

Changes of showKrepBCStoBC

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2021-12-29

When `SpaceGroupRep` \leq v1.0.4, there was a bug that the same LGIR label may give different LGIR matrices in certain cases. This case may occur for the H k-line of OrthBase lattice or the G, F, and U k-lines of OrthBody lattice. For example, the following two statements should give the same LGIR's, but they gave different LGIR's when `SpaceGroupRep` \leq v1.0.4.

```
showLGirepTab[39, "H", "abcOrBasVec" -> {a->2, b->3, c->4}, "rotmat" -> False]
showLGirepTab[39, "H", "abcOrBasVec" -> {a->3, b->2, c->4}, "rotmat" -> False]
```

The list of changes of `showKrepBCStoBC` are shown below.

No.24 , $I_{21}2_12_1$, BZ type (b)

| | | |
|-----------------|---|-----------------|
| LD1 1 G_1 A 1 | → | LD1 1 G_2 B 1 |
| LD2 1 G_2 B 1 | | LD2 1 G_1 A 1 |

(double)

| | | |
|----------------------------|---|----------------------------|
| -LD3 1 G_3 $^2\bar{E}$ 2 | → | -LD3 1 G_4 $^1\bar{E}$ 2 |
| -LD4 1 G_4 $^1\bar{E}$ 2 | | -LD4 1 G_3 $^2\bar{E}$ 2 |

No.24 , $I_{21}2_12_1$, BZ type (c)

| | | |
|-----------------|---|-----------------|
| DT1 1 U_2 B 1 | → | DT1 1 U_1 A 1 |
| DT2 1 U_1 A 1 | | DT2 1 U_2 B 1 |
| SM1 1 F_1 A 1 | → | SM1 1 F_2 B 1 |
| SM2 1 F_2 B 1 | | SM2 1 F_1 A 1 |

(double)

| | | |
|----------------------------|---|----------------------------|
| -DT3 1 U_4 $^1\bar{E}$ 2 | → | -DT3 1 U_3 $^2\bar{E}$ 2 |
| -DT4 1 U_3 $^2\bar{E}$ 2 | | -DT4 1 U_4 $^1\bar{E}$ 2 |
| -SM3 1 F_4 $^1\bar{E}$ 2 | → | -SM3 1 F_3 $^2\bar{E}$ 2 |
| -SM4 1 F_3 $^2\bar{E}$ 2 | | -SM4 1 F_4 $^1\bar{E}$ 2 |

No.39 , $A_{em}2$, BZ type (b)

| | | |
|--------------------|---|--------------------|
| H1 1 H_2 A'' 1 | → | H1 1 H_1 A' 1 |
| H2 1 H_1 A' 1 | | H2 1 H_2 A'' 1 |

(double)

| | | |
|---------------------------|---|---------------------------|
| -H3 1 H_3 $^2\bar{E}$ 2 | → | -H3 1 H_4 $^1\bar{E}$ 2 |
| -H4 1 H_4 $^1\bar{E}$ 2 | | -H4 1 H_3 $^2\bar{E}$ 2 |

No.41 , $A_{ea}2$, BZ type (b)

| | | |
|--------------------|---|--------------------|
| H1 1 H_1 A' 1 | → | H1 1 H_2 A'' 1 |
| H2 1 H_2 A'' 1 | | H2 1 H_1 A' 1 |

(double)

| | | |
|---------------------------|---|---------------------------|
| -H3 1 H_3 $^2\bar{E}$ 2 | → | -H3 1 H_4 $^1\bar{E}$ 2 |
| -H4 1 H_4 $^1\bar{E}$ 2 | | -H4 1 H_3 $^2\bar{E}$ 2 |

No.45 , $I_{ba}2$, BZ type (c)

| | | |
|---------------------|---|---------------------|
| DT1 1 U_2 A'' 1 | → | DT1 1 U_1 A' 1 |
| DT2 1 U_1 A' 1 | | DT2 1 U_2 A'' 1 |
| SM1 1 F_2 A'' 1 | → | SM1 1 F_1 A' 1 |
| SM2 1 F_1 A' 1 | | SM2 1 F_2 A'' 1 |

(double)

| | | |
|----------------------------|---|----------------------------|
| -DT3 1 U_3 $^2\bar{E}$ 2 | → | -DT3 1 U_4 $^1\bar{E}$ 2 |
| -DT4 1 U_4 $^1\bar{E}$ 2 | | -DT4 1 U_3 $^2\bar{E}$ 2 |
| -SM3 1 F_4 $^1\bar{E}$ 2 | → | -SM3 1 F_3 $^2\bar{E}$ 2 |
| -SM4 1 F_3 $^2\bar{E}$ 2 | | -SM4 1 F_4 $^1\bar{E}$ 2 |

No.46 , Ima2 , BZ type (b)

| | | |
|---------------------------------------|---|---------------------------------------|
| LD1 1 G ₃ A ₂ x | → | LD1 1 G ₁ A ₁ x |
| LD2 1 G ₁ A ₁ x | | LD2 1 G ₃ A ₂ x |
| LD3 1 G ₄ B ₂ x | | LD3 1 G ₂ B ₁ x |
| LD4 1 G ₂ B ₁ x | | LD4 1 G ₄ B ₂ x |

No.46 , Ima2 , BZ type (c)

| | | |
|----------------------------|---|----------------------------|
| DT1 1 F ₁ A' 1 | → | DT1 1 F ₂ A'' 1 |
| DT2 1 F ₂ A'' 1 | | DT2 1 F ₁ A' 1 |

(double)

| | | |
|---|---|---|
| -DT3 1 F ₄ ¹ Ē 2 | → | -DT3 1 F ₃ ² Ē 2 |
| -DT4 1 F ₃ ² Ē 2 | | -DT4 1 F ₄ ¹ Ē 2 |

No.64 , Cmce , BZ type (b)

| | | |
|--------------------------------------|---|--------------------------------------|
| H1 1 H ₄ B ₂ 1 | → | H1 1 H ₂ B ₁ 1 |
| H2 1 H ₂ B ₁ 1 | | H2 1 H ₄ B ₂ 1 |
| H3 1 H ₁ A ₁ 1 | | H3 1 H ₃ A ₂ 1 |
| H4 1 H ₃ A ₂ 1 | | H4 1 H ₁ A ₁ 1 |

No.67 , Cmme , BZ type (b)

| | | |
|--------------------------------------|---|--------------------------------------|
| H1 1 H ₁ A ₁ 1 | → | H1 1 H ₃ A ₂ 1 |
| H2 1 H ₃ A ₂ 1 | | H2 1 H ₁ A ₁ 1 |
| H3 1 H ₄ B ₂ 1 | | H3 1 H ₂ B ₁ 1 |
| H4 1 H ₂ B ₁ 1 | | H4 1 H ₄ B ₂ 1 |

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No.68 , Ccce , BZ type (b)

| | | |
|--------------------------------------|---|--------------------------------------|
| H1 1 H ₃ A ₂ 1 | → | H1 1 H ₁ A ₁ 1 |
| H2 1 H ₁ A ₁ 1 | | H2 1 H ₃ A ₂ 1 |
| H3 1 H ₂ B ₁ 1 | | H3 1 H ₄ B ₂ 1 |
| H4 1 H ₄ B ₂ 1 | | H4 1 H ₂ B ₁ 1 |

No.72 , Ibam , BZ type (c)

| | | |
|---------------------------------------|---|---------------------------------------|
| DT1 1 U ₃ A ₂ 1 | → | DT1 1 U ₁ A ₁ 1 |
| DT2 1 U ₁ A ₁ 1 | | DT2 1 U ₃ A ₂ 1 |
| DT3 1 U ₄ B ₂ 1 | | DT3 1 U ₂ B ₁ 1 |
| DT4 1 U ₂ B ₁ 1 | | DT4 1 U ₄ B ₂ 1 |

| | | |
|---------------------------------------|---|---------------------------------------|
| SM1 1 F ₃ A ₂ 1 | → | SM1 1 F ₁ A ₁ 1 |
| SM2 1 F ₁ A ₁ 1 | | SM2 1 F ₃ A ₂ 1 |
| SM3 1 F ₂ B ₁ 1 | | SM3 1 F ₄ B ₂ 1 |
| SM4 1 F ₄ B ₂ 1 | | SM4 1 F ₂ B ₁ 1 |

No.73 , Ibca , BZ type (b)

| | | |
|---------------------------------------|---|---------------------------------------|
| LD1 1 G ₃ A ₂ 1 | → | LD1 1 G ₄ B ₂ 1 |
| LD2 1 G ₁ A ₁ 1 | | LD2 1 G ₂ B ₁ 1 |
| LD3 1 G ₂ B ₁ 1 | | LD3 1 G ₁ A ₁ 1 |
| LD4 1 G ₄ B ₂ 1 | | LD4 1 G ₃ A ₂ 1 |

No.73 , Ibca , BZ type (c)

| | | |
|---------------------------------------|---|---------------------------------------|
| DT1 1 U ₄ B ₂ 1 | → | DT1 1 U ₃ A ₂ 1 |
| DT2 1 U ₂ B ₁ 1 | | DT2 1 U ₁ A ₁ 1 |
| DT3 1 U ₃ A ₂ 1 | | DT3 1 U ₄ B ₂ 1 |
| DT4 1 U ₁ A ₁ 1 | | DT4 1 U ₂ B ₁ 1 |
| SM1 1 F ₃ A ₂ 1 | → | SM1 1 F ₄ B ₂ 1 |
| SM2 1 F ₁ A ₁ 1 | | SM2 1 F ₂ B ₁ 1 |
| SM3 1 F ₂ B ₁ 1 | | SM3 1 F ₁ A ₁ 1 |
| SM4 1 F ₄ B ₂ 1 | | SM4 1 F ₃ A ₂ 1 |

No.74 , Imma , BZ type (b)

| | | |
|---------------------------------------|---|---------------------------------------|
| LD1 1 G ₁ A ₁ 1 | → | LD1 1 G ₂ B ₁ 1 |
| LD2 1 G ₃ A ₂ 1 | | LD2 1 G ₄ B ₂ 1 |
| LD3 1 G ₄ B ₂ 1 | | LD3 1 G ₃ A ₂ 1 |
| LD4 1 G ₂ B ₁ 1 | | LD4 1 G ₁ A ₁ 1 |

No.74 , Imma , BZ type (c)

| | | |
|---------------------------------------|---|---------------------------------------|
| DT1 1 U ₂ B ₁ 1 | → | DT1 1 U ₃ A ₂ 1 |
| DT2 1 U ₄ B ₂ 1 | | DT2 1 U ₁ A ₁ 1 |
| DT3 1 U ₁ A ₁ 1 | | DT3 1 U ₄ B ₂ 1 |
| DT4 1 U ₃ A ₂ 1 | | DT4 1 U ₂ B ₁ 1 |
| SM1 1 F ₁ A ₁ 1 | → | SM1 1 F ₄ B ₂ 1 |
| SM2 1 F ₃ A ₂ 1 | | SM2 1 F ₂ B ₁ 1 |
| SM3 1 F ₄ B ₂ 1 | | SM3 1 F ₁ A ₁ 1 |
| SM4 1 F ₂ B ₁ 1 | | SM4 1 F ₃ A ₂ 1 |