

Dynamics for Systems of Screw Dislocations

Original

Dynamics for Systems of Screw Dislocations / Blass, T.; Fonseca, I.; Leoni, Giovanni; Morandotti, M.. - In: SIAM JOURNAL ON APPLIED MATHEMATICS. - ISSN 0036-1399. - STAMPA. - 75:2(2015), pp. 393-419.
[10.1137/140980065]

Availability:

This version is available at: 11583/2722526 since: 2020-02-14T14:27:43Z

Publisher:

Society for Industrial and Applied Mathematics

Published

DOI:10.1137/140980065

Terms of use:

This article is made available under terms and conditions as specified in the corresponding bibliographic description in the repository

Publisher copyright

default_article_editorial [DA NON USARE]

-

(Article begins on next page)

DYNAMICS FOR SYSTEMS OF SCREW DISLOCATIONS*

T. BLASS[†], I. FONSECA[‡], G. LEONI[‡], AND M. MORANDOTTI[§]

Abstract. The goal of this paper is the analytical validation of a model of Cermelli and Gurtin [*Arch. Ration. Mech. Anal.*, 148 (1999), pp. 3–52] for an evolution law for systems of screw dislocations under the assumption of antiplane shear. The motion of the dislocations is restricted to a discrete set of glide directions, which are properties of the material. The evolution law is given by a “maximal dissipation criterion,” leading to a system of differential inclusions. Short time existence, uniqueness, cross-slip, and fine cross-slip of solutions are proved.

Key words. dislocation dynamics, screw dislocations, differential inclusions, Filippov systems, renormalized energy, variational methods

AMS subject classifications. 34A60, 74Bxx, 35J15, 49J40

DOI. 10.1137/140980065

1. Introduction. Dislocations are one-dimensional defects in crystalline materials [28]. Their modeling is of great interest in materials science since important material properties, such as rigidity and conductivity, can be strongly affected by the presence of dislocations. For example, large collections of dislocations can result in plastic deformations in solids under applied loads.

In this paper we study the motion of screw dislocations in cylindrical crystalline materials using a continuum model introduced by Cermelli and Gurtin [12]. One of our main contributions is the analytical validation to this model by proving local existence and uniqueness of solutions to the equations of motions for a system of dislocations. In particular, we prove rigorously the phenomena of cross-slip and fine cross-slip. We refer the reader to the work of Armano and Cermelli (see [4, 11]) for the case of a single dislocation.

Following the work of Cermelli and Gurtin [12], we consider an elastic body $B := \Omega \times \mathbb{R}$, where $\Omega \subset \mathbb{R}^2$ is a bounded simply connected open set with a $C^{2,\alpha}$ boundary. The body B undergoes *antiplane shear* deformations $\Phi : B \rightarrow B$ of the form

$$\Phi(x_1, x_2, x_3) := (x_1, x_2, x_3 + u(x_1, x_2)),$$

with $u : \Omega \rightarrow \mathbb{R}$. The deformation gradient \mathbf{F} is given by

$$(1.1) \quad \mathbf{F} := \nabla \Phi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{\partial u}{\partial x_1} & \frac{\partial u}{\partial x_2} & 1 \end{pmatrix} = \mathbf{I} + \mathbf{e}_3 \otimes \begin{pmatrix} \nabla u \\ 0 \end{pmatrix}.$$

*Received by the editors July 30, 2014; accepted for publication (in revised form) January 14, 2015; published electronically March 19, 2015. This research was partially supported by NSF grant DMS-0635983.

<http://www.siam.org/journals/siap/75-2/98006.html>

[†]Department of Mathematics, University of California, Riverside, Riverside, CA 92521 (timothy.blass@ucr.edu). This author’s research was supported by NSF PIRE grant OISE-0967140.

[‡]Department of Mathematical Sciences, Carnegie Mellon University, Pittsburgh, PA 15213 (fonseca@andrew.cmu.edu, giovanni@andrew.cmu.edu). The research of these authors was supported by NSF PIRE grant OISE-0967140. The second author’s research was also partially supported by NSF grant DMS-0905778. The third author’s research was also partially supported by NSF grant DMS-1007989.

[§]Mathematics Area, SISSA – Scuola Internazionale Superiore di Studi Avanzati, 34136 Trieste, Italy (morandot@sissa.it). This author’s research was partially supported by grant FCT-UTA/CMU/MAT/0005/2009.

The assumption of antiplane shear allows us to reduce the three-dimensional problem to a two-dimensional problem. We will consider *strain fields* \mathbf{h} that are defined on the cross-section Ω , taking values in \mathbb{R}^2 . In the absence of dislocations, the strain \mathbf{h} is the gradient of a function, $\mathbf{h} = \nabla u$. If dislocations are present, then the strain field is singular at the sites of the dislocations, and in the case of screw dislocations this will be a line singularity. In the antiplane shear setting, this line is parallel to the x_3 axis and the screw dislocation is represented as a point singularity on the cross-section Ω .

A screw dislocation is characterized by a position $\mathbf{z} \in \Omega$ and a vector $\mathbf{b} \in \mathbb{R}^3$, called the *Burgers vector*. The position $\mathbf{z} \in \Omega$ is a point where the strain field fails to be the gradient of a smooth function and the Burgers vector measures the severity of this failure. To be precise, a strain field associated with a system of N screw dislocations at positions

$$\mathcal{Z} := \{\mathbf{z}_1, \dots, \mathbf{z}_N\} \subset \Omega$$

with corresponding Burgers vectors

$$\mathcal{B} := \{b_1 \mathbf{e}_3, \dots, b_N \mathbf{e}_3\}$$

satisfies the relation

$$(1.2) \quad \operatorname{curl} \mathbf{h} = \sum_{i=1}^N b_i \delta_{\mathbf{z}_i} \quad \text{in } \Omega$$

in the sense of distributions. Here $\operatorname{curl} \mathbf{h}$ is the scalar $\operatorname{curl} \frac{\partial h_2}{\partial x_1} - \frac{\partial h_1}{\partial x_2}$, $\delta_{\mathbf{x}}$ is the Dirac mass at the point \mathbf{x} , and the scalar b_i is called the *Burgers modulus* for the dislocation at \mathbf{z}_i , and in view of (1.2) it is given by

$$b_i = \int_{\ell_i} \mathbf{h} \cdot \mathbf{t} \, ds,$$

where ℓ_i is any counterclockwise loop surrounding the dislocation point \mathbf{z}_i and no other dislocation points, \mathbf{t} is the tangent to ℓ_i , and ds is the line element.

Note that, following the classical construction of Volterra (see [27, sect. 3-2]), strain fields \mathbf{h} satisfying (1.2) can be obtained from a perfect cylinder by shear displacements in the z direction across the xz plane.

When dislocations are present, (1.1) is replaced with

$$\mathbf{F} = \mathbf{I} + \mathbf{e}_3 \otimes \begin{pmatrix} \mathbf{h} \\ 0 \end{pmatrix}.$$

To derive a motion law for the system of dislocations we need to introduce the free energy associated with the system. We work in the context of linear elasticity. The energy density W is given by

$$W(\mathbf{h}) := \frac{1}{2} \mathbf{h} \cdot \mathbf{L} \mathbf{h},$$

where the elasticity tensor \mathbf{L} is a symmetric, positive-definite matrix, which, in suitable coordinates, can be written in terms of the Lamé moduli λ, μ of the material as

$$\mathbf{L} := \begin{pmatrix} \mu & 0 \\ 0 & \mu \lambda^2 \end{pmatrix}.$$

We require $\mu > 0$, and the energy is isotropic if and only if $\lambda^2 = 1$. The energy of a strain field \mathbf{h} is given by

$$(1.3) \quad J(\mathbf{h}) := \int_{\Omega} W(\mathbf{h}(\mathbf{x})) \, d\mathbf{x},$$

and the equilibrium equation is

$$(1.4) \quad \operatorname{div} \mathbf{Lh} = 0 \quad \text{in } \Omega.$$

Equations (1.2) and (1.4) provide a characterization of strain fields describing screw dislocation systems in linearly elastic materials.

To be precise, we say that a strain field \mathbf{h} corresponds to a *system of dislocations* at the positions \mathcal{Z} with Burgers vectors \mathcal{B} if \mathbf{h} satisfies

$$(1.5) \quad \begin{cases} \operatorname{curl} \mathbf{h} = \sum_{i=1}^N b_i \delta_{\mathbf{z}_i} \\ \operatorname{div} \mathbf{Lh} = 0 \end{cases} \quad \text{in } \Omega$$

in the sense of distributions.

In analogy to the theory of Ginzburg–Landau vortices [6], no variational principle can be associated with (1.5) because the elastic energy of a system of screw dislocations is not finite (see, e.g., [13, 12, 28]), and therefore the study of (1.5) cannot be undertaken in terms of energy minimization. Indeed, the simultaneous requirements of finite energy and (1.2) are incompatible since if $\operatorname{curl} \mathbf{h} = \delta_{\mathbf{z}_0}$, $\mathbf{z}_0 \in \Omega$, and if $B_\varepsilon(\mathbf{z}_0) \subset\subset \Omega$, then

$$\int_{\Omega \setminus B_\varepsilon(\mathbf{z}_0)} |\mathbf{h}|^2 \, d\mathbf{x} = O(|\log \varepsilon|).$$

In the engineering literature (see, e.g., [12, 28]), this problem is usually overcome by regularizing the energy, namely, by replacing the energy J in (1.3) with a new energy J_ε obtained by removing small cores of size $\varepsilon > 0$ centered at the dislocations points \mathbf{z}_i . This allows one to obtain finite-energy strains \mathbf{h}_ε as minimizers of J_ε . It was shown in [7] (see also [2, 5, 13] and the references therein) that

$$(1.6) \quad J_\varepsilon(\mathbf{h}_\varepsilon) = C|\log \varepsilon| + U(\mathbf{z}_1, \dots, \mathbf{z}_N) + O(\varepsilon),$$

where U is the *renormalized energy* associated with the limiting strain

$$(1.7) \quad \mathbf{h}_0 = \lim_{\varepsilon \rightarrow 0} \mathbf{h}_\varepsilon,$$

satisfying (1.5). The renormalized energy U is a function only of the positions $\{\mathbf{z}_1, \dots, \mathbf{z}_N\}$ (and of the Burgers moduli) and can be written as the sum of three energy contributions: a “self” energy associated with the presence of a dislocation, an energy associated with the interaction between dislocations, and an energy associated to the elastic medium. See section IV in the supplementary materials file for this paper, which is linked from the main article webpage.

The force on a dislocation at \mathbf{z}_i due to the elastic strain is called the *Peach–Köhler force* and is denoted by \mathbf{j}_i (see [12, 29]). It is proved in [7] that \mathbf{j}_i is given by the negative gradient of the renormalized energy U with respect to \mathbf{z}_i . Specifically,

$$(1.8) \quad \mathbf{j}_i = -\nabla_{\mathbf{z}_i} U = \int_{\ell_i} \{W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0 \otimes (\mathbf{Lh}_0)\} \mathbf{n} \, ds,$$

where ℓ_i is a suitably chosen loop around \mathbf{z}_i , \mathbf{h}_0 is defined in (1.7), and \mathbf{n} is the outer unit normal to the set bounded by ℓ_i and containing \mathbf{z}_i . The quantity $W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)$ is the *Eshelby stress tensor*; see [17, 25].

To study the motion of dislocations it is more convenient to rewrite \mathbf{j}_i in the form

$$(1.9) \quad \mathbf{j}_i(\mathbf{Z}) = b_i \mathbf{J} \mathbf{L} \left[\sum_{j \neq i} \mathbf{k}_j(\mathbf{z}_i; \mathbf{z}_j) + \nabla u_0(\mathbf{z}_i; \mathbf{Z}) \right]$$

(see [7] for a proof of this derivation). Here $\mathbf{Z} := (\mathbf{z}_1, \dots, \mathbf{z}_N) \in \mathbb{R}^{2N}$, $\mathbf{k}_j(\cdot; \mathbf{z}_j)$ is the *fundamental singular strain* generated by the dislocation \mathbf{z}_j , where

$$(1.10) \quad \mathbf{k}_j(\mathbf{x}; \mathbf{y}) := \frac{b_j}{2\pi} \frac{\lambda \mathbf{J}^T(\mathbf{x} - \mathbf{y})}{|\Lambda(\mathbf{x} - \mathbf{y})|^2}, \quad (\mathbf{x}, \mathbf{y}) \in \mathbb{R}^2 \times \mathbb{R}^2, \mathbf{x} \neq \mathbf{y},$$

with

$$(1.11) \quad \mathbf{J} := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \Lambda := \begin{pmatrix} \lambda & 0 \\ 0 & 1 \end{pmatrix}.$$

Straightforward calculations show that, for $(\mathbf{x}, \mathbf{y}) \in \mathbb{R}^2 \times \mathbb{R}^2$, $\mathbf{x} \neq \mathbf{y}$, we have

$$(1.12a) \quad \operatorname{div}_{\mathbf{y}}(\mathbf{L} \nabla_{\mathbf{y}} \mathbf{k}_j(\mathbf{x}; \mathbf{y})) = \mathbf{0},$$

$$(1.12b) \quad \operatorname{div}_{\mathbf{x}}(\mathbf{L} \mathbf{k}_j(\mathbf{x}; \mathbf{y})) = 0,$$

and, for $(\mathbf{x}, \mathbf{y}) \in \mathbb{R}^2 \times \mathbb{R}^2$,

$$(1.12c) \quad \operatorname{curl}_{\mathbf{x}} \mathbf{k}_j(\mathbf{x}; \mathbf{y}) = b_j \delta_{\mathbf{y}}(\mathbf{x}).$$

Also, for fixed $\mathbf{z}_1, \dots, \mathbf{z}_N \in \Omega$, the function $u_0(\cdot; \mathbf{Z})$ is a solution of the Neumann problem

$$(1.13) \quad \begin{cases} \operatorname{div}_{\mathbf{x}}(\mathbf{L} \nabla_{\mathbf{x}} u_0(\mathbf{x}; \mathbf{Z})) = 0, & \mathbf{x} \in \Omega, \\ \mathbf{L}(\nabla_{\mathbf{x}} u_0(\mathbf{x}; \mathbf{Z}) + \sum_{i=1}^N \mathbf{k}_i(\mathbf{x}; \mathbf{z}_i)) \cdot \mathbf{n}(\mathbf{x}) = 0, & \mathbf{x} \in \partial\Omega. \end{cases}$$

The expression of (1.9) contains two contributions accounting for the two different kinds of forces acting on a dislocation when other dislocations are present: the interactions with the other dislocations and the interactions with $\partial\Omega$. The latter balances the tractions of the forces generated by all the dislocations. Indeed, the function $\nabla u_0(\mathbf{x}; \mathbf{Z})$ represents the elastic strain at the point $\mathbf{x} \in \Omega$ due to the presence of $\partial\Omega$ and the dislocations at \mathbf{z}_i with Burgers moduli b_i . For this reason, we refer to $\nabla u_0(\mathbf{x}; \mathbf{Z})$ as the *boundary-response strain* at \mathbf{x} due to \mathcal{Z} .

The formula (1.9) gives the force on the dislocation at \mathbf{z}_i , and it shows that, as a function of \mathbf{z}_i , the force \mathbf{j}_i is smooth in the interior of $\Omega \setminus \{\mathbf{z}_1, \dots, \mathbf{z}_{i-1}, \mathbf{z}_{i+1}, \dots, \mathbf{z}_N\}$. That is, provided \mathbf{z}_i is not colliding with another dislocation or with $\partial\Omega$, then the force is given by a smooth function. Of course, \mathbf{j}_i depends on the positions of *all* the dislocations, and the same reasoning applies to \mathbf{j}_i as a function of any \mathbf{z}_j .

In the study of the dynamics of the system \mathcal{Z} we will neglect inertia and any external body forces and consider only the Peach–Köhler force \mathbf{j}_i as given in (1.9).

The motion of dislocations (often called *dislocation glide*) in crystalline materials is restricted to a discrete set of crystallographic planes called *glide planes*, which are

spanned by \mathbf{e}_3 and vectors \mathbf{g} called *glide directions*, determined by the lattice structure of that material. We will consider the glide directions as a fixed finite collection of unit vectors in \mathbb{R}^2 , denoted by

$$(1.14) \quad \mathcal{G} := \{\mathbf{g}_1, \dots, \mathbf{g}_M\} \subset S^1,$$

with the requirement that if $\mathbf{g} \in \mathcal{G}$, then $-\mathbf{g} \in \mathcal{G}$.

We are interested in the physically realistic case where the span of the glide directions is all of \mathbb{R}^2 ; otherwise dislocations are restricted to one-dimensional motion and cannot abruptly change direction. Therefore, we assume that

$$(1.15) \quad \text{span}(\mathcal{G}) = \mathbb{R}^2.$$

The dislocation glide is restricted to the directions in \mathcal{G} , so the equation of motion for \mathbf{z}_i has the form

$$\dot{\mathbf{z}}_i = \mathcal{V}_i \mathbf{g}_i, \quad \mathbf{g}_i \in \mathcal{G},$$

and \mathcal{V}_i is a scalar velocity.

In [12] motion laws are proposed, where a variable mobility $M(\mathbf{g})$ and Peierls force $P(\mathbf{g})$ are incorporated to obtain equations of the form

$$(1.16) \quad \dot{\mathbf{z}}_i = M(\mathbf{g}_i) [\max\{\mathbf{j}_i \cdot \mathbf{g}_i - P(\mathbf{g}_i), 0\}]^p \mathbf{g}_i,$$

with the exponent $p > 0$ allowing for various “power-law kinetics.” The mobility function M favors some directions of dislocation glide. The Peierls force, $P \geq 0$, is a threshold force, acting as a static friction. If the Peach–Köhler force along \mathbf{g}_i is below the threshold, then the dislocation will not move. Glide initiates when $\mathbf{j}_i \cdot \mathbf{g}_i > P(\mathbf{g}_i)$. In this paper we will assume the simplest form of linear kinetics ($p = 1$) with vanishing Peierls force ($P \equiv 0$) and isotropic mobility ($M \equiv 1$). Thus (1.16) takes the form

$$(1.17) \quad \dot{\mathbf{z}}_i = (\mathbf{j}_i(\mathbf{Z}) \cdot \mathbf{g}_i) \mathbf{g}_i \quad \text{for } \mathbf{g}_i \in \mathcal{G}.$$

Following the model presented in [12], the choice of glide direction \mathbf{g}_i in (1.17) is determined by a *maximal dissipation inequality* for dislocation glide. At any point where $\mathbf{z}_i(t)$ is differentiable and where (1.17) is satisfied, we have $\dot{\mathbf{z}}_i = -(\nabla_{\mathbf{z}_i} U \cdot \mathbf{g}_i) \mathbf{g}_i$ (see (1.8)), and the energy dissipation inequality

$$(1.18) \quad \frac{d}{dt} U(\mathbf{Z}) = \sum_{i=1}^N \nabla_{\mathbf{z}_i} U \cdot \dot{\mathbf{z}}_i = - \sum_{i=1}^N (\nabla_{\mathbf{z}_i} U \cdot \mathbf{g}_i)^2 \leq 0$$

holds. The dissipation in (1.18) is maximal when \mathbf{g}_i maximizes $\{\mathbf{j}_i \cdot \mathbf{g} : \mathbf{g} \in \mathcal{G}\}$, that is,

$$(1.19) \quad \mathbf{j}_i(\mathbf{Z}) \cdot \mathbf{g}_i \geq \mathbf{j}_i(\mathbf{Z}) \cdot \mathbf{g} \quad \text{for all } \mathbf{g} \in \mathcal{G}.$$

When $\mathbf{j}_i(\mathbf{Z}) \neq 0$, there is either only one glide direction $\mathbf{g}_i = \mathbf{g}_i(\mathbf{Z})$ that satisfies (1.19) or two distinct glide directions, denoted by $\mathbf{g}_i^- = \mathbf{g}_i^-(\mathbf{Z})$ and $\mathbf{g}_i^+ = \mathbf{g}_i^+(\mathbf{Z})$, and in this case $\mathbf{j}_i(\mathbf{Z})$ is the bisector of the angle formed by $\mathbf{g}_i^-(\mathbf{Z})$ and $\mathbf{g}_i^+(\mathbf{Z})$. In the latter case (1.17) *becomes ill-defined* and should be replaced by the differential inclusion

$$(1.20) \quad \dot{\mathbf{z}}_i \in \{(\mathbf{j}_i(\mathbf{Z}) \cdot \mathbf{g}_i^+) \mathbf{g}_i^-, (\mathbf{j}_i(\mathbf{Z}) \cdot \mathbf{g}_i^-) \mathbf{g}_i^+\}.$$

Simple examples show that, in general, differential inclusions of the type (1.20) have no solutions. Thus, following the classical theory developed by Filippov [19], it is customary to replace the set $\{(\mathbf{j}_i(\mathbf{Z}) \cdot \mathbf{g}_i^+) \mathbf{g}_i^-, (\mathbf{j}_i(\mathbf{Z}) \cdot \mathbf{g}_i^+) \mathbf{g}_i^+\}$ with its convex envelope. Thus in place of (1.20) we consider the differential inclusion

$$(1.21) \quad \dot{\mathbf{z}}_i \in \text{the segment of endpoints } (\mathbf{j}_i(\mathbf{Z}) \cdot \mathbf{g}_i^+) \mathbf{g}_i^- \text{ and } (\mathbf{j}_i(\mathbf{Z}) \cdot \mathbf{g}_i^+) \mathbf{g}_i^+.$$

Local in time existence for the system of differential inclusions (1.21) is proved in Theorem 2.17 below. Uniqueness for differential inclusions is significantly more challenging (see, e.g., the recent paper [16] and the references contained therein). In this paper we consider only a special case; see Theorem 2.17 below and section I in the supplementary materials file.

It is important to observe that (1.21) allows for motion along directions which are not glide directions. If a dislocation point \mathbf{z}_i is moving in the direction \mathbf{g}_i (according to (1.17)) and the configuration $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_N)$ arrives at a point where \mathbf{g}_i^\pm are two glide directions that are equally favorable to \mathbf{z}_i , then \mathbf{z}_i could abruptly transition from motion along \mathbf{g}_i to motion along \mathbf{g}_i^- or \mathbf{g}_i^+ (in this case that motion is governed by (1.20)). Such a motion is called *cross-slip* (see Figure 1(a)). This phenomenon will be proved rigorously in Theorem 2.19 below. We refer the reader to Chapter 9 in [27] for a discussion of cross-slip in crystals.

Another possibility is that it is more convenient for the system to bounce at a faster and faster time scale between two glide directions following the motion law in (1.21). In this last situation, macroscopically, a dislocation is able to move along a direction which is not in \mathcal{G} but belongs to the convex hull of two glide directions (see Figure 1(b)). This phenomenon is called *fine cross-slip* and is studied analytically in Theorem 2.20 below (see also [4, 11]) for the case of a single dislocation). Fine cross-slip has been observed in aluminum and chromium (see footnote 13 in [12]).

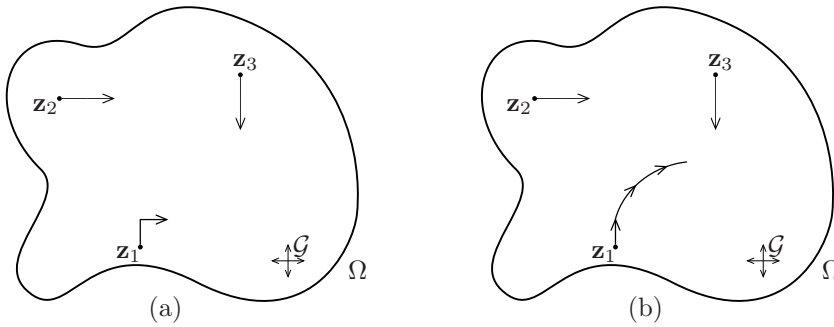


FIG. 1. *Cross-slip* (a) and *fine cross-slip* (b). The glide directions are $\mathcal{G} = \{\pm \mathbf{e}_1, \pm \mathbf{e}_2\}$, where \mathbf{e}_i is the i th basis vector. In (a), dislocation $\mathbf{z}_1 \in \Omega$ is undergoing cross-slip, switching direction from $\mathbf{g}_1^- = \mathbf{e}_2$ to $\mathbf{g}_1^+ = \mathbf{e}_1$, while dislocations \mathbf{z}_2 and \mathbf{z}_3 glide normally along directions $\mathbf{g}_2 = \mathbf{e}_1$ and $\mathbf{g}_3 = -\mathbf{e}_2$, respectively. In (b), dislocation $\mathbf{z}_1 \in \Omega$ is undergoing fine cross-slip, switching direction from $\mathbf{g}_1^- = \mathbf{e}_2$ to a curved one which is not in \mathcal{G} , while dislocations \mathbf{z}_2 and \mathbf{z}_3 glide normally along directions $\mathbf{g}_2 = \mathbf{e}_1$ and $\mathbf{g}_3 = -\mathbf{e}_2$, respectively. (Here, $N = 3$.)

Finally, it is important to remark that when many dislocations are present, the dynamics are nontrivial. Dislocations whose Burgers moduli have the same sign will repel each other, while attraction occurs if the Burgers moduli have opposite signs. This can be seen by investigating (1.9) in the case of two dislocations, and extended to an arbitrary number of dislocations by superposition, since the system (1.5) is linear. In section 3 below we will study the dynamics in some special cases, namely the unit disk, the half-plane, and the plane.

We conclude the introduction with a few remarks on previous work on the mathematical analysis of dislocations. The type of asymptotic expansion as in (1.6) was first proved by Bethuel, Brezis, and Hélein in [5] for Ginzburg–Landau vortices. The case of edge dislocations was studied in [13]. Asymptotic expansions of the type (1.6) can also be derived using Γ -convergence techniques (see, e.g., [3, 31] and the references therein for Ginzburg–Landau vortices, [15, 24, 21] for edge dislocations, and [1, 2, 9, 14, 20, 22, 23, 32] for other dislocations models). Finally, it is important to mention that here we ignore the *core energy*, that is, the energy contribution coming from the small cores that were removed to obtain J_ε . We refer the reader to [28, 34, 36] for a more detailed discussion of the core energy.

We refer the reader to [2, 8, 30, 35, 37] and the references contained therein for other results on the dynamics of dislocations. In particular, it is important to point out that, due to the discrete set of glide directions and the maximal dissipation criterion introduced in [25], our analysis significantly departs from that of Ginzburg–Landau vortices, where the motion of vortices is derived from a gradient flow (see the review paper of Serfaty [33]; see also [2]).

In forthcoming work and in collaboration with Thomas Hudson, we plan to study the behavior of dislocations as they approach the boundary and at collisions. In particular, preliminary results show that dislocations are attracted to the boundary.

The structure of this paper is as follows. Section 2 addresses the dynamics for a system of dislocations: a brief introduction on differential inclusion is presented in subsection 2.1, and the framework for the dynamics is presented in subsection 2.2. Local existence of the solutions to the dynamics problem is addressed in subsection 2.3, while subsection 2.4 deals with local uniqueness of the solution. A description of cross-slip and fine cross-slip is presented in subsection 2.5, where we give analytic proofs of the scenarios presented in [12]. In section 3 some special cases, namely the unit disk, the half-plane, and the plane, are discussed; in section 4 some numerical simulations are presented. Finally, we collect some technical proofs in the appendix.

In the supplementary materials file, we discuss the case of multiple dislocations simultaneously exhibiting fine cross-slip and how one can identify a fine cross-slip curve in the body cross-section, and we present the proof of Lemma 2.10.

2. Dislocation dynamics. We now turn our attention to the dynamics of the system \mathcal{Z} . As explained in the introduction, the direction of the motion of dislocations can change discontinuously, and this motivates its study using differential inclusions. We begin this section with some preliminaries on the theory developed by Filippov [19]. We introduce the setting for dislocation dynamics in subsections 2.1 and 2.2 and prove local existence and uniqueness in subsections 2.3 and 2.4, respectively.

2.1. Preliminaries on differential inclusions. The theory developed by Filippov [19] provides a notion of solution to an ordinary differential inclusion. Given an interval I and a set-valued function $H : D \rightarrow \mathcal{P}(\mathbb{R}^d)$, where $D \subset \mathbb{R}^{d+1}$ and $\mathcal{P}(\mathbb{R}^d)$ is the power set of \mathbb{R}^d , a *solution* on I of the differential inclusion

$$(2.1) \quad \dot{\mathbf{x}} \in H(t, \mathbf{x})$$

is an absolutely continuous function $\mathbf{x} : I \rightarrow \mathbb{R}^d$ such that $(t, \mathbf{x}(t)) \in D$ and $\dot{\mathbf{x}}(t) \in H(t, \mathbf{x}(t))$ for almost every $t \in I$.

In order to state a local existence theorem for (2.1), we need to introduce the definition of *upper semicontinuity* for a set-valued map (see [19]).

DEFINITION 2.1 (upper semicontinuity). *Given $D \subset \mathbb{R}^{d+1}$ and a set-valued function $H : D \rightarrow \mathcal{P}(\mathbb{R}^d)$, we say that H is upper semicontinuous if*

$$\sup_{\mathbf{a} \in H(\mathbf{y}_n)} \text{dist}(\mathbf{a}, H(\mathbf{y})) \rightarrow 0 \quad \text{for every } \mathbf{y}, \mathbf{y}_n \in D \text{ such that } \mathbf{y}_n \rightarrow \mathbf{y}.$$

The proof of the following theorem can be found in [19, p. 77].

THEOREM 2.2 (local existence). *Let $D \subset \mathbb{R}^{d+1}$ be open, and let $H : D \rightarrow \mathcal{P}(\mathbb{R}^d)$ be upper semicontinuous and such that $H(t, \mathbf{x})$ is nonempty, closed, bounded, and convex for every $(t, \mathbf{x}) \in D$. Then for every $(t_0, \mathbf{x}_0) \in D$ there exist $h > 0$ and a solution $\mathbf{x} : [t_0 - h, t_0 + h] \rightarrow \mathbb{R}^d$ of the problem*

$$(2.2) \quad \dot{\mathbf{x}}(t) \in H(t, \mathbf{x}(t)), \quad \mathbf{x}(t_0) = \mathbf{x}_0.$$

Moreover, if D contains a cylinder $C := [t_0 - T, t_0 + T] \times B_r(\mathbf{x}_0)$ for some $r, T > 0$, then $h \geq \min\{T, r/m\}$, where $m := \sup_{(t, \mathbf{x}) \in C} |H(t, \mathbf{x})|$.

Next we address uniqueness of solutions to (2.2). We say that *right uniqueness* holds for (2.2) at a point (t_0, \mathbf{x}_0) if there exists $t_1 > t_0$ such that any two solutions to the Cauchy problem (2.2) coincide on the subset of $[t_0, t_1]$ on which they are both defined. Similarly, we say that *left uniqueness* holds for (2.2) at a point (t_0, \mathbf{x}_0) if there exists $t_1 < t_0$ such that any two solutions to the Cauchy problem (2.2) coincide on the subset of $[t_1, t_0]$ on which they are both defined. We say that *uniqueness* holds for (2.2) at a point (t_0, \mathbf{x}_0) if both left and right uniqueness hold for (2.2) at (t_0, \mathbf{x}_0) .

Unlike the case of ordinary differential equations, for differential inclusions the question of uniqueness is significantly more delicate. We will consider here a very special case. Suppose that $V \subset \mathbb{R}^d$ is an open set and is separated into open domains V^\pm by a $(d - 1)$ -dimensional C^2 surface S . Let $\mathbf{f} : (a, b) \times (V \setminus S) \rightarrow \mathbb{R}^d$, and define $\mathbf{f}^\pm : (a, b) \times V^\pm \rightarrow \mathbb{R}^d$ as $\mathbf{f}^\pm(t, \mathbf{x}) := \mathbf{f}(t, \mathbf{x})$ for $\mathbf{x} \in V^\pm$. Assume that \mathbf{f}^\pm can both be extended in a C^1 way to $(a, b) \times V$, and denote these extensions by $\widehat{\mathbf{f}}^\pm$. Define

$$(2.3) \quad H(t, \mathbf{x}) := \begin{cases} \{\mathbf{f}(t, \mathbf{x})\} & \text{for } \mathbf{x} \notin S, \\ \text{co}\{\widehat{\mathbf{f}}^-(t, \mathbf{x}), \widehat{\mathbf{f}}^+(t, \mathbf{x})\} & \text{for } \mathbf{x} \in S, \end{cases}$$

and consider the differential inclusion (2.2). Here for a set $E \subset \mathbb{R}^d$ we denote by $\text{co}E$ the convex hull of E , that is, the smallest convex set that contains E .

It can be shown that the function H defined in (2.3) satisfies the conditions of Theorem 2.2, and local existence follows. In the following theorems, we denote by $\mathbf{n}(\mathbf{x}_0)$ the unit normal to S at $\mathbf{x}_0 \in S$ directed from V^- to V^+ . The following theorem can be found in [19, p. 110].

THEOREM 2.3 (local uniqueness). *Let $H : (a, b) \times V \rightarrow \mathcal{P}(\mathbb{R}^d)$ be given as in (2.3), where \mathbf{f} , V , and S are as above. If $(t_0, \mathbf{x}_0) \in (a, b) \times S$ is such that $\widehat{\mathbf{f}}^-(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) > 0$ or $\widehat{\mathbf{f}}^+(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) < 0$, then right uniqueness holds for (2.2) at the point (t_0, \mathbf{x}_0) .*

Similarly, if $\widehat{\mathbf{f}}^-(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) < 0$ or $\widehat{\mathbf{f}}^+(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) > 0$, then left uniqueness holds for (2.2) at the point (t_0, \mathbf{x}_0) .

Next we discuss cross-slip and fine cross-slip.

THEOREM 2.4 (cross-slip; Corollary 1, p. 107 in [19]). *Let $(t_0, \mathbf{x}_0) \in (a, b) \times S$ be such that $\widehat{\mathbf{f}}^-(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) > 0$ and $\widehat{\mathbf{f}}^+(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) > 0$. Then uniqueness holds for (2.2) at the point (t_0, \mathbf{x}_0) . Moreover, the unique solution \mathbf{x} to (2.2) passes from V^- to V^+ ; that is, there exists $t_1 < t_0 < t_2$ such that $\mathbf{x}(t)$ belongs to V^- for $t \in [t_1, t_0)$ and to V^+ for $t \in (t_0, t_2]$. Similarly, if $\widehat{\mathbf{f}}^-(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) < 0$ and $\widehat{\mathbf{f}}^+(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) < 0$,*

then uniqueness holds for (2.2) at the point (t_0, \mathbf{x}_0) and the unique solution passes from V^+ to V^- .

THEOREM 2.5 (Corollary 2, p. 108 in [19]). *Let $(t_0, \mathbf{x}_0) \in (a, b) \times S$ be such that*

$$(2.4) \quad \widehat{\mathbf{f}}^-(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) > 0 \quad \text{and} \quad \widehat{\mathbf{f}}^+(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0) < 0.$$

Then there exists $a \leq t_1 < t_0$ such that the problem (2.1) admits exactly one solution curve \mathbf{x}^- with $\mathbf{x}^-(t) \in V^-$ for $t \in (t_1, t_0)$ and $\mathbf{x}^-(t_0) = \mathbf{x}_0$ and exactly one solution curve \mathbf{x}^+ with $\mathbf{x}^+(t) \in V^+$ for $t \in (t_1, t_0)$ and $\mathbf{x}^+(t_0) = \mathbf{x}_0$.

LEMMA 2.6. *Assume that the conditions (2.4) hold for $(t_0, \mathbf{x}_0) \in (a, b) \times S$. Let $\mathbf{x}(t)$ be a solution to $\dot{\mathbf{x}} = \widehat{\mathbf{f}}^+(t, \mathbf{x})$ on an interval $[t_0, T]$ with $\mathbf{x}(t_0) = \mathbf{x}_0 \in S$. Then there exists $\delta > 0$ such that $\mathbf{x}(t) \in V^- \cap U$ for $t \in (t_0, t_0 + \delta)$. Similarly, if $\dot{\mathbf{x}} = \widehat{\mathbf{f}}^-(t, \mathbf{x})$ on an interval $[t_0, T]$ with $\mathbf{x}(t_0) = \mathbf{x}_0 \in S$, then there exists $\delta > 0$ such that $\mathbf{x}(t) \in V^+ \cap U$ for $t \in (t_0, t_0 + \delta)$.*

Proof. Let $h := \min\{-\widehat{\mathbf{f}}^+(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0), \widehat{\mathbf{f}}^-(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0)\}$. Then $h > 0$ by hypothesis, and therefore, by continuity of $\widehat{\mathbf{f}}^\pm$ and \mathbf{n} , there exist neighborhoods I_0 and U_0 of t_0 and \mathbf{x}_0 , respectively, such that $\widehat{\mathbf{f}}^+(t, \mathbf{x}) \cdot \mathbf{n}(\tilde{\mathbf{x}}) < -\frac{1}{2}h$ and $\widehat{\mathbf{f}}^-(t, \mathbf{x}) \cdot \mathbf{n}(\tilde{\mathbf{x}}) > \frac{1}{2}h$ for $(t, \mathbf{x}) \in I_0 \times U_0$ and $\tilde{\mathbf{x}} \in U_0 \cap S$.

We can write S locally as the graph of a function. Denoting points $\mathbf{x} = (\boldsymbol{\xi}, y) \in \mathbb{R}^{d-1} \times \mathbb{R}$, there is $r > 0$ such that we can write (without loss of generality) $S \cap B_r(\mathbf{x}_0) = \{(\boldsymbol{\xi}, y) \in B_r(\mathbf{x}_0) : y = \Phi(\boldsymbol{\xi})\}$ for some Φ of class C^2 . The sets V^\pm are locally defined as $V^+ \cap B_r(\mathbf{x}_0) = \{(\boldsymbol{\xi}, y) \in B_r(\mathbf{Z}_0) : y > \Phi(\boldsymbol{\xi})\}$ and $V^- \cap B_r(\mathbf{x}_0) = \{(\boldsymbol{\xi}, y) \in B_r(\mathbf{Z}_0) : y < \Phi(\boldsymbol{\xi})\}$. By rotating the coordinate axes, if necessary, we can assume that the tangent hyperplane to S at \mathbf{x}_0 is $\{(\boldsymbol{\xi}, y) : y = 0\}$ so that $\nabla\Phi(\boldsymbol{\xi}_0) = \mathbf{0}$, where $\mathbf{x}_0 = (\boldsymbol{\xi}_0, y_0)$. Then the unit normal to S at \mathbf{x}_0 is $\mathbf{n}(\mathbf{x}_0) = \mathbf{n}(\boldsymbol{\xi}_0, \Phi(\boldsymbol{\xi}_0)) = (\mathbf{0}, 1)$.

Consider the solution to $\dot{\mathbf{x}} = \widehat{\mathbf{f}}^+(t, \mathbf{x})$ with $\mathbf{x}(t_0) = \mathbf{x}_0$. Since \mathbf{x} is continuous, there is $\delta_1 > 0$ such that $\mathbf{x}(t) \in U_0$ for $t \in (t_0, t_0 + \delta_1)$, and in this interval it satisfies $\mathbf{x}(t) = \mathbf{x}_0 + \int_{t_0}^t \widehat{\mathbf{f}}^+(s, \mathbf{x}(s)) ds$. Hence,

$$(2.5) \quad y(t) = \mathbf{x}(t) \cdot \mathbf{n}(\mathbf{x}_0) = \mathbf{x}_0 \cdot \mathbf{n}(\mathbf{x}_0) + \int_{t_0}^t \widehat{\mathbf{f}}^+(s, \mathbf{x}(s)) \cdot \mathbf{n}(\mathbf{x}_0) ds < y_0 - \frac{h}{2}(t - t_0).$$

Writing $\mathbf{x}(t) = (\boldsymbol{\xi}(t), y(t))$, we have $\mathbf{x}(t) \cdot \mathbf{n}(\mathbf{x}_0) = y(t)$. Additionally, $\Phi(\boldsymbol{\xi}(t)) = \Phi(\boldsymbol{\xi}(t_0)) + \nabla\Phi(\boldsymbol{\xi}(t_0)) \cdot (\boldsymbol{\xi}(t) - \boldsymbol{\xi}(t_0)) + o(t - t_0) = y_0 + o(t - t_0)$. Therefore, (2.5) implies there is $\delta < \delta_1$ such that

$$y(t) < \Phi(\boldsymbol{\xi}(t)) - \frac{h}{2}(t - t_0) + o(t - t_0) < \Phi(\boldsymbol{\xi}(t))$$

for $t \in (t_0, t_0 + \delta)$. Thus, $\mathbf{x}(t) = (\boldsymbol{\xi}(t), y(t)) \in V^- \cap B_r(\mathbf{x}_0)$ for $t \in (t_0, t_0 + \delta)$. The proof of the result for solutions to $\dot{\mathbf{x}} = \widehat{\mathbf{f}}^-(t, \mathbf{x})$ is similar. \square

COROLLARY 2.7 (fine cross-slip). *Assume that the conditions (2.4) hold for $(t_0, \mathbf{x}_0) \in (a, b) \times S$. Then there exist $\delta > 0$ and a unique solution \mathbf{x} defined on $[t_0, t_0 + \delta)$ to the initial value problem (2.2) that is confined to S .*

Proof. Existence and uniqueness are consequences of Theorems 2.2 and 2.3. Let T be the maximal existence time provided by Theorem 2.2.

As in the proof of Lemma 2.6, there are neighborhoods I_0 and U_0 of t_0 and \mathbf{x}_0 , respectively, such that $\widehat{\mathbf{f}}^+(t, \mathbf{x}) \cdot \mathbf{n}(\tilde{\mathbf{x}}) < -\frac{1}{2}h$ and $\widehat{\mathbf{f}}^-(t, \mathbf{x}) \cdot \mathbf{n}(\tilde{\mathbf{x}}) > \frac{1}{2}h$ for $(t, \mathbf{x}) \in I_0 \times U_0$ and $\tilde{\mathbf{x}} \in U_0 \cap S$, with $h = \min\{-\widehat{\mathbf{f}}^+(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0), \widehat{\mathbf{f}}^-(t_0, \mathbf{x}_0) \cdot \mathbf{n}(\mathbf{x}_0)\}$. By continuity of $\mathbf{x}(t)$, there exists $\delta > 0$ such that $\mathbf{x}(t) \in U_0$ for $t \in (t_0, t_0 + \delta)$. Suppose there

is $t_1 \in (t_0, t_0 + \delta)$ such that $\mathbf{x}(t_1) \notin S$. Without loss of generality, we can assume $\mathbf{x}(t_1) \in V^+$, and we define

$$s_1 := \sup\{s \in [t_0, t_1) : \mathbf{x}(s) \notin V^+\};$$

i.e., s_1 is the last time $\mathbf{x}(t)$ belongs to S before entering V^+ and remaining in V^+ for $t \in (s_1, t_1]$. It follows that $\mathbf{x}(t)$ solves $\dot{\mathbf{x}} = \widehat{\mathbf{f}}^+(t, \mathbf{x})$ on $[s_1, t_1]$ with $\mathbf{x}(s_1) \in S$. Since the hypotheses of Lemma 2.6 are satisfied, there is a unique solution to $\dot{\mathbf{x}} = \widehat{\mathbf{f}}^+(t, \mathbf{x})$ on $[s_1, s_1 + \widehat{\delta}]$ for some $\widehat{\delta} > 0$, where $\mathbf{x}(t) \in V^-$ for $t \in (s_1, s_1 + \widehat{\delta})$. This contradicts the fact that $\mathbf{x}(t) \in V^+$ on $[s_1, t_1]$. We conclude that $\mathbf{x}(t) \in S$ for $t \in [t_0, t_0 + \delta)$. \square

Remark 2.8. In view of Corollary 2.7, the velocity field $\dot{\mathbf{x}}$ is tangent to S , and therefore it must be orthogonal to $\mathbf{n}(\mathbf{x})$ for $\mathbf{x} \in S$. Moreover, by (2.3), $\dot{\mathbf{x}}$ belongs to $\text{co}\{\widehat{\mathbf{f}}^-(t, \mathbf{x}), \widehat{\mathbf{f}}^+(t, \mathbf{x})\}$, and so

$$\dot{\mathbf{x}} = \mathbf{f}^0(t, \mathbf{x}) \in H(t, \mathbf{x}), \quad \text{where } \mathbf{f}^0(t, \mathbf{x}) := \alpha \widehat{\mathbf{f}}^+(t, \mathbf{x}) + (1 - \alpha) \widehat{\mathbf{f}}^-(t, \mathbf{x})$$

and $\alpha = \alpha(t, \mathbf{x}) \in (0, 1)$ is given by

$$\alpha = \frac{\widehat{\mathbf{f}}^-(t, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x})}{\widehat{\mathbf{f}}^-(t, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) - \widehat{\mathbf{f}}^+(t, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x})},$$

since $\mathbf{f}^0(t, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = 0$.

2.2. Setting for the dynamics. We now turn our attention to the dynamics of the system \mathcal{Z} . As described in the introduction (see (1.20)) the problem consists in solving the system of differential inclusions

$$\begin{cases} \dot{\mathbf{z}}_\ell \in F_\ell(\mathbf{Z}), \\ \mathbf{z}_\ell(0) = \mathbf{z}_{\ell,0}, \end{cases}$$

where

$$\mathbf{Z} := (\mathbf{z}_1, \dots, \mathbf{z}_N) \quad \text{and} \quad \mathbf{Z}_0 := (\mathbf{z}_{1,0}, \dots, \mathbf{z}_{N,0})$$

belong to $\Omega^N \subset \mathbb{R}^{2N}$ and, for $\ell = 1, \dots, N$,

$$(2.6) \quad F_\ell(\mathbf{Z}) := \left\{ (\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}) \mathbf{g} : \mathbf{g} \in \arg \max_{\mathbf{g}' \in \mathcal{G}} \{ \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}' \} \right\},$$

where we recall that

$$(2.7) \quad \mathbf{j}_i(\mathbf{z}_i) = b_i \mathbf{JL} \left[\sum_{j \neq i} \mathbf{k}_j(\mathbf{z}_i; \mathbf{z}_j) + \nabla u_0(\mathbf{z}_i; \mathbf{z}_1, \dots, \mathbf{z}_N) \right],$$

with \mathbf{k}_j and u_0 given in (1.10) and (1.13), respectively.

Setting

$$(2.8) \quad \mathcal{G}_\ell(\mathbf{Z}) := \arg \max_{\mathbf{g}' \in \mathcal{G}} \{ \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}' \},$$

the unit vectors $\mathbf{g} \in \mathcal{G}_\ell(\mathbf{Z})$ represent the glide directions *closest to* $\mathbf{j}_\ell(\mathbf{Z})$ (see [12]), that is,

$$(2.9) \quad \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g} \geq \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}' \quad \text{for all } \mathbf{g}' \in \mathcal{G}.$$

We recall that when $\mathbf{j}_\ell(\mathbf{Z}) \neq \mathbf{0}$, the set F_ℓ can either contain a single element, which we will call $\mathbf{g}_\ell(\mathbf{Z})$, or two distinct elements, denoted by $\mathbf{g}_\ell^-(\mathbf{Z})$ and $\mathbf{g}_\ell^+(\mathbf{Z})$, and in this case $\mathbf{j}_\ell(\mathbf{z}_\ell)$ is the bisector of the angle formed by \mathbf{g}_ℓ^- and \mathbf{g}_ℓ^+ .

Remark 2.9. Notice that if $\mathbf{j}_\ell(\mathbf{Z}) = \mathbf{0}$, then any glide direction $\mathbf{g} \in \mathcal{G}$ satisfies (2.9), and therefore $\mathcal{G}_\ell(\mathbf{Z}) = \mathcal{G}$.

In view of the comments above, we have

$$(2.10) \quad F_\ell(\mathbf{Z}) = \begin{cases} \{\mathbf{0}\} & \text{if } \mathbf{j}_\ell(\mathbf{Z}) = \mathbf{0}, \\ \{(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_\ell(\mathbf{Z})) \mathbf{g}_\ell(\mathbf{Z})\} & \text{if } \mathbf{j}_\ell(\mathbf{Z}) \neq \mathbf{0} \text{ and } \mathcal{G}_\ell(\mathbf{Z}) = \{\mathbf{g}_\ell(\mathbf{Z})\}, \\ \{(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_\ell^\pm(\mathbf{Z})) \mathbf{g}_\ell^\pm(\mathbf{Z})\} & \text{if } \mathbf{j}_\ell(\mathbf{Z}) \neq \mathbf{0} \text{ and } \mathcal{G}_\ell(\mathbf{Z}) = \{\mathbf{g}_\ell^\pm(\mathbf{Z})\}, \end{cases}$$

and the problem becomes

$$(2.11) \quad \begin{cases} \dot{\mathbf{Z}} \in F(\mathbf{Z}), \\ \mathbf{Z}(0) = \mathbf{Z}_0, \end{cases}$$

where

$$(2.12) \quad F(\mathbf{Z}) := F_1(\mathbf{Z}) \times \cdots \times F_N(\mathbf{Z}) \subset \mathbb{R}^{2N}.$$

The domain of the set-valued function F must be chosen in such a way that the forces $\mathbf{j}_\ell(\mathbf{Z})$ are well defined, and so collisions must be avoided. We denote by

$$(2.13) \quad \Pi_{jk} := \{\mathbf{Z} \in \Omega^N : \mathbf{z}_j = \mathbf{z}_k, j \neq k\}$$

the set where dislocations \mathbf{z}_j and \mathbf{z}_k collide, and we define the domain of F to be

$$(2.14) \quad \mathcal{D}(F) := \Omega^N \setminus \bigcup_{j < k} \Pi_{jk}.$$

Recall that the force \mathbf{j}_i is not defined for $\mathbf{z}_\ell \in \partial\Omega$. Since Ω is open, boundary collisions are also excluded from $\mathcal{D}(F)$.

2.3. Local existence. Following section 2.2, and in view of (2.11) and (2.12), we consider the differential inclusion

$$(2.15) \quad \begin{cases} \dot{\mathbf{Z}} \in \text{co } F(\mathbf{Z}), \\ \mathbf{Z}(0) = \mathbf{Z}_0. \end{cases}$$

The following lemma shows that the convex hull of $F(\mathbf{Z})$ is given by

$$(2.16) \quad \hat{F}(\mathbf{Z}) := (\text{co } F_1(\mathbf{Z})) \times \cdots \times (\text{co } F_N(\mathbf{Z})),$$

where, by (2.10),

$$(2.17) \quad \text{co } F_\ell(\mathbf{Z}) = \begin{cases} \{\mathbf{0}\} & \text{if } \mathbf{j}_\ell(\mathbf{Z}) = \mathbf{0}, \\ \{(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_\ell(\mathbf{Z})) \mathbf{g}_\ell(\mathbf{Z})\} & \text{if } \mathbf{j}_\ell(\mathbf{Z}) \neq \mathbf{0} \text{ and } \mathcal{G}_\ell(\mathbf{Z}) = \{\mathbf{g}_\ell(\mathbf{Z})\}, \\ \Sigma_\ell(\mathbf{Z}) & \text{if } \mathbf{j}_\ell(\mathbf{Z}) \neq \mathbf{0} \text{ and } \mathcal{G}_\ell(\mathbf{Z}) = \{\mathbf{g}_\ell^\pm(\mathbf{Z})\}, \end{cases}$$

with $\Sigma_\ell(\mathbf{Z})$ the segment of endpoints $(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_\ell^-(\mathbf{Z})) \mathbf{g}_\ell^-(\mathbf{Z})$ and $(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_\ell^+(\mathbf{Z})) \mathbf{g}_\ell^+(\mathbf{Z})$.

The proof is simple, and for the convenience of the reader it can be found in the supplementary materials file.

LEMMA 2.10. *Let $F_\ell(\mathbf{Z})$ be defined as in (2.6) for $\ell = 1, \dots, N$, and let $F(\mathbf{Z})$ be as in (2.12). Then $\text{co } F(\mathbf{Z}) = \hat{F}(\mathbf{Z})$, where $\hat{F}(\mathbf{Z})$ is defined in (2.16).*

Lemma 2.10 is useful for understanding the dynamics in Ω rather than in Ω^N . Each \mathbf{z}_i moves in some direction $\mathbf{g}_i \in \mathcal{G}$, unless the arg max in (2.8) is multivalued, in which case \mathbf{z}_i moves in a direction belonging to the convex hull of \mathbf{g}_i^+ and \mathbf{g}_i^- . Lemma 2.10 makes this precise and validates the use of (2.15) as our model for dislocation motion.

LEMMA 2.11. *Let $\mathcal{D}(F)$ be as defined in (2.14). Then the set-valued map $F : \mathcal{D}(F) \rightarrow \mathcal{P}(\mathbb{R}^{2N})$ defined in (2.12) is upper semicontinuous (according to Definition 2.1).*

Proof. Let $\mathbf{Z}_*, \mathbf{Z}_n \in \mathcal{D}(F)$ be such that $\mathbf{Z}_n \rightarrow \mathbf{Z}_*$ as $n \rightarrow \infty$. We need to show that

$$\sup_{\mathbf{Z} \in F(\mathbf{Z}_n)} \text{dist}(\mathbf{Z}, F(\mathbf{Z}_*)) \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

Since $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_N)$, $\mathbf{z}_\ell \in \mathbb{R}^2$, and $F(\mathbf{Z})$ is a Cartesian product (see (2.12)), it suffices to show that for every $\ell \in \{1, \dots, N\}$,

$$\sup_{\mathbf{z} \in F_\ell(\mathbf{Z}_n)} \text{dist}(\mathbf{z}, F_\ell(\mathbf{Z}_*)) \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

Fix $\ell \in \{1, \dots, N\}$. We consider the two cases $\mathbf{j}_\ell(\mathbf{Z}_*) = 0$ and $\mathbf{j}_\ell(\mathbf{Z}_*) \neq 0$.

If $\mathbf{j}_\ell(\mathbf{Z}_*) = 0$, then by (2.10), $F_\ell(\mathbf{Z}_*) = \{\mathbf{0}\}$. In turn, again by (2.10), the continuity of \mathbf{j}_ℓ (cf. (2.14)) shows that

$$\sup_{\mathbf{z} \in F_\ell(\mathbf{Z}_n)} \|\mathbf{z}\| \leq \|\mathbf{j}_\ell(\mathbf{Z}_n)\| \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

If $\mathbf{j}_\ell(\mathbf{Z}_*) \neq \mathbf{0}$, then, again by continuity of \mathbf{j}_ℓ , $\mathbf{j}_\ell(\mathbf{Z}_n) \neq \mathbf{0}$ for all $n \geq \bar{n}$ and for some $\bar{n} \in \mathbb{N}$. Taking \bar{n} larger, if necessary, we claim that $\mathbf{g}_\ell^-(\mathbf{Z}_n), \mathbf{g}_\ell^+(\mathbf{Z}_n) \in \{\mathbf{g}_\ell^-(\mathbf{Z}_*), \mathbf{g}_\ell^+(\mathbf{Z}_*)\}$ for $n \geq \bar{n}$. Arguing by contradiction, if the claim fails, since \mathcal{G} is finite, there exists $\mathbf{e} \in \mathcal{G} \setminus \{\mathbf{g}_\ell^\pm(\mathbf{Z}_*)\}$ such that $\mathbf{g}_\ell^-(\mathbf{Z}_n) = \mathbf{e}$ or $\mathbf{g}_\ell^+(\mathbf{Z}_n) = \mathbf{e}$ for infinitely many n . By (2.9) and (2.8), $\mathbf{j}_\ell(\mathbf{Z}_n) \cdot \mathbf{e} \geq \mathbf{j}_\ell(\mathbf{Z}_n) \cdot \mathbf{g}$ for all $\mathbf{g} \in \mathcal{G}$ and for infinitely many n . Letting $n \rightarrow \infty$ and using the continuity of \mathbf{j}_ℓ , it follows that $\mathbf{j}_\ell(\mathbf{Z}_*) \cdot \mathbf{e} \geq \mathbf{j}_\ell(\mathbf{Z}_*) \cdot \mathbf{g}$ for all $\mathbf{g} \in \mathcal{G}$, which implies that $\mathbf{e} \in \mathcal{G}_\ell(\mathbf{Z}_*)$, which is a contradiction. Thus the claim holds.

In particular, we have shown that $F_\ell(\mathbf{Z}_n) = \{(\mathbf{j}_\ell(\mathbf{Z}_n) \cdot \mathbf{g}_\ell^\pm(\mathbf{Z}_*)) \mathbf{g}_\ell^\pm(\mathbf{Z}_*)\}$ for $n \geq \bar{n}$, and hence

$$\sup_{\mathbf{z} \in F_\ell(\mathbf{Z}_n)} \text{dist}(\mathbf{z}, F_\ell(\mathbf{Z}_*)) \leq \|\mathbf{j}_\ell(\mathbf{Z}_n) - \mathbf{j}_\ell(\mathbf{Z}_*)\| \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

This concludes the proof. \square

COROLLARY 2.12. *Let $F : \mathcal{D}(F) \rightarrow \mathcal{P}(\mathbb{R}^{2N})$ be defined by (2.12) and (2.14), and consider the set-valued map $\text{co} F(\mathbf{Z})$, $\mathbf{Z} \in \mathcal{D}(G)$. Then $\text{co} F(\mathbf{Z})$ is nonempty, closed, and convex for every $\mathbf{Z} \in \mathcal{D}(F)$, and $\text{co} F$ is upper semicontinuous.*

Proof. For all $\mathbf{Z} \in \mathcal{D}(F)$, the set $\text{co} F(\mathbf{Z})$ is nonempty because $F(\mathbf{Z})$ is nonempty. By definition of convexification, $\text{co} F(\mathbf{Z})$ is closed and convex. By Lemma 2.11, the set-valued map F is upper semicontinuous, and therefore so is $\text{co} F$ (see Lemma 16, p. 66 in [19]). This corollary is proved. \square

Note that $\text{co} F$ is not bounded on $\mathcal{D}(F)$ because $|\mathbf{z}_i - \mathbf{z}_j|$ and $\text{dist}(\mathbf{z}_i, \partial\Omega)$ can become arbitrarily small, and thus \mathbf{j}_i can become unbounded (see (1.9) and (1.10)).

THEOREM 2.13 (local existence). *Let $\Omega \subset \mathbb{R}^2$ be a connected open set. Let $F : \mathcal{D}(F) \rightarrow \mathcal{P}(\mathbb{R}^{2N})$ be defined as in (2.12) and (2.14) with each F_ℓ as in (2.10),*

and let $\mathbf{Z}_0 \in \mathcal{D}(F)$ be a given initial configuration of dislocations. Then there exists a solution $\mathbf{Z} : [-T, T] \rightarrow \mathcal{D}(F)$ to (2.15), with $T \geq r_0/m_0$, where

$$(2.18) \quad 0 < r_0 < \text{dist}(\mathbf{Z}_0, \partial\mathcal{D}(F)) \text{ and } m_0 := \max_{\mathbf{Z} \in B(\mathbf{Z}_0, r_0)} \left(\sum_{\ell=1}^N |\mathbf{j}_\ell(\mathbf{Z})|^2 \right)^{1/2}.$$

Proof. The function F is bounded on the ball $B(\mathbf{Z}_0, r_0) \subset \mathcal{D}(F)$. Hence, by Corollary 2.12, the set-valued map $\text{co} F$ satisfies the conditions of Theorem 2.2 in $B(\mathbf{Z}_0, r_0)$, and thus local existence holds. \square

Remark 2.14. In view of (2.14) and (2.18), solutions to the problem (2.15) exist as long as dislocations stay away from $\partial\Omega$ and do not collide.

2.4. Local uniqueness. The set where dislocations can move in either of two different glide directions is called the *ambiguity set* and is denoted by \mathcal{A} . To be precise, we define

$$(2.19) \quad \mathcal{A} := \bigcup_{\ell=1}^N \mathcal{A}_\ell, \quad \text{where } \mathcal{A}_\ell := \{\mathbf{Z} \in \mathcal{D}(F) : \text{card}(\mathcal{G}_\ell(\mathbf{Z})) = 2\},$$

and $\mathcal{G}_\ell(\mathbf{Z})$ is defined in (2.8). On \mathcal{A}_ℓ the direction of the Peach–Köhler force \mathbf{j}_ℓ bisects two different glide directions that are closest to it. Note that $\mathbf{j}_\ell(\mathbf{Z}) \neq \mathbf{0}$ for $\mathbf{Z} \in \mathcal{A}_\ell$ because $\text{card}(\mathcal{G}) \geq 4$ by assumption (1.15) and since $\mathbf{g} \in \mathcal{G}$ implies $-\mathbf{g} \in \mathcal{G}$.

The uniqueness results in subsection 2.1 can only be applied at points $\mathbf{Z}_0 \in \mathcal{A}$ in which the ambiguity set \mathcal{A} is locally a $(2N - 1)$ -dimensional smooth surface separating $\mathcal{D}(F)$ into two open sets in a neighborhood of \mathbf{Z}_0 . In this subsection, we show that \mathcal{A} is a $(2N - 1)$ -dimensional smooth surface outside of a “singular set” and we estimate the Hausdorff dimension of this set.

LEMMA 2.15. *For all $\ell \in \{1, \dots, N\}$ the functions $\mathbf{j}_\ell(\mathbf{z}_1, \dots, \mathbf{z}_N)$ are analytic on any compact subset of $\mathcal{D}(F)$.*

Proof. Observe that if a smooth function v satisfies the partial differential equation $\text{div}(\mathbf{L}\nabla v) = 0$ in Ω , then the function $w(x_1, x_2) := v(\lambda x_1, x_2)$ satisfies the partial differential equation $\Delta w = 0$ in an open set U . Hence, without loss of generality, we may assume that $\lambda = 1$ (i.e., $\mathbf{L} = \mu\mathbf{I}$) so that (1.12a) and (1.13) reduce to

$$(2.20) \quad \Delta_{\mathbf{y}} \mathbf{k}_j(\mathbf{x}; \mathbf{y}) = \mathbf{0}, \quad (\mathbf{x}, \mathbf{y}) \in \mathbb{R}^2 \times \mathbb{R}^2, \mathbf{x} \neq \mathbf{y},$$

and, for fixed $\mathbf{z}_1, \dots, \mathbf{z}_N \in \Omega$,

$$(2.21) \quad \begin{cases} \Delta_{\mathbf{x}} u_0(\mathbf{x}; \mathbf{z}_1, \dots, \mathbf{z}_N) = 0, & \mathbf{x} \in \Omega, \\ \nabla_{\mathbf{x}} u_0(\mathbf{x}; \mathbf{z}_1, \dots, \mathbf{z}_N) \cdot \mathbf{n}(\mathbf{x}) = -\sum_{i=1}^N \mathbf{k}_i(\mathbf{x}; \mathbf{z}_i) \cdot \mathbf{n}(\mathbf{x}), & \mathbf{x} \in \partial\Omega. \end{cases}$$

A solution to (2.21) is given by

$$(2.22) \quad u_0(\mathbf{x}; \mathbf{z}_1, \dots, \mathbf{z}_N) = \int_{\partial\Omega} G(\mathbf{x}, \mathbf{y}) \sum_{i=1}^N \mathbf{k}_i(\mathbf{y}; \mathbf{z}_i) \cdot \mathbf{n}(\mathbf{y}) \, ds(\mathbf{y}),$$

where G is the Green’s function for the Neumann problem. Consider u_0 as a function in $\Omega^{N+1} \subset \mathbb{R}^{2N+2}$. Fix $K_i \subset\subset \Omega$ for $i = 0, \dots, N$. If $(\mathbf{x}, \mathbf{Z}) \in K := K_0 \times K_1 \times \dots \times K_N$, then the integrand in (2.22) is uniformly bounded, and we can find the derivatives of u_0 with respect to each $z_{i,m}$ by differentiating under the integral sign in (2.22).

Using (2.20), (2.21), and (2.22) we have

$$\begin{aligned} \Delta_{(\mathbf{x}, \mathbf{z})} u_0 &= \Delta_{\mathbf{x}} u_0 + \Delta_{\mathbf{z}_1} u_0 + \cdots + \Delta_{\mathbf{z}_N} u_0 \\ &= 0 + \sum_{i=1}^N \int_{\partial\Omega} G(\mathbf{x}, \mathbf{y}) \Delta_{\mathbf{z}_i} (\mathbf{k}_i(\mathbf{y}; \mathbf{z}_i) \cdot \mathbf{n}(\mathbf{y})) \, ds(\mathbf{y}) = 0. \end{aligned}$$

Observe that in a small ball around $(\mathbf{x}, \mathbf{Z}) \in K$, u_0 is a C^2 function in each variable because the formula (2.22) has singularities only on the boundary. Since a harmonic C^2 function on an open set is analytic in that set (cf. [18, Chapter 2]), we deduce that u_0 is analytic in the interior of Ω^{N+1} , and thus $u_0(\mathbf{z}_i; \mathbf{Z})$ is also analytic (though possibly no longer harmonic). By (2.7) we have that \mathbf{j}_ℓ is analytic away from the boundary and away from collisions because in this case each $\mathbf{k}_i(\mathbf{z}_\ell; \mathbf{z}_i)$ is harmonic in both \mathbf{z}_ℓ and \mathbf{z}_i . \square

Fix $\mathbf{Z}^* \in \mathcal{A}_\ell$. There are two maximizing glide directions for \mathbf{z}_ℓ , denoted by $\mathbf{g}_\ell^+(\mathbf{Z}^*)$ and $\mathbf{g}_\ell^-(\mathbf{Z}^*)$ (i.e., $\mathcal{G}_\ell(\mathbf{Z}^*) = \{\mathbf{g}_\ell^+(\mathbf{Z}^*), \mathbf{g}_\ell^-(\mathbf{Z}^*)\}$, as defined in (2.8)). For simplicity we will write $\mathbf{g}_\ell^\pm := \mathbf{g}_\ell^\pm(\mathbf{Z}^*)$. Let $B_h(\mathbf{Z}^*)$ be a ball around \mathbf{Z}^* with radius $h > 0$ small enough so that $B_h(\mathbf{Z}^*) \subset \mathcal{D}(F)$, and for any $\mathbf{Z} \in B_h(\mathbf{Z}^*)$ one of the following three possibilities holds: $\mathcal{G}_\ell(\mathbf{Z}) = \{\mathbf{g}_\ell^+\}$, $\mathcal{G}_\ell(\mathbf{Z}) = \{\mathbf{g}_\ell^-\}$, or $\mathcal{G}_\ell(\mathbf{Z}) = \{\mathbf{g}_\ell^+, \mathbf{g}_\ell^-\}$. Such an h exists because of the continuity of \mathbf{j}_ℓ and the fact that $\mathbf{j}_\ell(\mathbf{Z}^*) \neq \mathbf{0}$ (cf. the discussion following (2.19)). We denote by $\mathbf{g}_0 \in \mathbb{R}^2$ the vector

$$(2.23) \quad \mathbf{g}_0 := \mathbf{g}_\ell^+ - \mathbf{g}_\ell^-,$$

which is a well-defined constant vector for $\mathbf{Z} \in B_h(\mathbf{Z}^*)$ (see the proof of Lemma 2.11). Note that if $\partial^\beta \mathbf{j}_\ell(\mathbf{Z}^*) \cdot \mathbf{g}_0 \neq 0$ for some multi-index $\beta = (\beta_1, \dots, \beta_N) \in \mathbf{N}_0^N$ with $|\beta| = 1$, then \mathcal{A}_ℓ is locally a smooth manifold. With \mathbf{g}_0 as in (2.23), we define the *singular sets*

$$(2.24) \quad \mathcal{S}_\ell := \{\mathbf{Z} \in \mathcal{A}_\ell : \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0 = 0, \nabla_{\mathbf{Z}}(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0) = \mathbf{0}\}, \quad \ell = 1, \dots, N.$$

Each \mathcal{S}_ℓ contains the points where \mathcal{A}_ℓ could fail to be a manifold and is an obstruction to uniqueness of solutions to (2.15).

We now estimate the Hausdorff dimension of the singular sets. We adapt an argument from [26], which follows [10]; recall that $\mathcal{S}_\ell \subset \mathbb{R}^{2N}$, $\ell = 1, \dots, N$.

LEMMA 2.16. *Let \mathcal{S}_ℓ be defined as in (2.24). Then $\dim(\mathcal{S}_\ell) \leq 2N - 2$.*

Proof. Fix $\ell \in \{1, \dots, N\}$ and $\mathbf{Z}^* \in \mathcal{A}_\ell$. As in the discussion above, set $\mathbf{g}_0 := \mathbf{g}_\ell^+ - \mathbf{g}_\ell^- \in \mathbb{R}^2 \setminus \{\mathbf{0}\}$, where \mathbf{g}_ℓ^\pm are uniquely defined in $B_h(\mathbf{Z}^*)$ for $h > 0$ small enough.

We will be considering derivatives in all the \mathbf{z}_i directions except for $i = \ell$. For this purpose, we introduce the notations $\Delta_{\widehat{\mathbf{z}}_\ell}$, $\nabla_{\widehat{\mathbf{z}}_\ell}$, and $D_{\widehat{\mathbf{z}}_\ell}^2$ to denote the Laplacian, the gradient, and the Hessian with respect to $\mathbf{z}_1, \dots, \mathbf{z}_{\ell-1}, \mathbf{z}_{\ell+1}, \dots, \mathbf{z}_N$, respectively. We also write N_ℓ for the set of multi-indices α such that ∂^α does not contain any derivatives in the \mathbf{z}_ℓ directions, that is,

$$(2.25) \quad N_\ell := \{\alpha \in \mathbb{N}_0^{2N} : \alpha = (\alpha_1, \dots, \alpha_{\ell-1}, \mathbf{0}, \alpha_{\ell+1}, \dots, \alpha_N)\}.$$

For $m \geq 2$ we define

$$\begin{aligned} \widetilde{M}_\ell^m := \{ & \mathbf{Z} : \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0 = 0, \partial^\alpha(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0) = 0 \text{ for all } \alpha \in N_\ell \text{ such that } |\alpha| < m, \\ & \text{and } \partial^\alpha(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0) \neq 0 \text{ for some } \alpha \in N_\ell, \text{ with } |\alpha| = m \} \end{aligned}$$

and also

$$(2.26) \quad \widetilde{M}_\ell^\infty := \{\mathbf{Z} : \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0 = 0, \partial^\alpha(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0) = 0 \text{ for all } \alpha \in N_\ell\}.$$

Therefore

$$\mathcal{S}_\ell \subset \{\mathbf{Z} : \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0 = 0, \nabla_{\widehat{\mathbf{Z}}_\ell}(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0) = \mathbf{0}\} = \widetilde{M}_\ell^\infty \cup \left(\bigcup_{m \geq 2} \widetilde{M}_\ell^m \right).$$

By Lemma A.3 in the appendix, we have that $\widetilde{M}_\ell^\infty = \emptyset$.

Let $m \geq 2$, and let $\mathbf{Z}_0 \in \widetilde{M}_\ell^m$. Then there exists $\beta \in N_\ell$ such that $|\beta| = m - 2$, and

$$D_{\widehat{\mathbf{Z}}_\ell}^2(\partial^\beta \mathbf{j}_\ell(\mathbf{Z}_0) \cdot \mathbf{g}_0) \neq \mathbf{0}.$$

Thus, if we define $v(\mathbf{Z}) := \partial^\beta \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0$, then $D_{\widehat{\mathbf{Z}}_\ell}^2 v(\mathbf{Z}_0)$ is a symmetric matrix that is not identically zero, so it must have at least one nonzero eigenvalue, say λ_i .

Observe that $\text{Trace}(D_{\widehat{\mathbf{Z}}_\ell}^2 v(\mathbf{Z})) = \Delta_{\widehat{\mathbf{Z}}_\ell}(\partial^\beta \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0) = 0$ because $\Delta_{\widehat{\mathbf{Z}}_\ell}(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0) = 0$. But $\text{Trace}(D_{\widehat{\mathbf{Z}}_\ell}^2 v(\mathbf{Z}_0)) = \sum_{k=1}^{2N-2} \lambda_k$, where λ_k are the eigenvalues, and $\lambda_i \neq 0$, and so there is another nonzero eigenvalue, say λ_j . Define $w(\mathbf{Y}) := v(R\mathbf{Y})$, where R is a rotation matrix such that

$$D_{\widehat{\mathbf{Y}}_\ell}^2 w(\mathbf{Y}_0) = \begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_{2N-2} \end{pmatrix},$$

where $\mathbf{Y}_0 := R^{-1}\mathbf{Z}_0$. Since λ_i and λ_j are different from zero, there are two distinct multi-indices $\alpha_1, \alpha_2 \in N_\ell$ with $|\alpha_k| = 1$ such that

$$\nabla_{\widehat{\mathbf{Y}}_\ell} \partial^{\alpha_k} w(\mathbf{Y}_0) \neq \mathbf{0}, \quad k = 1, 2.$$

Hence, applying the implicit function theorem to $\partial^{\alpha_1} w$ and $\partial^{\alpha_2} w$, we conclude that $\mathcal{M} = \{\mathbf{Y} : \partial^{\alpha_1} w(\mathbf{Y}) = 0, \partial^{\alpha_2} w(\mathbf{Y}) = 0\}$ is a $(2N - 2)$ -dimensional manifold in a neighborhood of \mathbf{Y}_0 . Since $\widetilde{M}_\ell^m \subset \mathcal{M}$, we have that \mathcal{S}_ℓ is contained in a countable union of manifolds with dimension at most $2N - 2$. \square

We proved that the collection of *singular points*

$$\mathcal{E}_{\text{sing}} := \bigcup_{\ell=1}^N \mathcal{S}_\ell,$$

with \mathcal{S}_ℓ defined in (2.24), has dimension at most $2N - 2$. Further, each \mathcal{A}_ℓ is a $(2N - 1)$ -dimensional smooth manifold away from points on \mathcal{S}_ℓ , but, in general, the set \mathcal{A} defined in (2.19) will not be a manifold at points $\mathbf{Z} \in \mathcal{A}_\ell \cap \mathcal{A}_j$ for $\ell \neq j$. For this reason we need to exclude the set

$$(2.27) \quad \mathcal{E}_{\text{int}} := \{\mathbf{Z} \in \mathbb{R}^{2N} : \mathbf{Z} \in \mathcal{A}_\ell \cap \mathcal{A}_j \text{ for some } \ell, j \in \{1, \dots, N\}, \ell \neq j\}.$$

Uniqueness at points in \mathcal{E}_{int} is significantly more delicate and will be discussed in section I in the supplementary materials file.

If $\mathbf{Z} \in \mathcal{A}_\ell$, then $\mathbf{j}_\ell(\mathbf{Z}) \neq \mathbf{0}$, but it could be that $\mathbf{j}_i(\mathbf{Z}) = \mathbf{0}$ for some $i \neq \ell$. This would mean that the glide direction for \mathbf{z}_i would not be well defined at \mathbf{Z} and could cause an obstruction to uniqueness. In view of this, we set

$$\mathcal{E}_{\text{zero}} := \{\mathbf{Z} \in \mathcal{D}(F) : \mathbf{j}_k(\mathbf{Z}) = \mathbf{0} \text{ for some } k \in \{1, \dots, N\}\}.$$

Reasoning as in Lemma 2.16, $\dim(\mathcal{E}_{\text{zero}} \cap \{\nabla \mathbf{j}_k \text{ has rank } 0\}) \leq 2N - 2$. On the other hand, $\dim(\mathcal{E}_{\text{zero}} \cap \{\nabla \mathbf{j}_k \text{ has rank } 2\}) = 2N - 2$, by the implicit function theorem. The set $\mathcal{E}_{\text{zero}} \cap \{\nabla \mathbf{j}_k \text{ has rank } 1\}$ could have dimension at most $2N - 1$.

For each $\ell \in \{1, \dots, N\}$ define

$$(2.28) \quad \mathcal{I}_\ell := \mathcal{A}_\ell \setminus (\mathcal{S}_\ell \cup \mathcal{E}_{\text{int}} \cup \mathcal{E}_{\text{zero}}).$$

Let $\hat{\mathbf{Z}} \in \mathcal{I}_\ell$. Since $\hat{\mathbf{Z}} \notin \mathcal{S}_\ell$ (see (2.24)), there is an $r > 0$ so that $B_r(\hat{\mathbf{Z}}) \cap \mathcal{A}_\ell$ is a $(2N - 1)$ -dimensional smooth manifold, and \mathcal{A}_ℓ divides $B_r(\hat{\mathbf{Z}})$ into two disjoint, open sets V^\pm . Since the functions \mathbf{j}_k are continuous by Lemma 2.15 for all $k \in \{1, \dots, N\}$, and $\hat{\mathbf{Z}} \notin \mathcal{E}_{\text{zero}}$, by taking r smaller, if necessary, we can assume that $\mathbf{j}_k(\mathbf{Z}) \neq \mathbf{0}$ for all $\mathbf{Z} \in B_r(\hat{\mathbf{Z}})$ and for all $k \in \{1, \dots, N\}$. In turn, since $\hat{\mathbf{Z}} \notin \mathcal{E}_{\text{int}}$, again by continuity and by taking r even smaller, $\mathbf{g}_k(\mathbf{Z}) \equiv \mathbf{g}_k(\hat{\mathbf{Z}})$ for all $\mathbf{Z} \in B_r(\hat{\mathbf{Z}})$ and for all $k \neq \ell$, and $\mathbf{g}_\ell(\mathbf{Z}) \equiv \mathbf{g}_\ell^\pm(\hat{\mathbf{Z}})$ for $\mathbf{Z} \in V^\pm$. Now let $\mathbf{f} : B_r(\hat{\mathbf{Z}}) \setminus \mathcal{A}_\ell \rightarrow \mathbb{R}^{2N}$, $\mathbf{f} = (\mathbf{f}_1, \dots, \mathbf{f}_N)$, be the function defined by

$$(2.29) \quad \begin{aligned} \mathbf{f}_k(\mathbf{Z}) &:= (\mathbf{j}_k(\mathbf{Z}) \cdot \mathbf{g}_k(\hat{\mathbf{Z}}))\mathbf{g}_k(\hat{\mathbf{Z}}) && \text{if } k \neq \ell, \\ \mathbf{f}_\ell(\mathbf{Z}) &:= (\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_\ell^\pm(\hat{\mathbf{Z}}))\mathbf{g}_\ell^\pm(\hat{\mathbf{Z}}) && \text{if } \mathbf{Z} \in V^\pm. \end{aligned}$$

We define \mathbf{f}^\pm as the restrictions of \mathbf{f} to V^\pm , and we extend them smoothly to the ball $B_r(\hat{\mathbf{Z}})$ by setting $\hat{\mathbf{f}}_k^\pm(\mathbf{Z}) := \mathbf{f}_k(\mathbf{Z})$ if $k \neq \ell$ and $\hat{\mathbf{f}}_\ell^\pm(\mathbf{Z}) := (\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_\ell^\pm(\hat{\mathbf{Z}}))\mathbf{g}_\ell^\pm(\hat{\mathbf{Z}})$.

Let $\mathbf{n}(\hat{\mathbf{Z}})$ denote the unit normal vector to \mathcal{A}_ℓ at $\hat{\mathbf{Z}}$ directed from V^- to V^+ . Motions starting in V^+ will move towards or away from \mathcal{A}_ℓ according to whether $\hat{\mathbf{f}}^+(\hat{\mathbf{Z}}) \cdot \mathbf{n}(\hat{\mathbf{Z}}) < 0$ or $\hat{\mathbf{f}}^+(\hat{\mathbf{Z}}) \cdot \mathbf{n}(\hat{\mathbf{Z}}) > 0$. Similarly, motions starting in V^- will move towards or away from \mathcal{A}_ℓ according to whether $\hat{\mathbf{f}}^-(\hat{\mathbf{Z}}) \cdot \mathbf{n}(\hat{\mathbf{Z}}) > 0$ or $\hat{\mathbf{f}}^-(\hat{\mathbf{Z}}) \cdot \mathbf{n}(\hat{\mathbf{Z}}) < 0$.

We define the set of *source points*

$$\begin{aligned} \mathcal{E}_{\text{src}} &:= \{\mathbf{Z} \in \Omega^N : \mathbf{Z} \in \mathcal{I}_\ell \text{ for some } \ell \in \{1, \dots, N\}, \\ &\quad \hat{\mathbf{f}}^+(\mathbf{Z}) \cdot \mathbf{n}(\mathbf{Z}) > 0 \text{ and } \hat{\mathbf{f}}^-(\mathbf{Z}) \cdot \mathbf{n}(\mathbf{Z}) < 0\}. \end{aligned}$$

If $\hat{\mathbf{Z}} \in \mathcal{E}_{\text{src}}$, there are two solution curves originating at $\hat{\mathbf{Z}}$, one that moves into V^+ and one that moves into V^- . Thus there is no uniqueness at source points.

THEOREM 2.17 (local uniqueness). *Let $T > 0$, and let $\mathbf{Z} : [-T, T] \rightarrow \mathbb{R}^{2N}$ be a solution to (2.15). Assume that there exist $t_1 \in [-T, T]$ and $\mathbf{Z}_1 \in \mathcal{I}_\ell$, for some $\ell \in \{1, \dots, N\}$, such that $\mathbf{Z}(t_1) = \mathbf{Z}_1$ and*

$$(2.30) \quad \hat{\mathbf{f}}^-(\mathbf{Z}_1) \cdot \mathbf{n}(\mathbf{Z}_1) > 0 \quad \text{or} \quad \hat{\mathbf{f}}^+(\mathbf{Z}_1) \cdot \mathbf{n}(\mathbf{Z}_1) < 0,$$

where $\hat{\mathbf{f}}^\pm$ are the extensions of the functions \mathbf{f}^\pm defined in terms of the function \mathbf{f} given in (2.29) with $\hat{\mathbf{Z}} = \mathbf{Z}_1$. Then right uniqueness holds for (2.15) at the point (t_1, \mathbf{Z}_1) .

Proof. By (2.30), $\mathbf{Z}_0 \notin \mathcal{E}_{\text{src}}$, and therefore, by the previous discussion, the result follows from Theorem 2.3. \square

Remark 2.18. Existence time is limited by the possibility of collisions between dislocations, that is, $|\mathbf{z}_i - \mathbf{z}_j| \rightarrow 0$, or between a dislocation and $\partial\Omega$, that is, $\text{dist}(\mathbf{z}_i, \partial\Omega)$

approaches 0. Additionally, uniqueness is limited by possible intersections of $\mathbf{Z}(t)$ with $\mathcal{S}_\ell \cup \mathcal{E}_{\text{int}} \cup \mathcal{E}_{\text{zero}} \cup \mathcal{E}_{\text{src}}$. The ambiguity set \mathcal{A} is smooth except possibly on the singular sets \mathcal{S}_ℓ , which are at most $(2N - 2)$ -dimensional by Lemma 2.16, or points in \mathcal{E}_{int} .

2.5. Cross-slip and fine cross-slip. We expect to see two kinds of motion at points where the force is not single valued. If a dislocation point \mathbf{z}_ℓ is moving in the direction \mathbf{g}_ℓ^- and the configuration $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_N)$ arrives at a point on \mathcal{A}_ℓ where \mathbf{g}_ℓ^\pm are two glide directions that are equally favorable to \mathbf{z}_ℓ , then \mathbf{z}_ℓ could abruptly transition from motion along \mathbf{g}_ℓ^- to motion along \mathbf{g}_ℓ^+ . Such a motion is called *cross-slip* (see Figure 2(a)). Heuristically, cross-slip occurs when, on one side of \mathcal{A}_ℓ , the vector field F (see (2.15)) is pointing toward \mathcal{A}_ℓ , while the other side F is pointing away from \mathcal{A}_ℓ . If the configuration \mathbf{Z} is in the region where F points towards \mathcal{A}_ℓ , then \mathbf{Z} approaches \mathcal{A}_ℓ and arrives at it in a finite time. The configuration then leaves \mathcal{A}_ℓ , moving into the region where F points away from \mathcal{A}_ℓ .

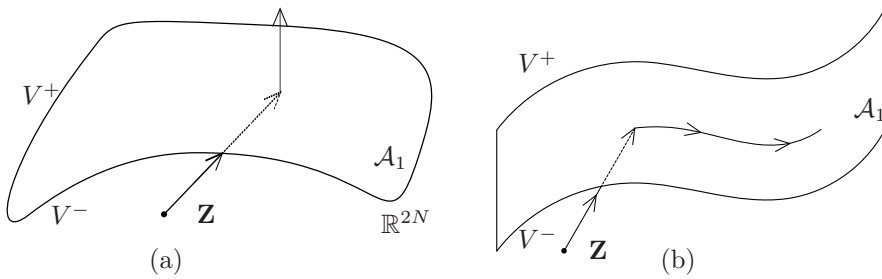


FIG. 2. *Cross-slip (a) and fine cross-slip (b) in \mathbb{R}^{2N} . The glide directions are $\mathcal{G} = \{\pm \mathbf{e}_1, \pm \mathbf{e}_2\}$, where \mathbf{e}_i is the i th basis vector. In (a) the motion of \mathbf{Z} changes direction while crossing the surface \mathcal{A}_1 , where the velocity field is multivalued. In (b) the motion of \mathbf{Z} , after hitting the surface \mathcal{A}_1 , continues on the surface following the tangent direction. (Here, $N = 3$.)*

Another possibility is that the vector field F points towards \mathcal{A}_ℓ on both sides of \mathcal{A}_ℓ . In this case, at a point on \mathcal{A}_ℓ , a motion by \mathbf{z}_ℓ in the \mathbf{g}_ℓ^+ direction will drive the configuration \mathbf{Z} to a region where \mathbf{j}_ℓ is most closely aligned with \mathbf{g}_ℓ^- , but then motion by \mathbf{z}_ℓ along \mathbf{g}_ℓ^- immediately forces \mathbf{Z} to intersect the surface \mathcal{A}_ℓ again. Motion by \mathbf{z}_ℓ along \mathbf{g}_ℓ^- then pushes \mathbf{Z} into a region where \mathbf{j}_ℓ is most closely aligned with \mathbf{g}_ℓ^+ , which forces \mathbf{Z} back to \mathcal{A}_ℓ . A motion such as this one on a finer and finer scale will appear as motion *along* the surface \mathcal{A}_ℓ . Following [12], such a motion is called *fine cross-slip*. See Figure 2(b), where the dislocation \mathbf{z}_1 is undergoing fine cross-slip. In part (a) it is shown how it follows a curve l rather than one of the glide directions $\mathbf{g} \in \mathcal{G}$. In part (b) the same phenomenon is shown in \mathbb{R}^{2N} ($N = 3$), where the point \mathbf{Z} hits \mathcal{A}_1 and starts moving along it.

The following theorems formalize the behaviors described above and provide an analytical validation of the notions of cross-slip and fine cross-slip introduced in [12]. We refer the reader to the discussion preceding Theorem 2.17 for the definitions of $\mathbf{n}(\mathbf{Z})$ and V^\pm for $\mathbf{Z} \in \mathcal{I}_\ell$.

THEOREM 2.19 (cross-slip). *Let $T > 0$, and let $\mathbf{Z} : [-T, T] \rightarrow \mathbb{R}^{2N}$ be a solution to (2.15). Assume that there exist $t_1 \in (-T, T)$ and $\mathbf{Z}_1 \in \mathcal{I}_\ell$, for some $\ell \in \{1, \dots, N\}$, such that $\mathbf{Z}(t_1) = \mathbf{Z}_1$ and*

$$(2.31) \quad \hat{\mathbf{f}}^-(\mathbf{Z}_1) \cdot \mathbf{n}(\mathbf{Z}_1) > 0 \quad \text{and} \quad \hat{\mathbf{f}}^+(\mathbf{Z}_1) \cdot \mathbf{n}(\mathbf{Z}_1) > 0,$$

where \mathbf{f} is the function defined in (2.29). Then uniqueness holds for (2.15) at the

point (t_1, \mathbf{Z}_1) , and the solution passes from V^- to V^+ . Similarly, if

$$(2.32) \quad \widehat{\mathbf{f}}^-(\mathbf{Z}_1) \cdot \mathbf{n}(\mathbf{Z}_1) < 0 \quad \text{and} \quad \widehat{\mathbf{f}}^+(\mathbf{Z}_1) \cdot \mathbf{n}(\mathbf{Z}_1) < 0,$$

then uniqueness holds for (2.15) at the point (t_1, \mathbf{Z}_1) and the solution passes from V^+ to V^- .

Proof. Since $\widehat{\mathbf{f}}^\pm$ are C^1 extensions of $\mathbf{f}^\pm := \mathbf{f}|_{V^\pm}$, the result follows from Theorem 2.4. \square

THEOREM 2.20 (fine cross-slip). *Let $T > 0$, and let $\mathbf{Z} : [-T, T] \rightarrow \mathbb{R}^{2N}$ be a solution to (2.15). Assume that there exist $t_1 \in (-T, T)$ and $\mathbf{Z}_1 \in \mathcal{I}_\ell$, for some $\ell \in \{1, \dots, N\}$, such that $\mathbf{Z}(t_1) = \mathbf{Z}_1$ and*

$$\widehat{\mathbf{f}}^-(\mathbf{Z}_1) \cdot \mathbf{n}(\mathbf{Z}_1) > 0 \quad \text{and} \quad \widehat{\mathbf{f}}^+(\mathbf{Z}_1) \cdot \mathbf{n}(\mathbf{Z}_1) < 0,$$

where \mathbf{f} is the function defined in (2.29). Then right uniqueness holds for (2.15) at the point (t_1, \mathbf{Z}_1) and there exists $\delta > 0$ such that \mathbf{Z} belongs to \mathcal{A}_ℓ and solves the ordinary differential equation for all $t \in [t_1, t_1 + \delta]$,

$$\dot{\mathbf{Z}} = \mathbf{f}^0(\mathbf{Z}) \in \text{co } F(\mathbf{Z}), \quad \text{where} \quad \mathbf{f}^0(\mathbf{Z}) := \alpha(\mathbf{Z})\widehat{\mathbf{f}}^+(\mathbf{Z}) + (1 - \alpha(\mathbf{Z}))\widehat{\mathbf{f}}^-(\mathbf{Z})$$

and $\alpha(\mathbf{Z}) \in (0, 1)$ is defined by

$$\alpha(\mathbf{Z}) := \frac{\widehat{\mathbf{f}}^-(\mathbf{Z}) \cdot \mathbf{n}(\mathbf{Z})}{\widehat{\mathbf{f}}^-(\mathbf{Z}) \cdot \mathbf{n}(\mathbf{Z}) - \widehat{\mathbf{f}}^+(\mathbf{Z}) \cdot \mathbf{n}(\mathbf{Z})}.$$

Proof. The result follows from Corollary 2.7. \square

Note that the cross-slip and fine cross-slip trajectories that we have described in Theorems 2.19 and 2.20 satisfy the conditions for right uniqueness in Theorem 2.17. Specifically, if (2.31) or (2.32) holds, then (2.30) holds (i.e., $\mathbf{Z}_1 \notin \mathcal{E}_{\text{src}}$).

3. Special cases. In this section we consider some special domains Ω for which the Peach–Köhler force can be explicitly determined (i.e., the solution to the Neumann problem (1.12) is known), specifically the unit disk B_1 , the half-plane \mathbb{R}_+^2 , and the plane \mathbb{R}^2 . The last two cases do not technically fit into our previous discussion because Ω is unbounded. However, the Neumann problem is well defined for these settings and we are able to discuss the dislocation dynamics.

In what follows we will use the fact that the boundary-response strains generated from each dislocation are “decoupled” in the following sense. Define u_0^i as

$$u_0^i(\mathbf{x}; \mathbf{z}_i) := \int_{\partial\Omega} G(\mathbf{x}, \mathbf{y}) \mathbf{Lk}_i(\mathbf{y}; \mathbf{z}_i) \cdot \mathbf{n}(\mathbf{y}) \, ds(\mathbf{y}),$$

where G is the Green’s function for the Neumann problem. Then $u_0^i(\cdot; \mathbf{z}_i)$ solves (1.12) with only one dislocation, i.e.,

$$\begin{cases} \operatorname{div}_{\mathbf{x}}(\mathbf{L}\nabla_{\mathbf{x}}u_0^i(\mathbf{x}; \mathbf{z}_i)) = 0, & \mathbf{x} \in \Omega, \\ \mathbf{L}(\nabla_{\mathbf{x}}u_0^i(\mathbf{x}; \mathbf{z}_i) + \mathbf{k}_i(\mathbf{x}; \mathbf{z}_i)) \cdot \mathbf{n}(\mathbf{x}) = 0, & \mathbf{x} \in \partial\Omega. \end{cases}$$

Thus the boundary-response strain at \mathbf{x} due to a dislocation at \mathbf{z}_i with Burgers modulus b_i is given by $\nabla_{\mathbf{x}}u_0^i(\mathbf{x}; \mathbf{z}_i)$, and the total boundary-response strain at \mathbf{x} due to the system \mathcal{Z} is $\nabla_{\mathbf{x}}u_0(\mathbf{x}; \mathbf{z}_1, \dots, \mathbf{z}_N) = \sum_{i=1}^N \nabla_{\mathbf{x}}u_0^i(\mathbf{x}; \mathbf{z}_i)$.

If we consider two dislocations \mathbf{z}_1 and \mathbf{z}_2 with Burgers moduli b_1 and b_2 , respectively, that collide in Ω , then by the definition of \mathbf{k}_j the boundary data in (1.12) satisfies

$$\mathbf{L}(\mathbf{k}_1(\mathbf{x}; \mathbf{z}_1) + \mathbf{k}_2(\mathbf{x}; \mathbf{z}_2)) \cdot \mathbf{n}(\mathbf{x}) \rightarrow \mathbf{L}\left(\mathbf{k}_1(\mathbf{x}; \mathbf{z}_1) + \frac{b_2}{b_1}\mathbf{k}_1(\mathbf{x}; \mathbf{z}_1)\right) \cdot \mathbf{n}(\mathbf{x}) \quad \text{as } \mathbf{z}_2 \rightarrow \mathbf{z}_1.$$

Notice that $\mathbf{k}_1(\cdot; \mathbf{z}_1) + (b_2/b_1)\mathbf{k}_1(\cdot; \mathbf{z}_1)$ is the singular strain generated by a single dislocation located at \mathbf{z}_1 with Burgers modulus $b_1 + b_2$. The same argument applies to an arbitrary number N of dislocation by linearity of (1.12). Thus, unlike the singular strain which becomes infinite if any two dislocations collide in Ω (see (1.9)), the boundary-response strain is oblivious to collisions between dislocations. Although the boundary-response strain is well defined when dislocations collide with each other, it is not well defined if a dislocation collides with $\partial\Omega$.

3.1. The unit disk. Consider the case $\Omega = B_1 = \{\mathbf{x} \in \mathbb{R}^2 : |\mathbf{x}| < 1\}$ and $\lambda = \mu = 1$ so that $\mathbf{L} = \mathbf{I}$. For $\mathbf{z} \in B_1$ we define $\bar{\mathbf{z}} \in B_1^c$ to be the reflection of \mathbf{z} across the unit circle ∂B_1 ,

$$\bar{\mathbf{z}} := \begin{cases} \frac{\mathbf{z}}{|\mathbf{z}|^2} & \text{if } \mathbf{z} \in B_1 \setminus \{\mathbf{0}\}, \\ \infty & \text{if } \mathbf{z} = \mathbf{0}. \end{cases}$$

For fixed $\mathbf{z}_i \in B_1$, it can be seen that the function

$$(3.1) \quad u_0^i(\mathbf{x}; \mathbf{z}_i) := \begin{cases} -\frac{b_i}{\pi} \arctan\left(\frac{x_2 - \bar{z}_{i,2}}{x_1 - \bar{z}_{i,1} + |\mathbf{x} - \bar{\mathbf{z}}_i|}\right) & \text{if } \mathbf{z} \neq \mathbf{0}, \\ 0 & \text{if } \mathbf{z} = \mathbf{0} \end{cases}$$

satisfies

$$\begin{cases} \Delta_{\mathbf{x}} u_0^i(\mathbf{x}; \mathbf{z}_i) = 0, & \mathbf{x} \in B_1, \\ \nabla_{\mathbf{x}} u_0^i(\mathbf{x}; \mathbf{z}_i) \cdot \mathbf{n}(\mathbf{x}) = -\mathbf{k}_i(\mathbf{x}; \mathbf{z}_i) \cdot \mathbf{n}(\mathbf{x}), & \mathbf{x} \in \partial B_1, \end{cases}$$

and

$$(3.2) \quad \nabla_{\mathbf{x}} u_0^i(\mathbf{x}; \mathbf{z}_i) = -\mathbf{k}_i(\mathbf{x}; \bar{\mathbf{z}}_i) \quad \text{for all } \mathbf{x} \in B_1.$$

Note that ∇u_0^i is singular only at the point $\mathbf{x} = \bar{\mathbf{z}}_i \notin B_1$.

As discussed at the beginning of section 3, for a system of dislocations given by \mathcal{Z} and \mathcal{B} , the solution to the Neumann problem (1.12) is given by

$$u_0(\mathbf{x}; \mathbf{z}_1, \dots, \mathbf{z}_N) = \sum_{i=1}^N u_0^i(\mathbf{x}; \mathbf{z}_i)$$

with u_0^i as in (3.1). Thus, combining (2.9) and (3.2), we have

$$(3.3) \quad \mathbf{j}_\ell(\mathbf{z}_1, \dots, \mathbf{z}_N) = b_\ell \mathbf{J} \left(\sum_{i \neq \ell} \mathbf{k}_i(\mathbf{z}_\ell; \mathbf{z}_i) - \sum_{i=1}^N \mathbf{k}_i(\mathbf{z}_\ell; \bar{\mathbf{z}}_i) \right).$$

Formula (3.3) greatly simplifies numerical simulations of the dislocation dynamics. Without an explicit formula, one must solve the Neumann problem at each time step.

From (3.3), we can see that the boundary of B_1 attracts dislocations. If $N = 1$ and $\mathbf{z}_1 \in B_1 \setminus \{\mathbf{0}\}$, then

$$\mathbf{j}_1(\mathbf{z}_1) = -b_1 \mathbf{J} \mathbf{k}_1(\mathbf{z}_1; \bar{\mathbf{z}}_1) = -\frac{b_1^2}{2\pi} \frac{\mathbf{z}_1 - \bar{\mathbf{z}}_1}{|\mathbf{z}_1 - \bar{\mathbf{z}}_1|^2} = \frac{b_1^2}{2\pi} \frac{\mathbf{z}_1}{(1 - |\mathbf{z}_1|^2)}$$

since $\mathbf{z} - \bar{\mathbf{z}} = \mathbf{z}(1 - |\mathbf{z}|^{-2})$. Thus, the force is directed radially outward (toward the nearest boundary point to \mathbf{z}_1) and diverges as $\mathbf{z}_1 \rightarrow \partial B_1$. If $\mathbf{z}_1 = \mathbf{0}$, then $\mathbf{j}_1 = \mathbf{0}$ and \mathbf{z}_1 will not move. Otherwise, a single dislocation in B_1 will be pulled to ∂B_1 and will collide with ∂B_1 in a finite time (assuming the glide directions span \mathbb{R}^2). If $N > 1$, then the other dislocations produce boundary forces that will pull on \mathbf{z}_ℓ in the directions $-b_\ell b_i(\mathbf{z}_\ell - \bar{\mathbf{z}}_i)$ for each i .

The sets \mathcal{A}_ℓ as given in (2.24) are smooth because they are locally given by $\mathbf{j}_\ell \cdot \mathbf{g}_0 = 0$ for a fixed vector \mathbf{g}_0 (cf. (2.28)), and by (3.3), $\mathbf{j}_\ell \cdot \mathbf{g}_0$ is a rational function with singularities only at collision points.

3.2. The half-plane. Although the theory developed in this paper applies only to bounded domains, the equation for the Peach–Köhler force (1.8) is still well defined, provided there is a weak solution to the Neumann problem (1.12). For the special cases of the half-plane and the plane we present an explicit expression for the Peach–Köhler force without resorting to the renormalized energy.

Let $\Omega = \mathbb{R}_+^2 := \{\mathbf{x} \in \mathbb{R}^2 : x_2 > 0\}$, and let $\lambda = \mu = 1$. The solution to (1.12) is given in terms of the inverse tangent, using a reflected point across $\partial \mathbb{R}_+^2 = \{x_2 = 0\}$. For all $\mathbf{z} = (z_1, z_2) \in \mathbb{R}^2$ define $\tilde{\mathbf{z}} := (z_1, -z_2)$. Then for $\mathbf{z}_i \in \mathbb{R}_+^2$,

$$(3.4) \quad u_0^i(\mathbf{x}; \mathbf{z}_i) := -\frac{b_i}{\pi} \arctan \left(\frac{x_2 - \tilde{z}_{i,2}}{x_1 - \tilde{z}_{i,1} + |\mathbf{x} - \tilde{\mathbf{z}}_i|} \right)$$

satisfies

$$\begin{cases} \Delta_{\mathbf{x}} u_0^i(\mathbf{x}; \mathbf{z}_i) = 0, & \mathbf{x} \in \mathbb{R}_+^2, \\ \nabla_{\mathbf{x}} u_0^i(\mathbf{x}; \mathbf{z}_i) \cdot \mathbf{n}(\mathbf{x}) = -\mathbf{k}_i(\mathbf{x}; \mathbf{z}_i) \cdot \mathbf{n}(\mathbf{x}), & \mathbf{x} \in \partial \mathbb{R}_+^2, \end{cases}$$

and

$$\nabla_{\mathbf{x}} u_0^i(\mathbf{x}; \mathbf{z}_i) = -\mathbf{k}_i(\mathbf{x}; \tilde{\mathbf{z}}_i) \quad \text{for all } \mathbf{x} \in \mathbb{R}_+^2.$$

Again, we have $u_0(\mathbf{x}; \mathbf{z}_1, \dots, \mathbf{z}_N) = \sum_{i=1}^N u_0^i(\mathbf{x}; \mathbf{z}_i)$ with u_0^i as in (3.4), and the Peach–Köhler force is

$$(3.5) \quad \mathbf{j}_\ell(\mathbf{z}_1, \dots, \mathbf{z}_N) = b_\ell \mathbf{J} \left(\sum_{i \neq \ell} \mathbf{k}_i(\mathbf{z}_\ell; \mathbf{z}_i) - \sum_{i=1}^N \mathbf{k}_i(\mathbf{z}_\ell; \tilde{\mathbf{z}}_i) \right).$$

From (3.5), it is again not difficult to see that a single dislocation \mathbf{z}_1 in \mathbb{R}_+^2 with Burgers modulus b_1 is attracted to $\partial \mathbb{R}_+^2$. As in the case of the disk, the ambiguity set \mathcal{A} is smooth except at the intersections of the \mathcal{A}_ℓ .

3.3. The plane. The case $\Omega = \mathbb{R}^2$ and $\lambda = \mu = 1$ is the simplest case. There is no boundary so that $u_0 \equiv 0$, and, by (1.8), the Peach–Köhler force is then

$$(3.6) \quad \mathbf{j}_\ell(\mathbf{z}_1, \dots, \mathbf{z}_N) = b_\ell \mathbf{J} \sum_{i \neq \ell} \mathbf{k}_i(\mathbf{z}_\ell; \mathbf{z}_i).$$

Even though the renormalized energy has not been defined for unbounded domains, in the case of the plane we can formally write $\mathbf{j}_\ell = -\nabla_{\mathbf{z}_\ell} U$, where, up to an additive constant,

$$U(\mathbf{z}_1, \dots, \mathbf{z}_N) = - \sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{b_i b_j}{2\pi} \log |\mathbf{\Lambda}(\mathbf{z}_i - \mathbf{z}_j)|,$$

with $\mathbf{\Lambda}$ defined in (1.10).

In general, it can be difficult to exhibit an example that shows analytically fine cross-slip (though it is regularly observed in numerical simulations). However, in the case $\Omega = \mathbb{R}^2$, this can be done with two dislocations as follows. Suppose we have a system of two dislocations $\mathbf{Z} = (\mathbf{z}, \mathbf{w}) \in \mathbb{R}^4$ with Burgers moduli $b_1 = -b_2 =: b > 0$, respectively. Under these assumptions, (3.6) reduces to

$$(3.7) \quad \mathbf{j}_1(\mathbf{z}, \mathbf{w}) = -\frac{b^2}{2\pi} \frac{\mathbf{z} - \mathbf{w}}{|\mathbf{z} - \mathbf{w}|^2} = -\mathbf{j}_2(\mathbf{z}, \mathbf{w}).$$

Assume that the glide directions are along the lines $x_2 = \pm x_1$,

$$(3.8) \quad \mathcal{G} = \{\pm \mathbf{g}_1, \pm \mathbf{g}_2\}, \quad \mathbf{g}_1 := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \mathbf{g}_2 := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

There are two cases of initial conditions $\mathbf{Z}_0 = (\mathbf{z}_0, \mathbf{w}_0)$ with $\mathbf{z}_0 = (z_{0,1}, z_{0,2})$, $\mathbf{w}_0 = (w_{0,1}, w_{0,2})$ to consider: either \mathbf{z}_0 and \mathbf{w}_0 are aligned along a vertical or horizontal line, or they are not. That is, either $z_{0,1} = w_{0,1}$ or $z_{0,2} = w_{0,2}$ (but not both), or $z_{0,i} \neq w_{0,i}$ for $i = 1, 2$.

We begin by considering the case $z_{0,2} = w_{0,2}$. Let $y := z_{0,2} = w_{0,2}$, and without loss of generality take $w_{0,1} > z_{0,1}$. From (3.7), we have

$$(3.9) \quad \mathbf{j}_1(\mathbf{Z}_0) = \mathbf{j}_1(z_{0,1}, y, w_{0,1}, y) = \frac{b^2}{2\pi} \frac{1}{w_{0,1} - z_{0,1}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\mathbf{j}_2(\mathbf{Z}_0).$$

Since $w_{0,1} - z_{0,1} > 0$, we see that $\mathbf{j}_1(\mathbf{Z}_0)$ is aligned with $(1, 0)$ and $\mathbf{j}_2(\mathbf{Z}_0)$ is aligned with $(-1, 0)$. Thus, the maximally dissipative glide directions for \mathbf{z} are \mathbf{g}_1 and \mathbf{g}_2 (see (3.8)) and the maximally dissipative glide directions for \mathbf{w} are $-\mathbf{g}_1$ and $-\mathbf{g}_2$. Define $\mathbf{g}_1^0 := \mathbf{g}_1 - \mathbf{g}_2 = (0, \sqrt{2})$ and $\mathbf{g}_2^0 := -\mathbf{g}_1 + \mathbf{g}_2 = -\mathbf{g}_1^0$ so that locally, near \mathbf{Z}_0 , the ambiguity surfaces are $\mathcal{A}_1 \cap B_r(\mathbf{Z}_0) = \{\mathbf{Z} : \mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_1^0 = 0\}$, $\mathcal{A}_2 \cap B_r(\mathbf{Z}_0) = \{\mathbf{Z} : \mathbf{j}_2(\mathbf{Z}) \cdot \mathbf{g}_2^0 = 0\}$ for some small $r > 0$. From (3.7), we see that $\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_1^0 = 0$ if and only if $z_2 = w_2$, and the same holds for $\mathbf{j}_2(\mathbf{Z}) \cdot \mathbf{g}_2^0 = 0$, so that

$$\mathcal{A}_1 \cap B_r(\mathbf{Z}_0) = \mathcal{A}_2 \cap B_r(\mathbf{Z}_0) = \{\mathbf{Z} = (\mathbf{z}, \mathbf{w}) \in B_r(\mathbf{Z}_0) : z_2 = w_2\}.$$

This is a degenerate situation since the ambiguity surfaces \mathcal{A}_1 and \mathcal{A}_2 coincide locally, and instead of having four vector fields near the intersection, we have two vector fields. That is, the fields $\mathbf{f}^{(+,+)}$ and $\mathbf{f}^{(-,-)}$ (see (3.1)) are defined on either side of the surface \mathcal{A}_1 , but since $\mathcal{A}_1 = \mathcal{A}_2$, there are no regions where the fields $\mathbf{f}^{(-,+)}$ or $\mathbf{f}^{(+,-)}$ are defined. We choose a sign for the normal to \mathcal{A}_1 and \mathcal{A}_2 at \mathbf{Z}_0 and set

$$(3.10) \quad \mathbf{n} := \frac{1}{\sqrt{2}}(0, 1, 0, -1).$$

Recall the convention that \mathcal{A}_1 (and \mathcal{A}_2) divides $B_r(\mathbf{Z}_0)$ into two regions, V^\pm and \mathbf{n} points from V^- to V^+ . A point in V^+ is of the form $\mathbf{Z}_0 + \varepsilon \mathbf{n} = (z_{0,1}, y + \varepsilon/\sqrt{2}, w_{0,1}, y - \varepsilon/\sqrt{2})$, and from (3.7),

$$\mathbf{j}_1(\mathbf{Z}_0 + \varepsilon \mathbf{n}) = \frac{b^2}{2\pi} \frac{1}{(z_{0,1} - w_{0,1})^2 + 2\varepsilon^2} \begin{pmatrix} w_{0,1} - z_{0,1} \\ -\sqrt{2}\varepsilon \end{pmatrix} = -\mathbf{j}_2(\mathbf{Z}_0 + \varepsilon \mathbf{n}),$$

so \mathbf{g}_2 is the maximally dissipative glide direction for \mathbf{z} , and $-\mathbf{g}_2$ is the maximally dissipative glide direction for \mathbf{w} if $\mathbf{Z} \in V^+$. Similarly, a point in V^- is of the form $\mathbf{Z}_0 - \varepsilon \mathbf{n} = (z_{0,1}, y - \varepsilon/\sqrt{2}, w_{0,1}, y + \varepsilon/\sqrt{2})$, and the maximally dissipative glide directions for \mathbf{z} and \mathbf{w} in this case are \mathbf{g}_1 and $-\mathbf{g}_1$, respectively. Thus, we have for $\mathbf{Z} \in B_r(\mathbf{Z}_0)$,

$$\begin{aligned} \mathbf{f}^{(+,+)}(\mathbf{Z}) &:= ((\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_2)\mathbf{g}_2, (\mathbf{j}_2(\mathbf{Z}) \cdot (-\mathbf{g}_2))(-\mathbf{g}_2)), \\ \mathbf{f}^{(-,-)}(\mathbf{Z}) &:= ((\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_1)\mathbf{g}_1, (\mathbf{j}_2(\mathbf{Z}) \cdot (-\mathbf{g}_1))(-\mathbf{g}_1)). \end{aligned}$$

Since $\mathbf{j}_1(\mathbf{Z}) = -\mathbf{j}_2(\mathbf{Z})$, we have

$$(3.11) \quad \mathbf{f}^{(+,+)}(\mathbf{Z}) := (\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_2)(\mathbf{g}_2, -\mathbf{g}_2), \quad \mathbf{f}^{(-,-)}(\mathbf{Z}) := (\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_1)(\mathbf{g}_1, -\mathbf{g}_1).$$

From (3.8) and (3.9), we have $\mathbf{j}_1(\mathbf{Z}_0) \cdot \mathbf{g}_1 = \mathbf{j}_1(\mathbf{Z}_0) \cdot \mathbf{g}_2 = \frac{b^2}{2\sqrt{2}\pi}(w_{0,1} - z_{0,1})^{-1} > 0$, and from (3.8) and (3.10), we have $\mathbf{n} \cdot (\mathbf{g}_2, -\mathbf{g}_2) = -1$ and $\mathbf{n} \cdot (\mathbf{g}_1, -\mathbf{g}_1) = 1$. Thus,

$$\mathbf{n} \cdot \mathbf{f}^{(+,+)}(\mathbf{Z}_0) = -\frac{b^2}{2\sqrt{2}\pi(w_{0,1} - z_{0,1})} < 0, \quad \mathbf{n} \cdot \mathbf{f}^{(-,-)}(\mathbf{Z}_0) = \frac{b^2}{2\sqrt{2}\pi(w_{0,1} - z_{0,1})} > 0,$$

so the fine cross-slip conditions (3.2) are satisfied (there are no conditions for $\mathbf{f}^{(+,-)}$ or $\mathbf{f}^{(-,+)}$ since locally $\mathcal{A}_1 = \mathcal{A}_2$). By (3.6), $\dot{\mathbf{Z}}$ must be a convex combination of $\mathbf{f}^{(+,+)}$ and $\mathbf{f}^{(-,-)}$, $\dot{\mathbf{Z}} = \alpha \mathbf{f}^{(+,+)}(\mathbf{Z}) + (1 - \alpha) \mathbf{f}^{(-,-)}(\mathbf{Z})$, and the trajectory $\mathbf{Z}(t) \in \mathcal{A}_1 = \mathcal{A}_2$ for some time interval $[0, T]$. Therefore, $\mathbf{Z}(t) = (\mathbf{z}(t), \mathbf{w}(t)) = (z_1(t), z_2(t), w_1(t), w_2(t))$ and $z_2(t) = w_2(t)$ for $t \in [0, T]$. From (3.11) and the fact that $\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_1 = \mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_2$ whenever $z_2 = w_2$, we have

$$\begin{aligned} \dot{\mathbf{Z}} &= \alpha(\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_2)(\mathbf{g}_2, -\mathbf{g}_2) + (1 - \alpha)(\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_1)(\mathbf{g}_1, -\mathbf{g}_1) \\ &= \frac{b^2}{4\pi(w_1 - z_1)} (1, 1 - 2\alpha, -1, 2\alpha - 1). \end{aligned}$$

The condition $\mathbf{n} \cdot \dot{\mathbf{Z}} = 0$ yields $\alpha = \frac{1}{2}$, so the equations of motion (3.6) are

$$\dot{\mathbf{Z}} = (\dot{z}_1, \dot{z}_2, \dot{w}_1, \dot{w}_2) = \frac{1}{2} \left(\mathbf{f}^{(+,+)}(\mathbf{Z}) + \mathbf{f}^{(-,-)}(\mathbf{Z}) \right) = \frac{b^2}{4\pi(w_1 - z_1)} (1, 0, -1, 0).$$

In particular, $\dot{z}_2 = 0$, $\dot{w}_2 = 0$, and $z_2(0) = y = w_2(0)$, so $z_2(t) = y = w_2(t)$ for $t \in [0, T]$. The equations for z_1 and w_1 are easily solved with

$$\begin{aligned} z_1(t) &= -\frac{1}{2} \left((w_{0,1} - z_{0,1})^2 - \frac{b^2}{\pi} t \right)^{\frac{1}{2}} + \frac{1}{2}(z_{0,1} + w_{0,1}), \\ w_1(t) &= \frac{1}{2} \left((w_{0,1} - z_{0,1})^2 - \frac{b^2}{\pi} t \right)^{\frac{1}{2}} + \frac{1}{2}(z_{0,1} + w_{0,1}). \end{aligned}$$

This implies that the trajectory $\mathbf{Z}(t)$ moves on $\mathcal{A}_1 = \mathcal{A}_2$ up to the maximal time $T = \frac{\pi}{b^2}(w_{0,1} - z_{0,1})^2$, and $z_1(t)$ increases from $z_{0,1}$ while $w_1(t)$ decreases from $w_{0,1}$, with the two meeting at $z_1(T) = w_1(T) = \frac{1}{2}(z_{0,1} + w_{0,1})$. At this collision, the dynamics are no longer well defined.

If the initial condition has \mathbf{z}_0 and \mathbf{w}_0 vertically aligned, then the same analysis applies, but the situation is rotated.

If \mathbf{z}_0 and \mathbf{w}_0 are not aligned vertically or horizontally, then a regular glide motion occurs until either $z_1 = w_1$ or $z_2 = w_2$, and then the above analysis applies. To see this, consider $\mathbf{z}_0 = (z_{0,1}, z_{0,2})$ and $\mathbf{w}_0 = (w_{0,1}, w_{0,2})$, and without loss of generality, assume that $w_{0,1} > z_{0,1}$ and $w_{0,2} > z_{0,2}$ (the other cases are similar). In this case

$$\mathbf{j}_1(\mathbf{Z}_0) = \frac{b^2}{2\pi|\mathbf{z}_0 - \mathbf{w}_0|^2} \begin{pmatrix} w_{0,1} - z_{0,1} \\ w_{0,2} - z_{0,2} \end{pmatrix} = -\mathbf{j}_2(\mathbf{Z}_0).$$

Since $w_{0,1} - z_{0,1} > 0$ and $w_{0,2} - z_{0,2} > 0$, the maximally dissipative glide directions for \mathbf{j}_1 and \mathbf{j}_2 are \mathbf{g}_1 and $-\mathbf{g}_1$, respectively. Thus, \mathbf{z} glides in the \mathbf{g}_1 direction so that z_1 and z_2 increase from $z_{0,1}$ and $z_{0,2}$, while \mathbf{w} glides in the $-\mathbf{g}_1$ direction so that w_1 and w_2 decrease from $w_{0,1}$ and $w_{0,2}$. At some time t_1 we must obtain either $z_1(t_1) = w_1(t_1)$ or $z_2(t_1) = w_2(t_1)$. If only one of these equalities holds, we are in the situations described above and fine cross-slip occurs. If both of these equalities hold, then \mathbf{z} and \mathbf{w} have collided and the dynamics is no longer defined.

Remark 3.1 (mirror dislocations). A direct inspection of (3.3) and (3.5) shows that the force on \mathbf{z}_ℓ in $\Omega = B_1$ and $\Omega = \mathbb{R}_+^2$ is the same as the force on \mathbf{z}_ℓ in \mathbb{R}^2 if one adds N dislocations with opposite Burgers moduli at the points $\bar{\mathbf{z}}_i$ in the case $\Omega = B_1$, and at $\bar{\mathbf{z}}_i$ in the case $\Omega = \mathbb{R}_+^2$, for $i = 1, \dots, N$.

4. Numerical simulations. The simulation of (2.20) may be undertaken using standard numerical ODE integrators, provided sufficient care is taken in resolving the evolution near the “ambiguity surfaces” \mathcal{A}_ℓ . A discrete time step leads to a numerical integration that oscillates back and forth across an attracting ambiguity surface in the case of fine cross-slip. On the macroscale, this appears as fine cross-slip since the small oscillations across the surface average out and what remains is motion approximately tangent to \mathcal{A}_ℓ . To compute the vector field, one must solve the Neumann problem (1.12) at each time step, so a fast elliptic PDE solver is needed in practice.

An example is shown in Figures 3 and 4, where we have simulated a system of $N = 12$ screw dislocations with each Burgers modulus $b_i = 1$ for $i = 1, \dots, 12$ and where the domain is the unit disk. The integration is done in $\Omega^{12} \subset \mathbb{R}^{24}$, but the graphics depict the path each \mathbf{z}_i takes in $\Omega \subset \mathbb{R}^2$. All but one dislocation exhibit normal glide motions, while the dislocation at the center exhibits fine cross-slip, as is visible in Figure 4. In this case, the solution to the Neumann problem is explicit (cf. (3.3)), so it is not difficult to simulate systems with more dislocations and observe more complicated behavior, such as multiple dislocations simultaneously exhibiting fine cross-slip, corresponding to motion along the intersection of multiple ambiguity surfaces in the full space Ω^N . The simulation depicted in Figures 3 and 4 was run until a dislocation collided with the boundary. Since all dislocations have positive Burgers moduli, they repel each other, and no collision between dislocations occurs, and the dynamics can be continued until a boundary collision.

Appendix. We collect some technical results that are needed in the proofs from section 2.

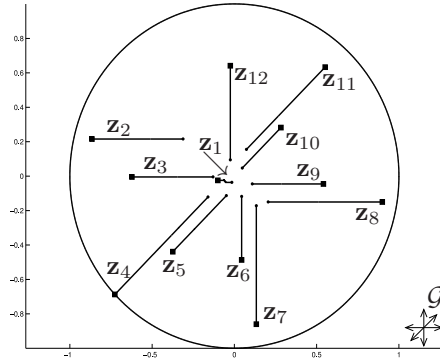


FIG. 3. The forces are repulsive, and the dislocations move mostly along the glide directions $\mathcal{G} = \{\pm \mathbf{e}_1, \pm \mathbf{e}_2, \pm \frac{1}{\sqrt{2}}(\mathbf{e}_1 + \mathbf{e}_2)\}$. All but one (the one at the center) move along a glide direction until one of them hits the boundary. The dislocation in the middle moves along $-\mathbf{e}_1$ but then exhibits fine cross-slip.

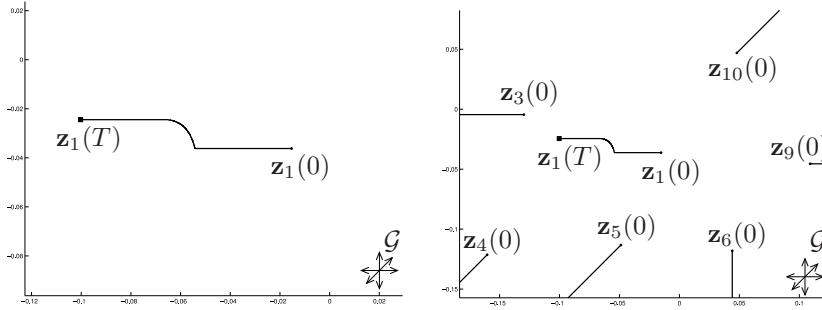


FIG. 4. These plots are magnified views of the motion of \mathbf{z}_1 . The motion begins at the dot on the right and ends at the square on the left. The motion abruptly begins to fine cross-slip and eventually moves back to a gliding motion as the fine cross-slip motion becomes aligned with $-\mathbf{e}_1$.

A.1. Lemmas on the singular set.

LEMMA A.1. The set $\mathcal{D}(F)$, as defined in (2.14), is open and connected.

Proof. From (2.14) and (2.13), it is clear that $\mathcal{D}(F)$ is open. We will now show that $\mathcal{D}(F)$ is path connected. Let $\mathbf{w}, \mathbf{z}_1, \dots, \mathbf{z}_N \in \Omega$ be distinct points, and let $\mathbf{Z}, \widehat{\mathbf{Z}} \in \mathcal{D}(F)$ be given by $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_N)$ and $\widehat{\mathbf{Z}} = (\mathbf{z}_1, \dots, \mathbf{z}_{\ell-1}, \mathbf{w}, \mathbf{z}_{\ell+1}, \dots, \mathbf{z}_N)$. We construct a continuous path $\gamma : [0, 1] \rightarrow \mathcal{D}(F)$ with $\gamma(0) = \mathbf{Z}$ and $\gamma(1) = \widehat{\mathbf{Z}}$ as follows.

Note that $\Omega \setminus \{\mathbf{z}_1, \dots, \mathbf{z}_{\ell-1}, \mathbf{z}_{\ell+1}, \dots, \mathbf{z}_N\}$ is path connected. Thus there is a path $\gamma_\ell : [0, 1] \rightarrow \Omega \setminus \{\mathbf{z}_1, \dots, \mathbf{z}_{\ell-1}, \mathbf{z}_{\ell+1}, \dots, \mathbf{z}_N\}$ with $\gamma_\ell(0) = \mathbf{z}_\ell$ and $\gamma_\ell(1) = \mathbf{w}$. Then setting $\gamma(t) = (\mathbf{z}_1, \dots, \mathbf{z}_{\ell-1}, \gamma_\ell(t), \mathbf{z}_{\ell+1}, \dots, \mathbf{z}_N)$ for each $t \in [0, 1]$ gives a path in $\mathcal{D}(F)$ from \mathbf{Z} to $\widehat{\mathbf{Z}}$.

We can now connect any vector $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_N) \in \mathcal{D}(F)$ to any other vector $\mathbf{W} = (\mathbf{w}_1, \dots, \mathbf{w}_N) \in \mathcal{D}(F)$ by first moving \mathbf{z}_1 to \mathbf{w}_1 as above, then \mathbf{z}_2 to \mathbf{w}_2 , and so on, until all the \mathbf{z}_i are moved to \mathbf{w}_i , producing a path from \mathbf{Z} to \mathbf{W} . \square

To prove the following lemma we will use the fact that the renormalized energy (see (1.6)) diverges logarithmically with the relative distance between the dislocations,

that is,

$$(A.1) \quad U(\mathbf{z}_1, \dots, \mathbf{z}_N) = - \sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{\mu \lambda b_i b_j}{4\pi} \log |\mathbf{\Lambda}(\mathbf{z}_i - \mathbf{z}_j)| + O(1)$$

as $|\mathbf{z}_i - \mathbf{z}_j| \rightarrow 0$. We refer the reader to [7] for a proof.

LEMMA A.2. *Fix $\ell \in \{1, \dots, N\}$, and let $\mathbf{e} \in \mathbb{R}^2 \setminus \{0\}$ be fixed. Then the set $V = \{\mathbf{Z} \in \mathcal{D}(F) : \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{e} = 0\}$ has an empty interior.*

Proof. The set V is closed because \mathbf{j}_ℓ is continuous. Suppose there is a ball $B \subset V$. From Lemma 2.15, we have that $\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{e}$ is analytic in B and is constant; therefore $\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{e}$ is constant in the largest connected component of $\mathcal{D}(F)$ containing B . Hence, by Lemma A.1, $\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{e} = 0$ in $\mathcal{D}(F)$. From (1.8), we have that

$$(A.2) \quad \nabla_{\mathbf{z}_\ell} U(\mathbf{Z}) \cdot \mathbf{e} = 0 \quad \text{in } \mathcal{D}(F),$$

so U is constant when \mathbf{z}_ℓ varies along the direction \mathbf{e} .

Consider a fixed $\mathbf{Z}^* = (\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N) \in \mathcal{D}(F)$. Let $h > 0$, and for $\delta \in (0, h]$ define $\mathbf{z}_\ell^\delta := \mathbf{z}_\ell + \delta \mathbf{e}$. We assume that h_0 is small enough so that $\mathbf{z}_\ell^\delta \in \Omega \setminus \{\mathbf{z}_1, \dots, \mathbf{z}_N\}$ for $\delta \in (0, h_0]$. Fix a $k \neq \ell$ and $h \in (0, h_0]$, and let \mathbf{Z}^h be the point in $\mathcal{D}(F)$ obtained by replacing \mathbf{z}_k in \mathbf{Z}^* with \mathbf{z}_ℓ^h , i.e.,

$$\mathbf{Z}^h := \{\mathbf{z}_1, \dots, \mathbf{z}_\ell, \dots, \mathbf{z}_{k-1}, \mathbf{z}_\ell^h, \mathbf{z}_{k+1}, \dots, \mathbf{z}_N\}.$$

Letting $\delta_n = (1 - \frac{1}{n})h$, we construct the sequence $\{\mathbf{Z}_n\} \subset \mathcal{D}(F)$ given by

$$\mathbf{Z}_n := \{\mathbf{z}_1, \dots, \mathbf{z}_\ell + \delta_n \mathbf{e}, \dots, \mathbf{z}_{k-1}, \mathbf{z}_\ell^h, \mathbf{z}_{k+1}, \dots, \mathbf{z}_N\}.$$

We have $\mathbf{Z}_1 = \mathbf{Z}^h$, and

$$\mathbf{Z}_n \rightarrow \mathbf{Z}_\infty := \{\mathbf{z}_1, \dots, \mathbf{z}_\ell^h, \dots, \mathbf{z}_{k-1}, \mathbf{z}_\ell^h, \mathbf{z}_{k+1}, \dots, \mathbf{z}_N\} \quad \text{as } n \rightarrow \infty.$$

Note that $\mathbf{Z}_\infty \notin \mathcal{D}(F)$ because \mathbf{z}_ℓ and \mathbf{z}_k are colliding as $n \rightarrow \infty$. In particular, by (A.1), $|U(\mathbf{Z}_n)| \rightarrow \infty$ as $n \rightarrow \infty$. On the other hand, in the sequence $\{\mathbf{Z}_n\}$, only the ℓ th dislocation is moving, and it is moving along the direction \mathbf{e} , so from (A.2), $U(\mathbf{Z}_n)$ remains constant for all n . We have reached a contradiction, and we conclude that V does not contain any ball. \square

LEMMA A.3. *The set $\widetilde{M}_\ell^\infty$, as defined in (2.26), is empty.*

Proof. Without loss of generality, let $\ell = 1$. Recall that

$$\widetilde{M}_1^\infty = \{\mathbf{Z} : \mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_0 = 0, \partial^\alpha(\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_0) = 0 \text{ for all } \alpha \in N_1\},$$

with N_1 defined in (2.25). Suppose that $\widetilde{M}_1^\infty \neq \emptyset$ and $\widetilde{\mathbf{Z}} = (\widetilde{\mathbf{z}}_1, \dots, \widetilde{\mathbf{z}}_N) \in \widetilde{M}_1^\infty$. Since $\mathbf{j}_1 \cdot \mathbf{g}_0$ is analytic and $\widetilde{\mathbf{Z}} \in \widetilde{M}_1^\infty$, we have that $\mathbf{j}_1(\mathbf{Z}) \cdot \mathbf{g}_0 = \mathbf{j}_1(\widetilde{\mathbf{Z}}) \cdot \mathbf{g}_0$ for $\mathbf{Z} \in \{\widetilde{\mathbf{z}}_1\} \times V$, where V is open in \mathbb{R}^{2N-2} . Take V to be the largest connected component of $\mathcal{D}(F)$ with $\mathbf{z}_1 = \widetilde{\mathbf{z}}_1$, which, by the same argument as in Lemma A.1, can be written as $\{\widetilde{\mathbf{z}}_1\} \times V = \{\mathbf{Z} \in \mathcal{D}(F) : \mathbf{z}_1 = \widetilde{\mathbf{z}}_1\}$. We cannot follow the energy approach of Lemma A.2 because that would require moving \mathbf{z}_1 , which is fixed. Instead, let $0 < \varepsilon_0 \ll 1$ and construct a sequence $\{\mathbf{Z}_n\} \subset V_0$, where

$$V_0 := \left\{ \mathbf{Z} \in V : \min_{i \in \{1, \dots, N\}} \text{dist}(\mathbf{z}_i, \partial\Omega) > \varepsilon_0 \right\}$$

(ε_0 is only required to ensure we do not have boundary collisions). To be precise, choose $\mathbf{z}_3, \dots, \mathbf{z}_N \in \Omega$ pairwise distinct and such that $\mathbf{z}_k \neq \tilde{\mathbf{z}}_1$ and $\text{dist}(\mathbf{z}_k, \partial\Omega) > \varepsilon_0$ for every $k = 3, \dots, N$. Therefore, for $n \geq 1$ and $\delta_0 > 0$ sufficiently small, $\mathbf{Z}_n := (\tilde{\mathbf{z}}_1, \tilde{\mathbf{z}}_1 + \delta_n \mathbf{g}_0, \mathbf{z}_3, \dots, \mathbf{z}_N)$ belongs to V_0 , where $\delta_n = \delta_0/n$. Then $\mathbf{j}_1(\mathbf{Z}_n) \cdot \mathbf{g}_0 = \mathbf{j}_1(\tilde{\mathbf{Z}}) \cdot \mathbf{g}_0$ by construction, but $\mathbf{Z}_\infty \notin \mathcal{D}(F)$, where $\mathbf{Z}_\infty = \lim_{n \rightarrow \infty} \mathbf{Z}_n$, because the first and second dislocations have collided.

For each n , all the components of \mathbf{Z}_n are a bounded distance from $\partial\Omega$. Thus, by (1.10), (1.13), and standard elliptic estimates, there exists $C > 0$ such that $|\nabla u(\tilde{\mathbf{z}}_1; \mathbf{Z}_n)| \leq C$ for all n . For each n , the singular strains $|\mathbf{k}_i(\tilde{\mathbf{z}}_1; \mathbf{z}_i)|$ are bounded for $i \geq 3$. However, $|\mathbf{k}_2(\tilde{\mathbf{z}}_1; \tilde{\mathbf{z}}_1 + \delta_n \mathbf{g}_0)| \geq c/\delta_n \rightarrow \infty$ as $n \rightarrow \infty$ for some $c > 0$. Thus, we see from (1.10) and (1.9) that for large n , the force $\mathbf{j}_1(\mathbf{Z}_n)$ will be large in magnitude and aligned closely with $b_1 b_2 (\tilde{\mathbf{z}}_1 - (\tilde{\mathbf{z}}_1 + \delta_n \mathbf{g}_0))$ (i.e., $\mathbf{j}_1(\mathbf{Z}_n)$ will be nearly parallel or antiparallel to \mathbf{g}_0). Therefore, $0 = \mathbf{j}_1(\tilde{\mathbf{Z}}) \cdot \mathbf{g}_0 = \mathbf{j}_1(\mathbf{Z}_n) \cdot \mathbf{g}_0 \geq c_1 |\mathbf{j}_1(\mathbf{Z}_n)| \cdot |\mathbf{g}_0| \rightarrow \infty$ as $n \rightarrow \infty$ for some $c_1 > 0$, which contradicts the fact that $\mathbf{j}_1(\mathbf{Z}_n) \cdot \mathbf{g}_0 = \mathbf{j}_1(\tilde{\mathbf{Z}}) \cdot \mathbf{g}_0$. We conclude that $\widetilde{M}_1^\infty = \emptyset$. \square

Acknowledgment. The authors warmly thank the Center for Nonlinear Analysis, where part of this research was carried out.

REFERENCES

- [1] R. ALICANDRO, M. CICALESE, AND M. PONSIGLIONE, *Variational equivalence between Ginzburg-Landau, XY spin systems and screw dislocations energies*, Indiana Univ. Math. J., 60 (2011), pp. 171–208.
- [2] R. ALICANDRO, L. DE LUCA, A. GARRONI, AND M. PONSIGLIONE, *Metastability and dynamics of discrete topological singularities in two dimensions: A Γ -convergence approach*, Arch. Ration. Mech. Anal., to appear.
- [3] R. ALICANDRO AND M. PONSIGLIONE, *Ginzburg-Landau functionals and renormalized energy: A revised Γ -convergence approach*, J. Funct. Anal., 266 (2014), pp. 4890–4907.
- [4] T. ARMANO AND P. CERMELLI, *Noncrystallographic motion of a dislocation as a fine mixture of rectilinear paths*, SIAM J. Appl. Math., 64 (2004), pp. 2121–2143.
- [5] F. BETHUEL, H. BREZIS, AND F. HÉLEIN, *Tourbillons de Ginzburg-Landau et énergie renormalisée*, C. R. Acad. Sci. Paris Sér. I Math., 317 (1993), pp. 165–171.
- [6] F. BETHUEL, H. BREZIS, AND F. HÉLEIN, *Ginzburg-Landau Vortices*, Progr. Nonlinear Differential Equations Appl. 13, Birkhäuser Boston, Boston, MA, 1994.
- [7] T. BLASS AND M. MORANDOTTI, *Renormalized Energy and Peach-Köhler Forces for Screw Dislocations with Antiplane Shear*, CNA Preprint 14-CNA-16, 2014.
- [8] S. CACACE, A. CHAMBOLLE, AND R. MONNEAU, *A posteriori error estimates for the effective Hamiltonian of dislocation dynamics*, Numer. Math., 121 (2012), pp. 281–335.
- [9] S. CACACE AND A. GARRONI, *A multi-phase transition model for the dislocations with interfacial microstructure*, Interfaces Free Bound., 11 (2009), pp. 291–316.
- [10] L. A. CAFFARELLI AND A. FRIEDMAN, *Partial regularity of the zero-set of solutions of linear and superlinear elliptic equations*, J. Differential Equations, 60 (1985), pp. 420–433.
- [11] P. CERMELLI AND T. ARMANO, *Fine cross-slip of a screw dislocation in anti-plane shear*, Rend. Semin. Mat. Univ. Politec. Torino, 65 (2007), pp. 249–259.
- [12] P. CERMELLI AND M. E. GURTIN, *The motion of screw dislocations in crystalline materials undergoing antiplane shear: Glide, cross-slip, fine cross-slip*, Arch. Ration. Mech. Anal., 148 (1999), pp. 3–52.
- [13] P. CERMELLI AND G. LEONI, *Renormalized energy and forces on dislocations*, SIAM J. Math. Anal., 37 (2005), pp. 1131–1160.
- [14] S. CONTI, A. GARRONI, AND S. MÜLLER, *Singular kernels, multiscale decomposition of microstructure, and dislocation models*, Arch. Ration. Mech. Anal., 199 (2011), pp. 779–819.
- [15] L. DE LUCA, A. GARRONI, AND M. PONSIGLIONE, *Γ -convergence analysis of systems of edge dislocations: The self energy regime*, Arch. Ration. Mech. Anal., 206 (2012), pp. 885–910.
- [16] L. DIECI, C. ELIA, AND L. LOPEZ, *A Filippov sliding vector field on an attracting co-dimension 2 discontinuity surface, and a limited loss-of-attractivity analysis*, J. Differential Equations, 254 (2013), pp. 1800–1832.

- [17] J. D. ESHELBY, *The force on an elastic singularity*, Philos. Trans. Roy. Soc. London. Ser. A., 244 (1951), pp. 84–112.
- [18] L. C. EVANS, *Partial Differential Equations*, 2nd ed., Grad. Stud. Math. 19, American Mathematical Society, Providence, RI, 2010.
- [19] A. F. FILIPPOV, *Differential Equations with Discontinuous Righthand Sides*, Math. Appl. (Soviet Ser.) 18, Kluwer Academic Publishers, Dordrecht, The Netherlands, 1988.
- [20] M. FOCARDI AND A. GARRONI, *A 1D macroscopic phase field model for dislocations and a second order Γ -limit*, Multiscale Model. Simul., 6 (2007), pp. 1098–1124.
- [21] A. GARRONI, G. LEONI, AND M. PONSIGLIONE, *Gradient theory for plasticity via homogenization of discrete dislocations*, J. Eur. Math. Soc. (JEMS), 12 (2010), pp. 1231–1266.
- [22] A. GARRONI AND S. MÜLLER, *Γ -limit of a phase-field model of dislocations*, SIAM J. Math. Anal., 36 (2005), pp. 1943–1964.
- [23] A. GARRONI AND S. MÜLLER, *A variational model for dislocations in the line tension limit*, Arch. Ration. Mech. Anal., 181 (2006), pp. 535–578.
- [24] M. G. D. GEERS, R. H. J. PEERLINGS, M. A. PELETIER, AND L. SCARDIA, *Asymptotic behaviour of a pile-up of infinite walls of edge dislocations*, Arch. Ration. Mech. Anal., 209 (2013), pp. 495–539.
- [25] M. E. GURTIN, *The nature of configurational forces*, Arch. Rational Mech. Anal., 131 (1995), pp. 67–100.
- [26] Q. HAN AND F.-H. LIN, *Nodal Sets of Solutions of Elliptic Differential Equations*, manuscript, 2013.
- [27] J. P. HIRTH AND J. LOTHE, *Theory of Dislocations*, 2nd ed., Krieger, Malabar, FL, 1992.
- [28] F. R. N. NABARRO, *Theory of Crystal Dislocations*, Internat. Ser. Monogr. Phys., Clarendon Press, Oxford, UK, 1967.
- [29] M. PEACH AND J. S. KÖHLER, *The forces exerted on dislocations and the stress fields produced by them*, Physical Rev. (2), 80 (1950), pp. 436–439.
- [30] Y.-P. PELLEGRINI, *Screw and edge dislocations with time-dependent core width: From dynamical core equations to an equation of motion*, J. Mech. Phys. Solids, 60 (2012), pp. 227–249.
- [31] E. SANDIER AND S. SERFATY, *Limiting vorticities for the Ginzburg-Landau equations*, Duke Math. J., 117 (2003), pp. 403–446.
- [32] L. SCARDIA AND C. I. ZEPPIERI, *Line-tension model for plasticity as the Γ -limit of a nonlinear dislocation energy*, SIAM J. Math. Anal., 44 (2012), pp. 2372–2400.
- [33] S. SERFATY, *Gamma-convergence of gradient flows on Hilbert and metric spaces and applications*, Discrete Contin. Dyn. Syst., 31 (2011), pp. 1427–1451.
- [34] E. B. TADMOR, M. ORTIZ, AND R. PHILLIPS, *Quasicontinuum analysis of defects in solids*, Philos. Mag. A, 73 (1996), pp. 1529–1563.
- [35] A. VAINCHTEIN, *Effect of nonlinearity on the steady motion of a twinning dislocation*, Phys. D, 239 (2010), pp. 1170–1179.
- [36] B. VAN KOTEN, X. H. LI, M. LUSKIN, AND C. ORTNER, *A computational and theoretical investigation of the accuracy of quasicontinuum methods*, in Numerical Analysis of Multiscale Problems, Lect. Notes Comput. Sci. Eng. 83, Springer, Heidelberg, 2012, pp. 67–96.
- [37] Y. ZHU, S. J. CHAPMAN, AND A. ACHARYA, *Dislocation motion and instability*, J. Mech. Phys. Solids, 61 (2013), pp. 1835–1853.