Exercise of HΦ

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(1) spin 1/2 dimer (fulldiag)
(2) spin 1/2 chain (Lanczos+LOBCG+Spectrum)
(3) J1-J2 Heisenberg model(Lanczos,TPQ)
(4) Kitaev model (Lanczos,TPQ)
(5) Hubbard chain (Lanczos,TPQ)
(6) Model Estimation using COMBO

(1) Heisenberg dimer, Hubbard dimer

$$H = J\vec{S}_0\vec{S}_1$$

$$H = -t(c^{\dagger}_{0\sigma}c_{1\sigma} + \text{h.c.}) + U(n_{0\uparrow}n_{0\downarrow} + n_{1\uparrow}n_{1\downarrow})$$

1. Calculate eigenvalues by full diagonalization method

   E_{min}=-3/4(singlet), E_{max}=1/4(triplet)

2. Change S as 1,2/3,2

   E_{min}=-S(S+1), E_{max}=S^2

3. Change the model to Hubbard model

(half filling , Sz=0)

$$E = 0, U, \frac{U}{2} \times (1 \pm \sqrt{1 + (4t/U)^2})$$

4. Try to use Lanczos or LOBCG methods

(2) Heisenberg chain

$$H = J \sum_{\langle i,j \rangle} S_i S_j$$

1. Calculate energies by Lanczos method (upto the lattice size L = 20)

→ Calculate energy gap Δ between the ground state and the first excited state.

→ Plot 1/L - Δ.

2. Do the same calculation on S=1 Heisenberg model. (Haldane gap)

3. Check the difference of eigenvalues obtained by Lanczos and LOBCG methods at high magnetic field.

4. Calculate the spectrum function: S(q, ω).

(3) J1-J2 Heisenberg model

$$H = J_1 \sum_{\langle i,j \rangle} S_i S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i S_j$$

1. Calculate energies by Lanczos method (L ~ 4×4)
2. Calculate specific heat by TPQ method (J2/J1~0.5)
3. Calculate spin-spin correlations.

Example script

```
L = 4
W = 4
model = "Spin"
method = "Lanczos"
lattice = "square lattice"
J = 2.0
J' = 1.0
2Sz = 0
```

(4) Kitaev model

$$H = -J_x \sum_{x-\mathrm{bond}} S_i^x S_j^x - J_y \sum_{y-\mathrm{bond}} S_i^y S_j^y - J_z \sum_{z-\mathrm{bond}} S_i^z S_j^z$$

1. Calculate energy by Lanczos method (L~18)
2. Calculate specific heat by TPQ
3. Calculate spin-spin correlation for nearest-neighbor bond (check the value becomes exactly 0).

Example script

```
W = 3
L = 3
model = "SpinGC"
method = "Lanczos"
lattice = "Honeycomb"
J0x = -1.0
J0y =  0.0
J0z =  0.0
J1x =  0.0
J1y = -1.0
J1z =  0.0
J2x =  0.0
J2y =  0.0
J2z = -1.0
```

(5) Hubbard chain

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

1. Calculate energies and double occupancy by Lanczos method (L = 8)
2. Calculate specific heat and double occupancy by TPQ method
3. Compare the results obtained by TPQ method with that obtained by Full diagonalization method.

Example script

```
L = 8
model = "FermionHubbard"
method = "Lanczos"
lattice = "chain"
t = 1.0
U = 8.0
nelec = 8
2Sz = 0
```

(6) Model estimation by using COMBO

One dimensional Heisenberg chain (12 sites)

$$H = \sum_{i=1}^{12} (J_1 S_i \cdot S_{i+1} + J_2 S_i \cdot S_{i+2} + J_3 S_i \cdot S_{i+3})$$

1. Calculate the magnetization curve by using Lanczos method at (J1, J2, J3) = (1.0, 0.5, 0.3).
2. To obtain the answer (J1, J2, J3) = (1.0, 0.5, 0.3) by comparing the magnetization curve for the parameter pair, model estimation using bayesian optimization library COMBO is performed.

For details, see python scripts ModelEstimation/model_estimation.py in HPhi-garally.

(1): Answer-1

1-1. Heisenberg dimer

```
L = 2
model = "Spin"
method = "FullDiag"
lattice = "chain"
J = 0.5
2Sz = 0
```

Set J=0.5, since J is double counted due to the periodic boundary condition.

1-2. spin-S Heisenberg dimer

```
L = 2
model = "Spin"
method = "FullDiag"
lattice = "chain"
J = 0.5
2Sz = 0
2S =2
```

If you set 2S=2, the model becomes S=1 spin model (The default value is 2S=1). Likewise, if you set 2S=3,2S=4, the model becomes S=3/2, S=2 spin model.

(1): Answer-II

1-3. Hubbard dimer

```
L = 2
model = "Hubbard"
method = "FullDiag"
lattice = "chain"
t = 0.5
U = 4
2Sz = 0
nelec = 2
```

Set t=0.5, since t is double counted due to the periodic boundary condition.

1-4. Heisenberg dimer

```
L = 2
model = "Spin"
method = "Lanczos"
lattice = "chain"
J = 0.5
2Sz = 0
```

```
L = 2
model = "Spin"
method = "CG"
lattice = "chain"
J = 0.5
2Sz = 0
```

By setting method=“Lanczos” (“CG”), calculation by Lanczos (LOBCG) method is done.
(*) Though Lanczos method gives exact eigenvalue, an error message appears since the Hilbert space is too small and the convergence condition is not satisfied.

(2): Answer-1

1-1. Heisenberg chain

```
L = 12
model = "Spin"
method = "Lanczos"
lattice = "chain"
J = 1.0
2Sz = 0
```

Results: output/zvo_Lanczos_Step.dat
E0＝-5.3873909174 ,E1= -5.0315434037

ΔE= E1-E0 ~0.355

(2) Answer-2

1-2. Heisenberg chain

```
L = 12
model = "Spin"
method = "Lanczos"
lattice = "chain"
J = 1.0
2Sz = 0
2S = 2
```

The L dependency of energy gap is left for practice.

(2): Answer-3

1-3. Heisenberg chain

```
L = 12
model = "SpinGC"
method = "Lanczos"
lattice = "chain"
J = 1.0
H = 10.0
```

```
L = 12
model = "SpinGC"
method = "CG"
lattice = "chain"
J = 1.0
H = 10.0
exct =4
```

H →SpinGC（Sz-free）

Lanczos → not correct (degeneracy appears)

```
stp = 74 -57.0000000000 -56.9998301292
stp = 76 -57.0000000000 -56.9999967206
stp = 78 -57.0000000000 -56.9999998797
```

CG → correct

```
i=    0 Energy=-57.000000 N= 12.000000
i=    1 Energy=-49.000000 N= 12.000000
i=    2 Energy=-48.866025 N= 12.000000
i=    3 Energy=-48.866025 N= 12.000000
```

(2):Answer-4

1-4. Calculation of S(q,ω)

https://github.com/issp-center-dev/HPhi-gallery/tree/master/Spin/HeisenbergSpectrum

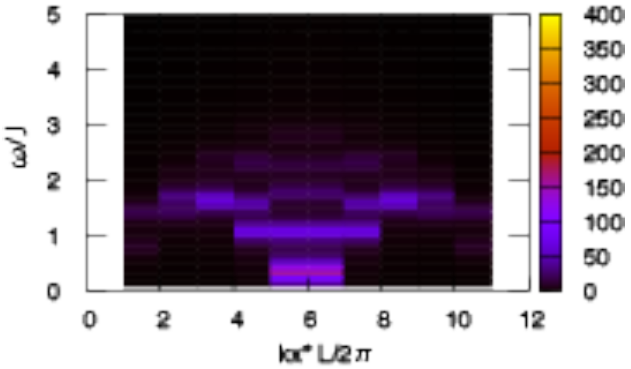
The spectrum function can be calculated by following steps.

1. Calculate the ground state.
2. Define excitation operators in the `pair.def` file.
3. Calculate spectrum function.

See the manual for details. To simply do above steps, we prepare the script file `spinchain_example.py`. In the following, we show the procedure to obtain the specrum function by using the script file.

1. Execute the script file (`spinchain_example.py`)
   ```
   $ python spinchain_example.py
   ```

3. Plot `spectrum.dat` by gnuplot.
   ```
   $ gnuplot
   ```
4. `$ set yrange [0:5]`
5. `$ set pm3d map`
6. `$ splot "./spectrum.dat" using 1:2:3`
7. You can see the right figure, where horizontal and vertical axises correspond to the index of wave vector and frequency, respectively.



(3): Answer-1

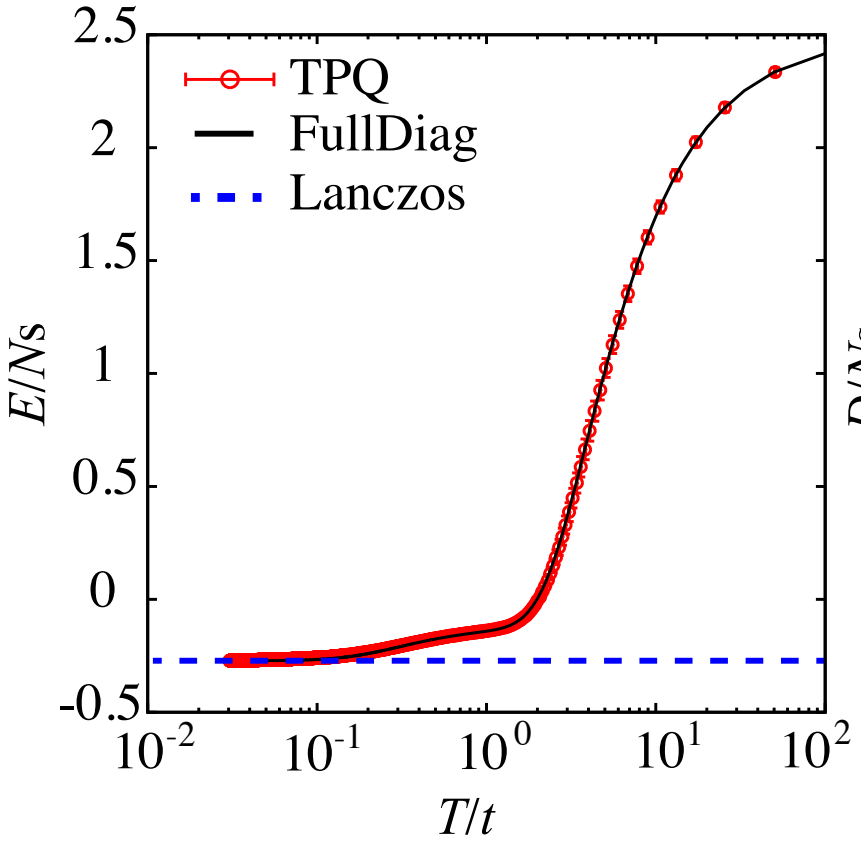
J_1-J_2 Heisenberg model, Ns=4×4, J_1=2.0
E. Dagotto and A. Moreo, PRB (R) 39 , 4744 (1989)

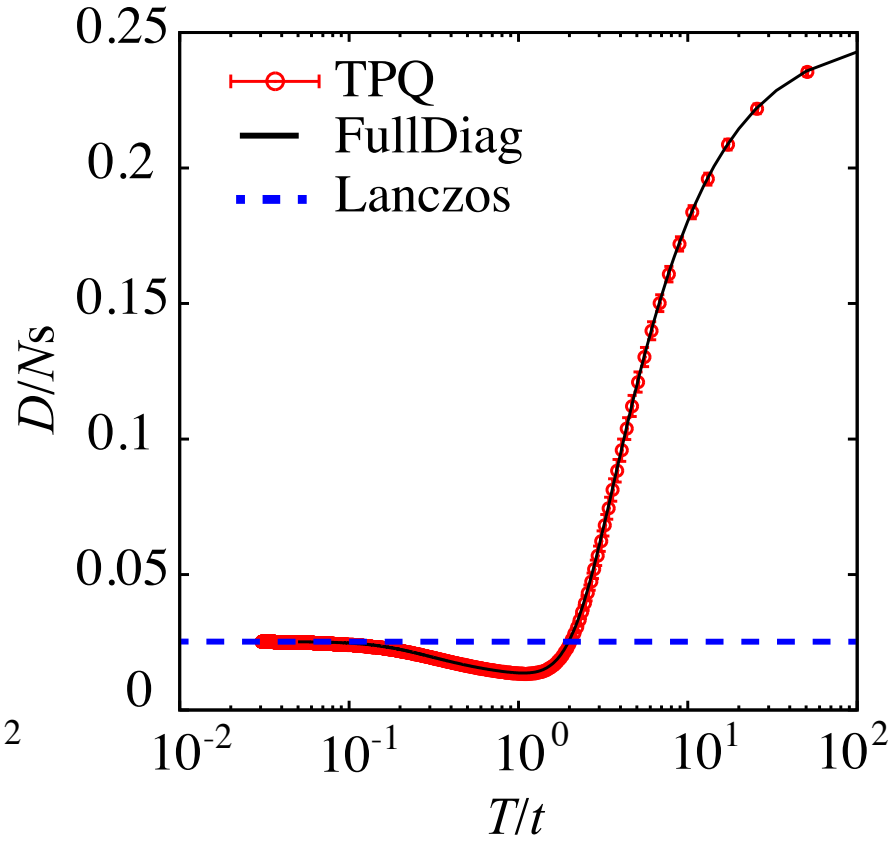
TABLE I. Ground-state energy (E_0) and first excited-state energy (E_1) per site (both singlets with zero momentum) of the 2D Heisenberg model with frustration as a function of J_2 on a 4×4 lattice. The error is in the last digit.

J_2	E_0	E_1
0.950	−1.065978	−1.0160
1.100	−1.047189	−1.0254
1.150	−1.047183	−1.0307
1.200	−1.051792	−1.0380
1.325	−1.089305	−1.0804
1.400	−1.127716	−1.1169
1.500	−1.188546	−1.1691
1.600	−1.254670	−1.2233
1.750	−1.358437	−1.3072

(5): Answer

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





TPQ method works well !