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APPLICATION OF SINGULARITY THEORY TO BIFURCATION OF BAND STRUCTURES IN CRYSTALS

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Abstract. Starting from the mean-field Hamiltonian of an electron in a crystal, we briefly review some known facts about its spectral structures and how singularities come into play in such spectral structures, and then provide our future perspective. We also estimate lower bounds of codimensions for the case where more than two bands to cross at a point.

1. Introduction

As in the song by Prof. Goo Ishikawa [10], singularity is everywhere. In this paper, we provide one example of such singularities appearing in solid-state physics [25]. Let

$$\hat{H} = -\frac{1}{2}\Delta + V(x) \tag{1}$$

be a Schrödinger operator on $L^2\left(\mathbb{R}^d\right)$, where $x = (x_1, \cdots, x_d) \in \mathbb{R}^d$, $\Delta = \sum_{i=1}^d \frac{\partial^2}{\partial x_i^2}$ is the Laplacian on $\mathbb{R}^d$, and $V\colon \mathbb{R}^d \to \mathbb{R}$. We assume there is a basis

$$\{\gamma_1, \ldots, \gamma_d\} \tag{2}$$

in $\mathbb{R}^d$ such that $V(x+\gamma_i) = V(x)$ holds for all $x \in \mathbb{R}^d$ and $i \in \{1, \ldots, d\}$. This Schrödinger operator appears in the following situation: an electron moving in a periodic potential in the bulk of a crystal ($d = 3$) or on the surface of a crystal ($d = 2$). A crystal consists of atoms and electrons interacting with each other. This Schrödinger operator is simplified to study the behavior of one of the electrons in the crystal; the effect of all the other electrons and atoms on the electron at $x \in \mathbb{R}^d$ is approximated by an averaged potential $V(x)$. One can also add a spin degree of freedom as in [15]. Some of mathematical justifications of this can be found in [13, 6, 5].

In Sec. 2, we briefly review what is known about spectral structures of the operator Eq. (1). There, band structures arise in the spectral structures as a consequence of the periodicity of the potential. Some of the topological features of the bands may be characterized by twisted-equivariant K-theory. Explaining the theory is beyond the scope of this paper but one of the established facts is that the bands cannot change their topology unless some of their band gaps close. Recently, it has become possible to manipulate band structures by changing the material properties of crystals and let some of the bands collide with each other [9]. To understand how such collisions trigger their topological changes, it is important to understand band geometries in neighborhoods of band crossings and their unfoldings. Having this goal in mind, in Sec. 3, we review our recent results on classification of band geometries in neighborhoods of band crossings in terms of the theory of singularities [25]. In Sec. 4, we discuss our future perspective along this direction.

2. Brief Review of Schrödinger operators with periodic potentials

In this section, we briefly review spectral properties of Schrödinger operators with periodic potentials by following [20, 16, 17]. For the definitions of terms in this section, see [21, 19, 20]. In this context, the basis in Eq. (2) is determined by the geometric structure of the crystal [2]. The lattice defined by

$$\Gamma = \left\{ \gamma \in \mathbb{R}^d \,\middle|\, \gamma = \sum_{j=1}^{d} n_j \gamma_j, (n_1, \cdots, n_d) \in \mathbb{Z}^d \right\} \tag{3}$$

is denoted as the Bravais lattice and its dual lattice

$$\Gamma^* = \left\{ k \in \mathbb{R}^d \,| k \cdot \gamma \in 2\pi\mathbb{Z}, \text{for all } \gamma \in \Gamma \right\} \tag{4}$$

is denoted as the inverse Bravais lattice. To fix the notation, we denote the centered fundamental domain of Γ by

$$Y = \left\{ x \in \mathbb{R}^d \,\middle|\, x = \sum_{j=1}^{d} \alpha_j \gamma_j, \text{for } \alpha_j \in \left[-\frac{1}{2}, \frac{1}{2} \right] \right\}, \tag{5}$$

and the centered fundamental domain of Γ^* by

$$Y^* = \left\{ k \in \mathbb{R}^d \,\middle|\, k = \sum_{j=1}^{d} \alpha_j \gamma_j^*, \text{for } \alpha_j \in \left[-\frac{1}{2}, \frac{1}{2} \right] \right\}, \tag{6}$$

where $\left\{\gamma_j^*\right\}_{j \in \{1,\cdots,d\}}$ is the dual basis to $\{\gamma_j\}_{j \in \{1,\cdots,d\}}$ such that $\gamma_i^* \cdot \gamma_j = 2\pi\delta_{i,j}$ holds for all $i, j \in \{1, \cdots, d\}$.

To investigate the spectral structure of the Schrödinger operator Eq. (1) on $L^2\left(\mathbb{R}^d\right)$, we show the operator is unitary equivalent to one decomposable by the direct integral decomposition. To do that, we introduce the following notation.

2.1. Constant Fiber Direct Integral and Direct Integral Decomposition.

Let $\mathcal{H}' = L^2\left(\mathbb{T}^d\right)$ be a Hilbert space on the torus $\mathbb{T}^d = \mathbb{R}^d/\Gamma$ with the inner product $(\cdot,\cdot)_{\mathcal{H}'}$, and let $L^2\left(Y^*, dk; \mathcal{H}'\right)$ be the set of measurable functions f on Y^* with values in $\mathcal{H}'$ which satisfy $\int_{Y^*} \|f(k)\|_{\mathcal{H}'}^2 dk < \infty$, where $\|\cdot\|_{\mathcal{H}'}$ is the norm induced from the inner product $(\cdot,\cdot)_{\mathcal{H}'}$. We call $\mathcal{H} = L^2\left(Y^*, dk; \mathcal{H}'\right)$ a constant fiber direct integral by following [20] and write

$$\mathcal{H} = \int_{Y^*}^{\oplus} \mathcal{H}' dk. \tag{7}$$

Note that $\mathcal{H}$ is a Hilbert space equipped with an inner product

$$(f, g)_{\mathcal{H}} = \int_{Y^*} (f(k), g(k))_{\mathcal{H}'} \, dk \tag{8}$$

for $f, g \in \mathcal{H}$.

Next we would like to introduce the direct integral decomposition of an operator associated with a constant fiber direct integral. Suppose $A(\cdot)$ is a function from Y^* to the set of self-adjoint operators on a Hilbert space $\mathcal{H}'$. The function is measurable if and only if the function $(A(\cdot) + i)^{-1}$ is measurable, where i is the operator multiplied by the imaginary number i. Note that the spectrum of a self-adjoint operator is on the real line and thus $-i$ is in the resolvent set of the operator. Therefore, the function $(A(\cdot) + i)^{-1}$ is a well-defined function from Y^* to the set of bounded operators on $\mathcal{H}'$, $\mathcal{L}(\mathcal{H}')$. Such a function is called measurable if for each $\phi, \psi \in \mathcal{H}'$, $\left(\phi, (A(\cdot)+i)^{-1}\psi\right)_{\mathcal{H}'}$ is measurable.

Let $A(\cdot)$ be a measurable function from Y^* with the Lebesgue measure to the set of self-adjoint operators on a Hilbert space $\mathcal{H}'$. We define an operator A on $\mathcal{H} = \int_{Y^*}^{\oplus} \mathcal{H}'\, dk$ having $A(\cdot)$ as direct sum components with domain

$$D(A) = \left\{ \psi \in \mathcal{H} \,\middle|\, \psi(k) \in D(A(k)) \text{ a.e. } k \in Y^*;\ \int_{Y^*} \|A(k)\psi(k)\|_{\mathcal{H}'}^2\, dk < \infty \right\} \tag{9}$$

by $(A\psi)(k) = A(k)\psi(k)$ for all $k \in Y^*$ and for $\psi \in D(A)$, where $D(A(k)) \subset \mathcal{H}'$ is the domain of the operator $A(k)$ for $k \in Y^*$. If an operator A on $\mathcal{H} = \int_{Y^*}^{\oplus} \mathcal{H}'\, dk$ can be decomposed in this form, we say that the operator A admits direct integral decomposition and write

$$A = \int_{Y^*}^{\oplus} A(k)\ dk. \tag{10}$$

Next, let us introduce the modified Bloch-Floquet transformation [28]. By using the transformation, the operator in Eq. (1) is shown to be unitary equivalent to one that admits direct integral decomposition.

2.2. **Modified Bloch-Floquet Transformation.** Let $\mathcal{S}(\mathbb{R}^d)$ be the set of rapid decreasing functions on $\mathbb{R}^d$, i.e.,

$$\mathcal{S}(\mathbb{R}^d) = \left\{ \psi \in C^\infty(\mathbb{R}^d) \,\middle|\, \|\psi\|_{\alpha,\beta} = \sup_{x\in\mathbb{R}^d} \left| x^\alpha D^\beta \psi(x) \right| < \infty, \text{for all } \alpha, \beta \in I_+^d \right\}, \tag{11}$$

where I_+^d is the set of all d-tuples of nonnegative integers, $x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_d^{\alpha_d}$ and

$$D^\beta \phi(x) = \frac{\partial^{|\beta|}\phi(x)}{\partial x_1^{\beta_1} \cdots \partial x_d^{\beta_d}} \quad \left(|\beta| = \sum_{j=1}^d \beta_d \right) \tag{12}$$

for $\alpha, \beta \in I_+^d$, and $|Y^*|$ is the volume of Y^*. Let $L^2_{\text{loc}}(\mathbb{R}^d)$ be the set of locally square-integrable functions on $\mathbb{R}^d$, i.e.,

$$L^2_{\text{loc}}(\mathbb{R}^d) = \left\{ \psi \colon \mathbb{R}^d \to \mathbb{C} \,\middle|\, \int_K |\psi|^2\ dx < \infty, \text{for any compact set } K \subset \mathbb{R}^d \right\}. \tag{13}$$

For $\psi \in \mathcal{S}(\mathbb{R}^d)$, we define the modified Bloch-Floquet transform

$$\tilde{\mathcal{U}}_{\text{BF}} \colon \mathcal{S}(\mathbb{R}^d) \to L^2_{\text{loc}}\left(\mathbb{R}^d, dk; L^2_{\text{loc}}(\mathbb{R}^d)\right) \tag{14}$$

as

$$\left(\tilde{\mathcal{U}}_{\text{BF}}\psi\right)(k,x) = \frac{1}{|Y^*|^{1/2}} \sum_{\gamma\in\Gamma} e^{-ik\cdot(x+\gamma)}\psi(x+\gamma) \tag{15}$$

for $x \in \mathbb{R}^d$ and $k \in \mathbb{R}^d$, where $|Y^*|$ is the volume of Y^*. In what follows, we construct $\mathcal{U}_{\text{BF}} \colon L^2(\mathbb{R}^d) \to \mathcal{H}$ from $\tilde{\mathcal{U}}_{\text{BF}} \colon \mathcal{S}(\mathbb{R}^d) \to L^2_{\text{loc}}\left(\mathbb{R}^d, dk; L^2_{\text{loc}}(\mathbb{R}^d)\right)$ by following [17].

First note that

$$\left(\tilde{\mathcal{U}}_{\text{BF}}\psi\right)(k, x+\gamma') = \left(\tilde{\mathcal{U}}_{\text{BF}}\psi\right)(k,x) \tag{16}$$

$$\left(\tilde{\mathcal{U}}_{\text{BF}}\psi\right)(k+\gamma^*, x) = e^{-i\gamma^*\cdot x}\left(\tilde{\mathcal{U}}_{\text{BF}}\psi\right)(k,x) \tag{17}$$

holds for all $\gamma' \in \Gamma$ and $\gamma^* \in \Gamma^*$ and the function is periodic in $x \in \mathbb{R}^d$, and thus $\left(\tilde{\mathcal{U}}_{\text{BF}}\phi\right)(k,\cdot)$ can be regarded as an element of $\mathcal{H}'$ for each $k \in \mathbb{R}^d$.

Next, by introducing a unitary representation of the group Γ^*, $\tau\colon \Gamma^* \to \mathcal{U}(\mathcal{H}')$, as $(\tau(\gamma^*)\phi)(x) = e^{i\gamma^*\cdot x}\phi(x)$ for $\phi \in \mathcal{H}'$, $x \in \mathbb{R}^d$, and $\gamma^* \in \Gamma^*$, the function

$$\left(\tilde{\mathcal{U}}_{\mathrm{BF}}\psi\right) \in L^2_{\mathrm{loc}}\left(\mathbb{R}^d, dk; \mathcal{H}'\right)$$

can be regarded as an element of the Hilbert space

(18)
$$\mathcal{H}_\tau = \left\{\psi \in L^2_{\mathrm{loc}}\left(\mathbb{R}^d, dk; \mathcal{H}'\right) \middle| \psi(k-\gamma^*, \cdot) = \tau(\gamma^*)\,\psi(k,\cdot), \text{for all } \gamma^* \in \Gamma^* \text{ for a.e. } k \in \mathbb{R}^d\right\}.$$

Since there is a natural isomorphism between $\mathcal{H}_\tau$ and $L^2(Y^*, dk; \mathcal{H}')$ given by restriction from $\mathbb{R}^d$ to Y^*, we get $\mathcal{H}_\tau \simeq \mathcal{H} = \int_{Y^*}^{\oplus} \mathcal{H}'\, dk$.

In addition, $\left(\tilde{\mathcal{U}}_{\mathrm{BF}}\psi_1, \tilde{\mathcal{U}}_{\mathrm{BF}}\psi_2\right)_{\mathcal{H}} = (\psi_1, \psi_2)_{L^2(\mathbb{R}^d)}$ holds for $\psi_1, \psi_2 \in \mathcal{S}\left(\mathbb{R}^d\right)$. This can be shown as follows: First, note that

$$\begin{aligned}\left(\tilde{\mathcal{U}}_{\mathrm{BF}}\psi_1, \tilde{\mathcal{U}}_{\mathrm{BF}}\psi_2\right)_{\mathcal{H}} &= \int_{Y^*} \left(\tilde{\mathcal{U}}_{\mathrm{BF}}\psi_1(k,\cdot), \tilde{\mathcal{U}}_{\mathrm{BF}}\psi_2(k,\cdot)\right)_{\mathcal{H}'} dk \\ &= \frac{1}{|Y^*|}\int_{Y^*}\int_{\mathbb{T}^d} \sum_{\gamma',\gamma\in\Gamma} e^{ik\cdot\left(x+\gamma'\right)-ik\cdot(x+\gamma)}\overline{\psi}_1(x+\gamma')\,\psi_2(x+\gamma)\; dxdk\end{aligned}$$

holds where $\bar{\cdot}$ is the complex conjugate of an operand. Since the sum in the integrand converges uniformly for all $x \in \mathbb{T}^d$ and $k \in Y^*$ and the domains of the integrations are compact, the sums and integrals can be interchanged to get

(19)
$$\frac{1}{|Y^*|}\sum_{\gamma',\gamma\in\Gamma}\int_{Y^*}\int_{\mathbb{T}^d} e^{ik\cdot\left(\gamma'-\gamma\right)}\overline{\psi}_1(x+\gamma')\,\psi_2(x+\gamma)\; dxdk.$$

By integrating it with respect to k and using

$$\frac{1}{|Y^*|}\int_{Y^*} e^{ik\cdot\left(\gamma'-\gamma\right)}dk = \delta_{\gamma',\gamma},$$

where $\delta_{\gamma',\gamma} = \begin{cases}1 & (\gamma' = \gamma)\\ 0 & (\gamma' \neq \gamma)\end{cases}$, we get

(20)
$$\sum_{\gamma\in\Gamma}\int_{\mathbb{T}^d} \overline{\psi}_1(x+\gamma)\,\psi_2(x+\gamma)\; dx.$$

This is equal to

(21)
$$(\psi_1,\psi_2)_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^d} \overline{\psi}_1(x)\,\psi_2(x)\; dx$$

and thus proves the claim. Since $\mathcal{S}\left(\mathbb{R}^d\right)$ is dense in $L^2\left(\mathbb{R}^d\right)$, the modified Bloch-Floquet operator can be extended to be a unitary operator $\mathcal{U}_{\mathrm{BF}}\colon L^2\left(\mathbb{R}^d\right) \to \mathcal{H}$ with inverse given by

(22)
$$\left(\mathcal{U}_{\mathrm{BF}}^{-1}\psi\right)(x) = \frac{1}{|Y|^{1/2}}\int_{Y^*}\psi(k,[x])\,e^{ik\cdot x}\; dk,$$

where $[\cdot]$ refers to the decomposition $x = \gamma_x + [x]$ with $\gamma_x \in \Gamma$ and $[x] \in Y$.

2.3. **Direct Integral Decomposition of Eq.** (1)**.** Suppose $d = 1, 2, 3$ and $V\colon \mathbb{R}^d \to \mathbb{R}$ is Γ-periodic and $V \in L^2_{\mathrm{loc}}\left(\mathbb{R}^d\right)$. Then,

$$\hat{H}_{\mathrm{BF}} = \mathcal{U}_{\mathrm{BF}} \hat{H} \mathcal{U}_{\mathrm{BF}}^{-1} = \int_{Y^*}^{\oplus} \hat{H}\left(k\right)\ dk \tag{23}$$

holds with fiber operator

$$\hat{H}\left(k\right) = \frac{1}{2}\left(-i\nabla_x + k\right)^2 + V\left(x\right) \tag{24}$$

for $k \in Y^*$ acting on the k-independent domain $D_0 = W^{2,2}\left(\mathbb{T}^d\right) \subset \mathcal{H}'$, where

$$W^{2,2}\left(\mathbb{T}^d\right) = \left\{\psi \in \mathcal{H}' \left| D^\alpha\psi \in \mathcal{H}', \text{for all } \left|\alpha\right| \le 2\right.\right\} \tag{25}$$

is the Sobolev space where $D^\alpha\psi$ is the differential of ψ in the weak sense, i.e., one satisfies

$$\int_{\mathbb{T}^d} \left(D^\alpha\psi\right)\left(x\right)\phi\left(x\right)\ dx = \left(-1\right)^{\left|\alpha\right|}\int_{\mathbb{T}^d} \psi\left(x\right)\left(D^\alpha\phi\right)\left(x\right)\ dx \tag{26}$$

for all $\phi \in C^\infty\left(\mathbb{T}^d\right)$.

To prove the claim in Eq. (23), let us show the following:

$$\mathcal{U}_{\mathrm{BF}}\left(-\Delta\right)\mathcal{U}_{\mathrm{BF}}^{-1} = \int_{Y^*}^{\oplus} \left(-i\nabla_x + k\right)^2 dk. \tag{27}$$

Let A be the operator on the right hand side of Eq. (27). The operator $A\left(k\right) = \left(-i\nabla_x + k\right)^2$ is self-adjoint for $k \in Y^*$ acting on the k-independent domain $D_0 = W^{2,2}\left(\mathbb{T}^d\right) \subset \mathcal{H}'$ and is measurable, therefore, **Theorem XIII.85 (a)** in [20] guarantees that the operator A is self-adjoint as well. We shall show that if $\psi \in \mathcal{S}\left(\mathbb{R}^d\right)$, then, $\mathcal{U}_{\mathrm{BF}}\psi \in D\left(A\right)$ and

$$\mathcal{U}_{\mathrm{BF}}\left(-\Delta\psi\right) = A\left(\mathcal{U}_{\mathrm{BF}}\psi\right).$$

Since $-\Delta$ is essentially self-adjoint on $\mathcal{S}\left(\mathbb{R}^d\right)$ and A is self-adjoint, Eq. (27) follows because this means that $-\Delta$ has the unique self-adjoint extension that should coincide with the self-adjoint operator $\mathcal{U}_{\mathrm{BF}}^{-1} A \mathcal{U}_{\mathrm{BF}}$. Take an arbitrary $\psi \in \mathcal{S}\left(\mathbb{R}^d\right)$. Then,

$$\mathcal{U}_{\mathrm{BF}}\left(-\Delta\psi\right)\left(k,x\right) = \frac{1}{\left|Y^*\right|^{1/2}}\sum_{\gamma\in\Gamma} e^{-ik\cdot\left(x+\gamma\right)}\left(-\Delta\psi\right)\left(x+\gamma\right) \tag{28}$$

$$= \frac{1}{\left|Y^*\right|^{1/2}}\sum_{\gamma\in\Gamma} \left(-i\nabla_x + k\right) e^{-ik\cdot\left(x+\gamma\right)}\left(-i\nabla_x\psi\right)\left(x+\gamma\right) \tag{29}$$

$$= \frac{1}{\left|Y^*\right|^{1/2}}\sum_{\gamma\in\Gamma} A\left(k\right) e^{-ik\cdot\left(x+\gamma\right)}\psi\left(x+\gamma\right) \tag{30}$$

holds. Since the sum converges uniformly for $x \in Y$, the sum and differential can be interchanged and we get

$$A\left(k\right)\frac{1}{\left|Y^*\right|^{1/2}}\sum_{\gamma\in\Gamma} e^{-ik\cdot\left(x+\gamma\right)}\psi\left(x+\gamma\right) \tag{31}$$

and this equals to $\left(A\left(\mathcal{U}_{\mathrm{BF}}\psi\right)\right)\left(k,x\right)$. For each $k \in Y^*$,

$$\left(A\left(\mathcal{U}_{\mathrm{BF}}\psi\right)\right)\left(k,x+\gamma\right) = \left(A\left(\mathcal{U}_{\mathrm{BF}}\psi\right)\right)\left(k,x\right) \tag{32}$$

for all $\gamma \in \Gamma$, thus $\left(A\left(\mathcal{U}_{\mathrm{BF}}\psi\right)\right)\left(k,\cdot\right) \in \mathcal{H}'$. This proves $\mathcal{U}_{\mathrm{BF}}\psi \in D\left(A\right)$. In the same manner, we can prove

$$\mathcal{U}_{\mathrm{BF}} V\left(x\right)\mathcal{U}_{\mathrm{BF}}^{-1} = \int_{Y^*}^{\oplus} V\left(x\right)\ dk. \tag{33}$$

Let B be the operator on the right hand side of Eq. (33). By noting that

$$|(\psi, V\psi)_{\mathcal{H}'}| \leq \|V\|_{\mathcal{H}'} (\psi, \psi)_{\mathcal{H}'} = 0 \times (\psi, A(k)\psi) + \beta (\psi, \psi)_{\mathcal{H}'} \tag{34}$$

holds for all $k \in Y^*$ and $\psi \in W^{2,2}(\mathbb{T}^d)$ where $\beta = \|V\|_{\mathcal{H}'}$ and using **Theorem XIII.85 (g)** in [20], we conclude that $\hat{H}_{\mathrm{BF}} = \int_{Y^*}^{\oplus} \hat{H}(k)\, dk$ is self-adjoint on $W^{2,2}(\mathbb{T}^d)$ as well and this proves the claim in Eq. (23).

Note that $\lambda \in \sigma\left(\hat{H}_{\mathrm{BF}}\right)$ if and only if

$$\left|\left\{k \middle| \sigma\left(\hat{H}(k)\right) \cap (\lambda - \epsilon, \lambda + \epsilon) \neq \emptyset\right\}\right| > 0 \tag{35}$$

holds for all $\epsilon > 0$, where $|\cdot|$ is the Lebesgue measure on Y^* by **Theorem XIII.85 (d)** in [20]. By using this fact, we can restore the spectrum of $\hat{H}_{\mathrm{BF}}$ from the spectrum of $\hat{H}(k)$ for each $k \in Y^*$.

2.4. **Spectral Structures of $\hat{H}(k)$.** Suppose $k \in Y^*$. We investigate the spectral structures of the operator $\hat{H}(k)$ on $\mathcal{H}'$. To do that, let us investigate the spectral structures of the unperturbed operator $\hat{H}_0(k) = \frac{1}{2}(-i\nabla_x + k)^2$ on $\mathcal{H}'$. This operator is self-adjoint on $W^{2,2}(\mathbb{T}^d)$ bounded from below, and has the complete set of eigenvectors $\phi_n(x) = \frac{1}{|Y^*|^{1/2}} e^{i\sum_{j=1}^d n_j \gamma_j^* \cdot x}$ with the eigenvalues $\frac{1}{2}\left(\sum_{j=1}^d n_j \gamma_j^* + k\right)^2$ for $n \in \mathbb{Z}^d$. From this information, we deduce the spectral structures of $\hat{H}(k)$ in what follows. First, note that $\hat{H}_0(k)$ has a compact resolvent, which can be shown by using **Theorem XIII.64** in [20]. Second, note that V is in $L^2(\mathbb{T}^d)$ and is symmetric and satisfies Eq. (34) for all $k \in Y^*$ and $\psi \in W^{2,2}(\mathbb{T}^d)$. Then, $\hat{H}(k) = \hat{H}_0(k) + V$ is self-adjoint and bounded from below as well and has a compact resolvent, which can be shown by using **Theorem XIII.68** in [20]. Then, by using **Theorem XIII.64** in [20], we conclude that $\hat{H}(k)$ has a complete set of eigenvectors with eigenvalues $E_0(k) \leq E_1(k) \leq \cdots$ where $E_j(k) \to \infty$ as $j \to \infty$. Since

$$H(k + \gamma^*) = \tau(\gamma^*)^{-1} H(k) \tau(\gamma^*) \tag{36}$$

holds for all $\gamma^* \in \Gamma^*$, $E_j(k)$ is Γ^*-periodic function of k for $j \in \mathbb{N} \cup \{0\}$. In the context of band theory in solid-state physics, the eigenvalues $E_j(k)$ parametrized by $k \in Y^*$ for each $j \in \mathbb{N} \cup \{0\}$ are called a band and we denote a band as a set of the eigenvalues parametrized by $k \in Y^*$ having a common index $j \in \mathbb{N} \cup \{0\}$.

3. Singularities in the spectral structures of the Schrödinger operator

In this section, we review our recent progress on classification of geometric structures of bands in a neighborhood of a band crossing in the bulk of a crystal ($d = 3$), under the condition that either time-reversal symmetry or space-inversion symmetry is broken [25]. Under this condition, band crossings, i.e, $E_j(k) = E_l(k)$ for $j \neq l$, occur only at a finite number of points $k \in Y^*$ in general. Among these band crossings, two-band crossings occur most generically and thus we first focus on a two-band crossing. Such band crossings are important because the band cannot change its topology unless its band gaps close.

Without loss of generality, we can assume a two-band crossing occurs at the origin $k = 0 \in \mathbb{R}^3$ in order to analyze the local geometry, and let $E_\pm(k)$ $(E_-(k) \leq E_+(k))$ be two bands involved in the crossing. Let $\sigma(k) = \{E_\pm(k)\}$ be the set of the eigenvalues. In addition, we assume that there exists an open neighborhood of the origin U $\left(\subset \mathbb{R}^d\right)$ in which the gap condition

$$\inf_{k \in U} d\left(\sigma(k), \sigma\left(\hat{H}(k)\right) \setminus \sigma(k)\right) > 0 \tag{37}$$

holds, where $d(\cdot,\cdot)$ is the Euclidean distance between the two sets. Under the gap condition, the projection operator $P(k): \mathcal{H}' \to \mathcal{H}'$ can be defined by using the Dunford integral such as

$$P(k) = -\frac{1}{2\pi i}\int_C \left(\hat{H}(k) - z\right)^{-1} dz, \tag{38}$$

where the integration path C on $\mathbb{C}$ is chosen so that it encloses $\sigma(k)$ $(k \in U)$ counterclockwise. Under this setting, by using **Proposition 2.1.** in [17], the map $k \mapsto P(k)$ is of class C^∞ from $\mathbb{R}^d$ to $\mathcal{L}(\mathcal{H}')$ equipped with the operator norm. This implies that there exists an open neighborhood $U_0 \subset U$ in which $\|P(k) - P(0)\| < 1$ holds. In the open neighborhood, we can use Nagy's formula [12]

$$W(k) = \left(1 - (P(k) - P(0))^2\right)^{-1/2} \left(P(k)P(0) + (1 - P(k))(1 - P(0))\right) \tag{39}$$

to get a smooth orthogonal frame $\chi_j(k) = W(k)\chi_j(0)$ $(j = 1,2)$ for

$$\mathrm{Ran}\, P(k) = \{\psi \in \mathcal{H}' \,|\text{There exists } \psi' \in \mathcal{H}' \text{ such that } \psi = P(k)\psi' \text{ holds.}\} \quad (k \in U_0) \tag{40}$$

where $\chi_j(0)$ $(j = 1,2)$ is an orthogonal basis spanning $\mathrm{Ran}\, P(0)$. By defining

$$H_{jl}(k) = \left(\chi_j(k), \hat{H}(k)\chi_l(k)\right)$$

for $j, l = 1, 2$, the map

$$H\colon k \mapsto \begin{pmatrix} H_{11}(k) & H_{12}(k) \\ H_{21}(k) & H_{22}(k) \end{pmatrix} \tag{41}$$

is a C^∞ map from U_0 to the set of 2×2 Hermite matrices and the two eigenvalues $E_\pm(k)$ can be written as

$$E_\pm(k) = \frac{H_{11}(k) + H_{22}(k) \pm \sqrt{(H_{11}(k) - H_{22}(k))^2 + \overline{H_{12}(k)}H_{21}(k)}}{2}. \tag{42}$$

If we consider the relative difference between the two eigenvalues, the trace part of the matrix

$$\frac{H_{11}(k) + H_{22}(k)}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{43}$$

is irrelevant and thus we subtract the trace part so that the target image of the map H is in the set of 2×2-traceless Hermite matrix $\mathrm{Herm}_0(2)$ for $k \in U_0$. Since we assume $E_+(0) = E_-(0)$, the map should satisfy $H_{11}(0) = H_{22}(0)$ and $\overline{H_{12}(0)}H_{21}(0) = |H_{21}(0)|^2 = 0$. In conjunction with $\mathrm{Trace}\, H(0) = H_{11}(0) + H_{22}(0) = 0$, we get $H(0) = O_2$ where O_2 is the 2×2 zero matrix. Under this setting, the map H can be written as $H\colon \left(\mathbb{R}^3, 0\right) \to (\mathrm{Herm}_0(2), O_2)$. Having this setting in mind, we introduce our framework [25, 11] to classify Hamiltonians in a neighborhood of a multi-band crossing in the next section.

3.1. **Settings.** Let $M_m(\mathbb{C})$ be the set of $m \times m$ complex matrices, $\mathrm{Herm}_0(m)$ be the set of $m \times m$ trace-less Hermite matrices

$$\mathrm{Herm}_0(m) = \left\{X \in M_m(\mathbb{C}) \,\middle|\, X^\dagger = X, \mathrm{Trace}\, X = 0\right\}, \tag{44}$$

and $SU(m)$ be the set of $m \times m$ special unitary matrices

$$SU(m) = \left\{X \in M_m(\mathbb{C}) \,\middle|\, X^\dagger X = XX^\dagger = I_m, \det X = 1\right\}, \tag{45}$$

where I_m is the $m \times m$ unit matrix. Let $H, H'\colon (\mathbb{R}^n, 0) \to (\mathrm{Herm}_0(m), O_m)$ be C^∞ map-germs where $n \in \mathbb{N}$ and O_m is the $m \times m$ zero matrix.

Definition 3.1. *We say that H and H' are $\mathcal{SU}(m)$-equivalent if there exists a map-germ $U\colon (\mathbb{R}^n, 0) \to (SU(m), U(0))$ and a diffeomorphism-germ $s\colon (\mathbb{R}^n, 0) \to (\mathbb{R}^n, 0)$ such that $H \circ s(k) = U(k) H'(k) U^\dagger(k)$ holds for all $k \in \mathbb{R}^n$.*

For example, the case where $m = 2$ and $n = 3$ corresponds to the geometric classification of Hamiltonians in the bulk of a crystal in a neighborhood of a two-band crossing. In this case, a map-germ $H\colon (\mathbb{R}^3, 0) \to (\mathrm{Herm}_0(2), O_2)$ can be written as

$$H\colon k \mapsto \begin{pmatrix} \delta(k) & \beta(k) - i\gamma(k) \\ \beta(k) + i\gamma(k) & -\delta(k) \end{pmatrix} \tag{46}$$

$$= \beta(k)\sigma_1 + \gamma(k)\sigma_2 + \delta(k)\sigma_3 \tag{47}$$

$$= (\beta(k), \gamma(k), \delta(k)) \cdot \sigma, \tag{48}$$

where $\beta, \gamma, \delta\colon (\mathbb{R}^3, 0) \to (\mathbb{R}, 0)$ are map-germs, $k = (k_1, k_2, k_3) \in \mathbb{R}^3$ a Bloch wavenumber,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \text{ and } \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{49}$$

are three Pauli matrices, $\sigma = (\sigma_1, \sigma_2, \sigma_3)$, and $(\beta(k), \gamma(k), \delta(k)) \cdot \sigma$ is an inner product between the two vectors $(\beta(k), \gamma(k), \delta(k))$ and σ. If one considers a map-germ

$$H'\colon k \mapsto U(k) H(k) U^\dagger(k)$$

where $U\colon (\mathbb{R}^n, 0) \to (SU(m), U(0))$, the image of the map-germ H' is also in $(\mathrm{Herm}_0(2), O_2)$ and $H'(k)$ and $H(k)$ are unitary equivalent for $k \in \mathbb{R}^3$. Therefore, it is natural to consider the two map-germs H' and H as equivalent in their geometric classification of bands. Contrastingly, the role that the diffeomorphism-germ $s\colon (\mathbb{R}^3, 0) \to (\mathbb{R}^3, 0)$ plays in the definition may be strange in this context because the source space $\mathbb{R}^3$ is spanned by a Bloch wavenumber k and introducing arbitrary nonlinear transformations to that space is not at all natural. Depending on which geometrical features one wants to preserve, one can have several other choices:

(1) Restrict a class of $s\colon (\mathbb{R}^3, 0) \to (\mathbb{R}^3, 0)$ to the set of orthogonal transformations.
(2) Relax a class of $s\colon (\mathbb{R}^3, 0) \to (\mathbb{R}^3, 0)$ to the set of homeomorphisms.

In case of 1, surely all the details of the graph of the eigenvalues against k are preserved. To understand a phenomenon such as in [7], in which the star-like shape of the Fermi surface is essential, it is important not to miss the details. However, if you restrict a class of

$$s\colon (\mathbb{R}^3, 0) \to (\mathbb{R}^3, 0)$$

to the set of orthogonal transformations, you will end up with infinitely many classes as many as all the possible graphs of the eigenvalues against k and this classification may be too fine to be useful. Contrastingly, if you relax a class of $s\colon (\mathbb{R}^3, 0) \to (\mathbb{R}^3, 0)$ to the set of homeomorphisms, you may end up with a finite number of classes up to a certain codimension but you will miss important information like multiplicity, which tells the maximum possible number of generic band crossings that can appear if you perturb the Hamiltonians smoothly [25]. Here, we set a class of $s\colon (\mathbb{R}^3, 0) \to (\mathbb{R}^3, 0)$ to the set of diffeomorphisms as in the definition so that we can get a finite number of classes up to a certain codimension and at the same time we do not miss important quantities like multiplicity and Chern number.

Let $\mathcal{E}_n = \{f\colon (\mathbb{R}^n, 0) \to (\mathbb{R}, f(0))\}$ be the ring of function-germs with the maximal ideal $\mathcal{M}_n$. Let $\mathcal{E}_{n,m} = \{H\colon (\mathbb{R}^n, 0) \to (\mathrm{Herm}_0(m), H(0))\}$ and

$$\mathcal{M}_n \mathcal{E}_{n,m} = \mathcal{M}_n \mathcal{E}_{n,m} = \{H\colon (\mathbb{R}^n, 0) \to (\mathrm{Herm}_0(m), O_m)\}.$$

For $\mathcal{SU}(m)$-equivalence, we define its tangent space $T\mathcal{SU}(m)$ at $H \in \mathcal{M}_n\mathcal{E}_{n,m}$ as the set of infinitesimal actions of map-germs U and s as

$$T\mathcal{SU}(m)(H) = \left\{ \left.\frac{\partial H_\epsilon(k)}{\partial \epsilon}\right|_{\epsilon=0} \middle| \begin{array}{c} H_\epsilon(k) = U_\epsilon(k)\, H \circ s_\epsilon(k)\, U_\epsilon^\dagger(k), \\ U_\epsilon\colon (\mathbb{R}^n, 0) \to (SU(m), U_\epsilon(0)), \\ s_\epsilon\colon (\mathbb{R}^n, 0) \to (\mathbb{R}^n, 0), \\ U_{\epsilon=0} = I_m, s_{\epsilon=0} = \mathrm{id}_n \end{array} \right\} (\subset \mathcal{E}_{n,m}), \tag{50}$$

where $\mathrm{id}_n\colon (\mathbb{R}^n, 0) \to (\mathbb{R}^n, 0)$ is the identity. In a similar manner, we define its extended tangent space as the set of infinitesimal actions of U and s that may map the origin to a point different from the origin as

$$T_e\mathcal{SU}(m)(H) = \left\{ \left.\frac{\partial H_\epsilon(k)}{\partial \epsilon}\right|_{\epsilon=0} \middle| \begin{array}{c} H_\epsilon(k) = U_\epsilon(k)\, H \circ s_\epsilon(k)\, U_\epsilon^\dagger(k), \\ U_\epsilon\colon (\mathbb{R}^n, 0) \to (SU(m), U_\epsilon(0)), \\ s_\epsilon\colon (\mathbb{R}^n, 0) \to (\mathbb{R}^n, s_\epsilon(0)), \\ U_{\epsilon=0} = I_m, s_{\epsilon=0} = \mathrm{id}_n \end{array} \right\} (\subset \mathcal{E}_{n,m}). \tag{51}$$

Note that the tangent space $T\mathcal{SU}(m)(H)$ and the extended tangent space $T_e\mathcal{SU}(m)(H)$ are modules over $\mathcal{E}_n$. We define the codimension of $H \in \mathcal{M}_n\mathcal{E}_{n,m}$ as $\dim_{\mathbb{R}} \dfrac{\mathcal{E}_{n,m}}{T_e\mathcal{SU}(m)(H)}$, which is the dimension of the quotient module $\dfrac{\mathcal{E}_{n,m}}{T_e\mathcal{SU}(m)(H)}$ regarded as a vector space over $\mathbb{R}$. For example, if $n = 3, m = 2$ as in the example above and $H(k) = \left(k_1, k_2, k_3^\ell\right) \cdot \sigma$ where $\ell \in \mathbb{N}$, its tangent space, extended tangent space, quotient module, and codimension are:

$$\begin{aligned} T\mathcal{SU}(m)(H) = \langle(-k_2, k_1, 0) \cdot \sigma, \left(k_3^\ell, 0, -k_1\right) \cdot \sigma, \left(0, -k_3^\ell, k_2\right) \cdot \sigma\rangle_{\mathcal{E}_n} \\ + \mathcal{M}_n\langle(1,0,0) \cdot \sigma, (0,1,0) \cdot \sigma, \left(0, 0, \ell k_3^{\ell-1}\right) \cdot \sigma\rangle_{\mathcal{E}_n}, \end{aligned} \tag{52}$$

$$\begin{aligned} T_e\mathcal{SU}(m)(H) = \langle(-k_2, k_1, 0) \cdot \sigma, \left(k_3^\ell, 0, -k_1\right) \cdot \sigma, \left(0, -k_3^\ell, k_2\right) \cdot \sigma, \\ (1,0,0) \cdot \sigma, (0,1,0) \cdot \sigma, \left(0, 0, \ell k_3^{\ell-1}\right) \cdot \sigma\rangle_{\mathcal{E}_n}, \end{aligned} \tag{53}$$

$$\frac{\mathcal{E}_{n,m}}{T_e\mathcal{SU}(m)(H)} = \langle(0,0,1) \cdot \sigma, (0,0,k_3) \cdot \sigma, \cdots, \left(0, 0, k_3^{\ell-2}\right) \cdot \sigma\rangle_{\mathbb{R}}, \tag{54}$$

and

$$\dim_{\mathbb{R}} \frac{\mathcal{E}_{n,m}}{T_e\mathcal{SU}(m)(H)} = \ell - 1,$$

respectively, where $\langle\cdots\rangle_A$ is the A-module generated by the elements in the bracket. Under this setting, we get the following classification of $\mathcal{M}_3\mathcal{E}_{3,2}$ under $\mathcal{SU}(m)$-equivalence [25]. In [25], the classes represented by the map-germs

$$\left(k_1, k_2k_3, k_2^2 \pm r k_3^{\ell+2}\right) \cdot \sigma \;\; (r > 0, \ell = 3, 4, 5) \tag{55}$$

are missing and we correct the result by adding the representatives to Table 1. The detail of the correction is reported in [26].

3.2. Classification of $\mathcal{M}_3\mathcal{E}_{3,2}$ under $\mathcal{SU}(2)$-equivalence.

Theorem 3.1 ([25])**.** *If the codimension of a map-germ in $\mathcal{M}_3\mathcal{E}_{2,3}$ is less than 8, the map-germ is $\mathcal{SU}(2)$-equivalent to one and only one of the map-germs listed in Table. 1.*

$\hat{H}(k)$	*ranges*	*mult*	*Ch*$_\pm$	*codim*
$(k_1, k_2, k_3) \cdot \sigma$		1	∓ 1	0
$\left(k_1, k_2, k_3^\ell\right) \cdot \sigma$	$\ell = 2, \cdots, 8$	ℓ	$\begin{cases} \mp 1 & (\ell\text{:}odd) \\ 0 & (\ell\text{:}even) \end{cases}$	$\ell - 1$
$\left(k_1, k_2^2, k_3^2 + rk_2^2\right) \cdot \sigma$	$r \in [0, \infty)$	4	0	5
$\left(k_1, k_2k_3, \frac{r}{2}\left(k_2^2 - k_3^2\right)\right) \cdot \sigma$	$r \in (0, 1)$	*4*	± 2	5
$\left(k_1, k_2k_3, k_2^2 + rk_3^{\ell+2}\right) \cdot \sigma$	$r \in (0, \infty), \ell = 1, 3$	$\ell + 4$	± 1	$\ell + 4$
$\left(k_1, k_2k_3, k_2^2 + rk_3^4\right) \cdot \sigma$	$r \in (0, \infty)$	6	0	6
$\left(k_1, k_2k_3, k_2^2 - rk_3^4\right) \cdot \sigma$	$r \in (0, \infty)$	6	± 2	6
$\left(k_1, k_2^2 - k_3^2 + rk_3^3, 2k_2k_3\right) \cdot \sigma$	$r \in (0, \infty)$	4	± 2	7
$\left(k_1, k_2^2 \pm k_3^2, rk_3^3\right) \cdot \sigma$	$r \in (0, \infty)$	6	0	7

TABLE 1. List of map-germs in each class of codimension less than 8 where "ranges" are possible ranges for the parameters r and ℓ, "mult" multiplicity, "Ch$_\pm$" Chern numbers of the upper and lower energy levels, and "codim" $\mathcal{SU}(2)_e$-codimension.

Here we define the multiplicity [14] and Chern number [27, 3, 23] as follows: Let

$$\hat{H}(k) = (\beta(k), \gamma(k), \delta(k)) \cdot \sigma \tag{56}$$

be a map-germ. Let $\langle \beta, \gamma, \delta \rangle_{\mathcal{E}_3}$ be the ideal in $\mathcal{E}_3$ generated by the matrix elements of the map-germ. We define the multiplicity of the map-germ as

$$\dim_{\mathbb{R}} \mathcal{E}_3 / \langle \beta, \gamma, \delta \rangle_{\mathcal{E}_3}, \tag{57}$$

i.e., the dimension of the quotient ring $\mathcal{E}_3 / \langle \beta, \gamma, \delta \rangle_{\mathcal{E}_3}$ regarded as a vector space over $\mathbb{R}$. Next, we define the Chern number. Here, we assume $\hat{H}(k) \neq (0,0,0) \cdot \sigma$ except for the origin $k = \mathbf{0}$. In this case, two eigenfunctions of the matrix, $\psi^{(\pm)}(k)$, can be chosen so that they depend smoothly on the Bloch wavenumber k $\left(\in \mathbb{R}^3\right)$ except for the origin $k = \mathbf{0}$. Let their corresponding eigenvalues be

$$E^{(\pm)}(k) \ \left(E^{(+)}(k) \geq E^{(-)}(k)\right). \tag{58}$$

Note that $\hat{H}(k)\psi^{(\pm)}(k) = E^{(\pm)}(k)\psi^{(\pm)}(k)$ holds. In terms of the two eigenfunctions, Berry curvatures are defined as

$$B^{(\pm)}(k) = i \sum_{j,j'=1}^{3} \frac{\partial}{\partial k_j} \left(\psi^{(\pm)}(k)^* \cdot \frac{\partial \psi^{(\pm)}(k)}{\partial k_{j'}}\right) dk_j \wedge dk_{j'}, \tag{59}$$

for $k \neq 0$. Note that the Berry curvature is well-defined except for the origin $k = \mathbf{0}$. Let S be an arbitrary 2-dimensional sphere enclosing the origin $k = \mathbf{0}$. Then, the Chern number is defined as

$$\mathrm{Ch}_\pm = \frac{1}{2\pi} \int_S B^{(\pm)}(k). \tag{60}$$

This number does not depend on how we choose the sphere S as long as the sphere encloses the origin. For the calculation of the multiplicity and Chern number, see [25].

In this classification, the class of codimension 0 is the most generic class and its normal form has a Weyl point at the origin $k = 0$. Other classes of higher codimension appear on verges of bifurcations. Bands cannot change their topology without colliding with others and these classes are expected to provide invaluable information on which types of geometric changes happen if two bands collide with each other.

When we presented this result in front of Prof. Goo Ishikawa in a workshop of differential geometry and singularity theory and their applications in Morioka, Japan, 2017,
Prof. Goo Ishikawa pointed out that band crossings among three or higher number of bands might be relevant for such a high codimension as 8. To answer Prof. Goo Ishikawa's question, we would like to show a list of lower bounds of codimensions of map-germs in $\mathcal{E}_{n,m}$ under $\mathcal{SU}(m)$-equivalence. The codimension of a map-germ in $\mathcal{E}_{n,m}$ having an m-fold degeneracy at the origin should be larger than this lower bound.

3.3. Lower bound of codimension of map-germs in $\mathcal{M}_n\mathcal{E}_{n,m}$ under $\mathcal{SU}(m)$-equivalence.

Let $\gamma_j \in \mathrm{Herm}_0(m)$ $\left(j = 1, \cdots, m^2-1\right)$ be bases of $\mathrm{Herm}_0(m)$.

Theorem 3.2. *Codimension of a C^∞ map-germ $H \in \mathcal{M}_n\mathcal{E}_{n,m}$ is equal to or greater than*

$$\max_{d\in\mathbb{N}\cup\{0\}} \left\{ \left(m^2-1\right) \frac{(n+d-1)!}{(n-1)!d!} - n\sum_{d'=0}^{d} \frac{(n+d'-1)!}{(n-1)!d'!} \right\}. \tag{61}$$

Proof. Take an arbitrary $H \in \mathcal{M}_n\mathcal{E}_{n,m}$ and $d \in \mathbb{N}\cup\{0\}$. We estimate the lower bound of its codimension. First note that

$$\dim_{\mathbb{R}} \frac{\mathcal{E}_{n,m}}{T_e\mathcal{SU}(m)(H)} \geq \dim_{\mathbb{R}} \frac{\mathcal{E}_{n,m}}{T_e\mathcal{SU}(m)(H) + \mathcal{M}_n^{d+1}\mathcal{E}_{n,m}} \tag{62}$$

holds.

Second note that $\dfrac{\mathcal{E}_{n,m}}{T_e\mathcal{SU}(m)(H) + \mathcal{M}_n^{d+1}\mathcal{E}_{n,m}}$ is isomorphic to

$$\frac{\mathcal{E}_{n,m}/\mathcal{M}_n^{d+1}\mathcal{E}_{n,m}}{\left(T_e\mathcal{SU}(m)(H) + \mathcal{M}_n^{d+1}\mathcal{E}_{n,m}\right)/\mathcal{M}_n^{d+1}\mathcal{E}_{n,m}} \tag{63}$$

by using **(2.6) Theorem. (Third isomorphism theorem)** in [1]. $\mathcal{E}_{n,m}/\mathcal{M}_n^{d+1}\mathcal{E}_{n,m}$ is an $\left(m^2-1\right)\left(\sum_{d'=0}^{d} \dfrac{(n+d'-1)!}{(n-1)!d'!}\right)$-dimensional vector space over $\mathbb{R}$.

$$\left(T_e\mathcal{SU}(m)(H) + \mathcal{M}_n^{d+1}\mathcal{E}_{n,m}\right)/\mathcal{M}_n^{d+1}\mathcal{E}_{n,m} \tag{64}$$

is a vector space over $\mathbb{R}$ spanned by

$$k_1^{d_1}k_2^{d_2}\cdots k_n^{d_n}\frac{\partial H(k)}{\partial k_j} + \mathcal{M}_n^{d+1}\mathcal{E}_{n,m}$$

for $j = 1, \cdots, n$ and $d_1 + d_2 + \cdots + d_n \leq d$ and $k_1^{d_1}k_2^{d_2}\cdots k_n^{d_n}\left[\gamma_j, H(k)\right] + \mathcal{M}_n^{d+1}\mathcal{E}_{n,m}$ for $j = 1, \cdots, n$ and $d_1 + d_2 + \cdots + d_n \leq d-1$ where $[A,B] = AB - BA$ for $A, B \in \mathrm{Herm}_0(m)$, which is a vector space in $\mathcal{E}_{n,m}/\mathcal{M}_n^{d+1}\mathcal{E}_{n,m}$ of dimension at most

$$\left(\left(m^2-1\right)\left(\sum_{d'=0}^{\max\{d-1,0\}} \frac{(n+d'-1)!}{(n-1)!d'!}\right) + n\sum_{d'=0}^{d} \frac{(n+d'-1)!}{(n-1)!d'!} \right).$$

Therefore,

$$\begin{aligned}(65)\quad \dim_{\mathbb{R}} \frac{\mathcal{E}_{n,m}/\mathcal{M}_n^{d+1}\mathcal{E}_{n,m}}{\left(T_e\mathcal{SU}\left(m\right)\left(H\right)+\mathcal{M}_n^{d+1}\mathcal{E}_{n,m}\right)/\mathcal{M}_n\mathcal{E}_{n,m}} &\geq \left(m^2-1\right)\left(\sum_{d'=0}^{d}\frac{(n+d'-1)!}{(n-1)!d'!}\right)\\ &-\left(\left(m^2-1\right)\left(\sum_{d'=0}^{\max\{d-1,0\}}\frac{(n+d'-1)!}{(n-1)!d'!}\right)+n\sum_{d'=0}^{d}\frac{(n+d'-1)!}{(n-1)!d'!}\right),\\ &=\left(m^2-1\right)\frac{(n+d-1)!}{(n-1)!d!}-n\sum_{d'=0}^{d}\frac{(n+d'-1)!}{(n-1)!d'!}\end{aligned}$$

holds. Since $d \in \mathbb{N}\cup\{0\}$ is arbitrary, this proves the theorem. □

If we set $n = 3$, we get lower bounds of codimensions for $m = 2, 3, 4, 5, 6$ in Table. 2. The results in Table 2 imply multiple band crossings may be less generic compared to two band crossings.

m	2	3	4	5	6
codimension ($\geq$)	0	20	180	840	2783

TABLE 2. Lower bounds of codimensions relative to $\mathcal{SU}(m)$-equivalence for $n = 3$ estimated by Eq. (61).

However, if we consider the codimension of a moduli family of map-germs, it can still have a small codimension. To investigate it, we need to classify $\mathcal{E}_{n,m}$ not based on the codimension of the extended tangent space in [25] but that substracted by the number of moduli parameters.

4. Future Perspectives

So far we have classified local geometric structures of bands in a neighborhood of a two-band crossing by classifying underlying Hamiltonians in the bulk of a crystal when either time-reversal symmetry or spacial inversion symmetry is broken. We have also estimated lower bounds of codimension for multi-band crossings. This should be the first step to understand global geometric structures of bands and their bifurcations. Steps further along this line of research are: Classification of local geometric structures of bands in a neighborhood of a multi-band crossing

(1) relative to a Fermi level.
(2) on a surface.
(3) in the bulk under time-reversal and spacial-inversion symmetries.

Point 1 is important to study the geometry of the Fermi surface, i.e., the intersection between bands and a Fermi level. For example, the geometry of a Fermi surface determines a type of semimetails [24]. This requires studying not only relative differences between bands, but also their differences relative to a Fermi level. We also need to take the trace part of Eq. (43) into account to classify geometric structures of Fermi surfaces.

Point 2 is important to understand geometric structures of bands on a surface, such as a Dirac-cone [7, 29, 4] and is also important for studying its engineering [9]. The geometric structures depend strongly on a crystallographic symmetry and the presence or absence of time-reversal symmetry and thus it is important to take these symmetries into account. This can be done if we extend our framework [25, 11] to an equivariant framework.

If the effective Hamiltonian of a crystal has a spin degree of freedom and symmetry as in Point 3, every band has two-fold degeneracy such as $E_0(k) = E_1(k) \leq E_2(k) = E_3(k) \leq \cdots$ for $k \in Y^*$ and it is important to take the degeneracy along with symmetries into account. Under this condition, band crossings that occur most generically are crossings of two pairs of bands. To classify geometric structures of such crossings, we need to classify 4×4 Hamiltonians instead of 2×2 ones because four bands are involved in the crossings. Such crossings appearing at time reversal invariant momentum (TRIM) points play a major role for topological properties of global band structures [8, 18]. Bifurcations occurring at TRIMs are shown to trigger topological changes in a lattice model in Chapter 3 in [22]. To study such bifurcations in our framework, we need to extend our framework [25, 11] to a framework in a multi-germ setting.

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