SAMB for “C4v1”

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- Group: No. 99 C_{4v}^{1} $P4mm$ [tetragonal]
- Associated point group: No. 13 C_{4v} $4mm$ [tetragonal]

- Generation condition
  - model type: `tight_binding`
  - time-reversal type: `electric`
  - irrep: `[A1]`
  - `spinful`

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

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 = 2

Table 2: Hilbert space for full matrix.

	No.	ket	No.	ket
	1	$(s,\uparrow)$@A_1	2	$(s,\downarrow)$@A_1

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S_1	A_1	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8]

- 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	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix}$ @ $\begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-2,5,-6]
	b_2	A_1	A_1	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[-3,4,-7,8]
B_2	b_3	A_1	A_1	1	2	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix}$ @ $\begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$	[1,2,3,4,5,6,7,8]

- SAMB:

$\boxed{\text{No. 1}}$ $\hat{\mathbb{Q}}_0^{(A_1)}$ $[\mathrm{M}_1, \mathrm{S}_1]$

$\hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1)}]$

$\hat{\mathbb{Z}}_1(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1)}]$

$\boxed{\text{No. 2}}$ $\hat{\mathbb{Q}}_0^{(A_1)}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b,A_1)}]$$

$$\hat{\mathbb{Z}}_2(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1)}]$$

$\boxed{\text{No. 3}}$ $\hat{\mathbb{Q}}_1^{(A_1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_3 = \frac{\sqrt{2}\mathbb{X}_2[\mathbb{M}_{1,0}^{(a,E)}(1,-1)] \otimes \mathbb{Y}_4[\mathbb{T}_{1,1}^{(b,E)}]}{2} - \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_{1,1}^{(a,E)}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{T}_{1,0}^{(b,E)}]}{2}$$

$$\hat{\mathbb{Z}}_3(\boldsymbol{k}) = \frac{\sqrt{2}\mathbb{X}_2[\mathbb{M}_{1,0}^{(a,E)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1)}] \otimes \mathbb{F}_3[\mathbb{T}_{1,1}^{(k,E)}]}{2} - \frac{\sqrt{2}\mathbb{X}_3[\mathbb{M}_{1,1}^{(a,E)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1)}] \otimes \mathbb{F}_2[\mathbb{T}_{1,0}^{(k,E)}]}{2}$$

$\boxed{\text{No. 4}}$ $\hat{\mathbb{Q}}_0^{(A_1)}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_1)}]$$

$$\hat{\mathbb{Z}}_4(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1)}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_1)}]$$

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
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_1)}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_2$	$\mathbb{M}_{1,0}^{(a,E)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{M}_{1,1}^{(a,E)}(1,-1)$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A_1)}$	S_1	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(b,A_1)}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{T}_{1,0}^{(b,E)}$	B_1	$\begin{pmatrix} 0 & i \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{T}_{1,1}^{(b,E)}$	B_1	$\begin{pmatrix} i & 0 \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{Q}_0^{(b,A_1)}$	B_2	$\begin{pmatrix} 1 \end{pmatrix}$

Table 8: Uniform SAMB.

symbol	type	cluster	form
$\mathbb{U}_1$	$\mathbb{Q}_0^{(s,A_1)}$	S_1	$\begin{pmatrix} 1 \end{pmatrix}$

Table 9: Structure SAMB.

symbol	type	cluster	form
$\mathbb{F}_1$	$\mathbb{Q}_0^{(k,A_1)}$	B_1	$c_{001} + c_{002}$
$\mathbb{F}_2$	$\mathbb{T}_{1,0}^{(k,E)}$	B_1	$\sqrt{2} s_{002}$
$\mathbb{F}_3$	$\mathbb{T}_{1,1}^{(k,E)}$	B_1	$\sqrt{2} s_{001}$
$\mathbb{F}_4$	$\mathbb{Q}_0^{(k,A_1)}$	B_2	$\sqrt{2} c_{003}$

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1)}$	0	A_1	–	–	1
2	$\mathbb{Q}_{1,0}^{(E)}$	1	E	–	0	x
3	$\mathbb{Q}_{1,1}^{(E)}$	1	E	–	1	y

Table 11: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_{1,0}^{(E)}$	1	E	–	0	X
2	$\mathbb{G}_{1,1}^{(E)}$	1	E	–	1	Y

- Group info.: Generator = $\{2_{001}|0\}$, $\{4^{+}_{001}|0\}$, $\{\mathrm{m}_{010}|0\}$

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

rep. SO	symmetry operations
$\{1\|0\}$	$\{1\|0\}$
$\{2_{001}\|0\}$	$\{2_{001}\|0\}$
$\{4^{+}_{001}\|0\}$	$\{4^{+}_{001}\|0\}$, $\{4^{-}_{001}\|0\}$
$\{m_{100}\|0\}$	$\{m_{100}\|0\}$, $\{m_{010}\|0\}$
$\{m_{110}\|0\}$	$\{m_{110}\|0\}$, $\{m_{1-10}\|0\}$

Table 13: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1\|0\}$	2	$\{2_{001}\|0\}$	3	$\{4^{+}_{001}\|0\}$	4	$\{4^{-}_{001}\|0\}$	5	$\{m_{100}\|0\}$
6	$\{m_{010}\|0\}$	7	$\{m_{110}\|0\}$	8	$\{m_{1-10}\|0\}$				

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

	1	2_{001}	4^{+}_{001}	m_{100}	m_{110}
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	1	−1	1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0

Table 15: Parity conversion.

$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$
A_1 (A_2)	B_1 (B_2)	E (E)	A_2 (A_1)	B_2 (B_1)

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

	A_1	A_2	B_1	B_2	E
A_1	A_1	A_2	B_1	B_2	E
A_2		A_1	B_2	B_1	E
B_1			A_1	A_2	E
B_2				A_1	E
E					$A_1 + B_1 + B_2$

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

A_1	A_2	B_1	B_2	E
$-$	$-$	$-$	$-$	A_2

Table 18: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix}2 & 1 & 0\end{pmatrix}$	2	$\begin{pmatrix}-2 & -1 & 0\end{pmatrix}$	3	$\begin{pmatrix}-1 & 2 & 0\end{pmatrix}$	4	$\begin{pmatrix}1 & -2 & 0\end{pmatrix}$
5	$\begin{pmatrix}-2 & 1 & 0\end{pmatrix}$	6	$\begin{pmatrix}2 & -1 & 0\end{pmatrix}$	7	$\begin{pmatrix}-1 & -2 & 0\end{pmatrix}$	8	$\begin{pmatrix}1 & 2 & 0\end{pmatrix}$

Table 19: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8
$\mathbb{Q}_0^{(A_1)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_{1,0}^{(E)}$	$\frac{\sqrt{5}}{5}$	$-\frac{\sqrt{5}}{5}$	$-\frac{\sqrt{5}}{10}$	$\frac{\sqrt{5}}{10}$	$-\frac{\sqrt{5}}{5}$	$\frac{\sqrt{5}}{5}$	$-\frac{\sqrt{5}}{10}$	$\frac{\sqrt{5}}{10}$
$\mathbb{Q}_{1,1}^{(E)}$	$\frac{\sqrt{5}}{10}$	$-\frac{\sqrt{5}}{10}$	$\frac{\sqrt{5}}{5}$	$-\frac{\sqrt{5}}{5}$	$\frac{\sqrt{5}}{10}$	$-\frac{\sqrt{5}}{10}$	$-\frac{\sqrt{5}}{5}$	$\frac{\sqrt{5}}{5}$
$\mathbb{Q}_2^{(B_1)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_2^{(B_2)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_{3,0}^{(E,1)}$	$\frac{\sqrt{5}}{10}$	$-\frac{\sqrt{5}}{10}$	$\frac{\sqrt{5}}{5}$	$-\frac{\sqrt{5}}{5}$	$-\frac{\sqrt{5}}{10}$	$\frac{\sqrt{5}}{10}$	$\frac{\sqrt{5}}{5}$	$-\frac{\sqrt{5}}{5}$
$\mathbb{Q}_{3,1}^{(E,1)}$	$-\frac{\sqrt{5}}{5}$	$\frac{\sqrt{5}}{5}$	$\frac{\sqrt{5}}{10}$	$-\frac{\sqrt{5}}{10}$	$-\frac{\sqrt{5}}{5}$	$\frac{\sqrt{5}}{5}$	$-\frac{\sqrt{5}}{10}$	$\frac{\sqrt{5}}{10}$
$\mathbb{Q}_4^{(A_2)}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$