Model for “kappaET”

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General Condition

- Basis type: `lgs`
- SAMB selection:
  - Type: `[Q, G]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_1, A_2, B_1, B_2]$
  - Spin (s): `[0, 1]`
- Max. neighbor: `10`
- Search cell range: `(-2, 3), (-2, 3), (-2, 3)`
- Toroidal priority: `false`

Group and Unit Cell

- Group: SG No. 32 C_{2v}^{8} $Pba2$ [orthorhombic]
- Associated point group: PG No. 32 C_{2v} $mm2$ [orthorhombic]
- Unit cell:
  $a =$ 1.00000, $b =$ 1.20000, $c =$ 1.00000, $\alpha =$ 90.0, $\beta =$ 90.0, $\gamma =$ 90.0
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ [1.00000, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [0.00000, 1.20000, 0.00000]
  $\boldsymbol{a}_3 =$ [0.00000, 0.00000, 1.00000]

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1\|0\}$	2	$\{2_{001}\|0\}$	3	$\{m_{010}\|\frac{1}{2}\frac{1}{2}0\}$	4	$\{m_{100}\|\frac{1}{2}\frac{1}{2}0\}$		

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_1)$	A_1	0	Q, T	-	-	1
2	$\mathbb{Q}_1(A_1)$	A_1	1	Q, T	-	-	z
3	$\mathbb{G}_2(A_1)$	A_1	2	G, M	-	-	$\sqrt{3}xy$
4	$\mathbb{G}_0(A_2)$	A_2	0	G, M	-	-	1
5	$\mathbb{G}_1(A_2)$	A_2	1	G, M	-	-	z
6	$\mathbb{G}_2(A_2, 2)$	A_2	2	G, M	2	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$\mathbb{Q}_2(A_2)$	A_2	2	Q, T	-	-	$\sqrt{3}xy$
8	$\mathbb{G}_1(B_1)$	B_1	1	G, M	-	-	y
9	$\mathbb{Q}_1(B_1)$	B_1	1	Q, T	-	-	x
10	$\mathbb{Q}_2(B_1)$	B_1	2	Q, T	-	-	$\sqrt{3}xz$
11	$\mathbb{G}_1(B_2)$	B_2	1	G, M	-	-	x
12	$\mathbb{Q}_1(B_2)$	B_2	1	Q, T	-	-	y
13	$\mathbb{Q}_2(B_2)$	B_2	2	Q, T	-	-	$\sqrt{3}yz$

Basis in full matrix

Table 3: dimension = 8

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$\lvert s,\uparrow\rangle$ @A(1)	1	$\lvert s,\downarrow\rangle$ @A(1)	2	$\lvert s,\uparrow\rangle$ @A(2)	3	$\lvert s,\downarrow\rangle$ @A(2)	4	$\lvert s,\uparrow\rangle$ @A(3)
5	$\lvert s,\downarrow\rangle$ @A(3)	6	$\lvert s,\uparrow\rangle$ @A(4)	7	$\lvert s,\downarrow\rangle$ @A(4)				

Table 4: Atomic basis (orbital part only)

orbital	definition
$\lvert s\rangle$	1

SAMB

28 (all 44) SAMBs

- 'A' site-cluster
  * bra: $\langle s,\uparrow\rvert$, $\langle s,\downarrow\rvert$
  * ket: $\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$
  * wyckoff: `4c`

$\boxed{\text{z1}}$ $\mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$

$\boxed{\text{z13}}$ $\mathbb{Q}_2^{(c)}(A_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_2^{(s)}(A_2)$

$\boxed{\text{z25}}$ $\mathbb{Q}_1^{(c)}(B_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(s)}(B_1)$

$\boxed{\text{z35}}$ $\mathbb{Q}_1^{(c)}(B_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(s)}(B_2)$

- 'A'-'A' bond-cluster
  * bra: $\langle s,\uparrow|\,,\ \langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle\,,\ |s,\downarrow\rangle$
  * wyckoff: `2a@2a`

$\boxed{\text{z2}}$ $\mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$

$\boxed{\text{z3}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_1) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$

$\boxed{\text{z4}}$ $\mathbb{G}_2^{(1,-1;c)}(A_1) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$

$\boxed{\text{z14}}$ $\mathbb{Q}_2^{(c)}(A_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_2^{(b)}(A_2)$

$\boxed{\text{z15}}$ $\mathbb{G}_0^{(1,-1;c)}(A_2) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$

$\boxed{\text{z16}}$ $\mathbb{G}_2^{(1,-1;c)}(A_2,2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$

$\boxed{\text{z26}}$ $\mathbb{Q}_1^{(1,-1;c)}(B_1) = -\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_2)$

$\boxed{\text{z36}}$ $\mathbb{Q}_1^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_1)$

- 'A'-'A' bond-cluster
  * bra: $\langle s,\uparrow|\,,\ \langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle\,,\ |s,\downarrow\rangle$
  * wyckoff: `4a@4c`

$\boxed{\text{z5}}$ $\mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$

$\boxed{\text{z6}}$ $\mathbb{Q}_0^{(1,-1;c)}(A_1) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{M}_1^{(b)}(A_2)$

$\boxed{\text{z7}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_1) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$

$\boxed{\text{z8}}$ $\mathbb{G}_2^{(1,-1;c)}(A_1) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$

$\boxed{\text{z17}}$ $\mathbb{Q}_2^{(c)}(A_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_2^{(b)}(A_2)$

$\boxed{\text{z18}}$ $\mathbb{G}_0^{(1,-1;c)}(A_2) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$

$\boxed{\text{z19}}$ $\mathbb{G}_1^{(1,-1;c)}(A_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$

$\boxed{\text{z20}}$ $\mathbb{G}_2^{(1,-1;c)}(A_2, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$

$\boxed{\text{z27}}$ $\mathbb{Q}_1^{(c)}(B_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(b)}(B_1)$

$\boxed{\text{z28}}$ $\mathbb{Q}_1^{(1,-1;c)}(B_1) = -\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_2)$

$\boxed{\text{z29}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_1) = \mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{M}_1^{(b)}(A_2)$

$\boxed{\text{z30}}$ $\mathbb{G}_1^{(1,-1;c)}(B_1) = \mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_0^{(b)}(A_1)$

$\boxed{\text{z37}}$ $\mathbb{Q}_1^{(c)}(B_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(b)}(B_2)$

$\boxed{\text{z38}}$ $\mathbb{Q}_1^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_1)$

$\boxed{\text{z39}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{M}_1^{(b)}(A_2)$

$\boxed{\text{z40}}$ $\mathbb{G}_1^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_0^{(b)}(A_1)$

* common SAMBs
`(z5, z9), (z6, z10), (z7, z11), (z8, z12), (z17, z21), (z18, z22), (z19, z23), (z20, z24), (z27, z31), (z28, z32), (z29, z33), (z30, z34), (z37, z41), (z38, z42), (z39, z43), (z40, z44)`

Atomic SAMB

- bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$

- ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$

$\boxed{\text{x1}}$ $\mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$

$\boxed{\text{x2}}$ $\mathbb{M}_1^{(1,-1;a)}(A_2) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$

$\boxed{\text{x3}}$ $\mathbb{M}_1^{(1,-1;a)}(B_1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$

$\boxed{\text{x4}}$ $\mathbb{M}_1^{(1,-1;a)}(B_2) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$

Cluster SAMB

- Site cluster

** Wyckoff: `4c`

$\boxed{\text{y1}}$ $\mathbb{Q}_0^{(s)}(A_1) = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$

$\boxed{\text{y2}}$ $\mathbb{Q}_2^{(s)}(A_2) = \left[\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y3}}$ $\mathbb{Q}_1^{(s)}(B_1) = \left[\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y4}}$ $\mathbb{Q}_1^{(s)}(B_2) = \left[\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right]$

- Bond cluster

** Wyckoff: `2a@2a`

$\boxed{\text{y5}}$ $\mathbb{Q}_0^{(s)}(A_1) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y6}}$ $\mathbb{Q}_2^{(s)}(A_2) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y7}}$ $\mathbb{T}_1^{(s)}(B_1) = \left[\frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2}\right]$

$\boxed{\text{y8}}$ $\mathbb{T}_1^{(s)}(B_2) = \left[\frac{\sqrt{2}i}{2}, -\frac{\sqrt{2}i}{2}\right]$

** Wyckoff: `4a@4c`

$\boxed{\text{y9}}$ $\mathbb{Q}_0^{(s)}(A_1) = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$

$\boxed{\text{y10}}$ $\mathbb{T}_0^{(s)}(A_1) = \left[\frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2}\right]$

$\boxed{\text{y11}}$ $\mathbb{M}_1^{(s)}(A_2) = \left[\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}\right]$

$\boxed{\text{y12}}$ $\mathbb{Q}_2^{(s)}(A_2) = \left[\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y13}}$ $\mathbb{Q}_1^{(s)}(B_1) = \left[\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y14}}$ $\mathbb{T}_1^{(s)}(B_1) = \left[\frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}\right]$

$\boxed{\text{y15}}$ $\mathbb{Q}_1^{(s)}(B_2) = \left[\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right]$

$\boxed{\text{y16}}$ $\mathbb{T}_1^{(s)}(B_2) = \left[\frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}, \frac{i}{2}\right]$

— Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`A`	$\vert s, \uparrow\rangle$, $\vert s, \downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	`A`	`A`	`[1,2,3]`	`[s]`	`[s]`

Site in Unit Cell

Sites in (conventional) cell (no plus set), SL = sublattice

Table 7: '`A`' (#1) site cluster (`4c`), `1`

SL	position ($\boldsymbol{s}$)	mapping
1	`[ 0.90000, 0.05000, 0.00000]`	`[1]`
2	`[ 0.10000, 0.95000, 0.00000]`	`[2]`
3	`[ 0.40000, 0.45000, 0.00000]`	`[3]`

continued ...

Table 7

SL	position ($\boldsymbol{s}$)	mapping
4	[0.60000, 0.55000, 0.00000]	[4]

Bond in Unit Cell

Bonds in (conventional) cell (no plus set): tail, head = (SL, plus set), (N)D = (non)directional (listed up to 5th neighbor at most)

Table 8: 1-th 'A'-'A' [1] (#1) bond cluster (2a@2a), ND, $|\boldsymbol{v}|$= 0.23324 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[0.20000,-0.10000, 0.00000]	[0.00000, 0.00000, 0.00000]	[1,-2]	(2,1)	(1,1)	[-1,1,0]
2	[0.20000, 0.10000, 0.00000]	[0.50000, 0.50000, 0.00000]	[3,-4]	(4,1)	(3,1)	[0,0,0]

Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (4a@4c), D, $|\boldsymbol{v}|$= 0.67082 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-0.30000,-0.50000, 0.00000]	[0.75000, 0.80000, 0.00000]	[1]	(4,1)	(1,1)	[0,1,0]
2	[0.30000, 0.50000, 0.00000]	[0.25000, 0.20000, 0.00000]	[2]	(3,1)	(2,1)	[0,-1,0]

continued ...

Table 9

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
3	[-0.30000, 0.50000, 0.00000]	[0.25000, 0.70000, 0.00000]	[3]	(2,1)	(3,1)	[0,0,0]
4	[0.30000,-0.50000, 0.00000]	[0.75000, 0.30000, 0.00000]	[4]	(1,1)	(4,1)	[0,0,0]

Table 10: 3-th 'A'-'A' [1] (#3) bond cluster (4a@4c), D, $|\boldsymbol{v}|$= 0.69311 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-0.50000, 0.40000, 0.00000]	[0.65000, 0.25000, 0.00000]	[1]	(3,1)	(1,1)	[0,0,0]
2	[0.50000,-0.40000, 0.00000]	[0.35000, 0.75000, 0.00000]	[2]	(4,1)	(2,1)	[0,0,0]
3	[-0.50000,-0.40000, 0.00000]	[0.15000, 0.25000, 0.00000]	[3]	(1,1)	(3,1)	[1,0,0]
4	[0.50000, 0.40000, 0.00000]	[0.85000, 0.75000, 0.00000]	[4]	(2,1)	(4,1)	[-1,0,0]