Question

1. 编写程序：计算正方格点上自旋1/2的反铁磁Heisenberg模型的自旋算符的期望值。将你得到的结果和quantum Monte Carlo 得到的结果进行比较， quantum Monte Carlo的结果需要自行查找。
2. 写出你的详细思路并对程序进行注释。
3. 本题满分10分，注意作业截止时间。

理论基础

Quantum Monte Carlo

This part is the results form an article[1]——Finite-size scaling of the ground-state parameters of the two-dimensional Heisenberg model, I'll compare my answer with its.

In this article, TABLE III gives some parameters of the ground state and FIG 6 givers the ground-energy and the L's relation, just as fellows:

Parameters	Value
Ground state energy E	-0.669437(5)
Sublattice magnetization M	0.3070(3)
Spin stiffness ρ_s	0.175(2)
Perpendicular susceptibility $\chi_\perp$	0.0625(9)
Spin-wave velocity c	1.673(7)
Leading size correction e_3	-2.405(10)
Subleading size correction e_4	4.00(6)
Size correction m_1	0.560(6)
Size correction m_2	1.08(5)

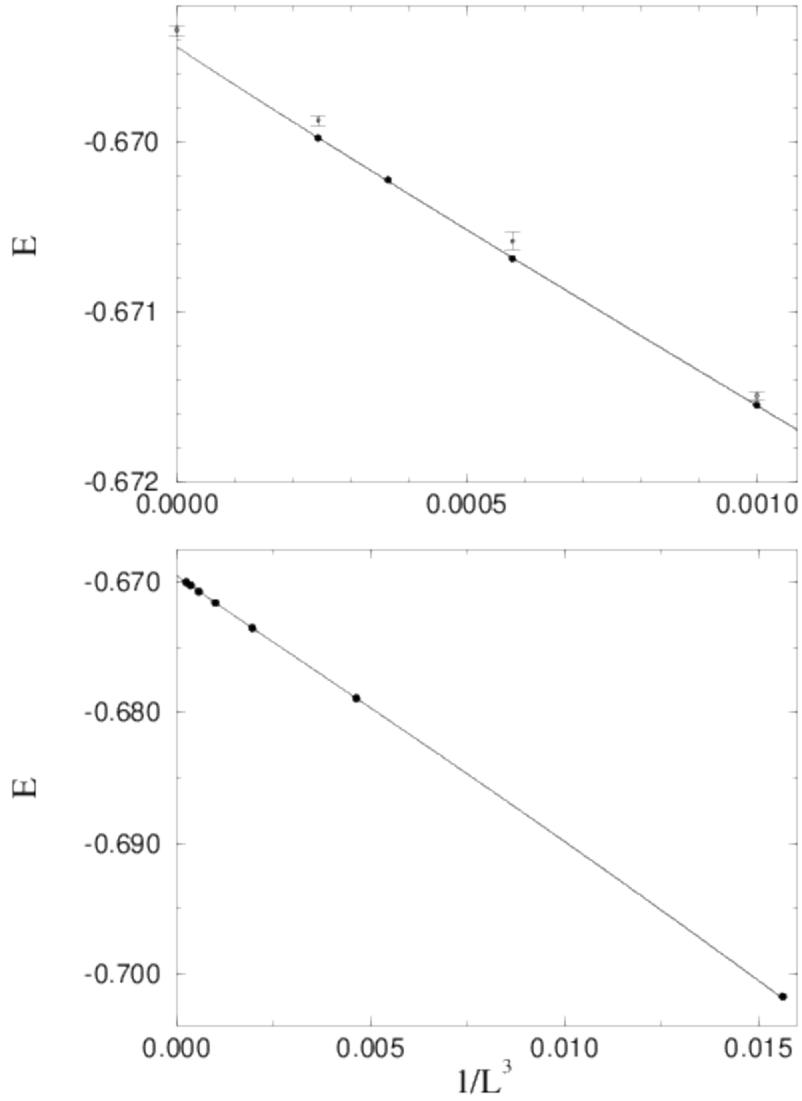


Fig. 6. A. W. Sandvik

磁矩[2]

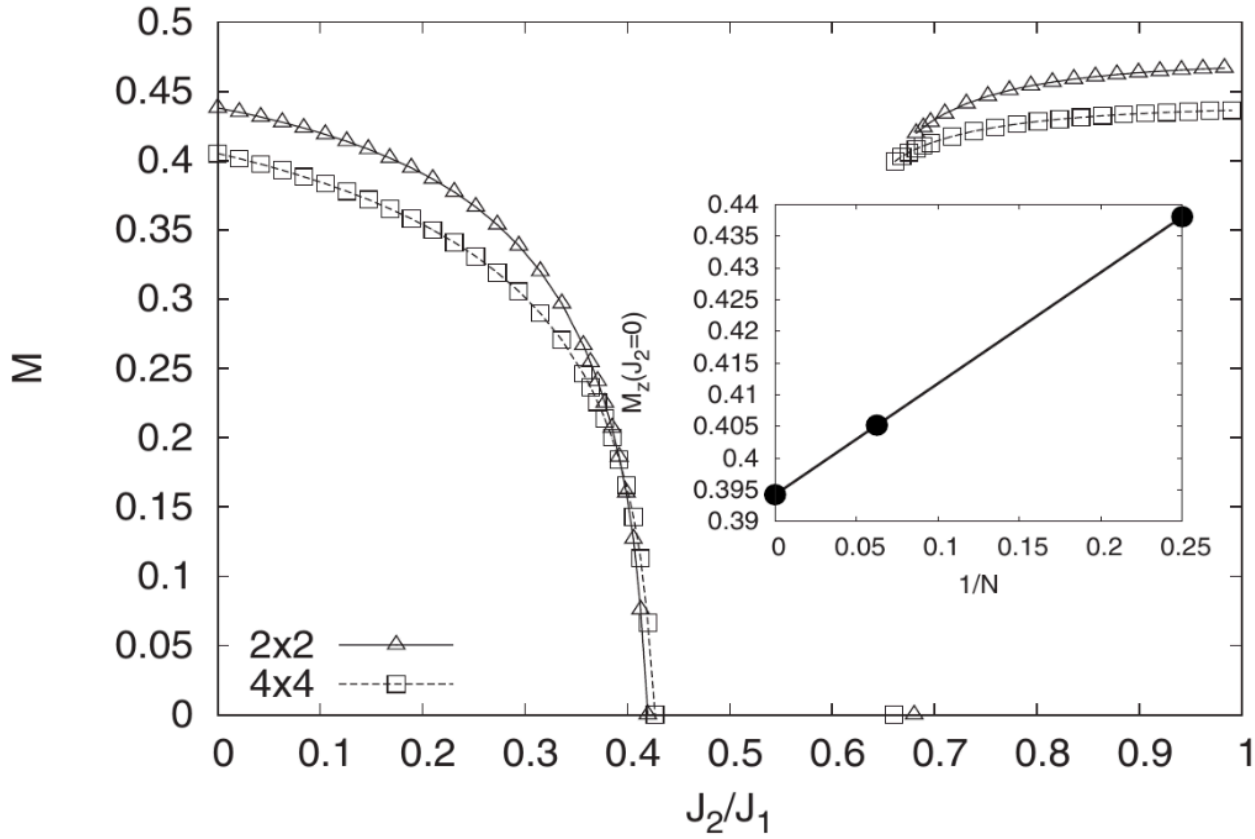


FIG. 9. Staggered magnetization M_{stag} for $J_2 \leq J_2^{c1}$ and collinear magnetization along the x direction, $M_{\text{col}}(x)$, for $J_2 \geq J_2^{c2}$ (for the 2×2 and 4×4 plaquette degrees of freedom), computed at the HF level. Notice the continuous phase transition at $J_2/J_1 \approx 0.42$ and a first-order transition at $J_2/J_1 \approx 0.68$ (2×2) and $J_2/J_1 \approx 0.66$ (4×4). The inset shows finite-size scaling of M_z at $J_2=0$.

But the M this aricle gives is very complex, it's divided into two types:

$$
\begin{aligned}
M_1^2(L) &= 3S(\pi,\pi)/L^2 \\
M_1^2(L) &= M^2 + \frac{m_1}{L} + \frac{m_2}{L^2} + \frac{m_3}{L^3} \\
M_2^2(L) &= 3C(L/2, L/2) \\
M_2^2(L) &= M^2 + \frac{n_1}{L} + \frac{n_2}{L^2} + \frac{n_3}{L^3}
\end{aligned}
$$

where has:

$$
\begin{aligned}
|\alpha(p)\rangle &= \prod_{i=1}^{p} \hat{H}_{a_i,b_i}|\alpha\rangle, \quad |\alpha(0)\rangle = |\alpha\rangle \\
S_i^z[p] &= \langle\alpha(p)|S_i^z|\alpha(p)\rangle \\
C(i,j) &= \left\langle \frac{1}{n+1}\sum_{p=0}^{n} S_i^z[p]S_j^z[p] \right\rangle \\
S(\pi,\pi) &= \frac{1}{N}\sum_{i,j}(-1)^{x_j-x_i+y_j-y_i}C(i,j)
\end{aligned}
$$

I can't fully understand these, so I find another definition in NTNU johnof's personal webpage[3]

> Let us next investigate the amount of magnetic order in the system. Thus we need to identify an order parameter for antiferromagnetic order. Note that the magnetization $M = (1/N)\sum_i \langle \mathbf{S_i} \rangle$can not be used since it is zero in the presence of antiferromagnetic order, because the two sublattices give equal-magnitude but opposite-sign contributions to M. Instead the natural order parameter is the so-called sublattice magnetization, defined by averaging $\langle \mathbf{S_i} \rangle$ only over the sites of one of the two sublattices. Without loss of generality, let's pick sublattice A, where the putative ordering is in the z direction. The magnitude of the sublattice magnetization is thus :
> $M_A = \frac{1}{N_A}\sum_{j\in A}\langle S_j^z \rangle$

mean-field method

首先，需要明确的是，我们一下的讨论完全是基于自旋为1/2的情况来的；因此，需要明确下述所有具体公式的适用范围。

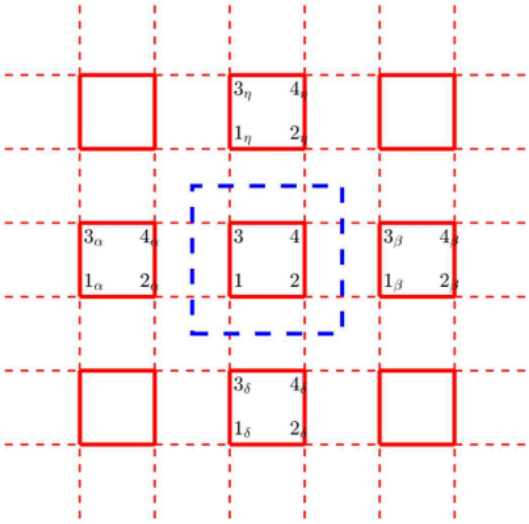
无论对于哪个粒子，均规定其自旋向上为第一个状态，则有：

$$
S^x = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad S^y = \frac{1}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad S^z = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
$$

下面是平均场近似的主要原理：

平均场计算磁化强度

设 $\mathcal{H}=\sum_{<ij>}\boldsymbol{S}_i\cdot\boldsymbol{S}_j$，用平均场理论计算该模型的磁化强度。这里假设设 S=1/2。



$$H=\sum_\sigma\langle S^\sigma_{2_\alpha}\rangle S^\sigma_1+\langle S^\sigma_{4_\alpha}\rangle S^\sigma_3+\left\langle S^\sigma_{1_\beta}\right\rangle S^\sigma_2+\left\langle S^\sigma_{3_\beta}\right\rangle S^\sigma_4$$
$$+\sum_\sigma\langle S^\sigma_{3_\delta}\rangle S^\sigma_1+\langle S^\sigma_{4_\delta}\rangle S^\sigma_2+\left\langle S^\sigma_{1_\eta}\right\rangle S^\sigma_3+\left\langle S^\sigma_{2_\eta}\right\rangle S^\sigma_4$$
$$+\boldsymbol{S}_1\cdot\boldsymbol{S}_2+\boldsymbol{S}_2\cdot\boldsymbol{S}_4+\boldsymbol{S}_3\cdot\boldsymbol{S}_4+\boldsymbol{S}_1\cdot\boldsymbol{S}_3$$

$$H=\sum_\sigma\alpha^\sigma_2S^\sigma_1+\alpha^\sigma_4S^\sigma_3+\beta^\sigma_1S^\sigma_2+\beta^\sigma_3S^\sigma_4$$
$$+\sum_\sigma\delta^\sigma_3S^\sigma_1+\delta^\sigma_4S^\sigma_2+\eta^\sigma_1S^\sigma_3+\eta^\sigma_2S^\sigma_4$$
$$+\boldsymbol{S}_1\cdot\boldsymbol{S}_2+\boldsymbol{S}_2\cdot\boldsymbol{S}_4+\boldsymbol{S}_3\cdot\boldsymbol{S}_4+\boldsymbol{S}_1\cdot\boldsymbol{S}_3$$

这里 $\sigma=x,y,z$

以期望值代替外部粒子对元胞的作用，根据对称性，外部粒子自旋的期望就是其对应内部粒子自旋的期望。

自旋的期望用迭代收敛的方式来计算，写出哈密顿量的矩阵表示（这个会在程序设计的时候提到），对角化以求出基态能量和其对应的本征态。开始时以随机数作为期望值，通过迭代得到收敛值。（当然，暂时我还无法证明是否会收敛，只能看计算结果了）。

设最后求出来的本征态为$|\psi\rangle$，则期望值$\langle S_i^\sigma\rangle=\langle\psi|\,S_i^\sigma\,|\psi\rangle$。

至此，思路很明显了，剩下的就是程序的编写了。因为论文涉及的点阵最小是4*4的，所以我打算写一个能计算n*n的程序。这在设计上会有一定的困难，但最坑的还是写好了只能算2*2的，3*3的可能也能算但比较勉强了。4*4是根本算不了（在没有优化算法的情况下，在利用对称性的情况下，有可能可以算）;因为我的内存根本无法分配65536*65536的矩阵。

程序编写

header file

1. a program to print a tensor

```
Function m_cprint(A: ComplexTensor, row_count: Integer,
 column_count: Integer)
 For i from 0 to row_count - 1
     For j from 0 to column_count - 1
         real_part = RealPart(A[(i * column_count) + j])
         imaginary_part = ImaginaryPart(A[(i * column_count) + j])
         Print(real_part, "+", "i", imaginary_part, "  ")
     End For
     Print(newline)  // Print a newline after each row
 End For
 Print(newline)  // Print a newline at the end of the tensor
 End Function
```

2. the Kronecher Product (Tensor Product)

```
Function m_KP(A: ComplexMatrix, B: ComplexMatrix, ARows:
 Integer, AColumns: Integer, BRows: Integer, BColumns: Integer,
  C: ComplexMatrix)
 For i from 0 to ARows - 1
     For j from 0 to AColumns - 1
         For k from 0 to BRows - 1
             For l from 0 to BColumns - 1
                 index = ((i * BRows) + k) * (AColumns *
                  BColumns) + ((j * BColumns) + l)
                 C[index] = A[(i * AColumns) + j] * B[(k *
                  BColumns) + l]
             End For
         End For
     End For
 End For
 End Function
```

3. get Hamiltonian

   伪代码这里就不给出来了，下面只简要介绍必须的约定。

   我们通过公式$H_{mn}=\langle m|\,H\,|n\rangle$来给出哈密顿量的矩阵。

   我们需要知道两件事——1.状态的规定。2.算符对状态的作用。我们一个一个说。

   首先是状态如何规定。我以0来代表状态$|\uparrow\rangle$（这样是为了与课上的规定相容），以1来代表状态$|\downarrow\rangle$。则对于4个粒子，状态$|0000\rangle=|0\rangle,|1111\rangle=|1*2^3+1*2^2+1*2^1+1*2^0\rangle=|15\rangle$（我们用计算机的天然语言来表示，其实也就是二进制）。同样，我们也可以算出给定状态对应的序号。可以以一个数组来存储原生状态，而通过代数式来表达序号。(见APPENDIX)

   下面，我们需要知道各算符对状态的作用。我们有$\hat{S}^+|\uparrow\rangle=0\,|\rangle,\hat{S}^-|\uparrow\rangle=|\downarrow\rangle,\hat{S}^+|\downarrow\rangle=|\uparrow\rangle,\hat{S}^-|\downarrow\rangle=0\,|\rangle$，于是有

$$\begin{aligned}\hat{S}^x|\uparrow\rangle&=0.5\,|\downarrow\rangle&\quad\hat{S}^x|\downarrow\rangle&=0.5\,|\uparrow\rangle\\\hat{S}^y|\uparrow\rangle&=0.5i\,|\downarrow\rangle&\quad\hat{S}^y|\downarrow\rangle&=-0.5i\,|\uparrow\rangle\\\hat{S}^z|\uparrow\rangle&=0.5\,|\uparrow\rangle&\quad\hat{S}^z|\downarrow\rangle&=-0.5\,|\downarrow\rangle\end{aligned}$$

   用序号表示则是：

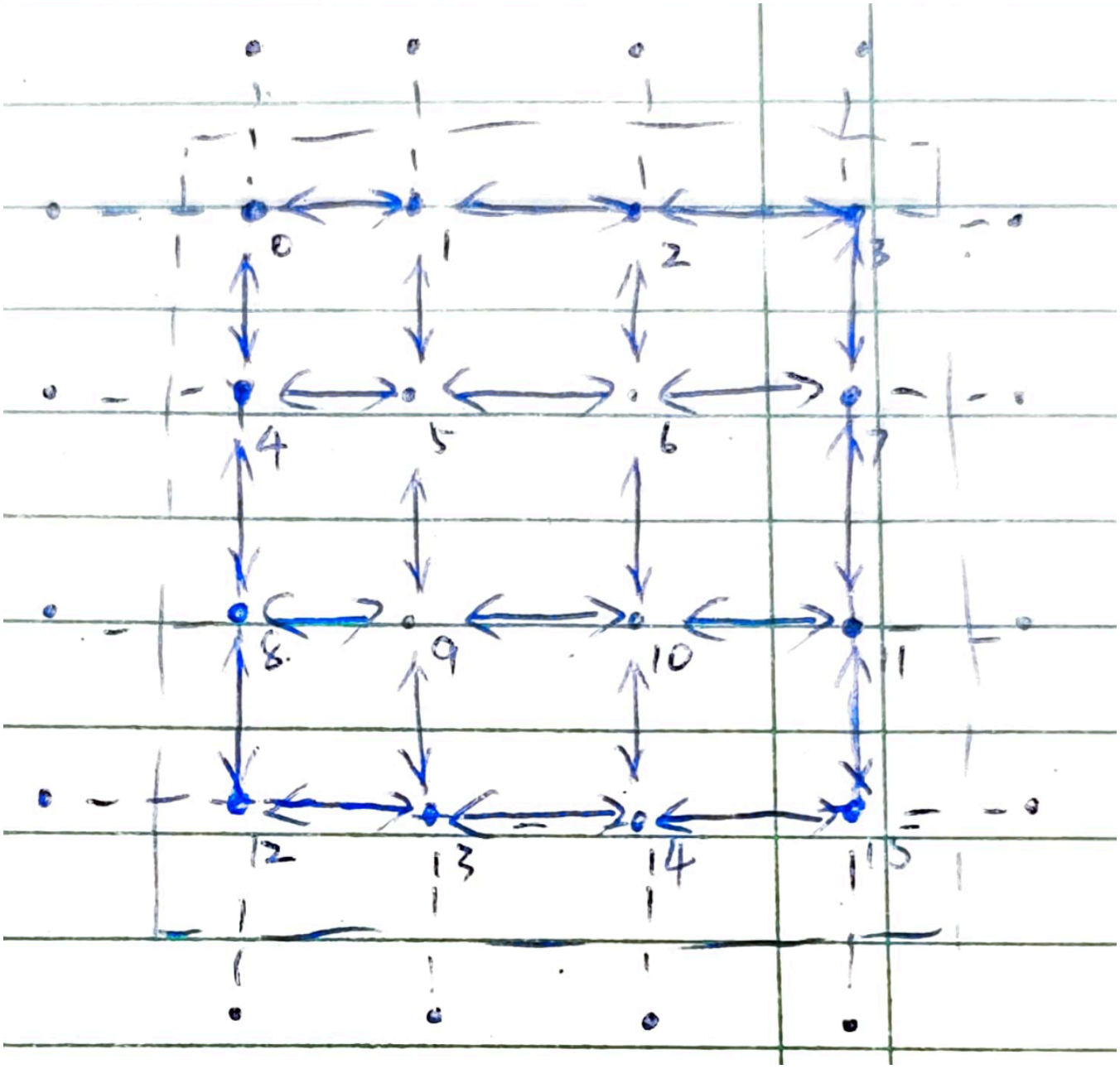
$$\begin{aligned}\hat{S}^x|0\rangle&=0.5\,|1\rangle&\quad\hat{S}^x|1\rangle&=0.5\,|0\rangle\\\hat{S}^y|0\rangle&=0.5i\,|1\rangle&\quad\hat{S}^y|1\rangle&=-0.5i\,|0\rangle\\\hat{S}^z|0\rangle&=0.5\,|0\rangle&\quad\hat{S}^z|1\rangle&=-0.5\,|1\rangle\end{aligned}$$

main function

首先需要做的就是给出哈密顿量的矩阵表示，这个直接用直乘也是可以的，但是对于较大的矩阵来说运算效率比较低下。同时由于自旋的期望是实数，将不对自旋进行整数化。

采取使用函数的办法来给出哈密顿量，形参应该有：子晶格大小L,自旋的期望值（我将以3*L*L的矩阵来存储它）。

如图（以4*4为例）：



需要分格点内外将耦合的自旋表达出来。我们对内部分行、列；外部分上下左右进行计算。

磁矩用期望值s来表示，有$M^2 = S_x^2 + S_y^2 + S_z^2 = s^2$

Results

根据下面的结果我们可以看到，能量算的是非常不错的，因为文献中算的是4*4的，而我的计算机最多只能跑3*3。但我们可以看到，随子格的尺度增加，能量是减小的。可以预期4*4的结果

会和文献中的差不多。
磁矩的计算结果和文献1中差异较大，但和文献3的2*2的结果符合的很好。

当L=2时，

1. No.1

```
the initial spin is :
0.1298+i0.0000  -0.0465+i0.0000  -0.4701+i0.0000  -0.4999+i0.0000
-0.4999+i0.0000  -0.1288+i0.0000  0.4523+i0.0000  -0.1297+i0.0000
-0.0216+i0.0000  -0.4340+i0.0000  -0.0851+i0.0000  -0.0501+i0.0000

the ground eigenvalue is:
-0.775951
the spin is :
0.0561+i-0.0000  -0.0561+i-0.0000  -0.0561+i0.0000  0.0561+i0.0000
-0.3947+i0.0000  0.3947+i-0.0000  0.3947+i-0.0000  -0.3947+i0.0000
0.1816+i0.0000  -0.1816+i0.0000  -0.1816+i0.0000  0.1816+i0.0000

the magnet moment M is:
0.4381
[1] + Done                       "/usr/bin/gdb" --interpreter=mi --tty=${DbgTe
```

2. No.2

```
the initial spin is :
-0.4042+i0.0000  -0.4824+i0.0000  -0.0222+i0.0000  0.3943+i0.0000
0.0386+i0.0000  -0.2183+i0.0000  0.2899+i0.0000  -0.1397+i0.0000
-0.1974+i0.0000  0.2291+i0.0000  -0.3189+i0.0000  -0.1692+i0.0000

the ground eigenvalue is:
-0.775951
the spin is :
0.3599+i-0.0000  -0.3599+i0.0000  -0.3599+i-0.0000  0.3599+i0.0000
-0.1292+i-0.0000  0.1292+i-0.0000  0.1292+i0.0000  -0.1292+i0.0000
-0.2138+i0.0000  0.2138+i0.0000  0.2138+i0.0000  -0.2138+i0.0000

the magnet moment M is:
0.4381
[1] + Done                       "/usr/bin/gdb" --interpreter=mi --tty=${DbgTe
```

3. No.3

```
the initial spin is :
0.3304+i0.0000  -0.4330+i0.0000  -0.2334+i0.0000  0.0043+i0.0000
0.0694+i0.0000  -0.3464+i0.0000  0.3289+i0.0000  0.4553+i0.0000
0.2850+i0.0000  0.3570+i0.0000  0.1711+i0.0000  -0.3016+i0.0000

the ground eigenvalue is:
-0.775951
the spin is :
0.3459+i0.0000  -0.3459+i-0.0000  -0.3459+i0.0000  0.3459+i0.0000
0.1958+i-0.0000  -0.1958+i-0.0000  -0.1958+i0.0000  0.1958+i0.0000
-0.1841+i0.0000  0.1841+i0.0000  0.1841+i0.0000  -0.1841+i0.0000

the magnet moment M is:
0.4381
[1] + Done                       "/usr/bin/gdb" --interpreter=mi --tty=${DbgTe
```

Parameters	Value
Ground state energy E	-0.775951
Sublattice magnetization M	0.4381

当n=3时

1. No.1

```
the initial spin is :
0.3147+i0.0000  0.2989+i0.0000  0.3544+i0.0000  0.2460+i0.0000  -0.2377+i0.000
-0.0801+i0.0000  0.1747+i0.0000  0.1587+i0.0000  0.1198+i0.0000  0.3082+i0.000
-0.2803+i0.0000  0.2609+i0.0000  0.4644+i0.0000  0.3798+i0.0000  -0.0676+i0.00

the ground eigenvalue is:
-0.732702
the spin is :
-0.2614+i-0.0000  0.2440+i-0.0000  -0.2613+i0.0000  0.2440+i-0.0000  -0.2292+i
0.1598+i0.0000  -0.1493+i-0.0000  0.1599+i0.0000  -0.1493+i-0.0000  0.1402+i-0
0.3129+i0.0000  -0.2922+i0.0000  0.3129+i0.0000  -0.2922+i0.0000  0.2745+i0.00

the magnet moment M is:
0.4379
[1] + Done                       "/usr/bin/gdb" --interpreter=mi --tty=${DbgTe
```

2. No.2

```
the initial spin is :
-0.2221+i0.0000  0.1412+i0.0000  -0.2827+i0.0000  0.1383+i0.0000  -0.4496+i0.0
-0.0545+i0.0000  -0.0705+i0.0000  -0.4984+i0.0000  0.3459+i0.0000  0.2450+i0.0
-0.0332+i0.0000  0.3961+i0.0000  -0.2112+i0.0000  -0.4202+i0.0000  0.1771+i0.0

the ground eigenvalue is:
-0.732702
the spin is :
-0.2637+i-0.0000  0.2463+i-0.0000  -0.2637+i-0.0000  0.2463+i0.0000  -0.2313+i
-0.3134+i-0.0000  0.2926+i-0.0000  -0.3134+i0.0000  0.2926+i-0.0000  -0.2749+i
-0.1550+i0.0000  0.1447+i0.0000  -0.1550+i0.0000  0.1447+i0.0000  -0.1359+i0.0

the magnet moment M is:
0.4379
[1] + Done                       "/usr/bin/gdb" --interpreter=mi --tty=${DbgTe
```

3. No.3

```
the initial spin is :
-0.0906+i0.0000  -0.1538+i0.0000  -0.1131+i0.0000  0.4182+i0.0000  0.1089+i0.0
-0.3727+i0.0000  -0.1175+i0.0000  0.2629+i0.0000  0.0821+i0.0000  -0.1040+i0.0
0.0542+i0.0000  -0.3327+i0.0000  -0.0741+i0.0000  -0.4146+i0.0000  0.3858+i0.0

the ground eigenvalue is:
-0.732702
the spin is :
-0.3052+i0.0000  0.2850+i-0.0000  -0.3051+i0.0000  0.2850+i0.0000  -0.2677+i0.
0.1784+i0.0000  -0.1666+i-0.0000  0.1785+i-0.0000  -0.1666+i-0.0000  0.1565+i-
0.2584+i0.0000  -0.2413+i0.0000  0.2584+i0.0000  -0.2413+i0.0000  0.2267+i0.00

the magnet moment M is:
0.4379
[1] + Done                       "/usr/bin/gdb" --interpreter=mi --tty=${DbgTe
```

Parameters	Value
Ground state energy E	-0.732702
Sublattice magnetization M	0.4379

APPENDIX

the state and it's correxponding number

$(|\uparrow\rangle, |\downarrow\rangle) \bigotimes (|\uparrow\rangle, |\downarrow\rangle)$

00	01	10	11
$\|\uparrow\uparrow\rangle$	$\|\uparrow\downarrow\rangle$	$\|\downarrow\uparrow\rangle$	$\|\downarrow\downarrow\rangle$
0	1	2	3

$(|\uparrow\rangle, |\downarrow\rangle) \bigotimes (|\uparrow\rangle, |\downarrow\rangle) \bigotimes (|\uparrow\rangle, |\downarrow\rangle)$

000	001	010	011	100	101	110	111
$\|\uparrow\uparrow\uparrow\rangle$	$\|\uparrow\uparrow\downarrow\rangle$	$\|\uparrow\downarrow\uparrow\rangle$	$\|\uparrow\downarrow\downarrow\rangle$	$\|\downarrow\uparrow\uparrow\rangle$	$\|\downarrow\uparrow\downarrow\rangle$	$\|\downarrow\downarrow\uparrow\rangle$	$\|\downarrow\downarrow\downarrow\rangle$
0	1	2	3	4	5	6	7

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1. Sandvik, Anders W. “Finite-Size Scaling of the Ground-State Parameters of the Two-Dimensional Heisenberg Model.” Physical Review B, vol. 56, no. 18, Nov. 1997, pp. 11678–90. Crossref, https://doi.org/10.1103/physrevb.56.11678. ↩
2. Isaev, Leonid, Gerardo Guzman Ortiz, Jagiellonian University, Bloomington, In, Usa, Instituto de Estructura de la Materia Csic, Madrid and Spain.. “Hierarchical mean-field approach to the J 1 -J 2 Heisenberg model on a square lattice.” Physical Review B 79 (2008): 024409. ↩
3. https://folk.ntnu.no/johnof/magnetism-2016.pdf ↩