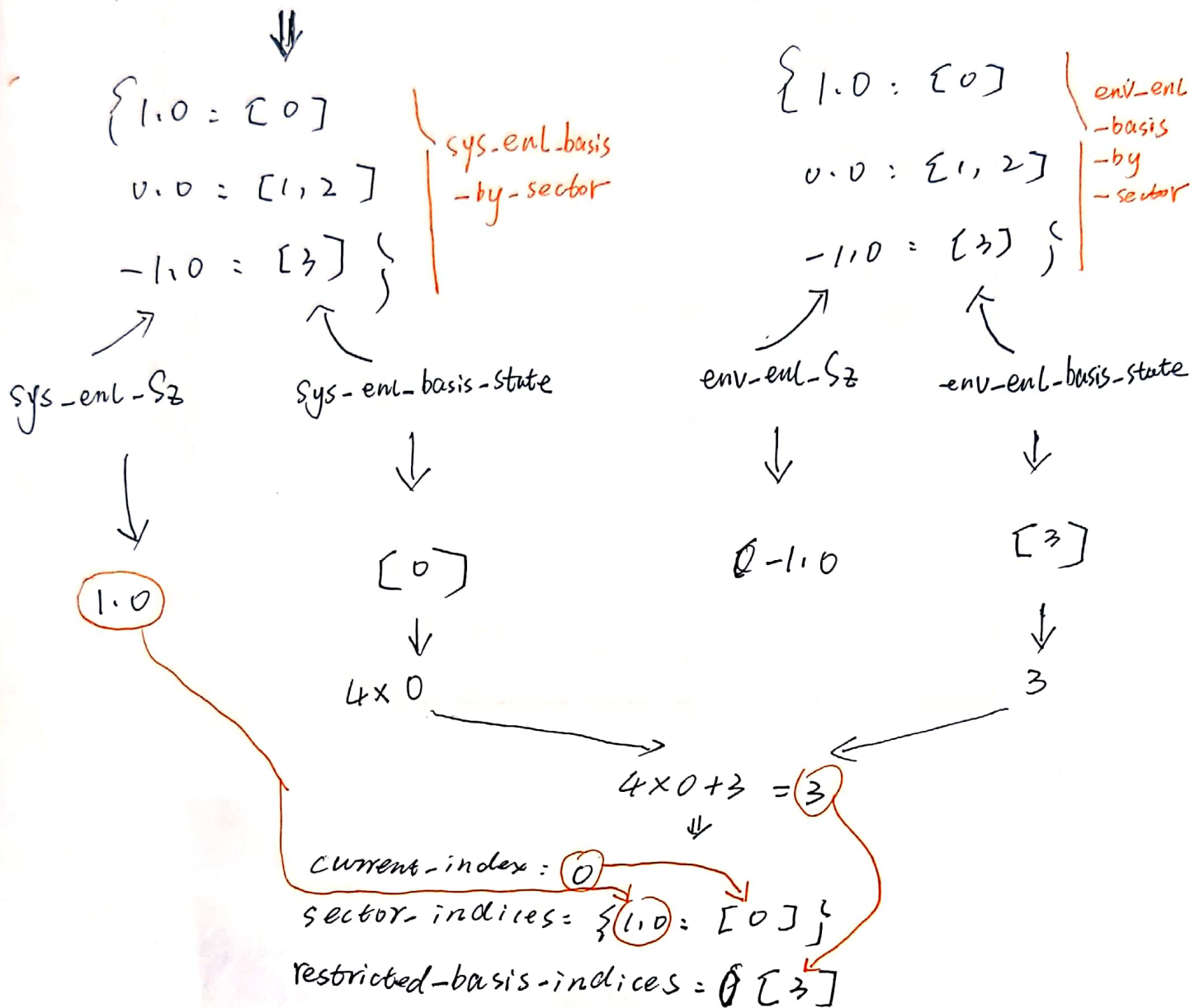
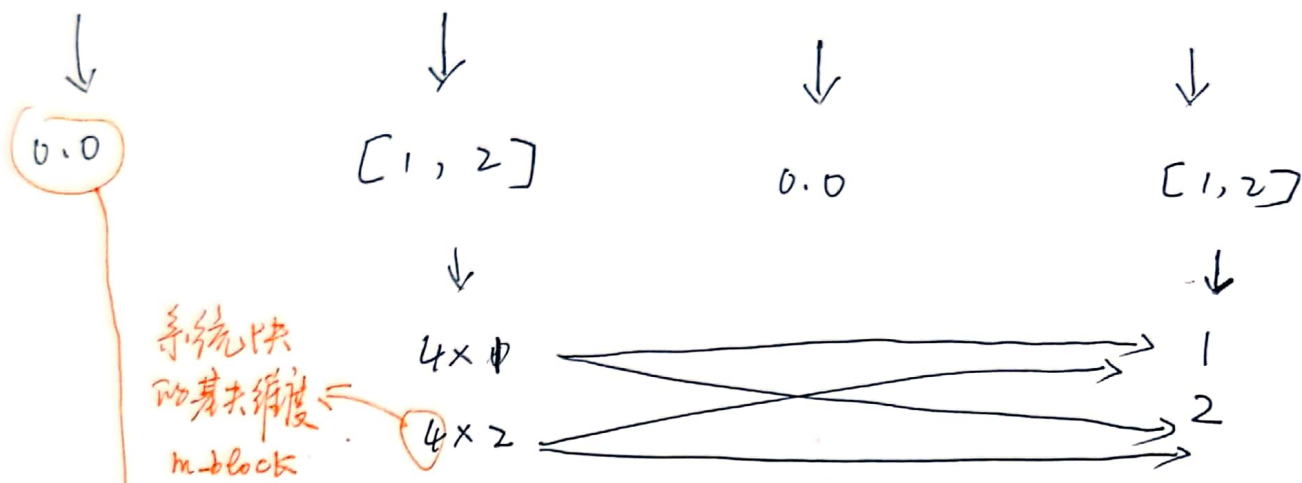
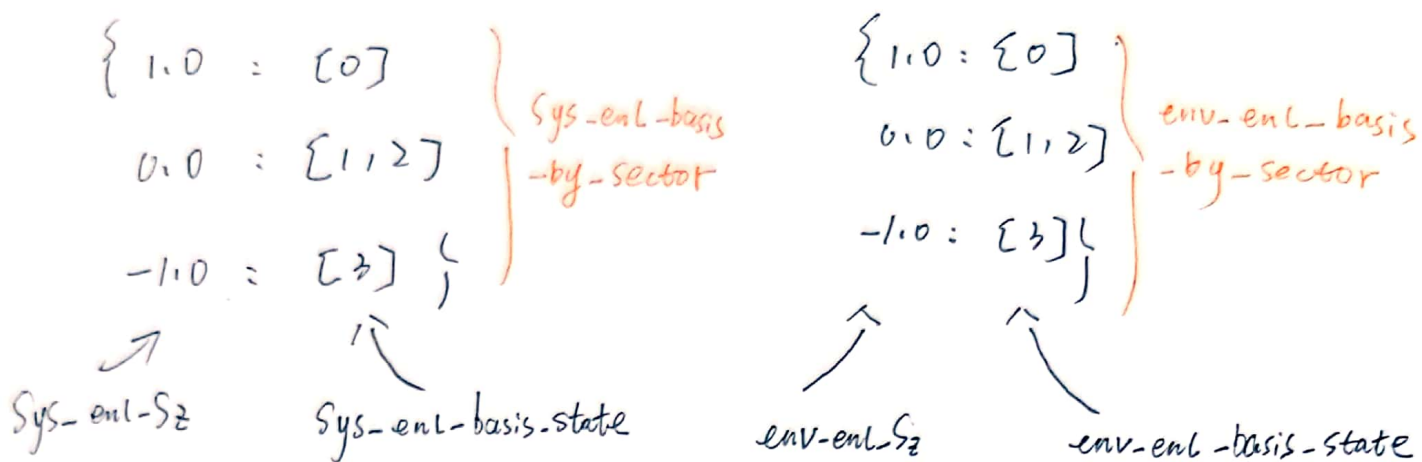


$$(0.5 \quad -0.5) \oplus (0.5, -0.5) \xrightarrow{\text{量子数之和.}} \Rightarrow (1, 0, 0, -1) \xrightarrow{\text{enlarge block}}$$



第一步. 系统块选择量子数 $S_z = 1$.
 对应的环境块选择量子数 $S_z = -1$





$$\Rightarrow \begin{aligned} 4 \times 1 + 1 &= 5, & 4 \times 1 + 2 &= 6 \\ 4 \times 2 + 1 &= 9, & 4 \times 2 + 2 &= 10 \end{aligned}$$

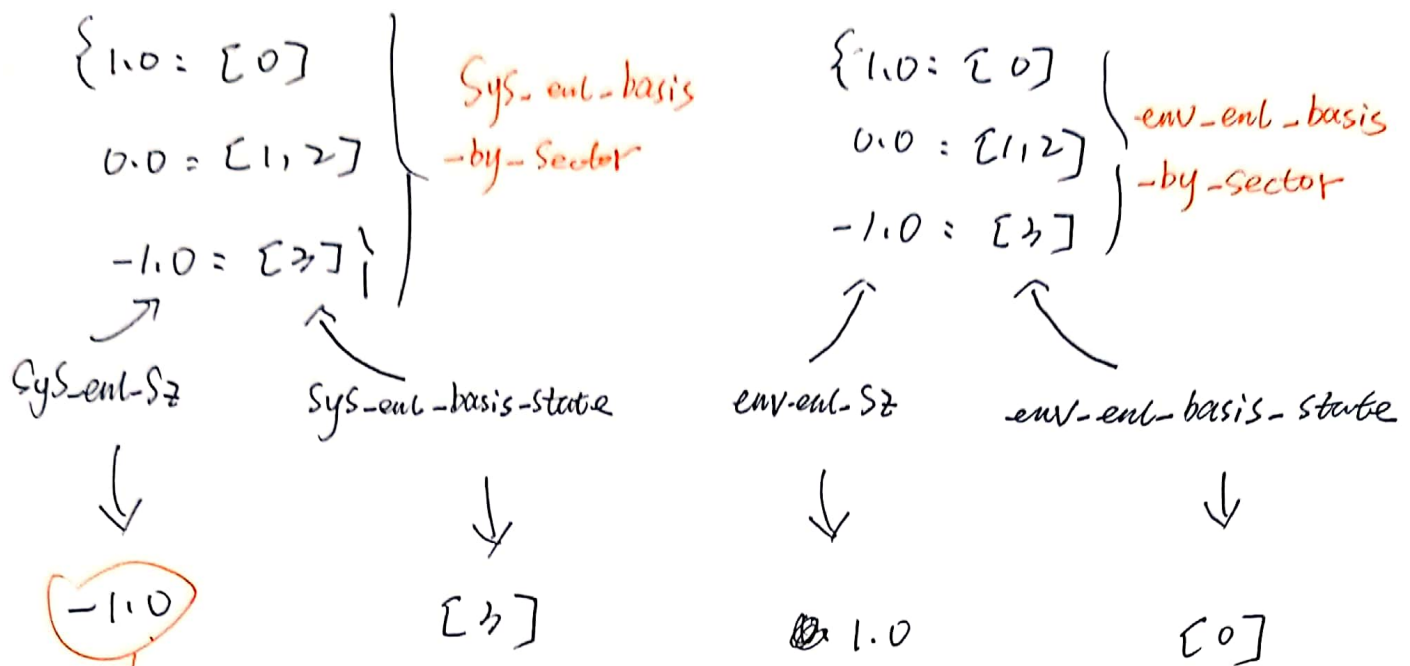
\Rightarrow ~~current-index = len~~
 restricted-basis-indices: $\{5, 6, 9, 10\}$

sector-indices: $\{1.0: [0], 0.0: [1, 2, 3, 4]\}$

current-index: $[len([0]), len([3, 5]), len([3, 5, 6]), len([3, 5, 6, 9])]$
 $= [1, 2, 3, 4]$

第二步: 系统快选择量子数 $S_z = 0$
 对应环境快选择量子数 $S_0 = 0$.





4×3

$$4 \times 3 + 0 = 12$$

\Rightarrow ~~current-index: [len([3]), len([3]), len([3, 5]), len([3, 5, 6]),~~
~~len([3, 5, 6, 9]), len([3, 5, 6, 9, 10])]~~
~~= [0, 1, 2, 3, 4, 5]~~

Current-index: [len([3, 5, 6, 9, 10])] = [5]

Sector-indices: { 1.0: [0], 0.0: [1, 2, 3, 4], -1.0: [5] }

Restricted-basis-indices: [3, 5, 6, 9, 10, 12]

第3步, 系统块选择量子数 $S_z = -1.0$ 时,
 对应的环境块选择量子数 $S_z = 1$.

(3)



扫描全能王 创建

系统

环境

$$\left\{ \begin{array}{l} 1.0 : [0] \\ 0.0 : [1, 2] \\ -1.0 : [3] \end{array} \right\}$$

$$\left\{ \begin{array}{l} 1.0 : [0] \\ 0.0 : [1, 2] \\ -1.0 : [3] \end{array} \right\}$$

superblock

$$\begin{array}{c} [0] [3] \\ \Downarrow \\ 3 \end{array}$$

$$\begin{array}{c} [1, 2] [1, 2] \\ \Downarrow \\ 5, 6, 9, 10 \end{array}$$

$$\begin{array}{c} [3] [0] \\ \Downarrow \\ 12 \end{array}$$

$$\begin{array}{c} \Downarrow \\ [0] \end{array}$$

$$\begin{array}{c} \Downarrow \\ [1, 2, 3, 4] \end{array}$$

$$\begin{array}{c} \Downarrow \\ [5] \end{array}$$

超块

$$\left\{ \begin{array}{l} 1.0 : [0] \\ 0.0 : [1, 2, 3, 4] \\ -1.0 : [5] \end{array} \right\}$$

超块中
对角块对应的基矢顺序

系统块
量子数



超快做对角化处理

①

$$\{ 1.0 : [0] \}$$

$$0.0 : [1, 2, 3, 4]$$

$$-1.0 : [5]$$

对角化

1.0	x x x
	x x x
0.0	x x x
	x x x
-1.0	x x x

能量
最低

psi-0

1.0	x
	x
0.0	x
	x
-1.0	x

用 psi-0 构造约化密度矩阵

$$\left\{ \begin{array}{l} \text{系统 } \{ 1.0 : [0] \\ 0.0 : [1, 2] \\ -1.0 : [3] \} \end{array} \right.$$

1.0	x	→ reshape [1, -1]
	x	
0.0	x	→ reshape [2, -1]
	x	
-1.0	x	→ reshape [1, -1]

⇒ 约化密度矩阵:

1.0	x	(1 by 1)
0.0	x x	(2 by 2)
	x x	
-1.0	x	(1 by 1)

对约化密度矩阵进行对角化处理

1.0	x	→ 对角化
	x x	
0.0	x x	→ 对角化
	x x	
-1.0	x	→ 对角化

分块对角化

本征值从大到小排序

1.0	x	eig ₀	evect ₀
	x x	eig ₁	evect ₁
0.0	x x	eig ₂	evect ₂
	x x		
-1.0	x	eig ₃	evect ₃

(2)



扫描全能王 创建

系统块的大小和约化密矩阵块的大小一致

系统块: $\begin{cases} 1.0 : [0] \\ 0.0 : [1, 2] \\ -1.0 : [3] \end{cases}$

约化密矩阵块

$$\begin{array}{c|cc} 1.0 & & \times \\ \hline 0.0 & \times & \times \\ & \times & \times \\ \hline -1.0 & & \times \end{array}$$

对约化密矩阵做分块对角化处理:

1.0	$[0]$	0 \times	eig_0	vec_0
0.0	$\begin{bmatrix} 1 \\ 2 \end{bmatrix}$	$\times \times$	eig_1	vec_1
		$\times \times$	eig_2	vec_2
-1.0	$[3]$	\times	eig_3	vec_3

特征值由大到小进行排序

特征值 特征态 $[eig_1, eig_2, eig_0, eig_3]$

构建转移矩阵:

$$vec_0 = \begin{bmatrix} \times \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$vec_1 = \begin{bmatrix} 0 \\ \times \\ \times \\ 0 \end{bmatrix}$$

$$vec_2 = \begin{bmatrix} 0 \\ \times \\ \times \\ 0 \end{bmatrix}$$

$$vec_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \times \end{bmatrix}$$

按 $[eig_1, eig_2, eig_0, eig_3]$ 的排序:

①

$$\begin{bmatrix} 0 & 0 & \times & 0 \\ \times & \times & 0 & 0 \\ \times & \times & 0 & 0 \\ 0 & 0 & 0 & \times \end{bmatrix}$$

如果截断到第3列, 只保留前3列即可

\Rightarrow Transform matrix 的量子数对应标也

$[0, 0, 1, -1]$ \rightarrow 将算符和快哈基顿重整化之后的量子数排序

③



扫描全能王 创建