Note: Checking the Calculations in arXiv:1907.09354 Classification of Surface States Using the Equivariant Thom Isomorphism

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May 31, 2026

Abstract

Motivated by discrepancies between the results of [2] and [1], I recalculated the classification tables in [1]. One example of such a discrepancy is the B representation of the magnetic point group $\bar{4}1'$ for spinful electrons. I have not yet checked whether [2] treats exactly the same classification problem. I found that the numerical calculations in [1] contained some errors. In other words, the error was not in the formulation of [1], but in the program implementation. The recalculated results are included in v2 of [1], namely the published version. Even after recalculation, some discrepancies with the results of [2] remain, for example the B representation of $\bar{4}1'$. For two examples, the spinful $\bar{4}1'$ B representation and the spinful $62'2'$ B representation, I also record hand calculations using the real-space AHSS in the latter half of this note. The real-space AHSS results are consistent with v2 of [1].

1 Checking the Formulation

The symmetry data consist of

- the group G,
- the action on real space $p_g \in O(3)$, $\boldsymbol{x} \mapsto p_g \boldsymbol{x}$,
- a factor system $z_{g,h}$,
- homomorphisms $\phi, c : G \to \mathbb{Z}_2 = \{\pm 1\}$.

The symmetry conditions are

$$u_g H(\boldsymbol{k}) u_g^{-1} = c_g H(\boldsymbol{k}), \quad u_g u_h = z_{g,h} u_{gh}, \quad u_g i u_g^{-1} = \phi_g i. \tag{1}$$

$$s_g = \det p_g \in \pm \tag{2}$$

Introduce this notation. Also write $p_g = I^{s_g} R_g$, where I is spatial inversion, and regard $R_g \in SO(3)$ as a rotation by θ_g around the axis $\boldsymbol{n}_g$. We fix the pair $(\boldsymbol{n}_g, \theta_g)$.

1.1 Construction of K_{AI}

Apply the Wigner criteria to the symmetry data (G, z, ϕ, c) and compute the K-group K_{AI} at the point-group center. For ϕ, c, decompose G as $G = G_0 + TG_0 + CG_0 + \Gamma G_0$. The lattice for K_{AI} is constructed by the following rules.

- For irreducible representations of G_0 with nontrivial classification, enter the representation dimension of the Hamiltonian.
- For representations that are mapped to one another, multiply by c_h.
- For $\mathbb{Z}_2$ classifications, take the absolute value.

These rules give

$$\begin{array}{ll} \mathrm{A}, \mathrm{AI} & (1) \\ \mathrm{A_T}, \mathrm{D_T} & (1,1) \\ \mathrm{A_C}, \mathrm{AI_C} & (1,-1) \\ \mathrm{A_{T,C}} & (1,1,-1,-1) \\ \mathrm{AII}, \mathrm{D}, \mathrm{BDI} & (2) \\ \mathrm{AII_C} & (2,-2) \end{array} \tag{3}$$

Let the matrices whose rows are the basis vectors of the $\mathbb{Z}$ and $\mathbb{Z}_2$ classifications be denoted respectively by

$$V_{\mathbb{Z}} = \begin{pmatrix} v_1 \\ \vdots \end{pmatrix}, \quad V_{\mathbb{Z}_2} = \begin{pmatrix} v_1 \\ \vdots \end{pmatrix} \tag{4}$$

1.2 Construction of K

Next, transform u_g into an internal symmetry by the method of Cornfeld–Chapman.

$$H(\boldsymbol{k}) = k_1\gamma_1 + k_2\gamma_2 + k_3\gamma_3 + m\Gamma_0 \tag{5}$$

Set

$$q_g := e^{\frac{\theta_g}{2}(n_{g1}\gamma_2\gamma_3 + n_{g2}\gamma_3\gamma_1 + n_{g3}\gamma_1\gamma_2)} \tag{6}$$

and define

$$\rho_g := (\gamma_1\gamma_2\gamma_3)^{\frac{1-s_g}{2}} q_g u_g \tag{7}$$

Then

$$\rho_g H(\boldsymbol{k})\rho_g^{-1} = c_g s_g H(\phi_g \boldsymbol{k}), \quad \rho_g\rho_h = \tilde{z}_{g,h}\rho_{gh}, \quad \rho_g i \rho_g^{-1} = \phi_g i. \tag{8}$$

Here the factor system $\tilde{z}_{g,h}$ is given by

$$\tilde{z}_{g,h} = z'_{g,h}(-1)^{\frac{1-c_g s_g}{2}\frac{1-s_h}{2}} z_{g,h}, \tag{9}$$

$$z'_{g,h} = q_h q_g q_{gh}^{-1} \in \pm 1 \tag{10}$$

Pay attention to the right action. The factor $z'_{g,h}$ is determined by $(\boldsymbol{n}_g, \theta_g)$ and does not necessarily coincide with the factor system for spinful electrons. Moreover, $z'_{g,h}$ is determined only by the unitary part, so in this respect also it differs from the factor system for spinful electrons when antiunitary symmetries are included. Apply the Wigner criteria to the data $(G, \tilde{z}, \tilde{c} = cs, \phi)$ and compute the K-group K. For $\tilde{c}, \phi$, decompose G as $G = G'_0 + T'G'_0 + C'G'_0 + \Gamma' G'_0$. The lattice for K is constructed by the following rules.

- If chiral symmetry is present and closes within an irreducible representation α of G'_0, choose one extension $\alpha+$ of the representation from the irreducible representations of $G'_0 + \Gamma' G'_0$.
- For irreducible representations with nontrivial classification, enter the representation dimension of the Hamiltonian.

- For representations that are mapped to one another, multiply by ϕ_h. The only relevant EAZ class is $\mathrm{AIII_T}$. Represent the mismatch between $T(\alpha+)$ and $(T\alpha)+$ by the sign η.
- For $\mathbb{Z}_2$ classifications, take the absolute value.

These rules give

$$\begin{array}{ll} \mathrm{AIII, DIII, AII} & (4) \\ \mathrm{CII, CI} & (8) \\ \mathrm{AIII_T} & (4, -\eta 4) \\ \mathrm{AII_C} & (4, 4) \end{array} \tag{11}$$

Let the matrices whose rows are the basis vectors of the $\mathbb{Z}$ and $\mathbb{Z}_2$ classifications be denoted respectively by

$$V'_{\mathbb{Z}} = \begin{pmatrix} v_1 \\ \vdots \end{pmatrix}, \quad V'_{\mathbb{Z}_2} = \begin{pmatrix} v_1 \\ \vdots \end{pmatrix} \tag{12}$$

1.3 The Third Isomorphism Theorem

$$f : K_{\mathrm{AI}} \to K \tag{13}$$

We want to compute this map. First rewrite the problem as a problem of integer lattices using the third isomorphism theorem. We want to compute $K/\mathrm{Im}\, f$. Write the extensions of the torsion parts of K and K_{AI} to $\mathbb{Z}$ as

$$H \to \tilde{K} \to K, \tag{14}$$

$$H_{\mathrm{AI}} \to \tilde{K}_{\mathrm{AI}} \to K_{\mathrm{AI}}, \tag{15}$$

respectively. Then for

$$\tilde{f} : \tilde{K}_{\mathrm{AI}} \to \tilde{K} \tag{16}$$

we note that

$$\mathrm{Im}\, f = (\mathrm{Im}\, \tilde{f} + H)/H \tag{17}$$

and the third isomorphism theorem gives

$$K/\mathrm{Im}\, f = \tilde{K}/(\mathrm{Im}\, \tilde{f} + H) \tag{18}$$

1.4 Computing $\tilde{f} : \tilde{K}_{\mathrm{AI}} \to \tilde{K}$

The computational method differs for $\mathbb{Z} \to \mathbb{Z}$, $\mathbb{Z} \to \mathbb{Z}_2$, and $\mathbb{Z}_2 \to \mathbb{Z}_2$. Note that all maps to $\mathbb{Z}_2$ take absolute values. First, for the Hamiltonian constructed from an irreducible representation α of G_0,

$$H = \boldsymbol{k} \cdot \boldsymbol{\gamma} + \boldsymbol{r} \cdot \boldsymbol{\Gamma} + m\Gamma_0 \tag{19}$$

restrict to $\boldsymbol{r} = \boldsymbol{0}$:

$$H = \boldsymbol{k} \cdot \boldsymbol{\gamma} + m\Gamma_0 \tag{20}$$

For this restricted Hamiltonian, construct the matrix δ_{w3} which computes the 3D winding number in the irreducible representation $\beta+$ of $G'_0 + \Gamma G'_0$, and the matrix $\delta_{\rm ir}$ which counts the number of irreducible representations β of G'_0.

$$[\delta_{w_3}]_{\alpha\beta} = 4 \times \frac{1}{|G'_0|} \sum_{g\in G} \delta_{\phi_g,1}\delta_{c_g,1}\delta_{s_g,-1}\chi^*_{\beta+}(g) 2\cos\frac{\theta_g}{2}\chi_\alpha(g), \tag{21}$$

$$[\delta_{\rm ir}]_{\alpha\beta} = 4 \times \frac{1}{|G'_0|} \sum_{g\in G} \delta_{\phi_g,1}\delta_{c_g,1}\delta_{s_g,1}\chi^*_{\beta}(g) 2\cos\frac{\theta_g}{2}\chi_\alpha(g). \tag{22}$$

These two matrices can be constructed independently of whether the classification in K is trivial or nontrivial. Since the decomposition of H may include irreducible representations whose $\mathbb{Z}_2$ classification is trivial, introduce the row vector $v'_{\mathbb{Z}_2}$ which assigns 1 only to the $\mathbb{Z}_2$ classifications in K and 0 otherwise, and define the matrix counting only the irreducible representations with nontrivial $\mathbb{Z}_2$ classification by

$$[\delta_{\mathbb{Z}_2}]_{\alpha\beta} := [\delta_{\rm ir}]_{\alpha\beta}[v'_{\mathbb{Z}_2}]_\beta \tag{23}$$

The matrices for $\mathbb{Z}\to\mathbb{Z}$, $\mathbb{Z}\to\mathbb{Z}_2$, $\mathbb{Z}_2\to\mathbb{Z}$, and $\mathbb{Z}_2\to\mathbb{Z}_2$ are as follows:

$$[\tilde f|_{\mathbb{Z}\to\mathbb{Z}}]_{\alpha\beta} = [V_{\mathbb{Z}}.\delta_{w_3}.(V'_{\mathbb{Z}})^+]_{\alpha\beta}, \tag{24}$$

$$[\tilde f|_{\mathbb{Z}\to\mathbb{Z}_2}]_{\alpha\beta} = [{\rm Abs}(V_{\mathbb{Z}}).\delta_{\mathbb{Z}_2}.(V'_{\mathbb{Z}_2})^+]_{\alpha\beta}, \tag{25}$$

$$[\tilde f|_{\mathbb{Z}_2\to\mathbb{Z}}]_{\alpha\beta} = 0, \tag{26}$$

$$[\tilde f|_{\mathbb{Z}_2\to\mathbb{Z}_2}]_{\alpha\beta} = [V_{\mathbb{Z}_2}.\delta_{\mathbb{Z}_2}.(V'_{\mathbb{Z}_2})^+]_{\alpha\beta}, \tag{27}$$

(28)

Here Abs takes the absolute value of each entry, and A^+ is the pseudoinverse of A. Since the pseudoinverse gives the zero matrix when the equation $A.x = b$ has no solution, one must check whether $V.\delta$ can be expanded in the basis V'. Concretely, it is enough to check $V.\delta = V.\delta.(V')^+.V'$. By construction the basis vectors of V' are independent, so the solution is unique.

Im $\tilde f$ is spanned by the row vectors of the matrix

$$\begin{pmatrix} \tilde f_{\mathbb{Z}\to\mathbb{Z}} & \tilde f|_{\mathbb{Z}\to\mathbb{Z}_2} \\ \tilde f_{\mathbb{Z}_2\to\mathbb{Z}} & \tilde f|_{\mathbb{Z}_2\to\mathbb{Z}_2} \end{pmatrix} \tag{29}$$

The space spanned by Im $\tilde f + H$ is obtained by adding (2) for the $\mathbb{Z}_2$ classifications of K'. In other words,

$${\rm Im}\,\tilde f + H = \begin{pmatrix} \tilde f_{\mathbb{Z}\to\mathbb{Z}} & \tilde f|_{\mathbb{Z}\to\mathbb{Z}_2} \\ \tilde f_{\mathbb{Z}_2\to\mathbb{Z}} & \tilde f|_{\mathbb{Z}_2\to\mathbb{Z}_2} \\ O & \mathbf{2} \end{pmatrix} =: M. \tag{30}$$

Taking the Smith normal form of the matrix M gives the quotient $K/{\rm Im}\, f$. For the computational results, see v2 of [1]. The Mathematica calculation file is named "Classification_Surface_State.nb".

References

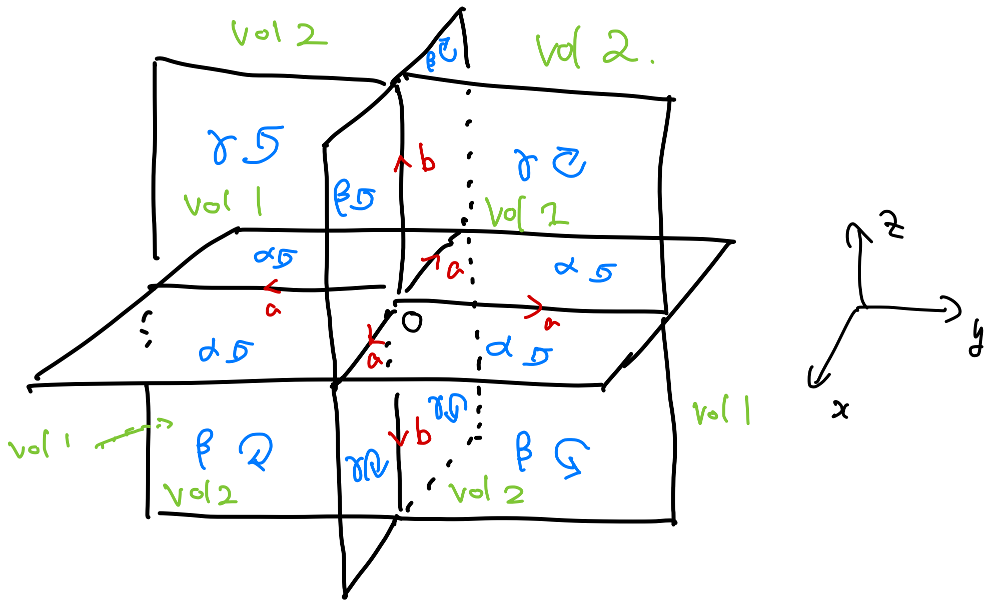
[1] Shiozaki, Ken. "The classification of surface states of topological insulators and superconductors with magnetic point group symmetry." arXiv:1907.09354v1 (2019).

[2] Zhang, Zhongyi, Jie Ren, and Chen Fang. "Classification of intrinsic topological superconductors jointly protected by time-reversal and point-group symmetries in three dimensions." arXiv:2109.14629v1 (2021).

平1', B表現　実空間AHSS.

$$(x, y, z) \overset{f}{\longmapsto} (y, -x, -z).$$

セル分割



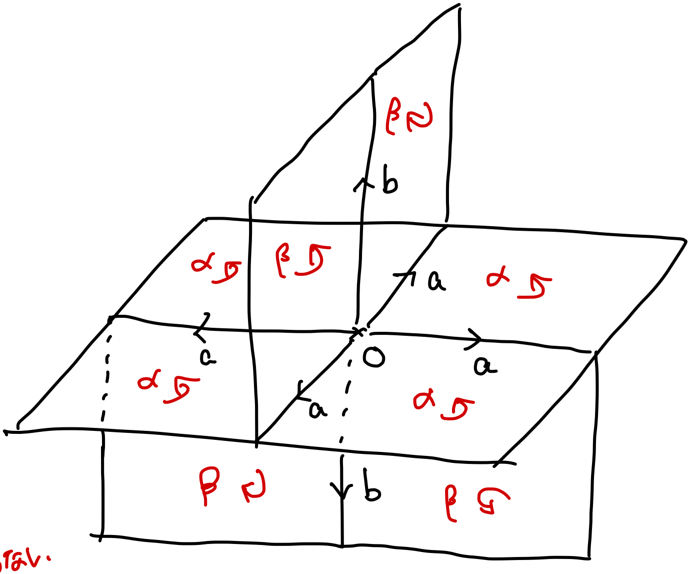
.... Vol はひとつにできるはず

面が余分だ.

⟶ γ or β が不要.

$E^1_{p,-n}$	$\{O\}$	$\{a, b\}$	$\{\alpha, \beta, \gamma\}$	$\{vol1, vol2\}$
	$p=0$	$p=1$	$p=2$	$p=3$

セル分割やり直し.



高次微分なし.

EA2の導出は次ページ.

	$A_{T,C}$	DIII $AIII_T$	DIII DIII	DIII
n=0	$\mathbb{Z}$	0		
n=1	0	$\mathbb{Z}_2+\mathbb{Z}$	$\mathbb{Z}_2+\mathbb{Z}_2$	
n=2		$\mathbb{Z}_2+0$ ⇇	$\mathbb{Z}_2+\mathbb{Z}_2$ ← 0	$\mathbb{Z}_2$
n=3			$\mathbb{Z}+\mathbb{Z}$ ← 0	$\mathbb{Z}$
$E^1_{p,-n}$	{O} p=0	{a, b} p=1	{α, β} p=2	{vol} p=3

2D DIII SC がキャンセル.

残る.

3D DIII SCは symと両立する.

⇓

局在位置が異なるので抜けない.

n=0	$\mathbb{Z}$	0		
n=1		$0+\mathbb{Z}$	$\mathbb{Z}_2+0$	
n=2		0	$\mathbb{Z}_2+0$	$\mathbb{Z}_2$
n=3				$\mathbb{Z}$
$E^2_{p,-n}$	p=0	p=1	p=2	p=3

$= E^{\infty}$ページ.

表面状態の分類は

$$\mathbb{Z}^2+\mathbb{Z}_2$$

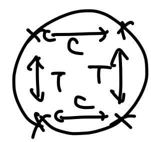
⇒ Cornfeld-Chapmanの結果と同一結果.

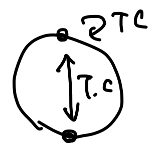
B-rep:

1	$\bar{4}^+$	2	$\bar{4}^-$
1	−1	1	−1

Sym. alg.

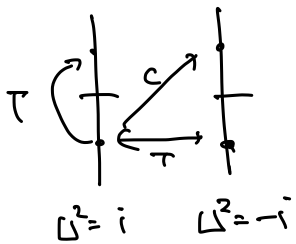
$$\begin{cases} U H(\mathbf{k}) U^{-1} = H(k_y, -k_x, -k_z), & U^4 = -1, \quad (U^2)^2 = -1. \\ T H(\mathbf{k}) T^{-1} = H(-\mathbf{k}), & T^2 = -1 \\ C H(\mathbf{k}) C^{-1} = -H(-\mathbf{k}), & C^2 = 1. \\ TU = UT, & CU = -UC. \end{cases}$$

U: 

U^2: 

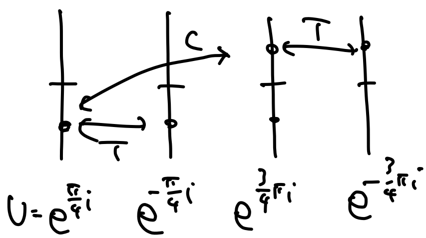
@ b

$AIII_T$



@ Γ

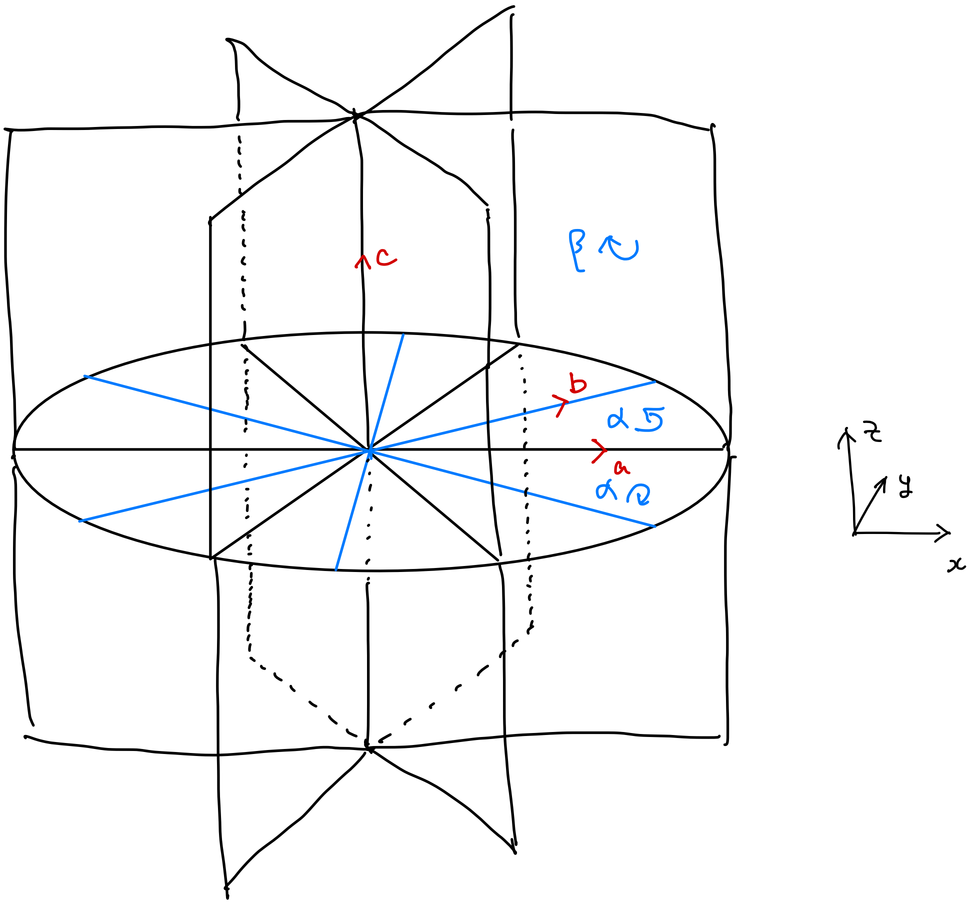
$A_{T,C}$



6 2'2'　B 表現　spinful

6 2'2'　:　$G^{\dagger}_{001}$, $2'_{100}$ で生成.

→ $|G| = 12$.



B rep

	1	6	3	2
B	1	−1	1	−1

$$C_2^x = -i\sigma^x$$
$$C_6^z = e^{-\frac{\pi}{3}i\sigma^z}$$
$$C_2^x C_6^z = -i\sigma^x e^{-\frac{\pi}{3}i\sigma^z} = e^{\frac{\pi}{3}i\sigma^z}(-i\sigma^x) = (C_6^z)^{-1} \cdot C_2^x$$

Sym. alg.

$$\begin{cases} (C_6^z)^6 = -1, \quad C C_6^z = -C_6^z C, \\ (C_2^x T)^2 = (C_2^x)^2 T^2 = 1, \quad C_2^x T \cdot C_6^z = (C_6^z)^{-1} \cdot C_2^x T. \end{cases}$$

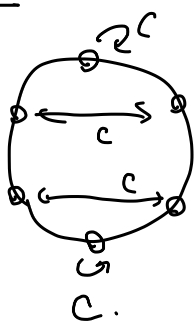
⇓

$C_6^z|\phi\rangle = \lambda|\phi\rangle$ aとき,

$$C_6^z C_2^x T|\phi\rangle = C_2^x T (C_6^z)^{-1}|\phi\rangle = C_2^x T \cdot \lambda^{-1}|\phi\rangle = \lambda C_2^x T|\phi\rangle.$$

⇒ 同一固有値.

@ C

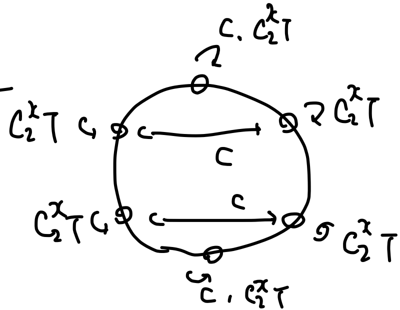


$\Rightarrow D^2 + A_C^2$.

@ a, b

$$\begin{cases} (C_2^x T)^2 = 1 \\ C^2 = 1 \end{cases} \Rightarrow \text{BDI}.$$

@ O



$\rightarrow \text{BDI}^2 + \text{AI}_C^2$.

E^1 ページ

	$BDI^2 + AI_c^2$	$BDI + BDI + D^2 + A_c^2$	$P + D$	D
$n=0$	$\mathbb{Z}_2^2 + \mathbb{Z}^2$	$\mathbb{Z}_2 + \mathbb{Z}_2 + \mathbb{Z}_2^2 + \mathbb{Z}^2$	$\mathbb{Z}_2 + \mathbb{Z}_2$	
$n=1$	$\mathbb{Z}^2 + 0 \leftarrow$	$\mathbb{Z} + \mathbb{Z} + (\mathbb{Z}_2^2 + 0)$	$0 \leftarrow (\mathbb{Z}_2) + (\mathbb{Z}_2)$	$\mathbb{Z}_2$
$n=2$		$0 + 0 + \mathbb{Z}^2 + \mathbb{Z}^2 \leftarrow$	$\mathbb{Z} + (\mathbb{Z})$	$\mathbb{Z}$
			$2 \leftarrow$	1
$n=3$			0	0
$E^1_{p,-n}$	$\{0\}$ $p=0$	$\{a, b, c\}$ $p=1$	$\{\alpha, \beta\}$ $p=2$	$\{vol\}$ $p=3$

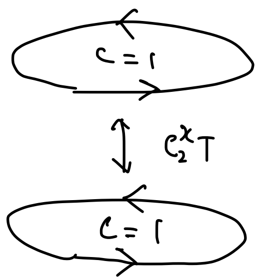
$$d^1_{2,-2} : \overset{\alpha}{\mathbb{Z}} + \overset{\beta}{\mathbb{Z}} \to \overset{c}{\mathbb{Z}^2 + \mathbb{Z}^2}$$

$(1,0) \mapsto 0.$

$(0,1) \mapsto (1,1,1,1)$ $p1.$

$$d^1_{3,-2} : \overset{vol}{\mathbb{Z}} \to \overset{\alpha}{\mathbb{Z}} + \overset{\beta}{\mathbb{Z}}$$

$1 \mapsto (2, 0)$



$$d^1_{2,-2} : \mathbb{Z}_2 + \overset{\beta}{\mathbb{Z}_2} \to \mathbb{Z} + \mathbb{Z} + \mathbb{Z}_2^2$$

$(1,0) \to 0$

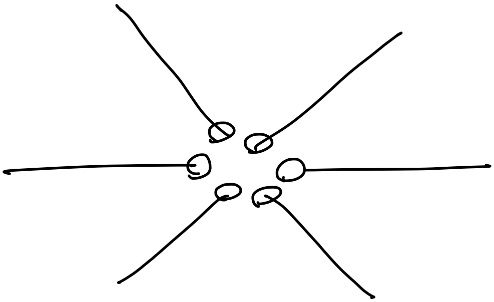
$(0,1) \mapsto (0, 0, 1, 1)$

$d^1_{1,-1}$: $\overset{a}{\mathbb{Z}} + \overset{b}{\mathbb{Z}} + \overset{c}{\mathbb{Z}_2^2} \longrightarrow \mathbb{Z}^2$

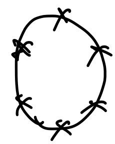
$(1,0,0) \longmapsto (1,1)$

$(0,1,0) \longmapsto (1,1)$ すなわち,

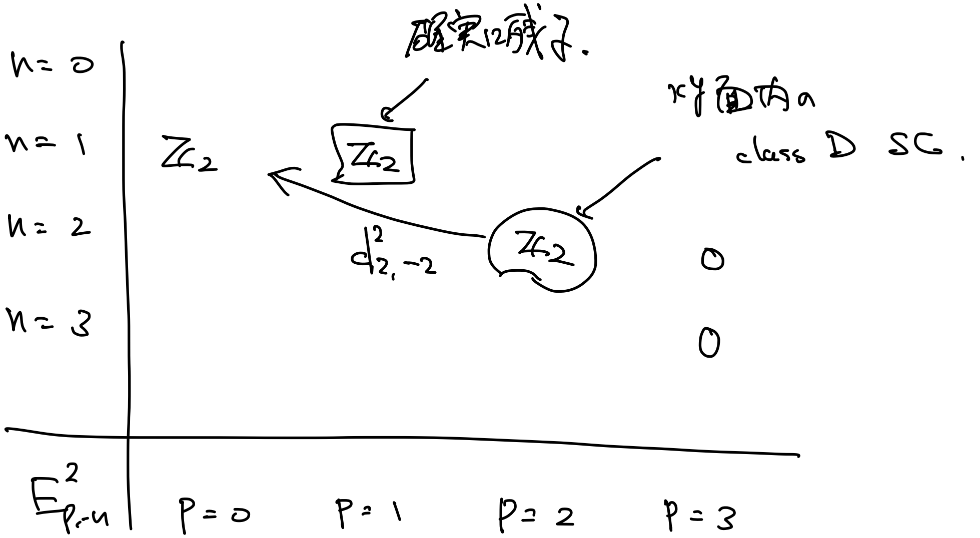
$\Rightarrow$ $\mathbb{Z}_2$ が残る.



C_6^2 固有値は,



E^2ページ



$\Rightarrow$ $\mathbb{Z}_2^2$ or $\mathbb{Z}_2$.

対角内の クラス D SC が、sym と compatible かどうか確認する.

$$H = k_x \tau_x - k_y \tau_y + m\tau_z,$$

$$= \begin{pmatrix} m & ke^{i\theta} \\ ke^{-i\theta} & -m \end{pmatrix}$$

$$C_\phi = e^{i\phi\tau_z/2} \sim \begin{pmatrix} 1 & \\ & e^{i\phi} \end{pmatrix}. \quad \to \quad C_{2\pi} = -\mathbb{I}.$$

$$C_\phi H(\theta) C_\phi^{-1} = \begin{pmatrix} 1 & \\ & e^{i\phi} \end{pmatrix}\begin{pmatrix} & e^{i\theta} \\ e^{-i\theta} & \end{pmatrix}\begin{pmatrix} 1 & \\ & e^{-i\phi} \end{pmatrix}$$

$$= \begin{pmatrix} & e^{i(\theta+\phi)} \\ e^{-i(\theta+\phi)} & \end{pmatrix} = H(\theta+\phi).$$

$\leadsto$ $C = \tau_x K$.

$\to$ $CC_\phi = \tau_x e^{-i\phi\tau_z/2} = e^{i\phi\tau_z/2}\tau_x = C_\phi C$.

…. C_6 の B-rep は両立しないぞ….

$\Rightarrow$ $d^2_{2,-2}$ は非自明.

$\Delta(k) = |\Delta| e^{in\phi}$ とすると…

$$H = \begin{pmatrix} m & k^n e^{in\phi} \\ k^n e^{-in\phi} & -m \end{pmatrix}.$$

Symmは $C_\phi = e^{in\phi\tau_z/2} \to C_{2\pi} = (-\mathbb{1})^n$.

$$C C_\phi = \tau_x e^{-in\phi\tau_z/2} = e^{in\phi\tau_z/2}\tau_x = C_\phi C.$$

… なので. B-rep はやりなし.

なので、 E^3 ページは以下.

$E^3_{p,-n}$	$p=0$	$p=1$	$p=2$	$p=3$
$n=0$				
$n=1$	0	$\mathbb{Z}_2$		
$n=2$			0	
$n=3$				0

⇒ 表面状態の分類は、$\mathbb{Z}_2$。//

(update した) Cornfeld-Chapman の結果と一致.

(arXiv の ver 1 は 計算間違いアリ)