

SAMB for “C4v1”

Generated on 2023-06-02 20:16 by MultiPie 1.1.2

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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
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- Unit cell:
 - $a = 1.0$, $b = 1.0$, $c = 1.0$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors:
 - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
 - $\mathbf{a}_2 = (0 \ 1.0 \ 0)$
 - $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

Table 1: High-symmetry line: Γ -X.

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

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- 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	$\#$	$\mathbf{b}@c$	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:

$$\boxed{\text{No. 1}} \quad \hat{Q}_0^{(A_1)} [M_1, S_1]$$

$$\hat{Z}_1 = \mathbb{X}_1[Q_0^{(a, A_1)}] \otimes \mathbb{Y}_1[Q_0^{(s, A_1)}]$$

$$\hat{Z}_1(\mathbf{k}) = \mathbb{X}_1[Q_0^{(a, A_1)}] \otimes \mathbb{U}_1[Q_0^{(s, A_1)}]$$

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

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

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

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

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

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

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

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

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

Table 5: Atomic SAMB group.

group	bra	ket
\mathbb{M}_1	$(s, \uparrow), (s, \downarrow)$	$(s, \uparrow), (s, \downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a, A_1)}$	\mathbb{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	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$
\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

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

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