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1 Introduction

This paper aims to provide a description of some lattice defects in terms of monodromy in the sense of W. Thurston [7, 8]. Although we mainly discuss lattice defects arising from edge dislocations, we hope that our method can be applied also to more general lattice defects in the future. We note that Kupferman–Maor [5] and Hamada–Matsutani–Nakagawa–Saeki–Uesaka [4] have previously described edge dislocations and screw dislocations respectively in terms of monodromy from different points of view. Kupferman–Maor discussed them using tools of differential geometry, such as connections and curvatures, and considered a sequence of manifolds with dislocation-type singularities. In this sense their description is given from a continuum perspective. We also note that Kupferman–Maor considered some specific coordinate change to describe monodromy. On the other hand, Hamada–Matsutani–Nakagawa–Saeki–Uesaka discussed screw dislocations using fiber bundles, and the monodromy is described using a bundle whose fiber is some discrete group, such as $\mathbb{Z}$. In this sense, their description is given from a discrete perspective. Our description inherits some features of Kupferman–Maor and Hamada–Matsutani–Nakagawa–Saeki–Uesaka: we describe lattice defects from a discrete perspective, and use specific coordinate changes to encode symmetries of lattices.

The basic idea of our description is as follows. A lattice defect is a configuration of points whose most parts look like usual lattice, such as $\mathbb{Z}^3$, but the lattice structure is broken somewhere. It can be hoped for a natural description of a given lattice defect to encode some symmetry emerging from the original symmetry of the usual lattice. In a suitable situation, this can be rephrased by saying that there are local charts of the graph corresponding to the lattice defects, and the coordinate change of the charts encodes the symmetry arising from the original lattice. This system of charts and coordinate changes can be understood using Thurston's monodromy.

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2 Thurston's monodromy

In this section we summarize Thurston's (G, X)-manifold and monodromy given in [7, 8] for reader's convenience. (We refer the reader also to Goldman [2].) Let X be a topological space and G be a group. Assume that G acts continuously on X. Namely, assume that we have a group homomorphism $\rho : G \to \mathrm{Homeo}(X)$, where $\mathrm{Homeo}(X)$ is the group of homeomorphisms on X. In

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fact, for our main purpose, we shall only need to consider the case that X is a C^ω-manifold, and ρ is the inclusion $\rho : G \hookrightarrow \mathrm{Diff}^\omega(X)$, where $\mathrm{Diff}^\omega(X)$ is the group of C^ω-diffeomorphisms on X.

Definition 2.1 ((G,X)-manifold [7,8])**.** Let M be a topological space

1. $\{(U_\alpha, \phi_\alpha)\}_\alpha$ is a (G,X)-*atlas* on M if
   - $\{U_\alpha\}_\alpha$ is an open covering of M,
   - each $\phi_\alpha : U_\alpha \to X$ is a homeomorphism onto its image, and
   - $\phi_\alpha \circ \phi_\beta^{-1}|_{\phi_\beta(U_\alpha \cap U_\beta)} : \phi_\beta(U_\alpha \cap U_\beta) \to \phi_\alpha(U_\alpha \cap U_\beta)$ is the restriction of an element of $\rho(G)$.
2. M equipped with a (G,X)-atlas is called a (G,X)-*manifold*. Each (U_α, ϕ_α) is called a (G,X)-*chart*.

Example 2.2. Let us consider the four pairs $(X,G) = (\mathbb{R}^n, \mathrm{Homeo}(\mathbb{R}^n))$, $(\mathbb{R}^n, \mathrm{Diff}(\mathbb{R}^n))$, $(\mathbb{C}^n, \mathrm{Hol}(\mathbb{C}^n))$, and $(\mathbb{H}^n, \mathrm{Isom}(\mathbb{H}^n))$. Here $\mathbb{H}^n$ is the hyperbolic space, $\mathrm{Diff}(\mathbb{R}^n)$, $\mathrm{Hol}(\mathbb{C}^n)$, and $\mathrm{Isom}(\mathbb{H}^n)$ are the groups of diffeomorphisms, biholomorphic maps, and isometries respectively. Then, corresponding to these four pairs, the notions of (G,X)-manifolds are equivalent to the notion of topological manifolds, smooth manifolds, complex manifolds, and hyperbolic manifolds respectively.

Henceforth assume that X is a C^ω-manifold, and $\rho : G \hookrightarrow \mathrm{Diff}^\omega(X)$ is the inclusion of the group of C^ω-diffeomorphisms. Then, for each (G,X)-manifold M, we can define the following group homomorphism which is called the *monodromoy*

$$\mathrm{Mon}_M : \pi_1(M, p_0) \to G,$$

where we fix a point $p_0 \in M$ and a (G,X)-chart (U_0, ϕ_0) near p_0. The construction of the monodromy map consists of the following four steps:

1. Take a loop $\gamma : [0,1] \to M$ with base point p_0.
2. Take (G,X)-charts $(U_1, \phi_1), \dots, (U_n, \phi_n)$ which cover the image of γ. (Note that the neighborhood of the base point is already covered by U_0.) Take the covers so that $U_i \cap U_{i+1}$ is non-empty and connected for each $i \in \{0, \dots, n-1\}$.
3. There exists a unique $g_i \in G$ such that g_i gives the coordinate change of (U_i, ϕ_i) and (U_{i+1}, ϕ_{i+1}). (Here, for the uniqueness, we need to assume that X is C^ω.)
4. One can show that $\mathrm{Mon}_M([\gamma]) := g_0 \cdots g_{n-1} \in G$ depends only on the homotopy class of γ (for the fixed chart (U_0, ϕ_0)).

If we take another base point p_0' and a chart (U_0', ϕ_0') near p_0', the monodoromy map is changed by conjugation. In particular, if G is abelian, we have a homomorphism

$$\mathrm{Mon}_M : \pi_1(M) \to G$$

which is independent of the choice of base points and charts near that.

3 Monodromy of dislocations

In this section we describe some dislocations in terms of Thurston's monodromy described in Section 2. Assume that we are given a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ realized in $\mathbb{R}^3$. We denote by $\mathcal{G}$ also the realization of the graph. Here $\mathcal{V}$ and $\mathcal{E}$ mean the sets of vertices and edges respectively. This situation can be rephrased as follows. Given a picture of a lattice defect of the type of dislocation, assume that

- we have the notion of “lattice point” (corresponding to vertices), and
- we also have the notion of “nearest lattice points” (corresponding to edges).

Define an open submanifold $M = M(\mathcal{G})$ of $\mathbb{R}^3$ as the “fat graph”:

$$M = M(\mathcal{G}) := \bigcup_{E \in \mathcal{E},\ p \in E} B_p(\epsilon_p), \tag{1}$$

where we regard an edge E as a (1-dimensional) subspace of $\mathbb{R}^3$, $\epsilon_p > 0$ is a sufficiently small number smoothly depending on p, and $B_p(\epsilon_p)$ is the open ball centered at p with radius ϵ_p. Here ϵ_p is taken so that the homotpy type of M coincides with that of $\mathcal{G}$ via a natural deformation retract which is obtained by multiplying $t \in [0, 1]$ to ϵ_p for any $B_p(\epsilon_p)$. If $\mathcal{G}$ is compact, of course, we can take ϵ_p so that it is common to any p. In some good situations, we can give a $(\mathbb{Z}^3, \mathbb{R}^3)$-manifold structure on M.

We first discuss 2-dimensional edge dislocation. A picture of an edge dislocation might be helpful for readers. See Guy [3] p. 153, for example. (It will be partially given in this paper.) We first consider a 2-dimensional model of edge dislocation. We assume that $\mathcal{G}$ is given as the 2-dimensional edge dislocation described as the left figure of Figure 1. More precisely, it is defined as follows. Let us regard $\mathbb{Z}^2$ as a graph in a usual way, and we write $\mathbb{Z}^2$ also for the realization of it. Let $L \subset \mathbb{Z}^2$ be the subgraph generated by $\{0\} \times \{\, n \le 0 \mid n \in \mathbb{Z}\,\} \subset \mathbb{Z}^2$. Let $\mathcal{G}'$ be the graph obtained by removing L from $\mathcal{G}$ and connecting the vertex written as $\{(-1, n)\}$ with $\{(1, n)\}$ by an edge of length 2 for each n. Let denote by $\mathcal{V}(\mathcal{G}')$ the set of vertices of the graph $\mathcal{G}'$. Let $f : \mathcal{V}(\mathcal{G}') \to \mathbb{R}^2$ be the injective map defined as follows. We write $\mathbb{Z}_{>0} := \{\, n > 0 \mid n \in \mathbb{Z}\,\}$ and $\mathbb{Z}_{\ge 0} := \{\, n \ge 0 \mid n \in \mathbb{Z}\,\}$, and similarly define $\mathbb{Z}_{<0}$ and $\mathbb{Z}_{\le 0}$.

- The restriction of f on $\mathbb{Z} \times \mathbb{Z}_{>0}$ is the identity map.
- The restriction of f on $\mathbb{Z}_{<0} \times \mathbb{Z}_{\le 0}$ is given as $f(m, n) := (m + 1/2, n)$.
- The restriction of f on $\mathbb{Z}_{>0} \times \mathbb{Z}_{\le 0}$ is given as $f(m, n) := (m - 1/2, n)$.

Then we can write down the definition of $\mathcal{G}$. Let $\mathcal{V} = \mathcal{V}(\mathcal{G})$ be the image $\mathcal{V}(\mathcal{G}')$ by f. We define the edges of $\mathcal{G}$ as follows: for given two vertices $V_1, V_2 \in \mathcal{V}$, there exists an edge between V_1 and V_2 if and only if the preimage of these vertices by f is connected by an edge. From this definition, we have a bijective map $\mathcal{E}(\mathcal{G}')$, the set of edges of $\mathcal{G}'$, to $\mathcal{E}(\mathcal{G})$. We also write $f : \mathcal{E}(\mathcal{G}') \to \mathcal{E}(\mathcal{G})$ for this map.

We now consider the fat graph M of $\mathcal{G}$. The manifold M is defined as (1), but we take ϵ_p to be common to any p, written as ϵ, and we use the two dimensional disk $B_p(\epsilon)$ instead of the three dimensional ball. We note that one can obtain a bijective between the realizations $f : \mathcal{G}' \to \mathcal{G}$ putting together $f : \mathcal{V}(G') \to \mathcal{V}(G)$ and $f : \mathcal{E}(\mathcal{G}') \to \mathcal{E}(\mathcal{G})$. We here take f so that the restriction of f to the realization of $E \in \mathcal{E}(\mathcal{G}')$ is an isometry if E is not the edge connecting $(-1, 0)$ and $(1, 0)$, and that is given by the natural affine map $[-1, 1] \times \{0\} \to [-1/2, 1/2] \times \{0\}$ if E is the edge connecting these two vertices. The map $f : \mathcal{E}(\mathcal{G}') \to \mathcal{E}(\mathcal{G})$ naturally induces a bijection between the fat graphs $f : M(\mathcal{G}') \to M(\mathcal{G})$.

We now give a $(\mathbb{Z}^2, \mathbb{R}^2)$-atlas on M, described in Figure 1. We first define an open subset U_+ of $\mathbb{R}^2$. For $V, V' \in \mathcal{V}(\mathcal{G}')$, let $E_{V,V'}$ be the (unique) edge connecting V with V', and define $\tilde{E}_{V,V'} := f(E_{V,V'})$. We define a subset $\tilde{E}^+_{(1,0),(-1,0)} \subset E_{(1,0),(-1,0)}$ as

$$\tilde{E}^+_{(1,0),(-1,0)} := \left\{\, (x, y) \in E_{(1,0),(-1,0)} \;\middle|\; x \ge 0 \,\right\}.$$

Set

$$U_+ := \bigcup_{p \in \tilde{E}_{(0,1),(1,1)} \cup \tilde{E}_{(1,1),(1,0)} \cup \tilde{E}^+_{(1,0),(-1,0)}} B_p(\epsilon_p).$$

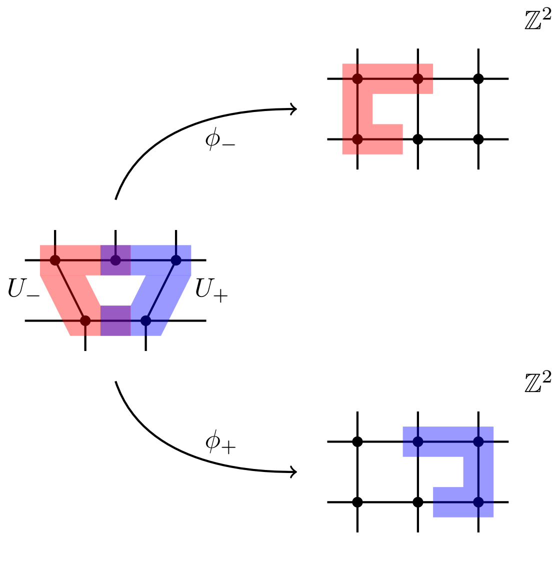

図 1: $(\mathbb{Z}^2, \mathbb{R}^2)$-charts on the edge dislocation

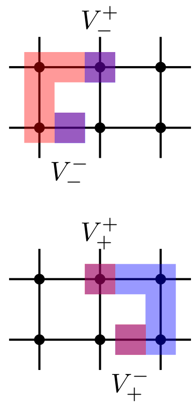

図 2: The coordinate changes between ϕ_+ and ϕ_-

The open subset U_+ of $\mathbb{R}^2$ is contained in $M = M(\mathcal{G})$, and therefore we can get the inverse map $f^{-1}|_{U_+} : U_+ \to f(U_+) \subset \mathbb{R}^2$. We define $\phi_+ : U_+ \to \mathbb{R}^2$ as this map $f^{-1}|_{U_+}$. We can define an open subset U_- of $\mathbb{R}^2$ by changing the sign of x-component in the above argument to construct U_+, and similarly define $\phi_- : U_- \to \mathbb{R}^2$. For the rest part $M \setminus (U_+ \cup U_-)$, one has obvious charts mapping to $\mathbb{R}^2$ respecting lattice structure. We thus get an atlas of M, and we shall conclude that this atlas is in fact a $(\mathbb{Z}^2, \mathbb{R}^2)$-atlas. To see it, we have to check that the coordinate change between (U_+, ϕ_+) and (U_-, ϕ_-) is controlled by $\mathbb{Z}^2$, which is described in Figure 2. Note that the intersection $U_+ \cap U_-$ has two connected components. Let U^+ be the component such that any element of it has a positive y-coordinate, and let U^- be the rest complement of $U_+ \cap U_-$. We define $V_\pm^+$ be the image of U^+ by $\phi_\pm$, and similarly define $V_\pm^-$. Then, $\phi_+^{-1} \circ \phi_-|_{V_-^+} : V_-^+ \to V_+^+$ is just the identity, and $\phi_+^{-1} \circ \phi_-|_{V_-^-} : V_-^- \to V_+^-$ is the addition of $(1, 0) \in \mathbb{Z}^2$. Other possibilities of coordinate changes are obviously just the identity, and therefore we deduce that our atlas on M is a $(\mathbb{Z}^2, \mathbb{R}^2)$-atlas.

We then can calculate the monodromy of with respect to the $(\mathbb{Z}^2, \mathbb{R}^2)$-structure on M. Since $\mathbb{Z}^2$ is abelian, we do not have to care about base points. Let γ be the loop in M consisting of the five edges which are completely contained in $U_- \cup U_+$. By the definition of monodromy in Section 2,

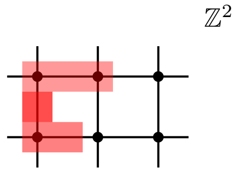

図 3: An example of a decomposition of U_-

the monodromy for this loop γ is given as the sum of coordinate changes between (U_+, ϕ_+) and (U_-, ϕ_-) calculated above: $\mathrm{Mon}_M(\gamma) = (0,0) + (1,0) = (1,0) \in \mathbb{Z}^2$.

Remark 3.1. Strictly speaking, to calculate the monodromy following the definition, we have to decompose the two U_+ and U_- so that the intersection of these charts is connected. See Figure 3 for an example of such a decomposition of U_-. (In Figure 3 it is illustrated as the corresponding decomposition of V_-.) However, the coordinate change between new two charts arising from the previous one chart, say U_-, is just the identity. The decompositions do not therefore give any change to the above calculation of the monodromy for γ.

Since M is homotopy equivalent to $\bigvee_{\mathbb{Z}} S^1$, we have $\pi_1(M) \cong *_{\mathbb{Z}}\mathbb{Z}$. The monodromy map

$$\mathrm{Mon}_M : \pi_1(M) \cong *_{\mathbb{Z}}\mathbb{Z} \to \mathbb{Z}^2 \tag{2}$$

is non-trivial since $\mathrm{Mon}_M(\gamma) = (1,0)$ as we have seen. On the other hand, let M_{std} be the fat graph of $\mathbb{Z}^2$. This manifold M_{std} obviously admits a $(\mathbb{Z}^2, \mathbb{R}^2)$-structure and $\pi_1(M_{\mathrm{std}}) \cong *_{\mathbb{Z}}\mathbb{Z}$, and therefore the domain and the range of the monodromy map

$$\mathrm{Mon}_{M_{\mathrm{std}}} : \pi_1(M_{\mathrm{std}}) \cong *_{\mathbb{Z}}\mathbb{Z} \to \mathbb{Z}^2$$

coincide with that of (2). However, $\mathrm{Mon}_{M_{\mathrm{std}}}$ is just the trivial homomorphism. This suggests that the monodromy reflects the difference between the usual lattice $\mathbb{Z}^2$ and the configuration arising from edge dislocation.

Remark 3.2. One can easily extend the above construction to a 3-dimensional model of edge dislocation. The model is given by the product of $\mathbb{Z}$ (regarded as a discrete subset of z-axis) and the previous 2-dimensional model. (See Guy [3] p. 153 for the picture.) For the fat graph M corresponding to the 3-dimensional edge dislocation, we can give a $(\mathbb{Z}^3, \mathbb{R}^3)$-manifold structure on it, and get the monodromy map

$$\mathrm{Mon}_M : \pi_1(M) \cong *_{\mathbb{Z}}\mathbb{Z} \to \mathbb{Z}^3.$$

One can again have a distinguished loop and the value of the loop by Mon_M is given by $(1,0,0) \in \mathbb{Z}^3$. Note that the non-trivial direction $(1,0,0)$ for monodromy is perpendicular to the dislocation line $\mathbb{R} \cdot (0,0,1)$. The non-trivial direction for monodromy can be regarded as some notion corresponding to the Burgers vector (see [6], for example). On the other hand, if we can give a $(\mathbb{Z}^3, \mathbb{R}^3)$-structrure for M corresponding to a given lattice defect, not necessary a dislocation, we can define the monodromy map Mon_M. This suggests that Mon_M may be regarded as a generalization of the Burgers vector.

Remark 3.3. We here mention screw dislocation. We refer Fig. 6.10 in Callister–Rethwisch [1] as a picture of a screw dislocation. In the figure, near the dislocation line, the graph corresponding to the screw dislocation cannot be regarded as a subgraph of $\mathbb{Z}^3$. We cannot therefore give $(\mathbb{Z}^3, \mathbb{R}^3)$-atlas for the whole fat graph. However, if we take M as the fat graph which is obtained by removing a neighborhood of the dislocation line in the original fat graph, we can give $(\mathbb{Z}^3, \mathbb{R}^3)$-atlas as the above one for an edge dislocation. If we take a loop γ in the graph having linking number one (up to sign) with the dislocation line, then we have $\mathrm{Mon}_M(\gamma)$ is parallel to the dislocation line. This is essentially only one non-trivial direction for monodromy. Therefore, also in the case of screw dislocation, the non-trivial direction for monodromy coincides with the Burgers vector as in Theorem 3.2.

Remark 3.4. We note that, as well as Burgers vectors, monodromy map can detect some difference between edge dislocations and screw dislocations, described in Theorems 3.2 and 3.3. This suggests that monodromy map may be regarded as a geometric invariant of lattice defects. To formulate this idea rigorously, we should first define a lattice defect as a mathematical object. We hope that monodromy map can give a guiding principle for the correct mathematical definition of lattice defects.

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