二维哈密顿量构建的思路

这一块的的整体框架是:

```
%pre-work 准备算符 ——— Part I
for row=1:L-1
  %pre-work 准备算符 ——— Part II

  for site=0:L-1
    %when site = 0 纵向哈密顿量

    if site>0
    %横向哈密顿量

    %为下一次循环准备算符
    %pre-work ———— Part III

end

row=L;  %对最后一行的处理:
```

对于2x2-spin系统，希伯尔特空间为$D = 2^4 = 16$, 最后的哈密顿量矩阵大小应该为: 16x16

我们一部分一部分来看，其中可能混杂一些对3x3-spin系统的讨论。

Pre-work Part II 横向哈密顿量的构造

在`row=1`时$II = I_{4\times4}$.

```
II=eye(2^(row*L),2^(row*L));
Sp0 = kron(II,sp);%row行的算符
Sz0 = kron(II,sz);
Sp1 = kron(II,sp);
Sz1 = kron(II,sz);
Id = eye(size(Sp0));
```

```
Sz0 =
    0.5000         0         0         0         0         0         0         0
         0   -0.5000         0         0         0         0         0         0
         0         0    0.5000         0         0         0         0         0
         0         0         0   -0.5000         0         0         0         0
         0         0         0         0    0.5000         0         0         0
         0         0         0         0         0   -0.5000         0         0
         0         0         0         0         0         0    0.5000         0
         0         0         0         0         0         0         0   -0.5000
```

```
Sz1 =
    0.5000         0         0         0         0         0         0         0
         0   -0.5000         0         0         0         0         0         0
         0         0    0.5000         0         0         0         0         0
         0         0         0   -0.5000         0         0         0         0
         0         0         0         0    0.5000         0         0         0
         0         0         0         0         0   -0.5000         0         0
         0         0         0         0         0         0    0.5000         0
         0         0         0         0         0         0         0   -0.5000
```

$$\text{II} = I_{2^2\times 2^2}, \rightarrow \text{Sz1,Sz0: } I_{4\times 4}\otimes S^z_{2\times 2} = I_{2\times 2}\otimes I_{2\times 2}\otimes S^z_{2\times 2} \tag{1}$$

与一维的情况有所不同，这里`Sp0,Sp1,Sz0,Sz1`的初始化我们在算符`sp,sz`上有所扩充

而在`row=1=L-1`的内部，对每个site和一维情况一样构建横向哈密顿量：

```
%outsite:
for site=0:L-1

%inside:
if site>0 %site starts from 1 to L-1
    h = 0.5*kron(Sp1, sp'); %kronecker 张量积
    H = H + h + h' + kron(Sz1,sz);%完成一个横向哈密顿量

  if L>2
    if site == L-1
        h = 0.5*kron(Sp0, sp');
        H = H + h + h' + kron(Sz0,sz);
    end

    if site < L-1
        Sp1 = kron(Id, sp);
        Sz1 = kron(Id, sz);

        Sp0 = kron(Sp0, id);
        Sz0 = kron(Sz0, id);
        Id = eye(size(Sz0));
    end
  end
end
```

1. For `site=1=L-1`

是$I_{4\times 4}\otimes S^z_{2\times 2}$这样一个矩阵作为一个整体`Sz1`和$S^z$进行张量积，在$L=2$的情况下，到这儿已经结束了。

也就是:

$$I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes S^z_{2\times2} \tag{2}$$

我们意识到，这不全啊，对于2x2-spin的横向哈密顿量，应该还有一项为:

$$S^z_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2} \tag{3}$$

也就是说， 对于横向哈密顿量来说，还有`row=0`的工作

```
row=0;
for site=1:L-1 %L-1
    h = 0.5*kron(Sp1, sp'); %kronecker 张量积,此时的Sp1是site-1的
    H = kron(H, id) + h + h' + kron(Sz1,sz);%完成一个哈密顿量 此时的Sz1是site-1的

    if L>2
        %对最后一个格点的处理
        if site == L-1
            h = 0.5*kron(Sp0, sp');
            H = H + h + h' + kron(Sz0,sz);
        end


        if site < L-1
            Sp1 = kron(Id, sp); %此时的Sp1是site的
            Sz1 = kron(Id, sz); %此时的Sz1是site的

            Sp0 = kron(Sp0, id);%此时的Sp0是site的
            Sz0 = kron(Sz0, id);%此时的Sz0是site的
            Id = eye(size(Sz0));
        end
    end
end
```

它的作用是产生:

$$S^z_{2\times2}\otimes S^z_{2\times2} \tag{4}$$

这一项呢，在后续`kron(H,id)`时会进行自动补全: $S^z_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}$.

我们可以继续看一下3x3-spin的情况，

对于2x2-spin system, `row=1:L-1=1:1`, For `row=1`,

$$\mathrm{II}=I_{2^2\times2^2},\rightarrow \text{Sz1,Sz0: } I_{4\times4}\otimes S^z_{2\times2}=I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2} \tag{5}$$

对于3x3-spin system, `row=1:L-1=1:2`, For `row=1,`

$$\mathrm{II}=I_{2^3\times2^3},\rightarrow \text{Sz1,Sz0: } I_{8\times8}\otimes S^z_{2\times2}=I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2} \tag{6}$$

For `row=2`,

$$\mathrm{II} = I_{2^6\times 2^6}, \rightarrow \mathrm{Sz1,Sz0}\text{: } I_{2^6\times 2^6} \otimes S^z_{2\times 2} \tag{7}$$

...

对于`row=0`，我们沿用一维时的哈密顿量构造方法能够成功构造出：

$$\begin{aligned} H = [&\frac{1}{2}(S_1^+ \otimes S_2^- \otimes I_3 + S_1^- \otimes S_2^+ \otimes I_3) + S_1^z \otimes S_2^z \otimes I_3 \\ &+\frac{1}{2}(I_1 \otimes S_2^+ \otimes S_3^- + I_1 \otimes S_2^- \otimes S_3^+) + I_1 \otimes S_2^z \otimes S_3^z \\ &+\frac{1}{2}(S_1^+ \otimes I_2 \otimes S_3^- + S_1^- \otimes I_2 \otimes S_3^+) + S_1^z \otimes I_2 \otimes S_3^z] \end{aligned} \tag{8}$$

在后续`kron(H,id)`时会进行自动补全。也就是在这里，实现了H_1, H_3, H_5.

现在先来看`row=1`, $II = I_{2^3\times 2^3}$.

我们知道

```
% Sz1 = kron(II,sz);
H = ... + kron(Sz1,sz);
```

先实现的是

$$I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes S^z_{2\times 2} \tag{9}$$

在`0<site<L-1=3-1=2`时：

```
Sz1 = kron(Id, sz);
Sz0 = kron(Sz0, id);
Id = eye(size(Sp0));
```

$$\begin{gathered} \mathrm{Sz1}\text{: } I_{16\times 16} \otimes S^z_{2\times 2}, \\ \mathrm{Sz0}\text{: } I_{8\times 8} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \end{gathered} \tag{10}$$

在外部再次经历：（此时`site=2=L-1`）

```
H = ... + kron(Sz1,sz);
```

$$I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes S^z_{2\times 2} \rightarrow 64\times 64 \text{ matrix} \tag{11}$$

符合条件`site=L-1`时，经历：

```
if site == L-1
    h = 0.5*kron(Sp0, sp');
    H = H + h + h' + kron(Sz0,sz);
end
```

$$I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \rightarrow 64\times 64 \text{ matrix} \tag{12}$$

此时实现了H_7, H_9, H_{11}.

然而，对于3x3-spin system, 还有`row=L-1=2`的循环，不难料到，这个循环可以实现H_{13}, H_{15}, H_{17}.

纵向哈密顿量的构造:

算符的准备 Part I:

```
for i=1:L
    Sp{i}=1
    Sz{i}=1
end
for i=1:L
for j=1:L
    if (j==i)
        Sp{j}=kron(Sp{j},sp)
        Sz{j}=kron(Sz{j},sz)
    else
        Sp{j}=kron(Sp{j},id)
        Sz{j}=kron(Sz{j},id)
    end
end
end
```

纵向哈密顿量这部分的介绍，我就直接以3x3-spin大小的系统进行举例了。

对于**3x3-spin**系统，输出的Sz为1x3数组，每个元素为8x8矩阵:

```
Sz =

  1×3 cell 数组

  {8×8 double}    {8×8 double}    {8×8 double}
```

```
Sz{1} =
    0.5000         0         0         0         0         0         0         0
         0    0.5000         0         0         0         0         0         0
         0         0    0.5000         0         0         0         0         0
         0         0         0    0.5000         0         0         0         0
         0         0         0         0   -0.5000         0         0         0
         0         0         0         0         0   -0.5000         0         0
         0         0         0         0         0         0   -0.5000         0
         0         0         0         0         0         0         0   -0.5000
```

It's:

$$\mathrm{Sz}(1) : S^z_{2\times 2} \otimes I_{4\times 4} = S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \tag{20}$$

```
Sz{2} =
    0.5000         0         0         0         0         0         0         0
         0    0.5000         0         0         0         0         0         0
         0         0   -0.5000         0         0         0         0         0
         0         0         0   -0.5000         0         0         0         0
         0         0         0         0    0.5000         0         0         0
         0         0         0         0         0    0.5000         0         0
         0         0         0         0         0         0   -0.5000         0
         0         0         0         0         0         0         0   -0.5000
```

$$\text{Sz}(2): I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2} \tag{21}$$

```
Sz{3} =
    0.5000         0         0         0         0         0         0         0
         0   -0.5000         0         0         0         0         0         0
         0         0    0.5000         0         0         0         0         0
         0         0         0   -0.5000         0         0         0         0
         0         0         0         0    0.5000         0         0         0
         0         0         0         0         0   -0.5000         0         0
         0         0         0         0         0         0    0.5000         0
         0         0         0         0         0         0         0   -0.5000
```

$$\text{Sz}(3): I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2} \tag{22}$$

在纵向哈密顿量构建过程中：

```
for i=1:L
    Sp{i}=kron(III,ssp{i});%row-1行的算符
    Sz{i}=kron(III,ssz{i});
end
% III=eye(2^(row*L-L),2^(row*L-L))
```

在`row=1`时$III = I_{2^0,2^0} = I_{1\times1}$。

1. For `site=0`:

```
kron(kron(Sz{site+1},eye(2^(site),2^(site)),sz)
```

$$\begin{aligned}&\text{Sz}(1)\otimes I_{1\times1}\\ \rightarrow\ & S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{1\times1}\\ \rightarrow\ & S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{1\times1}\otimes S^z_{2\times2}\rightarrow 16\times16\ \text{matrix}\end{aligned} \tag{23}$$

完成第一个纵向哈密顿量，这是在构建横向哈密顿量之前

2. For `site=1`

```
H = kron(H,id) +...+ kron(kron(Sz{site+1},eye(2^site,2^site)),sz)
```

$$
\begin{aligned}
&S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \\
&+I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2}
\end{aligned} \tag{24}
$$

gives 32x32 matrix.

3. For `site=2=L-1`

```
H = kron(H,id) +...+ kron(kron(Sz{site+1},eye(2^site,2^site)),sz)
```

$$
\begin{aligned}
&S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \\
&+I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \\
&+I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2}
\end{aligned} \tag{25}
$$

在`row=2=L-1`时$III = I_{2^3\times 2^3} = I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2}$

1. For `site=0`:

```
kron(kron(Sz{site+1},eye(2^(site),2^(site)),sz)
```

$$
\begin{aligned}
&I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes I_{1\times 1} \\
\rightarrow\ &I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \rightarrow 2^7 \times 2^7 \text{ matrix}
\end{aligned} \tag{26}
$$

2. For `site=1`

```
H = kron(H,id) +...+ kron(kron(Sz{site+1},eye(2^site,2^site)),sz)
```

$$
\begin{aligned}
&I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \\
&+I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2}
\end{aligned} \tag{27}
$$

gives $2^8 \times 2^8$ matrix.

3. For `site=2=L-1`

```
H = kron(H,id) +...+ kron(kron(Sz{site+1},eye(2^site,2^site)),sz)
```

$$
\begin{aligned}
&I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \\
&+I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \\
&+I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2} \otimes I_{2\times 2} \otimes I_{2\times 2} \otimes S^z_{2\times 2}
\end{aligned} \tag{28}
$$

Gives $2^9 \times 2^9$ matrix.

因此，我们总结`row = 1,2`时总的纵向哈密顿量:

$$
\begin{aligned}
&= S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{8\times8}\\
&+I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{8\times8}\\
&+I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{8\times8}\\
&+I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\\
&+I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\\
&+I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}
\end{aligned}
\tag{29}
$$

绿色是循环中`kron(H,id)`导致的补全，因此，我们看到，这部分代码的功能实现了$H_2, H_4, H_6, H_8, H_{10}, H_{12}$.

所以还有一部分呢，在`row=L`中实现：

For`row=L`

```
row = L
for i=1:L
    Sp{i}=kron(III,ssp{i});
    Sz{i}=kron(III,ssz{i});
end
% III=eye(2^(row*L-2*L),2^(row*L-2*L))
for i=1:L
    H = H + kron(ssz{i},Sz{i})
end
```

$$
III:(row-2)*L=3\rightarrow I_{2^3\times2^3} \tag{30}
$$

$$
\begin{aligned}
&\mathrm{kron}(\mathrm{ssz(i)},\mathrm{Sz(i)})\\
&S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\\
&+I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\\
&+I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes I_{2\times2}\otimes S^z_{2\times2}
\end{aligned}
\tag{31}
$$

因此，`row=L`实现了纵向哈密顿量的补全。

那么，不难看出，纵向哈密顿量这部分的构建，在row=1时构建第一行的纵向哈密顿量，在row=L-1时构建第L-1行纵向哈密顿量，在row=L时单独构建最后一行纵向哈密顿量，而最后一行哈密顿量是周期性地“连接”到第一行元素

Appendix 3x3-spin system

哈密顿量：

$$
\begin{aligned}
H_1 &= S_1 S_2 I_3 I_4 I_5 I_6 I_7 I_8 I_9 \\
H_2 &= S_1 I_2 I_3 S_4 I_5 I_6 I_7 I_8 I_9 \\
H_3 &= I_1 S_2 S_3 I_4 I_5 I_6 I_7 I_8 I_9 \\
H_4 &= I_1 S_2 I_3 I_4 S_5 I_6 I_7 I_8 I_9 \\
H_5 &= S_1 I_2 S_3 I_4 I_5 I_6 I_7 I_8 I_9 \\
H_6 &= I_1 I_2 S_3 I_4 I_5 S_6 I_7 I_8 I_9 \\
H_7 &= I_1 I_2 I_3 S_4 S_5 I_6 I_7 I_8 I_9 \\
H_8 &= I_1 I_2 I_3 S_4 I_5 I_6 S_7 I_8 I_9 \\
H_9 &= I_1 I_2 I_3 I_4 S_5 S_6 I_7 I_8 I_9 \\
H_{10} &= I_1 I_2 I_3 I_4 S_5 I_6 I_7 S_8 I_9 \\
H_{11} &= I_1 I_2 I_3 S_4 I_5 S_6 I_7 I_8 I_9 \\
H_{12} &= I_1 I_2 I_3 I_4 I_5 S_6 I_7 I_8 S_9 \\
H_{13} &= I_1 I_2 I_3 I_4 I_5 I_6 S_7 S_8 I_9 \\
H_{14} &= S_1 I_2 I_3 I_4 I_5 I_6 S_7 I_8 I_9 \\
H_{15} &= I_1 I_2 I_3 I_4 I_5 I_6 I_7 S_8 S_9 \\
H_{16} &= I_1 S_2 I_3 I_4 I_5 I_6 I_7 S_8 I_9 \\
H_{17} &= I_1 I_2 I_3 I_4 I_5 I_6 S_7 I_8 S_9 \\
H_{18} &= I_1 I_2 S_3 I_4 I_5 I_6 I_7 I_8 S_9
\end{aligned}
\tag{32}
$$