2(*t*-*t*' Hubbard)]。

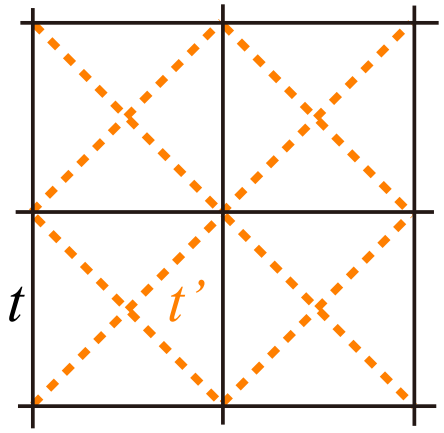
2. 平均場計算などで「面白い」ことがおきることを確認
→HPhiでその結果を確認する[論文4(extended Kitaev model)]

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

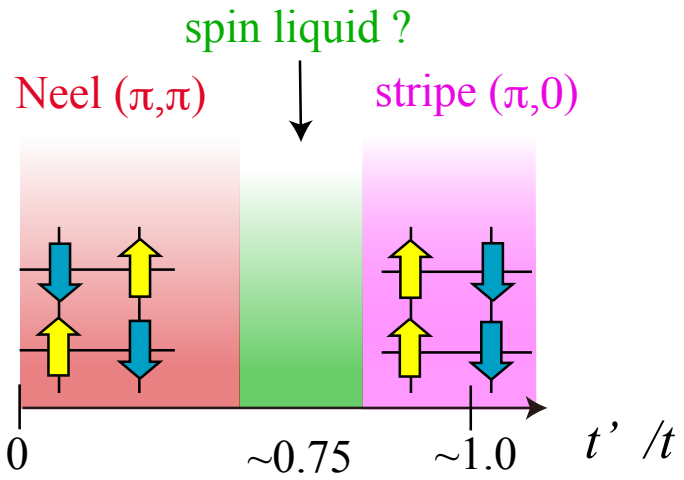
4. 新奇物質に対する現実的な有効模型の妥当性の確認,物性予測
(励起状態、有限温度、動的物理量)[Na_2IrO_3, Yamaji *et al.*]

Frustrated *t-t'* Hubbard model

Lattice geometry

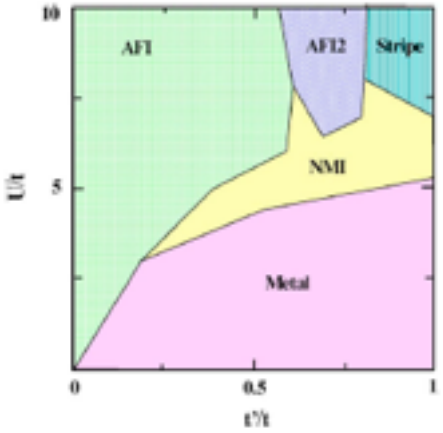


Schematic phase diagram

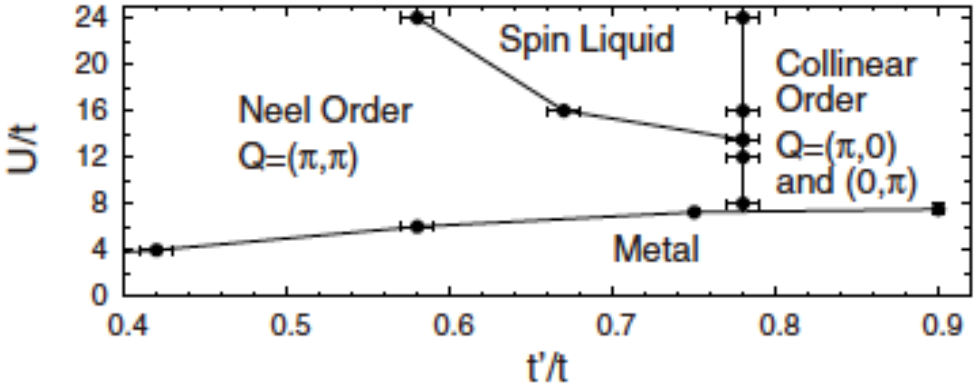


Previous studies

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

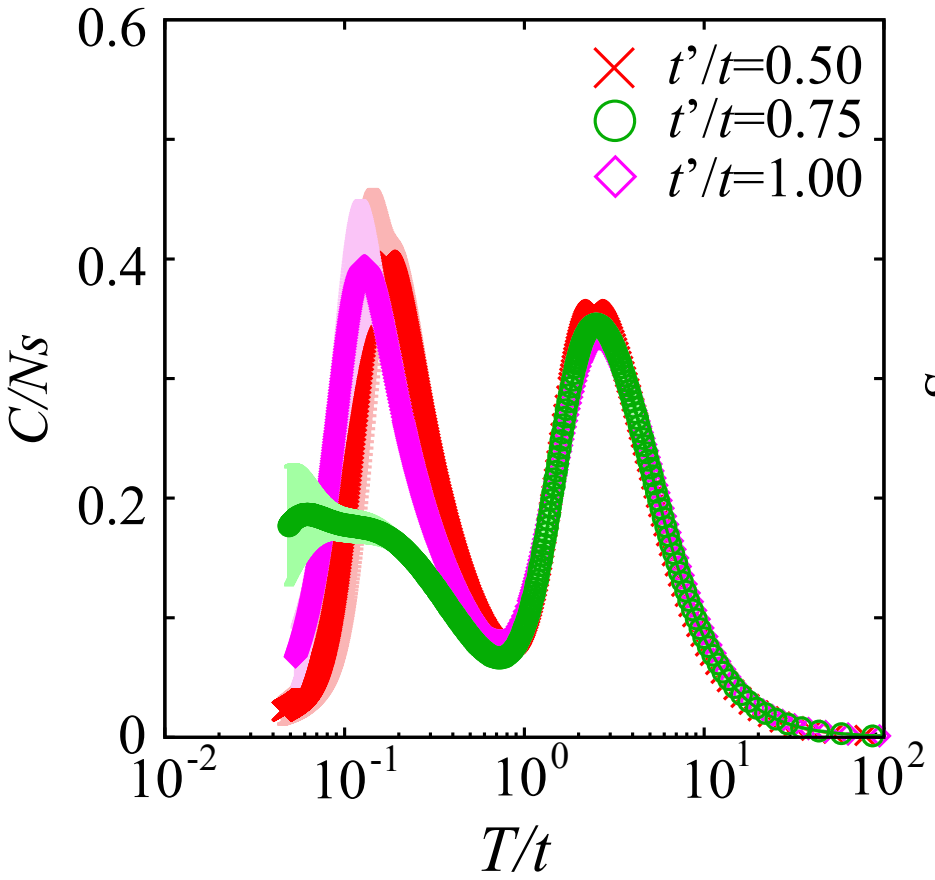
Input file

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

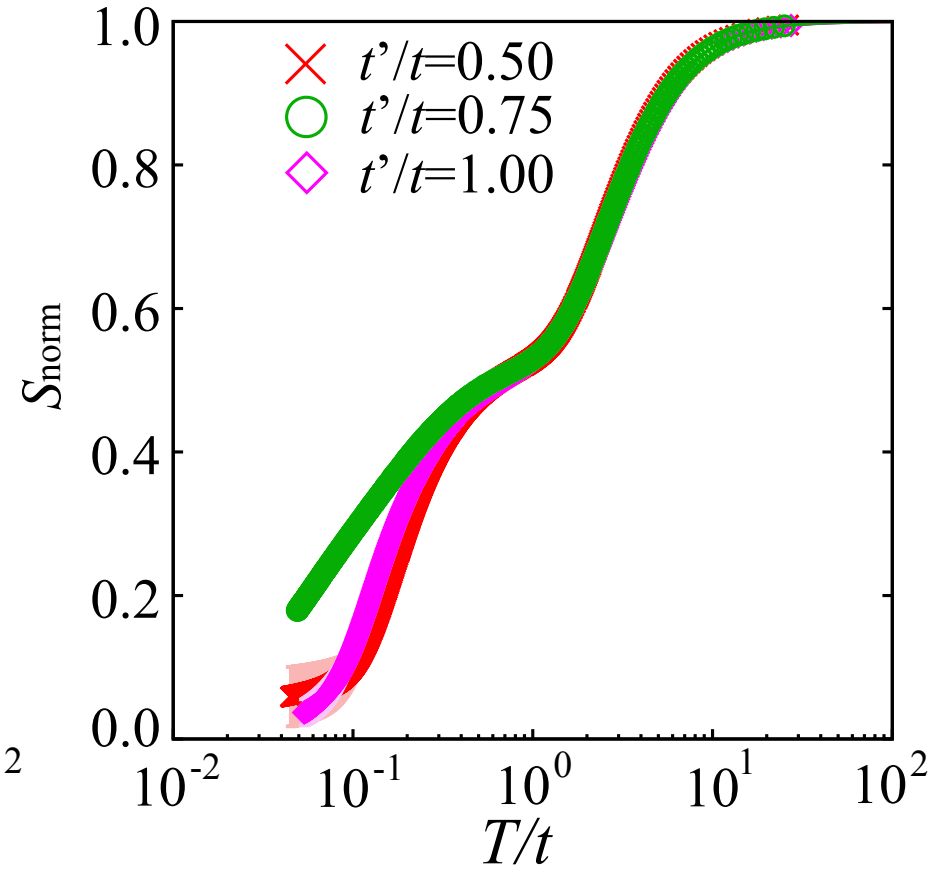
たった、これだけ！そのまま並列計算も可能

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