SAMB for “kappaET”

Generated on 2023-09-27 06:56 by MultiPie 1.1.14

- Group: No. 32 C_{2v}^{8} $Pba2$ [orthorhombic]
- Associated point group: No. 7 C_{2v} $mm2$ [orthorhombic]

- Generation condition
  - model type: `tight_binding`
  - time-reversal type: `electric`
  - irrep: `[A1]`
  - `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 = 8

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$(s,\uparrow)$@A_1	2	$(s,\downarrow)$@A_1	3	$(s,\uparrow)$@A_2	4	$(s,\downarrow)$@A_2	5	$(s,\uparrow)$@A_3
6	$(s,\downarrow)$@A_3	7	$(s,\uparrow)$@A_4	8	$(s,\downarrow)$@A_4				

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S_1 [4c: 1]	A_1	$\begin{pmatrix} \frac{9}{10} & \frac{1}{20} & 0 \end{pmatrix}$	[1]
	A_2	$\begin{pmatrix} \frac{1}{10} & \frac{19}{20} & 0 \end{pmatrix}$	[2]
	A_3	$\begin{pmatrix} \frac{2}{5} & \frac{9}{20} & 0 \end{pmatrix}$	[3]
	A_4	$\begin{pmatrix} \frac{3}{5} & \frac{11}{20} & 0 \end{pmatrix}$	[4]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\boldsymbol{b}$@$\boldsymbol{c}$	mapping
B_1 [2a: ..2]	b_1	A_2	A_1	1	1	$\begin{pmatrix} \frac{1}{5} & -\frac{1}{10} & 0 \end{pmatrix}$ @ $\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,-2]
	b_2	A_4	A_3	1	1	$\begin{pmatrix} \frac{1}{5} & \frac{1}{10} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[3,-4]
B_2 [4c: 1]	b_3	A_4	A_1	2	1	$\begin{pmatrix} -\frac{3}{10} & \frac{1}{2} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{3}{4} & \frac{3}{10} & 0 \end{pmatrix}$	[1]
	b_4	A_3	A_2	2	1	$\begin{pmatrix} \frac{3}{10} & -\frac{1}{2} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{4} & \frac{7}{10} & 0 \end{pmatrix}$	[2]
	b_5	A_3	A_2	2	1	$\begin{pmatrix} \frac{3}{10} & \frac{1}{2} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{4} & \frac{1}{5} & 0 \end{pmatrix}$	[-3]
	b_6	A_4	A_1	2	1	$\begin{pmatrix} -\frac{3}{10} & -\frac{1}{2} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{3}{4} & \frac{4}{5} & 0 \end{pmatrix}$	[-4]
B_3 [4c: 1]	b_7	A_3	A_1	3	1	$\begin{pmatrix} \frac{1}{2} & \frac{2}{5} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{3}{20} & \frac{1}{4} & 0 \end{pmatrix}$	[1]

continued ...

Table 4

bond	tail	head	n	#	$\boldsymbol{b}$@$\boldsymbol{c}$	mapping
b_{8}	A_{4}	A_{2}	3	1	$\begin{pmatrix} -\frac{1}{2} & -\frac{2}{5} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{17}{20} & \frac{3}{4} & 0 \end{pmatrix}$	[2]
b_{9}	A_{3}	A_{1}	3	1	$\begin{pmatrix} -\frac{1}{2} & \frac{2}{5} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{13}{20} & \frac{1}{4} & 0 \end{pmatrix}$	[-3]
b_{10}	A_{4}	A_{2}	3	1	$\begin{pmatrix} \frac{1}{2} & -\frac{2}{5} & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{7}{20} & \frac{3}{4} & 0 \end{pmatrix}$	[-4]

- SAMB:

$\boxed{\text{No. 1}}$ $\hat{\mathbb{Q}}_{0}^{(A_1)}$ $[\mathrm{M}_1, \mathrm{S}_1]$

$$\hat{\mathbb{Z}}_{1} = \mathbb{X}_{1}[\mathbb{Q}_{0}^{(a,A_1)}] \otimes \mathbb{Y}_{1}[\mathbb{Q}_{0}^{(s,A_1)}]$$

$\boxed{\text{No. 2}}$ $\hat{\mathbb{Q}}_{0}^{(A_1)}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{2} = \mathbb{X}_{1}[\mathbb{Q}_{0}^{(a,A_1)}] \otimes \mathbb{Y}_{2}[\mathbb{Q}_{0}^{(b,A_1)}]$$

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

$$\hat{\mathbb{Z}}_{3} = -\frac{\sqrt{2}\mathbb{X}_{3}[\mathbb{M}_{1}^{(a,B_1)}(1,-1)] \otimes \mathbb{Y}_{3}[\mathbb{T}_{1}^{(b,B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{4}[\mathbb{M}_{1}^{(a,B_2)}(1,-1)] \otimes \mathbb{Y}_{4}[\mathbb{T}_{1}^{(b,B_2)}]}{2}$$

$\boxed{\text{No. 4}}$ $\hat{\mathbb{G}}_{2}^{(A_1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{4} = \frac{\sqrt{2}\mathbb{X}_{3}[\mathbb{M}_{1}^{(a,B_1)}(1,-1)] \otimes \mathbb{Y}_{3}[\mathbb{T}_{1}^{(b,B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{4}[\mathbb{M}_{1}^{(a,B_2)}(1,-1)] \otimes \mathbb{Y}_{4}[\mathbb{T}_{1}^{(b,B_2)}]}{2}$$

$\boxed{\text{No. 5}}$ $\hat{\mathbb{Q}}_{0}^{(A_1)}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{5} = \mathbb{X}_{1}[\mathbb{Q}_{0}^{(a,A_1)}] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{0}^{(b,A_1)}]$$

$\boxed{\text{No. 6}}$ $\hat{\mathbb{Q}}_{1}^{(A_1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{6} = -\frac{\sqrt{2}\mathbb{X}_{3}[\mathbb{M}_{1}^{(a,B_1)}(1,-1)] \otimes \mathbb{Y}_{6}[\mathbb{T}_{1}^{(b,B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{4}[\mathbb{M}_{1}^{(a,B_2)}(1,-1)] \otimes \mathbb{Y}_{7}[\mathbb{T}_{1}^{(b,B_2)}]}{2}$$

$\boxed{\text{No. 7}}$ $\hat{\mathbb{G}}_{2}^{(A_1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{7} = \frac{\sqrt{2}\mathbb{X}_{3}[\mathbb{M}_{1}^{(a,B_1)}(1,-1)] \otimes \mathbb{Y}_{6}[\mathbb{T}_{1}^{(b,B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{4}[\mathbb{M}_{1}^{(a,B_2)}(1,-1)] \otimes \mathbb{Y}_{7}[\mathbb{T}_{1}^{(b,B_2)}]}{2}$$

$\boxed{\text{No. 8}}$ $\hat{\mathbb{Q}}_{2}^{(A_1,2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{8} = -\mathbb{X}_{2}[\mathbb{M}_{1}^{(a,A_2)}(1,-1)] \otimes \mathbb{Y}_{8}[\mathbb{T}_{2}^{(b,A_2)}]$$

$\boxed{\text{No. 9}}$ $\hat{\mathbb{Q}}_{0}^{(A_1)}$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{9} = \mathbb{X}_{1}[\mathbb{Q}_{0}^{(a,A_1)}] \otimes \mathbb{Y}_{9}[\mathbb{Q}_{0}^{(b,A_1)}]$$

$\boxed{\text{No. 10}}$ $\hat{\mathbb{Q}}_{1}^{(A_1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{10} = -\frac{\sqrt{2}\mathbb{X}_{3}[\mathbb{M}_{1}^{(a,B_1)}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_{1}^{(b,B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{4}[\mathbb{M}_{1}^{(a,B_2)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{1}^{(b,B_2)}]}{2}$$

$\boxed{\text{No. 11}}$ $\hat{\mathbb{G}}_{2}^{(A_1)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{11} = \frac{\sqrt{2}\mathbb{X}_{3}[\mathbb{M}_{1}^{(a,B_1)}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_{1}^{(b,B_1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{4}[\mathbb{M}_{1}^{(a,B_2)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{1}^{(b,B_2)}]}{2}$$

$\boxed{\text{No. 12}}$ $\hat{\mathbb{Q}}_{2}^{(A_1,2)}(1,-1)$ $[\mathrm{M}_1, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_{12} = -\mathbb{X}_{2}[\mathbb{M}_{1}^{(a,A_2)}(1,-1)] \otimes \mathbb{Y}_{12}[\mathbb{T}_{2}^{(b,A_2)}]$$

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
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_1)}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{M}_1^{(a,A_2)}(1,-1)$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{M}_1^{(a,B_1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{M}_1^{(a,B_2)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A_1)}$	S_1	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(b,A_1)}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{T}_1^{(b,B_1)}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{T}_1^{(b,B_2)}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2} \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{Q}_0^{(b,A_1)}$	B_2	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{T}_1^{(b,B_1)}$	B_2	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{T}_1^{(b,B_2)}$	B_2	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{T}_2^{(b,A_2)}$	B_2	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{Q}_0^{(b,A_1)}$	B_3	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_{10}$	$\mathbb{T}_1^{(b,B_1)}$	B_3	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} & \frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{11}$	$\mathbb{T}_1^{(b,B_2)}$	B_3	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
$\mathbb{Y}_{12}$	$\mathbb{T}_2^{(b,A_2)}$	B_3	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & \frac{i}{2} \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1)}$	0	A_1	–	–	1
2	$\mathbb{Q}_1^{(B_1)}$	1	B_1	–	–	x
3	$\mathbb{Q}_1^{(B_2)}$	1	B_2	–	–	y
4	$\mathbb{Q}_2^{(A_2)}$	2	A_2	–	–	$\sqrt{3}xy$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A_2)}$	1	A_2	–	–	Z
2	$\mathbb{G}_1^{(B_1)}$	1	B_1	–	–	Y
3	$\mathbb{G}_1^{(B_2)}$	1	B_2	–	–	X

- Group info.: Generator = $\{2_{001}|0\}$, $\{\mathrm{m}_{010}|\frac{1}{2}\frac{1}{2}0\}$

Table 10: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1|0\}$	$\{1|0\}$
$\{2_{001}|0\}$	$\{2_{001}|0\}$
$\{\mathrm{m}_{010}|\frac{1}{2}\frac{1}{2}0\}$	$\{\mathrm{m}_{010}|\frac{1}{2}\frac{1}{2}0\}$
$\{\mathrm{m}_{100}|\frac{1}{2}\frac{1}{2}0\}$	$\{\mathrm{m}_{100}|\frac{1}{2}\frac{1}{2}0\}$

Table 11: Symmetry operations.

	No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
	1	$\{1\|0\}$	2	$\{2_{001}\|0\}$	3	$\{m_{010}\|\frac{1}{2}\frac{1}{2}0\}$	4	$\{m_{100}\|\frac{1}{2}\frac{1}{2}0\}$		

Table 12: Character table (point-group part).

	1	2_{001}	m_{010}	m_{100}
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

Table 13: Parity conversion.

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

Table 14: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A_1	A_2	B_1	B_2
A_1	A_1	A_2	B_1	B_2
A_2		A_1	B_2	B_1
B_1			A_1	A_2
B_2				A_1

Table 15: Anti-symmetric product, $[\Gamma \otimes \Gamma]_-$.

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

Table 16: 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 17: Virtual-cluster basis.

symbol	1	2	3	4
$\mathbb{Q}_0^{(A_1)}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$\mathbb{Q}_1^{(B_1)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$
$\mathbb{Q}_1^{(B_2)}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$
$\mathbb{Q}_2^{(A_2)}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$