# CLASSIFICATION OF EIGENMODES IN A SIDE-COUPLED STRUCTURE ACCORDING TO THE SPACE GROUP REPRESENTATIONS

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## Abstract

The geometric symmetry of an rf structure can be expressed by a group of symmetry operations that keep the configuration invariant [1]. For a periodic structure, the geometric symmetry is described by a space group containing translations, reflections, and other operations. Eigenmodes in the structure can be classified according to the irreducible representations of the space group of the structure. In this paper, we apply this method to a sidecoupled structure (SCS) [2] which is widely used for proton accelerators.

## **INTRODUCTION**

Many periodic accelerating structures have both translational and other geometric symmetries. An entire symmetry of a given structure can be expressed by a group of symmetry operations that keep the structure invariant. The symmetry group of the structure has several irreducible representations that can express the fundamental patterns of transformations induced by the symmetry operations. Eigenmodes in the structure can be classified according to these irreducible representations. This approach provides a general method of classifying the eigenmodes in any cavities.

For a periodic structure, its geometric symmetry can be expressed by a space group containing translations, reflections, and other operations. The application of space groups to rf problems was partly discussed in [3]. In this paper, we apply this method to the side-coupled structure which is widely used for proton accelerators. This example is practically important as well as interesting because it has a non-symmorphic space group. First, we find the symmetry group of this structure, and derive its irreducible representations. Then, we classify some of its eigenmodes according to these irreducible representations.

## SYMMETRY GROUP OF THE SCS

A typical configuration of the side-coupled structure is depicted in Fig. 1. The SCS is usually operated under a phase difference of  $\pi/2$  between adjacent acceleratingand coupling-cells. It has a fundamental period of *d*. We take the Cartesian coordinates as shown in Fig. 1. To simplify the analysis, we assume that the structure contains *N* fundamental periods where *N* is a huge integer, and assume the periodic boundary conditions at the ends of the structure.

Let us denote an operation, which takes a point **r** to  $(\alpha \mathbf{r}+\mathbf{b})$ , by a symbol  $\{\alpha|\mathbf{b}\}$ , where  $\alpha$  is any of rotations or reflections. Then, the translational symmetry of the structure can be expressed by a translation group,

 $T = \left\{ \left\{ \varepsilon \mid \mathbf{t}_n \right\} \mid n = 0, 1, ..., N - 1 \right\}, \text{ where } \varepsilon \text{ is an identity} \\ \text{operation, } \mathbf{t}_n \ ( \equiv nd\hat{\mathbf{z}} \text{ ) denote the primitive translation} \\ \text{vectors, and } \hat{\mathbf{z}} \text{ is the unit vector in the positive } z \text{ direction.} \\ \text{An entire symmetry of the structure is expressed by a space group,}$ 

$$G = R_1 T + R_2 T + \dots + R_8 T , \qquad (1)$$

where the *G* has been expressed by a union of the cosets of *T*. The coset representatives, *R*<sub>1</sub> to *R*<sub>8</sub>, are given by  $\{\varepsilon \mid \mathbf{0}\}, \{C_2 \mid \mathbf{\tau}\}, \{C_2^y \mid \mathbf{\tau}\}, \{C_2^x \mid \mathbf{0}\}, \{I \mid \mathbf{0}\}, \{\sigma_z \mid \mathbf{\tau}\}, \{\sigma_y \mid \mathbf{\tau}\}, \text{ and } \{\sigma_x \mid \mathbf{0}\}, \text{ where } C_2, C_2^y, \text{ and } C_2^x \text{ are the rotations through } \pi \text{ about the } z, y \text{ and } x \text{ axes, respectively,}$ 

*I* is the space inversion,  $\sigma_z$ ,  $\sigma_y$ , and  $\sigma_x$  are the mirror reflections in the *x*-*y*, *z*-*x*, and *y*-*z* planes, respectively, and  $\tau (\equiv d\hat{z}/2)$  is a non-primitive translation vector. We can notice that this group contains several operations involving the non-primitive translations. Space groups involving such operations (screws or glides) are called the non-symmorphic space groups [4].



Figure 1: A sketch of the side-coupled structure.

## **IRREDUCIBLE REPRESENTATIONS**

We next derive the irreducible representations of the space group G of the SCS. This is done in three steps. First, we present the irreducible representations of the translation group, and define the wavevector **k**. Next, we define the group of the wavevector **k**,  $G(\mathbf{k})$ , and derive its irreducible representations. Finally, we derive the irreducible representations of the entire space group G.

## Translation Group

Because the translation group T is a cyclic group of order N, it has N one-dimensional irreducible representations. Their characters are given by

$$\chi^{\mathbf{k}}\left(\left\{\boldsymbol{\varepsilon} \mid \mathbf{t}_{n}\right\}\right) = \exp\left(i\mathbf{k}\cdot\mathbf{t}_{n}\right),\tag{2}$$

where the wavevector **k** is given by  $\mathbf{k} = ((2p/N)-1)\pi\hat{\mathbf{z}}/d$ , and *p* is an integer ranging from 1 to *N*. Because *N* is a huge integer, the wavevector takes almost continuous values inside the first Brillouin zone,  $-\pi/d < k_z \le \pi/d$ .

If an eigenmode,  $\mathbf{E}_{\mathbf{k}}$ , belongs to an irreducible representation that is specified by a wavevector  $\mathbf{k}$ , it is transformed by a translation by

$$\{\varepsilon \mid \mathbf{t}_n\} \mathbf{E}_{\mathbf{k}}(\mathbf{r}) \equiv \mathbf{E}_{\mathbf{k}}(\mathbf{r} - \mathbf{t}_n) = \exp(i\mathbf{k} \cdot \mathbf{t}_n) \mathbf{E}_{\mathbf{k}}(\mathbf{r}) .$$
(3)  
This relation is known as the Floquet's theorem.

The first Brillouin zone is shown in Fig. 2. Following the solid state physics, we give notations to three specific points in the Brillouin zone: a point  $\Gamma$  at the origin,  $\mathbf{k}_{\Gamma} =$ (0, 0, 0); points  $\Delta$  at  $\mathbf{k}_{\Delta} = (0, 0, k_z)$  with  $0 < |k_z| < \pi/d$ ; and a point X at  $\mathbf{k}_X = (0, 0, \pi/d)$ .



Figure 2: The first Brillouin zone in one dimension.

#### The Groups of the Wavevector $\boldsymbol{k}$

For each wavevector **k** in the Brillouin zone, we can define a subgroup,  $G(\mathbf{k})$ , of *G*. This subgroup consists of operations that keep the **k** vector invariant by allowing a difference by a reciprocal vector **K** ( $\equiv 2\pi \hat{\mathbf{z}}/d$ ). For the  $\Gamma$  and X points,  $G(\mathbf{k})$  coincides with the entire space group. For the  $\Delta$  point, the  $G(\mathbf{k}_{\Delta})$  is given by

$$G(\mathbf{k}_{\Delta}) = \{ \varepsilon \mid \mathbf{0} \} T + \{ C_2 \mid \mathbf{\tau} \} T + \{ \sigma_y \mid \mathbf{\tau} \} T + \{ \sigma_x \mid \mathbf{0} \} T . (4)$$

Note that the  $G(\mathbf{k})$  is non-symmorphic in every case.

To derive the irreducible representations of  $G(\mathbf{k})$ , we need separate treatments for two cases: (i) when the  $\mathbf{k}$  is located inside the Brillouin zone, and (ii) when the  $\mathbf{k}$  is located on the Brillouin zone boundary. In the case (i), the

irreducible representation matrices of  $G(\mathbf{k})$  are given by

$$\hat{D}^{\mathbf{k}}\left(\left\{\boldsymbol{\alpha} \,|\, \mathbf{b}\right\}\right) = \exp\left(i\mathbf{k}\cdot\mathbf{b}\right)\hat{\Gamma}(\boldsymbol{\alpha}), \qquad (5)$$

where,  $\hat{\Gamma}(\alpha)$  is an irreducible representation matrix of a point group  $G_0(\mathbf{k})$ , which is composed of the rotational parts,  $\alpha$ , of the operations  $\{\alpha | \mathbf{b}\}$  of  $G(\mathbf{k})$ . We can apply this relation for the  $\Gamma$  and  $\Delta$  points.

At the  $\Gamma$  point, the point group  $G_0(\mathbf{k}_{\Gamma})$  is given by  $D_{2h} \equiv \left\{ \varepsilon, C_2, C_2^y, C_2^x, I, \sigma_z, \sigma_y, \sigma_x \right\}$ , where the standard Schönflies symbol has been used for the point group. Using the irreducible representations of this group [4], we can deduce the irreducible representations of  $G_0(\mathbf{k}_{\Gamma})$ , as given in Table 1.

At the  $\Delta$  point, the point group  $G_0(\mathbf{k}_{\Delta})$  is given by  $C_{2v} \equiv \{\varepsilon, C_2, \sigma_y, \sigma_x\}$ . From its irreducible representations, the irreducible representations of  $G(\mathbf{k}_{\Delta})$  are deduced, as shown in Table 2.

At the X point (the case (ii)), we cannot apply Eq. 5 to the non-symmorphic group, therefore, we apply the Herring's method for deriving the irreducible representations of  $G(\mathbf{k}_X)$ . We can carry out this procedure in a similar manner as that described in Chapter 11 of [4] for a rutile crystal structure. As a result, we obtain two two-dimensional representations,  $X_1$  and  $X_2$ , as given in Table 3.

Table 2: Irreducible representation matrices of the  $G(\mathbf{k}_{\Delta})$  at the  $\Delta$  point. The irreducible representations are named after those of  $C_{2v}$ .

Irr. Rep.	$\left\{ \boldsymbol{\varepsilon}   \mathbf{t}_{n} \right\}$	$\left\{ C_{2} \mid \mathbf{\tau} \right\}$	$\left\{ \sigma_{y}   \mathbf{\tau} \right\}$	$\{\sigma_x \mid 0\}$
A <sub>1</sub>	$e^{i \mathbf{k} \cdot \mathbf{t}_n}$	$e^{i{f k}\cdot {f  au}}$	$e^{i\mathbf{k}\cdot\mathbf{ au}}$	1
A <sub>2</sub>	$e^{i \mathbf{k} \cdot \mathbf{t}_n}$	$e^{i{f k}\cdot{f  au}}$	$-e^{i\mathbf{k}\cdot\boldsymbol{\tau}}$	-1
<b>B</b> <sub>1</sub>	$e^{i \mathbf{k} \cdot \mathbf{t}_n}$	$-e^{i\mathbf{k}\cdot\mathbf{\tau}}$	$e^{i\mathbf{k}\cdot\mathbf{ au}}$	-1
<b>B</b> <sub>2</sub>	$e^{i \mathbf{k} \cdot \mathbf{t}_n}$	$-e^{i\mathbf{k}\cdot\mathbf{\tau}}$	$-e^{i\mathbf{k}\cdot\mathbf{\tau}}$	1

## Space Group

At the  $\Gamma$  and X points, the irreducible representations of the space group are given by Tables 1 and 3, respectively. At the  $\Delta$  point, we can decompose the space group into the cosets of  $G(\mathbf{k}_{\Delta})$  as

Table 1: Irreducible representation matrices of  $G(\mathbf{k}_{\Gamma})$ , and of the space group G, at the  $\Gamma$  point. The irreducible representations are named after those of  $D_{2h}$ .

Irr. Rep.	$\left\{ \boldsymbol{\varepsilon}   \mathbf{t}_{n} \right\}$	$\left\{ C_{2} \mid \mathbf{\tau} \right\}$	$\left\{C_2^{y} \mid \mathbf{\tau} ight\}$	$\left\{ C_{2}^{x}\mid0 ight\}$	$\{I \mid 0\}$	$\{\sigma_z   \mathbf{\tau}\}$	$\left\{ \sigma_{y}   \mathbf{\tau} \right\}$	$\{\sigma_x \mid 0\}$
Ag	1	1	1	1	1	1	1	1
$B_{1g}$	1	1	-1	-1	1	1	-1	-1
B <sub>2g</sub>	1	-1	1	-1	1	-1	1	-1
B <sub>3g</sub>	1	-1	-1	1	1	-1	-1	1
A <sub>u</sub>	1	1	1	1	-1	-1	-1	-1
B <sub>1u</sub>	1	1	-1	-1	-1	-1	1	1
$B_{2u}$	1	-1	1	-1	-1	1	-1	1
B <sub>3u</sub>	1	-1	-1	1	-1	1	1	-1

Irr. Rep.	$\left\{ \mathcal{E}   \mathbf{t}_n \right\}$	$\left\{ C_{2} \mid \mathbf{\tau} \right\}$	$\left\{C_2^{y} \mid \mathbf{\tau} ight\}$	$\left\{C_2^x \mid 0\right\}$	$\{I \mid 0\}$	$\left\{ \pmb{\sigma}_{_{z}}   \pmb{ au}  ight\}$	$\left\{ \sigma_{y}   \mathbf{\tau} \right\}$	$\{\sigma_x \mid 0\}$
X <sub>1</sub>	$\begin{pmatrix} (-1)^n & \\ & (-1)^n \end{pmatrix}$	$\begin{pmatrix} i \\ & -i \end{pmatrix}$	$\begin{pmatrix} & i \\ -i & \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\begin{pmatrix} & i \\ -i & \end{pmatrix}$	$\begin{pmatrix} i & \\ & -i \end{pmatrix}$	$\begin{pmatrix} 1 \\ & 1 \end{pmatrix}$
X <sub>2</sub>	$\begin{pmatrix} (-1)^n & \\ & (-1)^n \end{pmatrix}$	$\begin{pmatrix} i \\ -i \end{pmatrix}$	$\begin{pmatrix} -i \\ i \end{pmatrix}$	$\begin{pmatrix} -1 \\ -1 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\begin{pmatrix} i \\ -i \end{pmatrix}$	$\begin{pmatrix} -i \\ i \end{pmatrix}$	$\begin{pmatrix} -1 \\ & -1 \end{pmatrix}$

Table 3: Irreducible representation matrices of  $G(\mathbf{k}_X)$ , and of the space G, at the X point.

			-		-	• •	-	
Irr. Rep.	$\{\boldsymbol{\varepsilon}   \mathbf{t}_n\}$	$\left\{ C_{2} oldsymbol{ au} ight\}$	$\left\{C_2^y \mid \mathbf{ au} ight\}$	$\left\{C_2^x \mid 0\right\}$	$\{I \mid 0\}$	$\{\sigma_{_z} \mathbf{ au}\}$	$\left\{ \pmb{\sigma}_{_{y}}   \pmb{ au}  ight\}$	$\{\sigma_x   0\}$
A <sub>1</sub>	$\begin{pmatrix} e^{i\mathbf{k}\cdot\mathbf{t}_n} & \\ & e^{-i\mathbf{k}\cdot\mathbf{t}_n} \end{pmatrix}$	$egin{pmatrix} e^{i{f k}\cdot{f  au}}&&\ &e^{-i{f k}\cdot{f  au}} \end{pmatrix}$	$\begin{pmatrix} e^{i\mathbf{k}\cdot\boldsymbol{\tau}} \\ e^{-i\mathbf{k}\cdot\boldsymbol{\tau}} \end{pmatrix}$	$\begin{pmatrix} 1\\1 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\begin{pmatrix} e^{i\mathbf{k}\cdot\boldsymbol{\tau}} \\ e^{-i\mathbf{k}\cdot\boldsymbol{\tau}} \end{pmatrix}$	$egin{pmatrix} e^{i{f k}\cdot {f  au}} & \ & e^{-i{f k}\cdot {f  au}} \end{pmatrix}$	$\begin{pmatrix} 1 \\ & 1 \end{pmatrix}$
A <sub>2</sub>	$\begin{pmatrix} e^{i\mathbf{k}\cdot\mathbf{t}_n} & \\ & e^{-i\mathbf{k}\cdot\mathbf{t}_n} \end{pmatrix}$	$\begin{pmatrix} e^{i\mathbf{k}\cdot\boldsymbol{\tau}} & \\ & e^{-i\mathbf{k}\cdot\boldsymbol{\tau}} \end{pmatrix}$	$\begin{pmatrix} -e^{i\mathbf{k}\cdot\boldsymbol{\tau}} \\ -e^{-i\mathbf{k}\cdot\boldsymbol{\tau}} \end{pmatrix}$	$\begin{pmatrix} -1 \\ -1 \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} e^{i\mathbf{k}\cdot\boldsymbol{\tau}} \\ e^{-i\mathbf{k}\cdot\boldsymbol{\tau}} \end{pmatrix}$	$\begin{pmatrix} -e^{i\mathbf{k}\cdot\mathbf{\tau}} & \\ & -e^{-i\mathbf{k}\cdot\mathbf{\tau}} \end{pmatrix}$	$\begin{pmatrix} -1 \\ & -1 \end{pmatrix}$
B <sub>1</sub>	$\begin{pmatrix} e^{i\mathbf{k}\cdot\mathbf{t}_n} & \\ & e^{-i\mathbf{k}\cdot\mathbf{t}_n} \end{pmatrix}$	$\begin{pmatrix} -e^{i\mathbf{k}\cdot\mathbf{\tau}} & \\ & -e^{-i\mathbf{k}\cdot\mathbf{\tau}} \end{pmatrix}$	$\begin{pmatrix} e^{i\mathbf{k}\cdot\mathbf{\tau}} \\ e^{-i\mathbf{k}\cdot\mathbf{\tau}} \end{pmatrix}$	$\begin{pmatrix} -1 \\ -1 \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} & -e^{i\mathbf{k}\cdot\mathbf{\tau}} \\ -e^{-i\mathbf{k}\cdot\mathbf{\tau}} & \end{pmatrix}$	$egin{pmatrix} e^{i{f k}\cdot  au} & \ & e^{-i{f k}\cdot  au} \end{pmatrix}$	$\begin{pmatrix} -1 \\ & -1 \end{pmatrix}$
<b>B</b> <sub>2</sub>	$\begin{pmatrix} e^{i\mathbf{k}\cdot\mathbf{t}_n} & \\ & e^{-i\mathbf{k}\cdot\mathbf{t}_n} \end{pmatrix}$	$\begin{pmatrix} -e^{i\mathbf{k}\cdot\mathbf{\tau}} & \\ & -e^{-i\mathbf{k}\cdot\mathbf{\tau}} \end{pmatrix}$	$\begin{pmatrix} & -e^{i\mathbf{k}\cdot\mathbf{\tau}} \\ -e^{-i\mathbf{k}\cdot\mathbf{\tau}} & \end{pmatrix}$	$\begin{pmatrix} 1\\ 1 \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} & -e^{i\mathbf{k}\cdot\mathbf{\tau}} \\ -e^{-i\mathbf{k}\cdot\mathbf{\tau}} & \end{pmatrix}$	$\begin{pmatrix} -e^{i\mathbf{k}\cdot\mathbf{\tau}} & \\ & -e^{-i\mathbf{k}\cdot\mathbf{\tau}} \end{pmatrix}$	$\begin{pmatrix} 1 \\ & 1 \end{pmatrix}$

Table 4: Irreducible representation matrices of the space group G at the 
$$\Delta$$
 point.

$$G = \left\{ \varepsilon \mid \mathbf{0} \right\} G(\mathbf{k}_{\Delta}) + \left\{ I \mid \mathbf{0} \right\} G(\mathbf{k}_{\Delta}) .$$
 (6)

Since we have obtained the irreducible representations of  $G(\mathbf{k}_{\Delta})$ , the irreducible representations of *G* are given by induced representations of them onto the *G*. Results are given in Table 4.

## **CLASSIFICATION OF EIGENMODES**

For each **k** vector in the Brillouin zone, the eigenmodes in the structure can be classified according to the corresponding irreducible representations (i.e., Tables 1, 4, and 3 for the  $\Gamma$ ,  $\Delta$ , and X points, respectively). For onedimensional representations, each representation matrix (scalar) expresses an eigenvalue for each operation. When two eigenmodes,  $\mathbf{E}_1^{(\lambda)}$  and  $\mathbf{E}_2^{(\lambda)}$ , belong to a twodimensional representation  $\lambda$ , they are transformed by an operation { $\alpha$ |**b**} according to a relation,

$$\left(\left\{\boldsymbol{\alpha} \mid \mathbf{b}\right\}\mathbf{E}_{1}^{(\lambda)} \quad \left\{\boldsymbol{\alpha} \mid \mathbf{b}\right\}\mathbf{E}_{2}^{(\lambda)}\right) = \left(\mathbf{E}_{1}^{(\lambda)} \quad \mathbf{E}_{2}^{(\lambda)}\right) D^{(\lambda)}\left(\left\{\boldsymbol{\alpha} \mid \mathbf{b}\right\}\right),$$

where  $D^{(\lambda)}$  is a representation matrix for  $\{\alpha | \mathbf{b}\}$ . Note that the representation matrices are arbitrary within a similarity transformation.

An example of numerical calculations of dispersion curves for the SCS is shown in Fig. 3. The dimensions of the SCS were taken from a cold model [5] for the former Japanese Hadron Project. By looking at field distributions, these eigenmodes have been labeled by the irreducible representations, as shown in the figure.

## CONCLUSIONS

We analyzed a symmetry group of the side-coupled structure, and derived the irreducible representations of the space group of the structure. The eigenmodes in the structure can be classified according to these irreducible representations.



Figure 3: A dispersion relation of the side-coupled structure. Only the lowest passband is shown.

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