SAMB for “`C2h1`”

Generated on 2023-06-01 17:38 by MultiPie 1.1.2

- Group: No. 10 C_{2h}^{1} $P2/m$ (b-axis setting) [monoclinic]
- Associated point group: No. 5 C_{2h} $2/m$ (b-axis setting) [monoclinic]

- Generation condition
  - model type: `tight_binding`
  - time-reversal type: `electric`
  - irrep: `[Ag]`
  - `spinful`

- Unit cell:
  $a = 1.0,\ b = 1.2,\ c = 1.0,\ \alpha = 90.0,\ \beta = 90.0,\ \gamma = 90.0$
- Lattice vectors:
  $\boldsymbol{a}_1 = \begin{pmatrix} 1.0 & 0 & 0 \end{pmatrix}$
  $\boldsymbol{a}_2 = \begin{pmatrix} 0 & 1.2 & 0 \end{pmatrix}$
  $\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 1.0 \end{pmatrix}$

Table 1: High-symmetry line: Γ-X.

	symbol	position	symbol	position
	Γ	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	X	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$

- Kets: dimension = 4

Table 2: Hilbert space for full matrix.

	No.	ket	No.	ket	No.	ket	No.	ket
	1	$(s,\uparrow)$@A$_1$	2	$(s,\downarrow)$@A$_1$	3	$(s,\uparrow)$@B$_1$	4	$(s,\downarrow)$@B$_1$

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S$_1$	A$_1$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4]
S$_2$	B$_1$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[1,2,3,4]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\boldsymbol{b}$@$\boldsymbol{c}$	mapping
B$_1$	b$_1$	A$_1$	A$_1$	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[1,-2,-3,4]
B$_2$	b$_2$	A$_1$	A$_1$	1	2	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix}$ @ $\begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$	[1,-2,-3,4]
B$_3$	b$_3$	B$_1$	B$_1$	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$ @ $\begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,-3,4]
B$_4$	b$_4$	B$_1$	B$_1$	1	2	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[1,-2,-3,4]
B$_5$	b$_5$	A$_1$	B$_1$	1	1	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0 \end{pmatrix}$	[1]
	b$_6$	A$_1$	B$_1$	1	1	$\begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{3}{4} & \frac{1}{4} & 0 \end{pmatrix}$	[2]
	b$_7$	A$_1$	B$_1$	1	1	$\begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{3}{4} & \frac{3}{4} & 0 \end{pmatrix}$	[3]
	b$_8$	A$_1$	B$_1$	1	1	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{4} & \frac{3}{4} & 0 \end{pmatrix}$	[4]

- SAMB:

$\boxed{\text{No. 1}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{S}_1]$

$\hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_g)}]$

$\hat{\mathbb{Z}}_1(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}]$

$\boxed{\text{No. 2}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{S}_2]$

$\hat{\mathbb{Z}}_2 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_g)}]$

$\hat{\mathbb{Z}}_2(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_g)}]$

$\boxed{\text{No. 3}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$\hat{\mathbb{Z}}_3 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_g)}]$

$\hat{\mathbb{Z}}_3(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_g)}]$

$\boxed{\text{No. 4}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$\hat{\mathbb{Z}}_4 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_g)}]$

$\hat{\mathbb{Z}}_4(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_2[\mathbb{Q}_0^{(k,A_g)}]$

$\boxed{\text{No. 5}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$\hat{\mathbb{Z}}_5 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_g)}]$

$\hat{\mathbb{Z}}_5(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_3[\mathbb{Q}_0^{(k,A_g)}]$

$\boxed{\text{No. 6}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{B}_4]$

$\hat{\mathbb{Z}}_6 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_g)}]$

$$\hat{\mathbb{Z}}_6(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_g)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 7}}$ $\hat{\mathbb{Q}}_0^{(A_g)}$ $[\mathrm{M}_1, \mathrm{B}_5]$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{Y}_7[\mathbb{Q}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_7(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_g)}] \otimes \mathbb{U}_3[\mathbb{Q}_0^{(u,A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 8}}$ $\hat{\mathbb{G}}_1^{(A_g)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$$\hat{\mathbb{Z}}_8 = \mathbb{X}_2[\mathbb{M}_1^{(a,A_g)}(1,-1)] \otimes \mathbb{Y}_8[\mathbb{T}_0^{(b,A_g)}]$$

$$\hat{\mathbb{Z}}_8(\boldsymbol{k}) = \mathbb{X}_2[\mathbb{M}_1^{(a,A_g)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_g)}] \otimes \mathbb{F}_5[\mathbb{Q}_0^{(k,A_g)}]$$

$\boxed{\text{No. 9}}$ $\hat{\mathbb{G}}_1^{(A_g)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_3[\mathbb{M}_1^{(a,B_g,1)}(1,-1)] \otimes \mathbb{Y}_9[\mathbb{T}_2^{(b,B_g,2)}]$$

$$\hat{\mathbb{Z}}_9(\boldsymbol{k}) = \mathbb{X}_3[\mathbb{M}_1^{(a,B_g,1)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_g)}] \otimes \mathbb{F}_6[\mathbb{Q}_2^{(k,B_g,2)}]$$

$\boxed{\text{No. 10}}$ $\hat{\mathbb{Q}}_2^{(A_g,2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_5]$

$$\hat{\mathbb{Z}}_{10} = -\mathbb{X}_4[\mathbb{M}_1^{(a,B_g,2)}(1,-1)] \otimes \mathbb{Y}_9[\mathbb{T}_2^{(b,B_g,2)}]$$

$$\hat{\mathbb{Z}}_{10}(\boldsymbol{k}) = -\mathbb{X}_4[\mathbb{M}_1^{(a,B_g,2)}(1,-1)] \otimes \mathbb{U}_4[\mathbb{T}_0^{(u,A_g)}] \otimes \mathbb{F}_6[\mathbb{Q}_2^{(k,B_g,2)}]$$

Table 5: Atomic SAMB group.

group	bra	ket
M_1	$(s,\uparrow),(s,\downarrow)$	$(s,\uparrow),(s,\downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_g)}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{M}_1^{(a,A_g)}(1,-1)$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{M}_1^{(a,B_g,1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{M}_1^{(a,B_g,2)}(1,-1)$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A_g)}$	S_1	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(s,A_g)}$	S_2	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{Q}_0^{(b,A_g)}$	B_1	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{Q}_0^{(b,A_g)}$	B_2	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{Q}_0^{(b,A_g)}$	B_3	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{Q}_0^{(b,A_g)}$	B_4	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{Q}_0^{(b,A_g)}$	B_5	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{T}_0^{(b,A_g)}$	B_5	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{T}_2^{(b,B_g,2)}$	B_5	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$

Table 8: Uniform SAMB.

symbol	type	cluster	form
$\mathbb{U}_1$	$\mathbb{Q}_0^{(s,A_g)}$	S_1	$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$
$\mathbb{U}_2$	$\mathbb{Q}_0^{(s,A_g)}$	S_2	$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$
$\mathbb{U}_3$	$\mathbb{Q}_0^{(u,A_g)}$	B_5	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{U}_4$	$\mathbb{T}_0^{(u,A_g)}$	B_5	$\begin{pmatrix} 0 & \frac{\sqrt{2}i}{2} \\ -\frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$

Table 9: Structure SAMB.

symbol	type	cluster	form
$\mathbb{F}_1$	$\mathbb{Q}_0^{(k,A_g)}$	B_1	$\sqrt{2}c_{001}$
$\mathbb{F}_2$	$\mathbb{Q}_0^{(k,A_g)}$	B_2	$\sqrt{2}c_{002}$
$\mathbb{F}_3$	$\mathbb{Q}_0^{(k,A_g)}$	B_3	$\sqrt{2}c_{003}$
$\mathbb{F}_4$	$\mathbb{Q}_0^{(k,A_g)}$	B_4	$\sqrt{2}c_{004}$
$\mathbb{F}_5$	$\mathbb{Q}_0^{(k,A_g)}$	B_5	$c_{005} + c_{006}$
$\mathbb{F}_6$	$\mathbb{Q}_2^{(k,B_g,2)}$	B_5	$c_{005} - c_{006}$

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_g)}$	0	A_g	–	–	1

continued ...

Table 10

No.	symbol	rank	irrep.	mul.	comp.	form
2	$\mathbb{Q}_2^{(B_g,2)}$	2	B_g	2	$-$	$\sqrt{3}xy$

Table 11: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A_g)}$	1	A_g	$-$	$-$	Y
2	$\mathbb{G}_1^{(B_g,1)}$	1	B_g	1	$-$	X
3	$\mathbb{G}_1^{(B_g,2)}$	1	B_g	2	$-$	Z

- Group info.: Generator = $\{2_{010}|0\}$, $\{-1|0\}$

Table 12: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1|0\}$	$\{1|0\}$
$\{2_{010}|0\}$	$\{2_{010}|0\}$
$\{-1|0\}$	$\{-1|0\}$
$\{m_{010}|0\}$	$\{m_{010}|0\}$

Table 13: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1\|0\}$	2	$\{2_{010}\|0\}$	3	$\{-1\|0\}$	4	$\{m_{010}\|0\}$		

Table 14: Character table (point-group part).

	1	2_{010}	-1	m_{010}
A_g	1	1	1	1
B_g	1	-1	1	-1
A_u	1	1	-1	-1
B_u	1	-1	-1	1

Table 15: Parity conversion.

$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$
A_g (A_u)	B_g (B_u)	A_u (A_g)	B_u (B_g)

Table 16: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A_g	B_g	A_u	B_u
A_g	A_g	B_g	A_u	B_u
B_g		A_g	B_u	A_u
A_u			A_g	B_g
B_u				A_g

Table 17: Anti-symmetric product, $[\Gamma \otimes \Gamma]_{-}$.

A_g	B_g	A_u	B_u
–	–	–	–

Table 18: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix}1 & 1 & 0\end{pmatrix}$	2	$\begin{pmatrix}-1 & 1 & 0\end{pmatrix}$	3	$\begin{pmatrix}-1 & -1 & 0\end{pmatrix}$	4	$\begin{pmatrix}1 & -1 & 0\end{pmatrix}$

Table 19: Virtual-cluster basis.

symbol	1	2	3	4
$\mathbb{Q}_0^{(A_g)}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$\mathbb{Q}_1^{(A_u)}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$
$\mathbb{Q}_1^{(B_u,1)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$
$\mathbb{Q}_2^{(B_g,2)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$