

DYNAMICS OF DISCRETE SCREW DISLOCATIONS ON GLIDE DIRECTIONS

R. ALICANDRO, L. DE LUCA, A. GARRONI, AND M. PONSIGLIONE

ABSTRACT. We consider a simple discrete model for screw dislocations in crystals. Using a variational discrete scheme we study the motion of a configuration of dislocations toward low energy configurations. We deduce an effective fully overdamped dynamics that follows the maximal dissipation criterion introduced in [15] and predicts motion along the glide directions of the crystal.

Introduction. Dislocations are one-dimensional defects in the periodic structure of crystals, and their motion represents the microscopic mechanism of plastic flow in metals. In view of this fundamental role, dislocations have been extensively studied by theoretical, experimental and computational means. Classical models are mainly based on the so-called continuum theory of dislocations, in the context of linearized elasticity (see [30] and [27] for a comprehensive treatment). In recent years considerable efforts have been made in order to improve those models by including more information from the microscopic scale. Much insight has been gained on the microscopic structure of dislocations through fine numerical simulations (see e.g. [12] and the references therein), and new phenomenological models accounting for microscopic effects have been proposed (e.g. [25, 42]), while a variety of rigorous mathematical analyses has been done to bridge different scales (see [40, 26, 17] and the references therein). A major issue behind those approaches is the formulation of a simple and efficient discrete model for dislocations that should be the starting point of a multi-scale analysis.

In this paper we consider a two dimensional model for screw dislocations that is inspired by the Frenkel-Kontorova model for dislocation dynamics ([23]). We consider an antiplane discrete setting in which atoms can only move vertically and interact through a two-body periodic potential, a prototypical example being a piecewise quadratic function with wells at the integers. Such Peierls potentials have been successfully exploited to describe basic mechanisms of plastic slips ([13, 38, 24, 27, 28]). Periodic potentials show up naturally starting from a three-dimensional two-particle interaction energy of Lennard-Jones type and assuming anti-plane deformations. We derive their specific form for some precise crystalline structures (as BCC, FCC and HCP lattices), assuming first neighbor interactions.

Our model relies on the general approach developed in [6]. We adopt the formalism therein to introduce the notion of elastic and plastic strain defined on each bond of the lattice, and the notion of discrete dislocations associated to each cell of the lattice. One of the advantages of considering a genuine discrete model is that it does not need any artificial regularization of the core, which is otherwise common in linear continuum (or rather *semi-discrete*) theories.

According to the low-energy dislocation structure assumption (LEDS, [32]), dislocations move following a steepest-descent criterion. Nevertheless, it is well known

that at zero temperature discrete dislocations are pinned by the energy barriers due to the lattice structure. This has been proved analytically for the model under consideration in [28, 29, 2, 19]. Clearly the depinning mechanism is governed by fluctuations of the system or by external forces that can tilt the potential allowing dislocations to overcome the energy barriers.

Here we adopt a variational approach to describe the depinning and motion of dislocations toward states with lower energy by considering a discrete in time (and space) scheme, already proposed in [7, 2]. Precisely, at each time step we minimize the elastic energy stored in the crystal plus a term that accounts for the energy dissipated in moving dislocations from a site to another. A rate-independent dissipation in the presence of a time dependent load, in the spirit of [7], would lead to a quasi-static evolution (see e.g. [34] for a rate-independent evolution law for edge dislocations). Here we consider the case of a rate-dependent quadratic dissipation that leads to a fully overdamped dynamics.

We derive an effective dynamics, the so-called *discrete dislocation dynamics*, by means of a multi-scale analysis of the discrete elastic energy stored in the crystal (see also [26]). It turns out ([16, 2, 19]) that, in the limit as the lattice spacing tends to zero, the elastic energy can be decomposed into a self energy, which scales logarithmically in the core radius, plus an interaction energy $W(x_1, \dots, x_M)$ depending on the dislocation positions x_i . The latter is determined by the behaviour of the discrete periodic interaction potential at the bottom of the wells. In this respect, we validate the harmonic approximation of the far field as predicted by the continuum linear theory (see [41, 35]).

We would like to remark that this analysis has many similarities with other theories in which the presence of topological defects plays an important role ([1]). This is the case of the Ginzburg-Landau model for vortices in super-conductors ([8, 39]). Borrowing the terminology from that context we refer to the interaction energy between dislocations $W(x_1, \dots, x_M)$ as the *renormalized energy*. The gradient of the renormalized energy is nothing but the Peach-Koehler force j between dislocations; namely, $j_i = -\nabla_{x_i} W$ is the force acting on the dislocation at x_i . The corresponding overdamped dynamics is then driven by the Peach-Koehler force (see [22]).

A crucial issue in the time-discrete scheme is the specific choice of the dissipation potential. Choosing a quadratic isotropic dissipation, one recovers an implicit Euler scheme for the renormalized energy, and hence, in the limit of the time step to zero, the fully overdamped discrete dislocation dynamics $\dot{x}_i = j_i$ (see [2]).

Here we make a different choice. We consider a crystalline dissipation that accounts for the specific lattice structure and that is minimal exactly on the preferred glide directions (that in this model are considered as a given material property of the crystal). As a consequence of this choice, we derive an effective dynamics that forces the motion along the glide directions, and follows the *maximal energy dissipation criterion* postulated in [15]. Indeed, dislocations move along the glide direction that maximizes the scalar product with the force $j = -\nabla W$. Clearly this direction could be not unique, so that dislocations can rapidly move from a glide direction to another. This effective dynamics may also predict cross-slip and fine cross-slip, according to [15] and the analysis performed in the recent papers [9, 10]. In view of this lack of uniqueness of the velocity field of the dislocations, the effective dynamics turns out to be described by a differential inclusion rather than a differential equation (see [21]).

Our discrete variational scheme provides a simple and natural model to describe the depinning and the dynamics of screw dislocations, taking into account the preferred glide directions. Moreover it provides an approximation of the effective dynamics proposed by [15], highlighting its gradient flow structure.

1. ANTI-PLANE ELASTICITY IN COMPLEX LATTICES WITH DEFECTS

In this section we will introduce our discrete models for screw dislocations in the framework of anti-plane elasticity. To this purpose, it is convenient to fix some notation for the discrete reference configuration we deal with.

A *Bravais lattice* \mathcal{BL} in \mathbb{R}^d is a discrete set of points in \mathbb{R}^d of the form

$$\mathcal{BL} := \left\{ \sum_{l=1}^d z_l v_l, z_l \in \mathbb{Z} \right\},$$

where v_1, \dots, v_d are given d linearly independent vectors in \mathbb{R}^d , referred to as *primitive vectors*.

A *complex lattice* \mathcal{CL} in \mathbb{R}^d is defined as the union of a finite number of translations of a given Bravais lattice. Namely, \mathcal{CL} is of the form

$$(1.1) \quad \mathcal{CL} := \bigcup_{k=1}^M \mathcal{BL} + \tau_k,$$

where τ_1, \dots, τ_M are M given translation vectors in \mathbb{R}^d .

In the sequel, we will denote by \mathcal{L} any complex (and in particular Bravais) lattice in \mathbb{R}^3 , and by Λ any complex (and in particular Bravais) lattice in \mathbb{R}^2 . The vectors of the canonical basis in \mathbb{R}^3 will be denoted by e_1, e_2 , and e_3 .

In our model Λ is the projection of \mathcal{L} onto a plane orthogonal to the vector v_3 , which we assume to be parallel to e_3 . In view of our discrete-to-continuum asymptotic analysis, we scale the lattice \mathcal{L} by a small parameter $\varepsilon > 0$, representing the lattice spacing, and we consider the portion of $\varepsilon\mathcal{L}$ contained in an infinite cylinder $\Omega \times \mathbb{R}$, where Ω is a bounded open set in \mathbb{R}^2 . Then, our discrete reference configuration is given by $\varepsilon\Lambda \cap \Omega$.

Next, we will introduce a discrete model for anti-plane elasticity suited to describe the presence of screw dislocations, according to the formalism introduced in [6].

1.1. The anti-plane energy. We introduce a class of energy functionals defined on any vertical displacement $u e_3$, with $u : \varepsilon\Lambda \cap \Omega \rightarrow \mathbb{R}$. Let $\{f_{i,j}\}_{i,j \in \Lambda}$ be a family of continuous, 1-periodic interaction potentials vanishing on \mathbb{Z} . We also assume that

$$(1.2) \quad f_{i,j}(t) = c_{i,j} t^2 + o(t^2),$$

for some constants $c_{i,j} \geq 0$. This condition is satisfied by our main examples (see Subsection 1.3).

For every positive ε , the energy functionals $F_{\varepsilon,\Lambda}$ are defined by

$$(1.3) \quad F_{\varepsilon,\Lambda}(u) = \sum_{\substack{\varepsilon i, \varepsilon j \in \varepsilon\Lambda \cap \Omega \\ i \neq j}} f_{i,j}(u(\varepsilon i) - u(\varepsilon j)).$$

A prototypical example is given by the piecewise quadratic energy

$$(1.4) \quad \sum_{\substack{\varepsilon i, \varepsilon j \in \varepsilon \Lambda \cap \Omega \\ i \neq j}} c_{i,j} \operatorname{dist}^2(u(\varepsilon i) - u(\varepsilon j), \mathbb{Z}),$$

which is a Frenkel-Kontorova type energy ([23]), already used by several authors in order to study dislocation dynamics (see e.g. [14, 24, 38]).

Discrete two-dimensional interaction energies as in (1.3) can be justified starting from three-dimensional elastic models for crystals governed by Lennard-Jones type interactions and assuming anti-plane deformations, as described below (see also [28]).

1.2. Formal derivation of the energy. We now present some heuristic arguments that give a more solid ground to our choice for the energy. We will also use these arguments to identify some explicit examples of two dimensional lattice structures and their corresponding energies.

To simplify matter, we work in an infinite complex lattice \mathcal{L} in \mathbb{R}^3 as defined in (1.1) and we will assume that the primitive vector v_3 of the Bravais lattice \mathcal{BL} is e_3 . Moreover, we assume that e_3 is the minimal vertical translation for which the lattice is invariant.

We consider a pair potential $J : (0, +\infty) \rightarrow \mathbb{R}$ of Lennard-Jones type and we assume that the infinite lattice \mathcal{L} has minimal energy with respect to local vertical perturbations.

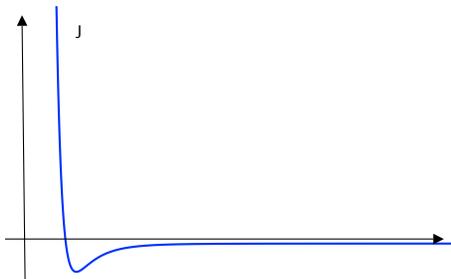


Figure 1. A Lennard-Jones type interaction potential.

Precisely, for any deformation $v : \mathcal{L} \rightarrow \mathbb{R}^3$ with $v = Id$ outside a compact set we define the residual energy

$$E(v) := \sum_{\substack{\tilde{i}, \tilde{j} \in \mathcal{L}, \tilde{i} \neq \tilde{j}}} J(|v(\tilde{i}) - v(\tilde{j})|) - J(|\tilde{i} - \tilde{j}|)$$

and we assume that for every $u : \mathcal{L} \rightarrow \mathbb{R}$ with compact support

$$(1.5) \quad E(Id + ue_3) \geq E(Id) = 0.$$

Notice that with some mild assumptions on the decay at infinity of the potential J , the above energies are finite whenever u is injective. The projected lattice along the direction e_3 is defined by $\Lambda := \Pi(\mathcal{L})$, where $\Pi(x^1, x^2, x^3) := (x^1, x^2)$ for every $(x^1, x^2, x^3) \in \mathbb{R}^3$. Since $\Pi(v_3) = 0$, it is straightforward to check that Λ is a complex lattice in \mathbb{R}^2 , and it is a Bravais lattice whenever \mathcal{L} is a Bravais lattice.

The anti-plane discrete elastic energy is defined on the projected lattice Λ as the energy stored in the cylindrical crystal per unit length. Precisely, we compute the

energy for any vertical displacement that do not depend on the vertical direction e_3 . To this end, fix $u : \Lambda \rightarrow \mathbb{R}$ with compact support, and for every $h > 0$ consider $u_h : \mathcal{L} \rightarrow \mathbb{R}^3$ defined by $u_h(\tilde{i}) = u(\Pi(\tilde{i}))e_3$ if $|\tilde{i}_3| \leq h$ and $u_h(\tilde{i}) = 0$ otherwise. Assume that $Id + u_h$ is injective, so that it has finite energy for every h . Then we can define the anti-plane energy as

$$E^{ap}(u) = \lim_{h \rightarrow +\infty} \frac{1}{2h} E(Id + u_h e_3).$$

Loosely speaking, we are computing the elastic energy per unit length stored in a cylinder whose cross section is much smaller than the height h . This is the classical formal computation used to derive anti-plane models from three dimensional elasticity. A more rigorous derivation, in terms of Γ -convergence, should rely on some assumptions of Cauchy-Born type with respect to the vertical direction.

Note that, in view of (1.5), $E^{ap}(u) \geq 0$ and equality holds true for $u \equiv 0$. For every $i, j \in \Lambda$, with $i \neq j$, and for every $t \in \mathbb{R}$, set

$$\bar{J}(i, j, t) := \sum_{z \in \mathbb{Z}} (J(|\tilde{i} - \tilde{j} + (t+z)e_3|) - J(|\tilde{i} - \tilde{j} + ze_3|)),$$

where \tilde{i}, \tilde{j} are (arbitrarily chosen) points in \mathcal{L} projecting on i, j , respectively.

From the definition of $E^{ap}(u)$ we deduce that

$$E^{ap}(u) = \sum_{i, j \in \Lambda, i \neq j} \bar{J}(i, j, u(i) - u(j)),$$

which corresponds to our model (1.3) choosing $f_{i,j}(t) = \bar{J}(i, j, t)$.

Periodicity. Notice that the interaction of two rows of atoms through the pairwise interaction potential J is invariant under a translation of one row by an integer multiple of e_3 (which restores the lattice). As a consequence of this invariance, the anti-plane interaction potential \bar{J} turns out to be 1-periodic, i.e.,

$$(1.6) \quad \bar{J}(i, j, t) = \bar{J}(i, j, t + z) \quad \text{for every } i, j \in \Lambda, i \neq j, t \in \mathbb{R}, z \in \mathbb{Z}.$$

In particular, by the minimality property (1.5) and by the periodicity (1.6), we have that

$$(1.7) \quad E^{ap}(\zeta) = E^{ap}(0) \leq E^{ap}(u)$$

for every $\zeta : \Lambda \rightarrow \mathbb{Z}$ and $u : \Lambda \rightarrow \mathbb{R}$ with compact support.

Linearization. Let $\zeta : \Lambda \rightarrow \mathbb{Z}$ and let $u : \Lambda \rightarrow \mathbb{R}$ with compact support. By (1.7) we have

$$\frac{d}{d\delta} \Big|_{\delta=0} E^{ap}(\zeta + \delta u) = 0.$$

The next term in the Taylor expansion of E^{ap} represents the linearized anti-plane elastic energy. Indeed, for every $\zeta : \Lambda \rightarrow \mathbb{Z}$ and for every $u : \Lambda \rightarrow \mathbb{R}$ with compact support

$$(1.8) \quad E^{ap}(\zeta + \delta u, \Omega) = \delta^2 \sum_{i, j \in \Lambda, i \neq j} c_{i,j} |u(i) - u(j)|^2 + o(\delta^2),$$

where the constants $c_{i,j}$ are given by $\frac{1}{2} \frac{d^2}{dt^2} \bar{J}(i, j, t) \Big|_{t=0}$ for every $i, j \in \Lambda$, with $i \neq j$. Such constants can be computed using the very definition of \bar{J}

$$(1.9) \quad c_{i,j} = \frac{1}{2} \sum_{z \in \mathbb{Z}} J''(|\tilde{i} - \tilde{j} + ze_3|) \frac{|\tilde{i}^3 - \tilde{j}^3 + z|^2}{|\tilde{i} - \tilde{j} + ze_3|^2} + J'(|\tilde{i} - \tilde{j} + ze_3|) \frac{|i - j|^2}{|\tilde{i} - \tilde{j} + ze_3|^3},$$

where \tilde{i}, \tilde{j} are points in \mathcal{L} projecting on i, j , respectively. If \mathcal{L} is a Bravais lattice, it can be easily seen that the coefficients $c_{i,j}$ in (1.9) depend only on $i - j$.

The expansion (1.8) justifies the use of the prototypical piecewise quadratic model (1.4), which is also very convenient for computational purposes (see [7]). Moreover, we will see that the effective dynamics of dislocations in the limit $\varepsilon \rightarrow 0$ is governed by the Peach-Koehler forces, determined only by the constants $c_{i,j}$ and the crystalline structure Λ .

For the specific choice of the elastic potential J in the main crystal structures described in the following, we will assume that the constants $c_{i,j}$ are positive for short range (either nearest neighbor or next-to-nearest neighbor) interactions, and zero otherwise. This is consistent with the assumption that all the relevant interactions are between particles whose distance is in the convex region of the potential J (and this property is clearly preserved under small deformations).

1.3. The crystal structures. Here we illustrate some examples of crystal lattices: Body-Centered Cubic (BCC), Face-Centered Cubic (FCC), Hexagonal Close-Packed (HCP), and Simple Cubic (SC), and we compute the corresponding coefficients $c_{i,j}$ in (1.9) for very special Lennard-Jones potentials. For BCC, FCC and HCP crystals we assume nearest neighbor interactions and that the distance between nearest neighbors in the undeformed lattice is at the minimum point of the Lennard-Jones potential J , that we fix to be equal to 1. Clearly we have $J'(1) = 0$ and assume $J''(1) > 0$. Let $i, j \in \Lambda$ be the projection of nearest neighbors \tilde{i}, \tilde{j} in \mathcal{L} . A straightforward computation yields

$$(1.10) \quad c_{i,j} = \begin{cases} \frac{1}{2}J''(1)|\tilde{i}^3 - \tilde{j}^3|^2 & \text{if } |\tilde{i}^3 - \tilde{j}^3| \neq \frac{1}{2}; \\ \frac{1}{4}J''(1) & \text{if } |\tilde{i}^3 - \tilde{j}^3| = \frac{1}{2}. \end{cases}$$

If i, j are not projection of nearest neighbors in \mathcal{L} , then $c_{i,j} = 0$.

Finally, we will consider also the Simple Cubic structure (SC). In this case, assuming nearest neighbor interaction would provide a degenerate energy. Hence, we compute the linearized energy in the case of next-to-nearest neighbor interactions.

The BCC lattice. We consider the following unitary linearly independent vectors

$$v_1 := (\sqrt{\frac{8}{9}}, 0, -\frac{1}{3}), \quad v_2 := (\sqrt{\frac{2}{9}}, \sqrt{\frac{2}{3}}, \frac{1}{3}), \quad v_3 := (0, 0, 1)$$

and we define the BCC lattice as the Bravais lattice \mathcal{L}_B generated by v_1, v_2, v_3 . Namely v_1, v_2, v_3 represent three vectors that connect the center of the cube (here given by $(0, 0, 0)$) in the BCC crystal with three neighboring vertices. The class of nearest neighbors $\mathcal{N}\text{-}\mathcal{N}_{\mathcal{L}_B}^0$ to the origin in \mathcal{L}_B is then given by

$$\mathcal{N}\text{-}\mathcal{N}_{\mathcal{L}_B}^0 := \{\pm v_1, \pm v_2, \pm v_3, \pm(v_1 - v_2 + v_3)\}.$$

Projecting the lattice \mathcal{L}_B along the direction v_3 we obtain the hexagonal Bravais lattice Λ_B , generated by

$$w_1 := (\sqrt{\frac{8}{9}}, 0), \quad w_2 := (\sqrt{\frac{2}{9}}, \sqrt{\frac{2}{3}}).$$

The class of nearest neighbors of the origin in Λ_B is given by the projection of the nearest neighbors of the origin in \mathcal{L}_B (see Figure 2), i.e.,

$$\mathcal{N}\text{-}\mathcal{N}_{\Lambda_B}^0 := \{\pm w_1, \pm w_2, \pm(w_1 - w_2)\}.$$

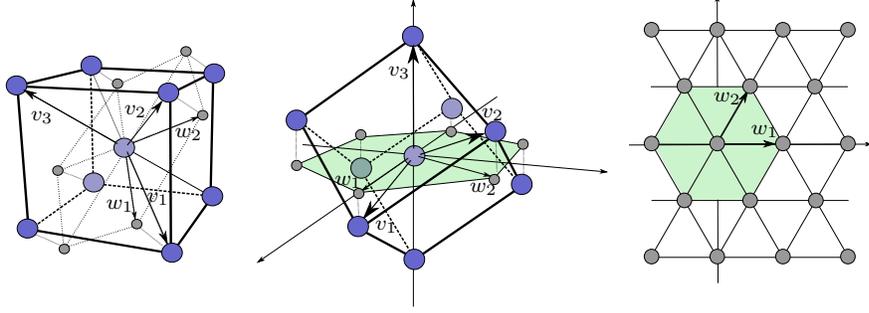


Figure 2. Left: the primitive cell in the BCC lattice. Center: the primitive cell oriented according to the anti-plane direction. Right: the projected hexagonal lattice.

Recalling (1.10), a straightforward computation yields

$$c_{i,j} = c_{0,j-i} = \begin{cases} \frac{J''(1)}{18} & \text{if } j-i \in \{\pm w_1, \pm w_2, \pm(w_1 - w_2)\} \\ 0 & \text{otherwise.} \end{cases}$$

1.3.1. *The FCC lattice.* We consider the following unitary linearly independent vectors

$$v_1 := \left(\frac{\sqrt{2}}{2}, -\frac{1}{2}, \frac{1}{2}\right), \quad v_2 := \left(\frac{\sqrt{2}}{2}, \frac{1}{2}, \frac{1}{2}\right), \quad v_3 := (0, 0, 1)$$

and we define the FCC lattice as the Bravais lattice \mathcal{L}_F generated by v_1, v_2, v_3 .

The class of nearest neighbors $\mathcal{N}\text{-}\mathcal{N}_{\mathcal{L}_F}^0$ to the origin in \mathcal{L}_F is given by

$$\mathcal{N}\text{-}\mathcal{N}_{\mathcal{L}_F}^0 := \{\pm v_1, \pm v_2, \pm v_3, \pm(v_1 - v_2), \pm(v_1 - v_3), \pm(v_2 - v_3)\}.$$

The projected lattice Λ_F along the direction v_3 is the rhombic (centered rectangular) Bravais lattice (see Figure 3) generated by

$$w_1 := \left(\frac{\sqrt{2}}{2}, -\frac{1}{2}\right), \quad w_2 := \left(\frac{\sqrt{2}}{2}, \frac{1}{2}\right).$$

The class of nearest neighbors $\mathcal{N}\text{-}\mathcal{N}_{\Lambda_F}^0$ to the origin is given by

$$\mathcal{N}\text{-}\mathcal{N}_{\Lambda_F}^0 := \{\pm w_1, \pm w_2\}.$$

One can check that for every $i, j \in \Lambda_B$

$$c_{i,j} = c_{0,j-i} = \begin{cases} \frac{J''(1)}{4} & \text{if } j-i \in \{\pm w_1, \pm w_2\} \\ 0 & \text{otherwise.} \end{cases}$$

Notice that, even if $\mathcal{N}\text{-}\mathcal{N}_{\Lambda_F}^0 \neq \Pi(\mathcal{N}\text{-}\mathcal{N}_{\mathcal{L}_F}^0)$, $c_{i,j}$ vanishes for $i-j \notin \mathcal{N}\text{-}\mathcal{N}_{\Lambda_F}^0$.

1.3.2. *The HCP lattice.* Set

$$v_1 := \left(\frac{\sqrt{3}}{2}, 0, \frac{1}{2}\right), \quad v_2 := \left(0, \sqrt{\frac{8}{3}}, 0\right), \quad v_3 := (0, 0, 1), \quad \tau := \left(\frac{\sqrt{3}}{6}, \sqrt{\frac{2}{3}}, \frac{1}{2}\right).$$

Let \mathcal{L}'_H be the Bravais lattice generated by v_1, v_2, v_3 ; we define the HCP lattice as the complex lattice given by

$$\mathcal{L}_H := \mathcal{L}'_H \cup (\mathcal{L}'_H + \tau).$$

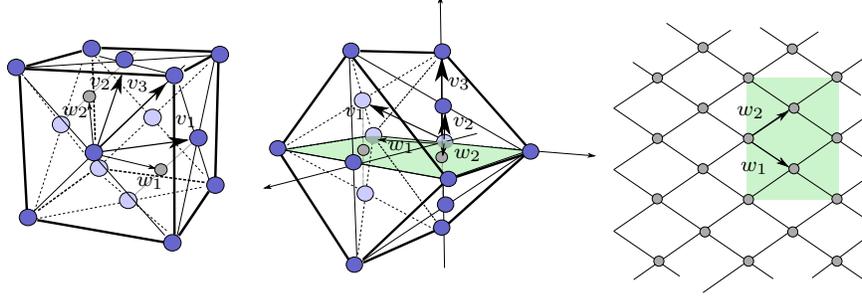


Figure 3. Left: the primitive cell in the FCC lattice. Center: the primitive cell oriented according with the anti-plane direction. Right: the projected rhombic lattice.

The class $\mathcal{N}\text{-}\mathcal{N}_{\mathcal{L}_H}^{\tilde{i}}$ of nearest neighbors to $\tilde{i} \in \mathcal{L}_H$ is given by

$$\begin{aligned} \mathcal{N}\text{-}\mathcal{N}_{\mathcal{L}_H}^{\tilde{i}} &:= \{\tilde{i} \pm v_1, \tilde{i} \pm v_3, \tilde{i} \pm (v_1 - v_3), \tilde{i} + \tau, \tilde{i} + \tau - v_1, \tilde{i} + \tau - v_2, \tilde{i} + \tau - v_3, \\ &\quad \tilde{i} + \tau - v_1 - v_2, \tilde{i} + \tau - v_2 - v_3\} \text{ if } \tilde{i} \in \mathcal{L}'_H \\ \mathcal{N}\text{-}\mathcal{N}_{\mathcal{L}_H}^{\tilde{i}} &:= \{\tilde{i} \pm v_1, \tilde{i} \pm v_3, \tilde{i} \pm (v_1 - v_3), \tilde{i} - \tau, \tilde{i} - \tau + v_1, \tilde{i} - \tau + v_2, \tilde{i} - \tau + v_3, \\ &\quad \tilde{i} - \tau + v_1 - v_2, \tilde{i} - \tau - v_2 + v_3\} \text{ if } \tilde{i} \in \mathcal{L}'_H + \tau. \end{aligned}$$

The projected lattice along v_3 is the complex lattice

$$\Lambda_H = \Lambda'_H \cup (\Lambda'_H + \eta),$$

where Λ'_H is the Bravais lattice generated by the vectors

$$w_1 := \left(\frac{\sqrt{3}}{2}, 0\right), \quad w_2 := \left(0, \sqrt{\frac{8}{3}}\right),$$

and

$$\eta = \left(\frac{\sqrt{3}}{6}, \sqrt{\frac{2}{3}}\right).$$

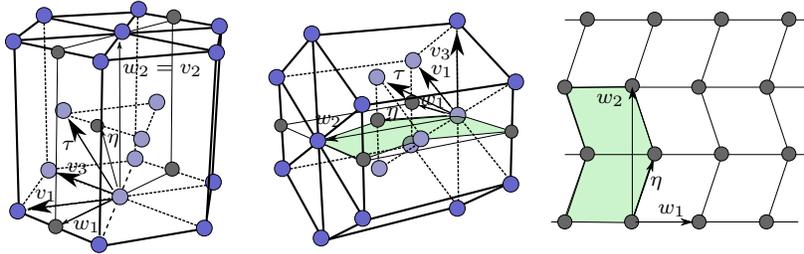


Figure 4. Left: the primitive cell in the HCP lattice. Center: the primitive cell oriented according to the anti-plane direction. Right: the (complex) projected lattice.

The class $\mathcal{N}\text{-}\mathcal{N}_{\Lambda_H}^i$ of nearest neighbors to $i \in \Lambda_H$ is given by the projection of $\mathcal{N}\text{-}\mathcal{N}_{\mathcal{L}_H}^i$ (see Figure 4), i.e.,

$$\begin{aligned}\mathcal{N}\text{-}\mathcal{N}_{\Lambda_H}^i &:= \{i \pm w_1, i + \eta, i + \eta - w_2\} && \text{if } i \in \Lambda'_H \\ \mathcal{N}\text{-}\mathcal{N}_{\Lambda_H}^i &:= \{i \pm w_1, i - \eta, i - \eta + w_2\} && \text{if } i \in \Lambda'_H + \eta.\end{aligned}$$

One can check that for every $i, j \in \Lambda_H$

$$c_{i,j} = \begin{cases} \frac{J''(1)}{4} & \text{if } j \in \mathcal{N}\text{-}\mathcal{N}_{\Lambda_H}^i \\ 0 & \text{otherwise.} \end{cases}$$

1.3.3. The SC lattice. The SC lattice is the Bravais lattice \mathcal{L}_S generated by the vectors of the canonical basis e_1, e_2, e_3 , namely $\mathcal{L}_S := \mathbb{Z}^3$. Hence the projected lattice is the square lattice $\Lambda_S = \mathbb{Z}^2$.

Since all the nearest neighbors in the cubic lattice are either parallel or orthogonal to e_3 , by (1.10) we deduce that $c_{i,j} \equiv 0$ for any $i, j \in \Lambda_S$ with $|i-j| = 1$: considering only nearest neighbor interactions would give degenerate linearized energy. It can be indeed checked that a system of harmonic springs connecting only nearest neighbors in a cubic lattice and subject to a vertical simple shear of size δ gives an energy response of order δ^4 .

In order to get a non-trivial linearized energy, we are led to consider next-to-nearest-neighbors. In this case, recalling (1.9) we have that for every $i \in \Lambda_S$

$$c_{i,j} = c_{0,i-j} = \begin{cases} \frac{1}{2}(J''(\sqrt{2}) + \frac{J'(\sqrt{2})}{\sqrt{2}} + J'(1)) & \text{if } |i-j| = 1, \\ \frac{J'(\sqrt{2})}{2\sqrt{2}} & \text{if } |i-j| = \sqrt{2}, \\ 0 & \text{otherwise.} \end{cases}$$

1.4. Identification of screw dislocations. Classically, dislocations can be detected through so-called *Burgers circuits*, measuring the *geometrically necessary dislocations* in a planar region of the crystal surrounded by a given closed path. The corresponding density of dislocations is nothing but the *Nye's density measure* [36]. Following [6], we will consider elementary Burgers circuits, defined on the boundary of elementary cells of the crystal. In such a way, we obtain a measure of dislocations with a resolution of the order of the lattice spacing. This point of view is very suited to the variational approaches to dislocations, in particular in the asymptotic analysis of the energy stored by discrete dislocations as the atomic distance tends to zero. For screw dislocations and nearest neighbor interactions, this formalism has been adopted for instance in [37], for cubic crystals, and in [28], for BCC crystals.

We first need to fix some additional notation. Let Λ be a complex lattice in \mathbb{R}^2 and denote by \mathcal{T} a Delaunay triangulation of Λ . The class of ε -triangles is defined by

$$\Omega_{\varepsilon,\Lambda}^2 := \{T \in \varepsilon\mathcal{T} : T \subset \Omega\}.$$

The edges of the triangles in $\Omega_{\varepsilon,\Lambda}^2$ are the bonds of the lattice, and are identified by a pair (i, j) , where i and j are vertices of a triangle. Clearly (i, j) and (j, i) identify the same bond. We fix an arbitrary orientation on such bonds: to each bond $(i, j) = (j, i)$, we associate an oriented vector $\ell_{i,j} = \ell_{j,i}$ which either coincides with $i-j$ or with $j-i$.

We now introduce the notion of discrete screw dislocations in our model. Let $P : \mathbb{R} \rightarrow \mathbb{Z}$ be the projection to the closest integer, i.e.

$$(1.11) \quad |t - P(t)| = \min \{|t - s| : s \in \mathbb{Z}\},$$

with the convention that, if the minimizer is not unique (namely if $t \in \frac{1}{2} + \mathbb{Z}$), we choose the minimal one. The discrete plastic strain β_u , associated to any displacement u , is defined on the oriented bonds of the triangulation by $\beta_u(\ell_{i,j}) = P(u(j) - u(i))$ if $\ell_{i,j} = j - i$ (and hence $\beta_u(\ell_{i,j}) = P(u(i) - u(j))$ if $\ell_{i,j} = i - j$). In accordance with the additive decomposition of the strain in elastic and plastic part, following in particular the discrete approach of [6], we have that the elastic strain on $\ell_{i,j} = j - i$ is given by $u(j) - u(i) - \beta_u(\ell_{i,j})$. Since the interaction potentials $f_{i,j}$ are 1-periodic, the elastic energy defined in (1.3) depends only on the elastic strain.

Given $T \in \Omega_{\varepsilon,\Lambda}^2$, let (i, j, k) denote a triple of vertices of T defining a counter-clockwise orientation of T . We introduce the discrete *Burgers circulation* of u around T as

$$\alpha_u(T) := \ell_{i,j} \cdot \frac{j-i}{|j-i|^2} \beta_u(\ell_{i,j}) + \ell_{j,k} \cdot \frac{k-j}{|k-j|^2} \beta_u(\ell_{j,k}) + \ell_{k,i} \cdot \frac{i-k}{|i-k|^2} \beta_u(\ell_{k,i}).$$

Notice that the sign in front of any contribution $\beta_u(\ell_{i,j})$ depends on the relative orientation of the bond $\ell_{i,j}$ and the counter-clockwise orientation of the triangle T . This ensures that, whenever we sum the Burgers circulation around two adjacent triangles, then the plastic contribution on the common bond cancels. The resulting total dislocation is given by the Burgers circulation around the union of the two triangles.

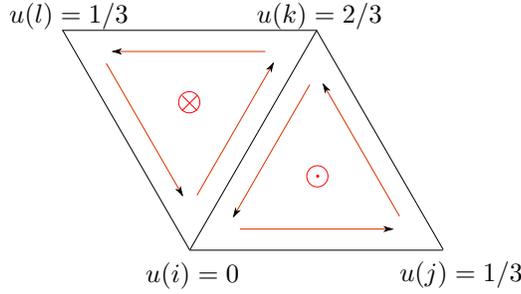


Figure 5. Discrete Burgers Circuit: According to the definition of α_u , the discrete circulation of u along the edges of the triangle (i, j, k) equals 1 and along the edges of the triangle (i, k, l) equals -1 .

It is easy to see that α_u takes values in $\{-1, 0, 1\}$. The values $+1$ and -1 for α_u correspond to the presence of a screw dislocation in the triangle T pointing upward and downward respectively. We now introduce a discrete version of the Nye's dislocation density by means of the measure

$$(1.12) \quad \mu(u) := \sum_{T \in \Omega_{\varepsilon,\Lambda}^2} \alpha_u(T) \delta_{b(T)},$$

where $b(T)$ is the barycenter of the triangle T . By its very definition, for every subset A of Ω which is union of ε -triangles we have that $\mu(u)(A)$ depends only on the values of u on ∂A and represents the geometrically necessary dislocations in A .

Note that different choices for the orientation of the bonds (as well as for the projection P whenever it is not unique) may slightly vary the position of the dislocation cores associated to a given displacement u , but they would not affect the asymptotic analysis that we will describe in the sequel. In particular, assigning two different orientations to the bonds does not affect the definition of the Burgers circulation, except on two adjacent triangles where the elastic strain on the common bond is equal to $\pm 1/2$. In this case, the specific choice of the orientation of the common bond has the effect of switching the dislocation from a triangle to the adjacent one. Clearly, for periodic structures, one could in principle assign the orientation of the bonds using some conventional periodic rule (as done in [2, 28]).

The set of all configurations of discrete dislocations in Ω is identified with

$$(1.13) \quad X_{\varepsilon, \Lambda}(\Omega) := \left\{ \mu = \sum_i d_i \delta_{b(T_i)}, T_i \in \Omega_{\varepsilon, \Lambda}^2, d_i \in \{-1, 0, 1\} \right\}.$$

For any distribution of dislocations $\mu \in X_{\varepsilon, \Lambda}(\Omega)$ we can consider the elastic energy $\mathcal{F}_{\varepsilon, \Lambda}(\mu)$ induced by μ by minimizing the energy $F_{\varepsilon, \Lambda}(u)$ (defined in (1.3)) over all displacements u compatible with μ , i.e.,

$$(1.14) \quad \mathcal{F}_{\varepsilon, \Lambda}(\mu) := \inf \{ F_{\varepsilon, \Lambda}(u) : u : \varepsilon \Lambda \cap \Omega \rightarrow \mathbb{R}, \mu(u) = \mu \}.$$

It is well known that diluted dislocations induce an elastic energy that scales logarithmically in the core radius, i.e., proportional to $|\log \varepsilon|$, while short dipoles may store energy of order one. This means that, in our asymptotic analysis, a logarithmic bound on the total energy does not provide a uniform bound on the number of short dipoles. Hence, it is convenient to introduce a distance between different configurations of dislocations, which vanishes on annihilating dipoles (in fact, it vanishes on the statistically stored dislocations). A natural choice is the distance induced by the flat norm

$$\|\mu\|_{\text{flat}} := \min \left\{ \sum_l |m_l| |p_l - q_l| : m_l \in \mathbb{Z}, p_l, q_l \in \bar{\Omega}, \sum_{p_l, q_l \in \Omega} m_l (\delta_{q_l} - \delta_{p_l}) = \mu \right\},$$

i.e., the length of the minimal connection joining positive and negative masses. Note that if $\mu := \delta_x - \delta_y$, then

$$\|\mu\|_{\text{flat}} \leq |x - y|$$

with equality whenever $|x - y|$ is smaller than the distance of x and y from $\partial\Omega$. This distance turns out to be very suited in our analysis of the effective dynamics, which for $\varepsilon = 0$ (i.e., in the continuous description of the crystal) involves only the geometrically necessary dislocations.

2. DYNAMICS OF DISCRETE SCREW DISLOCATIONS

According to the so-called low-energy dislocation structure hypothesis (LEDS, [32]), a relevant mechanism in plastic deformations is the motion of configurations of dislocations toward low energy configurations, following the steepest descent of the interaction energy.

Discrete systems, however, are often characterized by the presence of many metastable configurations. In the specific case of the model introduced above this has been proved in [2, 28, 29, 19]. In order to move, discrete dislocations have to

overcome energy barriers, and without external forcing terms or fluctuations they are pinned. As a consequence, the gradient flow of the discrete energy $\mathcal{F}_{\varepsilon,\Lambda}$ is stuck.

In order to describe an effective dynamics driven by the sole minimization of the elastic energy we follow a discrete in time scheme, in the spirit of [7]. Precisely, we introduce a notion of discrete gradient flow (see [2]), defined through a step-by-step minimization of a total energy given by the sum of the elastic energy $\mathcal{F}_{\varepsilon,\Lambda}$ and a suitable dissipation. This method corresponds to the Euler implicit scheme for convex energies, which has been generalized to infinite dimensional problems and to non regular and non convex functionals. In the mathematical community, such a general variational approach is known as *minimizing movements* (see [4] and the references therein).

2.1. Dissipations. Here we introduce a class of dissipation functionals, that will measure the energy spent to move a configuration of dislocations during the discrete gradient flow.

Assume for a while that the dislocation configuration at two different time steps t_1, t_2 is given by a single Dirac mass $\delta_{x(t)}$ centered at $x(t)$. Then, we assume that the energy spent to move the dislocation from $x(t_1)$ to $x(t_2)$ can be expressed as $\phi^2(x(t_1) - x(t_2))$, for a suitable norm ϕ , which depends on the material properties of the crystal, taking into account the specific glide directions. In our applications, ϕ is minimal on the slip directions, so we can think that its unit ball is given by a polygon whose vertices coincide with the glide directions of the crystal.

We define our dissipation in two steps. First assume that all the dislocations have the same sign. More precisely, let $\nu_1 = \sum_{i=1}^{N_1} d_i^1 \delta_{x_i^1}$ and $\nu_2 = \sum_{j=1}^{N_2} d_j^2 \delta_{x_j^2}$ with $d_i^1, d_j^2 \in \mathbb{N}$ and set

$$\tilde{D}_\phi(\nu_1, \nu_2) := \min \left\{ \sum_l \phi^2(q_l - p_l) : q_l, p_l \in \bar{\Omega}, \sum_{q_l \in \Omega} \delta_{q_l} = \nu_1, \sum_{p_l \in \Omega} \delta_{p_l} = \nu_2 \right\}.$$

Namely, we minimize the quantity $\sum_l \phi^2(q_l - p_l)$ over all connections between the masses of ν_1 with the masses of ν_2 and possibly with $\partial\Omega$. Actually, $\tilde{D}_\phi(\nu_1, \nu_2)$ can be rewritten as

$$\tilde{D}_\phi(\nu_1, \nu_2) = \min_\lambda \int_{\bar{\Omega} \times \bar{\Omega}} \phi^2(x - y) d\lambda(x, y),$$

where the minimum is taken over all positive measures λ which are sums of Dirac deltas in $\bar{\Omega} \times \bar{\Omega}$ with integer coefficients, and have marginals restricted to Ω given by ν_1 and ν_2 . In other words, the dissipation \tilde{D}_ϕ computed on probability measures is the square of a 2-Wasserstein type metric for a cost function given by the distance induced by ϕ .

For the general case of $\mu_1 = \sum_{i=1}^{N_1} d_i^1 \delta_{x_i^1}$ and $\mu_2 = \sum_{j=1}^{N_2} d_j^2 \delta_{x_j^2}$ with $d_i^1, d_j^2 \in \mathbb{Z}$ we set

$$(2.1) \quad D_\phi(\mu_1, \mu_2) := \tilde{D}_\phi(\mu_1^+ + \mu_2^-, \mu_2^+ + \mu_1^-),$$

where μ_l^+ and μ_l^- are the positive and the negative part of μ_l . This definition encodes the fact that we are connecting in an optimal way dipoles belonging to the same measure, and dislocations with the same sign, belonging to different measures, and has been used to deal with evolution of signed measures in [5, 2].

2.2. Discrete in time and space dynamics. We are now in a position to introduce the discrete gradient flow of $\mathcal{F}_{\varepsilon,\Lambda}$ with respect to the dissipation D_ϕ , fixing a time step $\tau > 0$ and constructing iteratively a discrete in time evolution. To this purpose, first notice that a given dipole $\delta_x - \delta_y$ induces an elastic energy which blows up as $|\log \varepsilon|$ as $\varepsilon \rightarrow 0$. This fact can be formalized in terms of Γ -convergence (see [37, 2]). It is therefore clear that, for ε small enough, it is always convenient to annihilate (in a single time step) such a pair of dislocations, paying a finite dissipated energy (independent of ε), while gaining an amount of elastic energy of order $|\log \varepsilon|$. This suggests that the scheme needed in order to define our discrete gradient flow cannot be based on a global minimization argument, that would lead to instantaneous collision. It is then convenient to consider local minimizers of the total energy instead of global minimizers. To this purpose, we introduce a length scale δ , and we look for minimizers in a δ -neighborhood of the configuration at the previous time step. While it is essential to fix such a length scale, it turns out that its specific choice does not affect at all the dynamics: dislocations move with finite velocity, and hence at each time step they make a “jump” of order τ , which for small τ is smaller than any fixed δ .

Fix a length scale $\delta > 0$, the lattice spacing ε and a time step $\tau > 0$. We define a discrete dynamics, starting from a given initial condition $\mu_0 = \sum_1^M d_{i,0} \delta_{x_{i,0}}$ (with multiplicities $d_{i,0} = \pm 1$), through an iterative minimization process. Namely the discrete dynamics (gradient flow) is given by the measures $\{\mu_{\varepsilon,k}^\tau\}$, with $k \in \mathbb{N} \cup \{0\}$, satisfying $\mu_{\varepsilon,0}^\tau = \mu_0$ and for $k \in \mathbb{N}$, $\mu_{\varepsilon,k}^\tau$ is a solution of

$$(2.2) \quad \min \left\{ \mathcal{F}_{\varepsilon,\Lambda}(\mu) + \frac{D_\phi(\mu, \mu_{\varepsilon,k-1}^\tau)}{2\tau} : \mu \in X_{\varepsilon,\Lambda}(\Omega), \|\mu - \mu_{\varepsilon,k-1}^\tau\|_{\text{flat}} \leq \delta \right\}.$$

Notice that the existence of a minimizer is obvious, since μ lies in X_ε which is a finite set.

If $\phi(x) = |x|^2$, the step-by-step minimization (2.2) is nothing but the Euler implicit scheme for the fully overdamped dynamics governed by the gradient flow $v = -\nabla \mathcal{F}_{\varepsilon,\Lambda}$, where v represents the velocity of the dislocations. We will see that the effect of this minimization problem will be a discrete in time “relaxation of the system”, in the sense that dislocations of opposite sign tend to annihilate, while dislocations near the boundary tend to escape from the domain, as it is expected.

During this process, there might be the emergence of new dislocations in form of short dipoles. Nevertheless, studying the asymptotics as the lattice spacing ε tends to zero, we can show that the discrete evolution $\mu_{\varepsilon,k}^\tau$ is given by the motion of the initial dislocations μ_0 , plus the possible presence of short dipoles that do not affect the dynamics of the geometrically necessary dislocations.

The limit effective dynamics has still a gradient flow structure, with respect to a metric which depends on the specific dissipation norm ϕ and an effective interaction energy.

3. EFFECTIVE DYNAMICS

Our approach in constructing the effective dynamics is based on the assumption that the elastic energy can be decomposed, for ε small, into a self energy, concentrated around each dislocation, and an interaction energy W , referred to as *renormalized energy*, governing the dynamics. It turns out that, for ε much

smaller than the time step τ , the dislocations overcome the energetic barriers and the dynamics is described by a gradient flow of such a renormalized energy.

Actually, we will see that, as $\varepsilon \rightarrow 0$, the sequence $\mu_{\varepsilon,k}^\tau$ converges (up to a subsequence) to some $\mu_k^\tau = \sum_1^M d_{i,0} \delta_{x_i^{k,\tau}}$, whose singularities have the same multiplicity of those of the initial datum, and that solve a step-by-step minimum problem similar to (2.2), but with $\mathcal{F}_{\varepsilon,\Lambda}$ replaced by the renormalized energy (see (3.6)).

Finally, letting $\tau \rightarrow 0$, we obtain a differential inclusion, proposed in [15] and analyzed in [9], which can be interpreted as the gradient flow of the renormalized energy with respect to a metric related with the specific choice of the dissipation functional.

3.1. Renormalized energy. Here we introduce the renormalized energy, which governs the dynamics of dislocations as ε tends to zero. Under suitable assumptions on the periodic potentials $f_{i,j}$, the energy functionals behave as

$$(3.1) \quad \mathcal{F}_{\varepsilon,\Lambda}(\mu) \approx \lambda_{\text{self}} M |\log \varepsilon| + \mathbb{W}_\Lambda(\mu) + M\gamma.$$

The first term is the so-called self energy, \mathbb{W}_Λ is an interaction energy (the renormalized energy) and γ is a finite core energy. Our standing assumption to study the dynamics of dislocations will be to assume that the energy induced by dislocations satisfies the expansion (3.1) in terms of Γ -convergence. For nearest and next-to-nearest neighbor interactions, this Γ -convergence analysis has been developed in [2] and [19].

We now introduce the renormalized energy. Let $M \in \mathbb{N}$ be fixed, representing the number of dislocations, and let $\mathbf{d} = (d_1, \dots, d_M) \in \{-1, +1\}^M$, representing the signs of the dislocations. Once fixed these parameters, the renormalized energy can be expressed in terms of the sole position of the dislocations: it is a smooth function

$$W_{\Lambda,\mathbf{d}} : \Omega^M \setminus \{(x_1, \dots, x_M) : x_i = x_j \text{ for some } i \neq j\} \rightarrow \mathbb{R}.$$

Given $\mu := \sum_{i=1}^M z_i \delta_{x_i} \in X(\Omega)$, we set

$$\mathbb{W}_\Lambda(\mu) := W_{\Lambda,\mathbf{d}}(x_1, \dots, x_M).$$

We will give a formal derivation of the different terms in the asymptotic expansion (3.1), following the classical core radius approach as described in [8] in the context of vortices, and recently developed for variational models of dislocations (see for instance [16, 2, 19, 9]). We first assume that no dislocations are present. In this case, under suitable assumptions on the pair interaction potentials $f_{i,j}$, one can expect that the discrete energy stored in the crystal can be approximated, as $\varepsilon \rightarrow 0$, by a continuous energy, which is quadratic in the small strain regime, i.e.,

$$E_{\text{elastic}}(u, \Omega) \approx \int_{\Omega} \langle A_\Lambda \nabla u, \nabla u \rangle dx,$$

for some suitable macroscopic positive symmetric matrix A_Λ , which depend only on the lattice Λ and the linearization of the energy $F_{\varepsilon,\Lambda}$ (see 1.2). The self energy associated to a dislocation can be described as the continuous energy stored in a fixed ball around such a dislocation, once a disk of radius ε centered at the dislocation position is removed. As $\varepsilon \rightarrow 0$, this quantity blows up logarithmically.

The logarithmic prefactor λ_{self} is then given by

$$\lambda_{\text{self}} := \lim_{\varepsilon \rightarrow 0} \frac{1}{|\log \varepsilon|} \int_{B_1 \setminus B_\varepsilon} \langle A_\Lambda \beta, \beta \rangle \, dx,$$

where β is the strain induced on the plane $\{x_3 = 0\}$ by a screw dislocation centered at the origin with Burgers vector e_3 . If $A_\Lambda = Id$, we have $\beta(x) = \frac{1}{2\pi} \nabla \theta(x)$, where $\theta(x) := \arctan \frac{x_2}{x_1}$, and $\lambda_{\text{self}} = \frac{1}{2\pi}$. In general (by a change of variable) $\beta = \frac{1}{2\pi} A_\Lambda^{-\frac{1}{2}} \nabla \theta(A_\Lambda^{-\frac{1}{2}} x)$, and

$$\lambda_{\text{self}} = \frac{1}{2\pi} \sqrt{\det A_\Lambda}.$$

Since in general the matrix A_Λ is not a multiple of the identity matrix, it is more appropriate to identify the cores of the singularities with ellipses instead of balls, whose ellipticity is suitably determined by the matrix A_Λ . More precisely, set

$$(3.2) \quad B_\Lambda := \frac{A_\Lambda}{\sqrt{\det A_\Lambda}},$$

and for any $\sigma > 0$ let $D_\sigma(x) := B_\Lambda^{-\frac{1}{2}}(B_\sigma(B_\Lambda^{\frac{1}{2}}(x)))$. With such a notation, the core energy γ measures the asymptotic discrepancy between the continuous and the discrete energy around each dislocation x_i in the elliptic annulus $D_1(x_i) \setminus D_\varepsilon(x_i)$. Loosely speaking, if $E_\varepsilon^{\text{disc}}$ denotes the minimal discrete energy stored in $D_1(x_i)$ and induced by a dislocation in its center, and $E_\varepsilon^{\text{cont}}$ denotes its continuous counterpart (stored in $D_1(x_i) \setminus D_\varepsilon(x_i)$), then $\gamma := \lim_{\varepsilon \rightarrow 0} E_\varepsilon^{\text{disc}} - E_\varepsilon^{\text{cont}}$. We refer to [2, 19] for the formal definition of γ .

Finally the renormalized energy $\mathbb{W}_\Lambda(\mu)$ is nothing but the finite continuous energy stored in Ω once the self energy is removed. More precisely, let $\sigma > 0$ and let Ω_σ be the perforated domain obtained removing the ellipses $D_\sigma(x_i)$ from Ω . Then

$$W_{\Lambda, \mathbf{d}}(x_1, \dots, x_M) = \lim_{\sigma \rightarrow 0} \left(E_{\text{elastic}}(u, \Omega_\sigma) - \lambda_{\text{self}} \log \frac{1}{\sigma} \right),$$

where u is the displacement induced by the presence of the dislocations. This is an interaction energy, depending on the mutual positions of the dislocations, and it is responsible for their dynamics. It can be described in terms of the following Dirichlet problem

$$\begin{cases} \operatorname{div}(A_\Lambda \nabla \Phi) = \sqrt{\det A_\Lambda} \sum_i d_i \delta_{x_i} & \text{in } \Omega, \\ \Phi = 0 & \text{on } \partial\Omega. \end{cases}$$

Let

$$(3.3) \quad R_\Lambda(x) := \Phi(x) - \sum_{i=1}^M d_i \log |B_\Lambda^{-\frac{1}{2}}(x - x_i)|$$

be the regular part of the singular potential Φ , which accounts for the interaction with the boundary of Ω . Then, the following formula for the renormalized energy holds

$$(3.4) \quad W_{\Lambda, \mathbf{d}}(x_1, \dots, x_M) := -\lambda_{\text{self}} \left(\sum_{i \neq j} d_i d_j \log |B_\Lambda^{-\frac{1}{2}}(x_i - x_j)| + \sum_{i=1}^M d_i R_\Lambda(x_i) \right).$$

It can be seen that the derivative of the renormalized energy measures the force exerted by the elastic strain to the dislocations (see [16, 10, 9]), i.e.,

$$(3.5) \quad j_i := -\nabla_{x_i} W_{\Lambda, \mathbf{d}}(x_1, \dots, x_M)$$

is the *Peach-Koehler* force on the dislocation at x_i . In dislocation dynamics the Peach-Koehler force is the driving force for the motion of the dislocations ([27]).

In the Appendix A we will give some explicit examples of the quantities λ_{self} and the singular part of $W_{\Lambda, \mathbf{d}}$ for different crystalline structures, namely BCC, FCC, HCP (assuming nearest neighbor interactions) and SC (assuming next-to-nearest-neighbor interactions). The computation of the regular part $R_{\Lambda}(x)$, which accounts for the interaction with the boundary of the domain Ω , can be obtained numerically or explicitly for very special domains, for which the Green function of the Laplacian is explicit.

3.2. Asymptotic dynamics. In view of the asymptotic expansion (3.1) we can derive a limit dynamics as the lattice spacing ε tends to zero. If the dissipation introduced in the scheme (2.2) is differentiable, such a limit dynamics can be described by a finite difference equation for the positions of the evolving M dislocation points. Here we are interested in considering crystalline dissipations, and hence not differentiable (see Figure 6). Therefore we obtain a finite difference inclusion rather than a finite difference equation for the positions of the dislocations.

Denote by $\mathbf{x}_0 = (x_{1,0}, \dots, x_{M,0})$ the initial positions of the dislocations and by $\mathbf{d}_0 = (d_{1,0}, \dots, d_{M,0})$ the corresponding multiplicities. The limiting (as $\varepsilon \rightarrow 0$) discrete in time evolution is defined by solving the step-by-step minimization problem

$$(3.6) \quad \min \left\{ W_{\Lambda, \mathbf{d}_0}(\mathbf{x}) + \sum_{i=1}^M \frac{\phi^2(x_i - x_{i,k-1}^\tau)}{2\tau} : \mathbf{x} \in \Omega^M, \sum_{i=1}^M |x_i - x_{k-1,i}^\tau| \leq \delta \right\},$$

with $\mathbf{x} = (x_1, \dots, x_M) \in \Omega^M$ and $W_{\Lambda, \mathbf{d}_0}(\mathbf{x}) = \mathbb{W}_{\Lambda}(\sum_{i=1}^M d_{i,0} \delta_{x_i})$. We refer to the solutions $\mathbf{x}_k^\tau := (x_{1,k}^\tau, \dots, x_{M,k}^\tau)$ as the *discrete gradient flow* of the renormalized energy $W_{\Lambda, \mathbf{d}_0}$ with dissipation ϕ^2 . These trajectories represent the limit of the trajectories $\mu_{\varepsilon, k}^\tau$ (see (2.2)) as $\varepsilon \rightarrow 0$. Such result has been proved in [2] in the case of a dissipation proportional to the square of the Euclidean distance and will appear in [3] for the crystalline case.

The trajectories defined in (3.6) also satisfy a finite difference inclusion. Indeed if δ is chosen smaller than the relative distance between the dislocations and the boundary of the domain, it can be seen that $\sum |x_i - x_{i,k-1}^\tau| < C\tau$, and hence for τ small enough the constraint is not active for all k up to a time step $k_\delta \approx \frac{1}{\tau}$. We are then led to compute the Euler-Lagrange equation for the minimization problem (3.6). To this end we notice that the function ϕ^2 might be not differentiable (and this will be the case of the examples treated in Section 4), but it is convex, and that $W_{\Lambda, \mathbf{d}_0}$ is regular as far as the dislocations do not collide or reach the boundary of the domain. Therefore the minimality of \mathbf{x}_k^τ yields

$$(3.7) \quad 0 \in \nabla_{x_i} W_{\Lambda, \mathbf{d}_0}(\mathbf{x}_k^\tau) + \frac{1}{2\tau} \partial^- \phi^2(x_{i,k}^\tau - x_{i,k-1}^\tau),$$

where $\partial^- g$ denotes the subdifferential of a function g , which always exists for convex g , and is given by

$$(3.8) \quad \partial^- g(x) = \{v \in \mathbb{R}^2 : g(y) \geq g(x) + v \cdot (y - x) \quad \forall y\}.$$

The differential inclusion (3.7) can be rewritten using the homogeneity of ϕ (precisely the 1-homogeneity of $\partial^- \phi^2$) as follows

$$(3.9) \quad -\nabla_{x_i} W_{\Lambda, \mathbf{d}_0}(\mathbf{x}_k^\tau) \in \partial^- \frac{\phi^2}{2} \left(\frac{x_{i,k}^\tau - x_{i,k-1}^\tau}{\tau} \right).$$

Now, by a classical argument of convex analysis (see e.g. [20], Corollary 5.2) we have that

$$\xi \in \partial^- \frac{\phi^2}{2}(z) \quad \iff \quad z \in \partial^- \left(\frac{\phi^2}{2} \right)^*(\xi),$$

where $(\frac{\phi^2}{2})^*$ is the polar function of $\frac{\phi^2}{2}$ defined by

$$\psi^*(\xi) := \max_{\eta \in \mathbb{R}^2} \langle \xi, \eta \rangle - \psi(\eta).$$

We can conclude that the discrete gradient flow \mathbf{x}_k^τ satisfies the finite difference inclusion

$$(3.10) \quad \frac{x_{i,k}^\tau - x_{i,k-1}^\tau}{\tau} \in \partial^- \left(\frac{\phi^2}{2} \right)^* \left(-\nabla_{x_i} W_{\Lambda, \mathbf{d}_0}(\mathbf{x}_k^\tau) \right).$$

The effective dynamics can be then obtained by taking the limit as the time step τ tends to zero. To this end, we denote by $\mathbf{x}^\tau(t) = (x_1^\tau(t), \dots, x_M^\tau(t))$ the piecewise affine interpolation in time of $\{\mathbf{x}_k^\tau\}$, and, using classical results on differential inclusions (see [21], Chapter 2, paragraphs 6 and 7), we can show that there exists a positive time T such that $\mathbf{x}^\tau(t)$ converges uniformly in $[0, T]$ to a trajectory $\mathbf{x} = \mathbf{x}(t)$ which is a solution of

$$(3.11) \quad \begin{cases} \dot{\mathbf{x}}_i(t) \in \partial^- \left(\frac{\phi^2}{2} \right)^* \left(-\nabla_{x_i} W_{\Lambda, \mathbf{d}_0}(\mathbf{x}(t)) \right) & \text{for } i = 1, \dots, M \\ \mathbf{x}(0) = \mathbf{x}_0. \end{cases}$$

Summarizing we start from a discrete system governed by a periodic interaction potential and we construct a discrete in time evolution for dislocations which converges to a solution of the differential inclusion (3.11). Such result is obtained by taking first the limit as the space parameter ε tends to zero and then by letting the time step τ tend to zero.

Notice that, letting first $\tau \rightarrow 0$ and then $\varepsilon \rightarrow 0$ the evolution would be pinned by the local minima of the discrete energy. This means that there are at least two regimes for $\tau_\varepsilon \gg \varepsilon$ and $\tau_\varepsilon \ll \varepsilon$, for which the effective dynamics is either described by (3.10) or is stuck. A natural question is whether there are other relevant regimes for ε and τ tending to zero. We believe that a critical regime is $\varepsilon \sim \tau$ where the pinning/depinning threshold could be determined by the intensity of the Peach-Koehler force.

In the next section we will specialize the effective dynamics (3.11) for some specific crystalline dissipations, giving rise to a motion along glide directions, according to the maximal dissipation principle stated in [15]. The corresponding differential inclusion has been analyzed in [9], showing existence as long as dislocations stay away from the boundary of Ω and from collision. In [9] it is also shown that this equation may exhibit the occurrence of cross slip and fine cross slip effects.

4. MOTION ALONG GLIDE DIRECTIONS

Here we introduce a natural class of crystalline dissipations taking into account the glide directions of the crystal, that are assumed to be a known material property. Let ξ_1, \dots, ξ_m be m vectors in \mathbb{R}^2 , representing the glide directions in the lattice Λ . We define the norm

$$(4.1) \quad \phi(\xi) := \inf \left\{ \sum_{i=1}^m |\alpha_i| : \sum_{i=1}^m \alpha_i \xi_i = \xi \right\}.$$

We notice that the unit ball in the metric ϕ is given by the convex hull of the polygon whose vertices are $\pm \xi_i$. Notice also that we do not require that all ξ_i have all the same norm, so that some glide directions could turn out to be more preferable than others. One can compute the polar function of $\frac{\phi^2}{2}$ and get

$$(4.2) \quad \left(\frac{\phi^2}{2} \right)^* (\eta) = \frac{1}{2} \max_i \langle \eta, \xi_i \rangle^2.$$

This is again a 2-homogeneous function whose level sets are convex polygons dual to the level sets of ϕ^2 . Notice that, for any fixed $\eta \in \mathbb{R}^2$, we may have either a unique ξ_{\max} , or a pair, $\xi_{\max,1}, \xi_{\max,2}$ which maximize $\langle \eta, \xi_i \rangle^2$ (the set of η in which the maximizers are not unique is called the *ambiguity set*). In the first case, we have that also the subdifferential contains a single vector, precisely

$$(4.3) \quad \partial^- \left(\frac{\phi^2}{2} \right)^* (\eta) = \nabla \left(\frac{\phi^2}{2} \right)^* (\eta) = \langle \eta, \xi_{\max} \rangle \xi_{\max}.$$

In the second case, which corresponds to the vertices of the dual polygons, we have

$$(4.4) \quad \partial^- \left(\frac{\phi^2}{2} \right)^* (\eta) = \langle \eta, \xi_{\max,1} \rangle \text{co}(\{\xi_{\max,1}, \xi_{\max,2}\}),$$

where $\text{co}(\{\xi_{\max,1}, \xi_{\max,2}\})$ is the convex hull of the set $\{\xi_{\max,1}, \xi_{\max,2}\}$ (see Figure 6).

With this choice of a crystalline dissipation the differential inclusion (3.11) recovers the dynamics proposed in [15], according to the maximal dissipation of energy criterion. If the Peach-Koehler force (3.5) acting on a dislocation belongs to the set in which the subdifferential is single valued, then the dislocation moves in the direction prescribed by (4.3). Otherwise, if the Peach-Koehler force lies in the ambiguity set, the dislocation can move along any direction of the convex hull in (4.4) and cross slip and fine cross slip may occur. This is clarified by the following examples.

Example 4.1 (The square lattice). For the square lattice $\Lambda_S = \mathbb{Z}^2$ it is reasonable to assume that the preferred glide directions are given by e_1, e_2 .

In this case $\phi(\xi) = \|\xi\|_1 := |\xi^1| + |\xi^2|$, where $\xi = (\xi^1, \xi^2)$, and therefore

$$(4.5) \quad \left(\frac{\phi^2}{2} \right)^* (\eta) = \frac{1}{2} \max\{|\eta^1|^2, |\eta^2|^2\}.$$

Moreover, for every η such that $|\eta^1| \neq |\eta^2|$, we have

$$(4.6) \quad \partial^- \left(\frac{\phi^2}{2} \right)^* (\eta) = \begin{cases} (\eta^1, 0) & \text{if } |\eta^1| > |\eta^2|, \\ (0, \eta^2) & \text{if } |\eta^2| > |\eta^1|, \end{cases}$$

while in the ambiguity set $\{|\eta^1| = |\eta^2|\}$ we have

$$\partial^- \left(\frac{\phi^2}{2} \right)^* (\eta) = \text{co}(\{(\eta^1, 0), (0, \eta^2)\}).$$

In particular we deduce that in equation (3.11) the dislocation at position $x_i(t)$ moves along the slip directions e_1 or e_2 whenever $|\partial_{x_i^1} W_{\lambda, \mathbf{d}_0}(\mathbf{x}(t))| > |\partial_{x_i^2} W_{\lambda, \mathbf{d}_0}(\mathbf{x}(t))|$ or $|\partial_{x_i^1} W_{\lambda, \mathbf{d}_0}(\mathbf{x}(t))| < |\partial_{x_i^2} W_{\lambda, \mathbf{d}_0}(\mathbf{x}(t))|$, respectively.

Example 4.2 (The hexagonal lattice). For the hexagonal lattice

$$\Lambda_B := \{z_1(1, 0) + z_2(\frac{1}{2}, \frac{\sqrt{3}}{2}) : z_1, z_2 \in \mathbb{Z}\}$$

we assume that the preferred glide directions are given by the vectors $\xi_1 = (1, 0)$, $\xi_2 := (\frac{1}{2}, \frac{\sqrt{3}}{2})$ and $\xi_3 := (\frac{1}{2}, -\frac{\sqrt{3}}{2})$. By the very definition of $(\frac{\phi^2}{2})^*$ in (4.2), for any $\eta = (\eta^1, \eta^2) \in \mathbb{R}^2$ we have

$$\left(\frac{\phi^2}{2} \right)^* (\eta) = \frac{1}{2} \max_{i=1,2,3} \langle \eta, \xi_i \rangle^2 = \frac{1}{2} \max \left\{ |\eta^1|^2, \left| \frac{\eta^1}{2} + \frac{\sqrt{3}\eta^2}{2} \right|^2, \left| \frac{\eta^1}{2} - \frac{\sqrt{3}\eta^2}{2} \right|^2 \right\}.$$

Moreover, for every $\eta \in \mathbb{R}^2$ with $\eta^1 \notin \{-\sqrt{3}\eta^2, 0, \sqrt{3}\eta^2\}$, we have

$$(4.7) \quad \partial^- \left(\frac{\phi^2}{2} \right)^* (\eta) = \begin{cases} \left(\frac{\eta^1}{2} - \frac{\sqrt{3}\eta^2}{2} \right) \xi_3 & \text{if } -\sqrt{3} < \frac{\eta^1}{\eta^2} < 0, \\ \left(\frac{\eta^1}{2} + \frac{\sqrt{3}\eta^2}{2} \right) \xi_2 & \text{if } 0 < \frac{\eta^1}{\eta^2} < \sqrt{3}, \\ \eta^1 \xi_1 & \text{if } -\sqrt{3}|\eta^2| < \eta^1 < \sqrt{3}|\eta^2|, \end{cases}$$

while in the critical cases we get

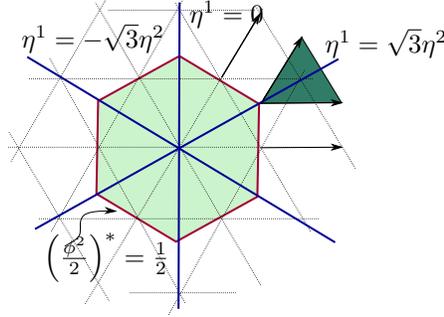


Figure 6. The red hexagon represents a level set of the function $(\frac{\phi^2}{2})^*$. The blue lines represent the ambiguity set where the subdifferential is not single valued. Outside this region the function $(\frac{\phi^2}{2})^*$ is differentiable and the differential is orthogonal to the level set, while on the blue lines, which correspond to the corners of the level sets, the subdifferential is obtained by the convex combination of the differentials on the adjacent edges.

$$(4.8) \quad \partial^- \left(\frac{\phi^2}{2} \right)^* (\eta) = \begin{cases} \eta^1 \text{co}(\{\xi_1, \xi_3\}), & \text{if } \eta^1 = -\sqrt{3}\eta^2 \\ \frac{\sqrt{3}\eta^2}{2} \text{co}(\{\xi_2, -\xi_3\}) & \text{if } \eta^1 = 0, \\ \eta^1 \text{co}(\xi_1, \xi_2) & \text{if } \eta^1 = \sqrt{3}\eta^2. \end{cases}$$

The structure of the subdifferential is described in Figure 6.

CONCLUSIONS

We have introduced a simple discrete setting of anti-plane elasticity in crystals governed by periodic potentials, accounting for the presence of screw dislocations. A multi-scale analysis of this model highlights concentration of energy around the cores, and the emergence of an interaction far field energy, referred to as the renormalized energy, governing the dynamics of dislocations.

In order to model depinning and dynamics of dislocations toward lower energy configurations, we have considered a step-by-step minimization scheme. The dissipations involved in this process encode fundamental material properties of the crystal, such as the preferred glide directions. We show that our effective dynamics satisfies the so-called maximum dissipation criterion: dislocations move according to the glide directions that maximize the scalar product with the Peach-Koehler force, i.e., follow a steepest descent of the renormalized energy along glide directions. We remark that this criterion is not imposed to the model as a constraint, but arises as a consequence of energy balance arguments. On the other hand, enforcing such a constraint in the discrete in time (but continuous in space) scheme would lead to the same evolution law. Enforcing the class of admissible velocity directions in the purely discrete scheme would require a fine analysis of formation and annihilation of short dipoles.

The effective dynamics has a gradient flow structure, and is parabolic in time. It describes a fast dynamics of dislocations toward ground states that could be coupled with a slow rate independent dynamics, driven by time dependent external forces or boundary conditions. This would correspond to one-homogeneous instead of quadratic dissipation functionals.

In our model we neglect thermal effects, or any kind of statistical fluctuation of the system. Our time discretization mimics these effects with a simpler mechanism, allowing dislocations to overcome energy barriers and move. This happens whenever the time step is much larger than the lattice space. We believe that the regime when these two scales are of the same order is somehow critical, leading to a threshold depinning criterion.

APPENDIX A. SOME EXAMPLE OF EXPLICIT RENORMALIZED ENERGIES

A rigorous derivation of the asymptotic expansion (3.1) in terms of Γ -convergence can be done under quite general assumptions for the interaction potentials $f_{i,j}$.

We now review such conditions on the potentials $f_{i,j}$ and we compute explicitly the renormalized energy if the lattice structures is given by $\Lambda_B, \Lambda_F, \Lambda_H$ (see Subsection 1.3), and $f_{i,j} \equiv 0$ whenever $|i - j| > \min_{i,j \in \Lambda, i \neq j} |i - j|$. This corresponds to considering nearest neighbors in the three dimensional BCC, FCC and HCP lattices. To this purpose, we first fix a linear (indeed piecewise-affine for Λ_H) application mapping such lattices into \mathbb{Z}^2 , by setting

$$L_{\Lambda_B} \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} := \frac{3}{2\sqrt{2}} \begin{pmatrix} 1 & 1/\sqrt{3} \\ 0 & 2/\sqrt{3} \end{pmatrix} \begin{pmatrix} x^1 \\ x^2 \end{pmatrix},$$

$$L_{\Lambda_F} \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} := \begin{pmatrix} \sqrt{2}/2 & -1 \\ \sqrt{2}/2 & 1 \end{pmatrix} \begin{pmatrix} x^1 \\ x^2 \end{pmatrix},$$

$$L_{\Lambda_H} \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} := \begin{cases} \begin{pmatrix} \frac{2}{\sqrt{3}}x^1 - \frac{x^2 - 2k\sqrt{\frac{2}{3}}}{\sqrt{6}} \\ \sqrt{\frac{3}{2}}x^2 \end{pmatrix} & \text{if } 2k\sqrt{\frac{2}{3}} \leq x^2 \leq (2k+1)\sqrt{\frac{2}{3}} \\ \begin{pmatrix} \frac{2}{\sqrt{3}}x^1 + \frac{x^2 - 2k\sqrt{\frac{2}{3}}}{\sqrt{6}} \\ \sqrt{\frac{3}{2}}x^2 \end{pmatrix} & \text{if } (2k-1)\sqrt{\frac{2}{3}} \leq x^2 \leq 2k\sqrt{\frac{2}{3}}. \end{cases}$$

For every $\Lambda \in \{\Lambda_B, \Lambda_F, \Lambda_H\}$ there exists a linear application $\bar{L}_\Lambda : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ such that the piecewise-affine functions $L_{\varepsilon, \Lambda}$ mapping $\varepsilon\Lambda$ into $\varepsilon\mathbb{Z}^2$ defined by

$$(A.1) \quad L_{\varepsilon, \Lambda}(x) := \varepsilon L_\Lambda(x/\varepsilon)$$

satisfy $\|L_{\varepsilon, \Lambda} - \bar{L}_\Lambda\|_{L^\infty(\Omega)} \leq \bar{C}\varepsilon$ for some constant $\bar{C} > 0$. In particular $\bar{L}_\Lambda = L_\Lambda$ if $\Lambda \in \{\Lambda_B, \Lambda_F, \Lambda_S\}$, while

$$\bar{L}_{\Lambda_H} \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} := \begin{pmatrix} 2/\sqrt{3} & 0 \\ 0 & \sqrt{3/2} \end{pmatrix} \begin{pmatrix} x^1 \\ x^2 \end{pmatrix}.$$

We assume that the potentials $f_{i,j}$ depend only on $i-j$ (and that $f_{i,j} = f_{j,i}$), i.e., there exists a family of functions $\{g_\xi\}_{\xi \in \{\pm e_1, \pm e_2, \pm(e_1+e_2)\}}$ such that $f_{i,j} = g_{L_\Lambda(i-j)}$ for every pair of nearest neighbors (i, j) . By virtue of the nearest neighbor assumption, we have that $g_{e_1+e_2} \neq 0$ only for the BCC lattice, while it is zero otherwise.

In [19] the Γ -convergence result for (3.1) is proven under the following assumptions: For every $\xi \in \{e_1, e_2, e_1 + e_2\}$ there exists $c_\xi \geq 0$, strictly positive for $\xi = e_1, e_2$, such that the potentials g_ξ satisfy

$$g_\xi(t) \geq \frac{c_\xi}{4\pi^2}(1 - \cos(2\pi t)), \quad g_\xi(t) = c_\xi t^2 + o(t^2).$$

To ease the computations, we assume an isotropy condition for our potentials $f_{i,j}$, which reads as $g_{e_1} = g_{e_2}$ for every $\Lambda \in \{\Lambda_B, \Lambda_F, \Lambda_H\}$, and $g_{e_1+e_2} = g_{e_1}$ for the BCC lattice. We set

$$c := c_{e_1} = c_{e_2}, \quad c_d := c_{e_1+e_2}.$$

Then, $c_d = 0$ for every Λ except for the BCC lattice, where $c_d = c$. These choices are coherent with the derivation of linearized anti-plane elasticity done in Section 1.2.

Now we compute the renormalized energy $W_{\Lambda, \mathbf{d}}$ in (3.4) under the assumptions above. To this purpose, we need to know the explicit formula of the matrix A_Λ used in its definition. We first notice that, in the case of the square lattice with interactions along the directions e_1, e_2, e_1+e_2 , the linearized effective elastic energy is obtained by interpolating the displacement field and the corresponding elasticity matrix A' is given by

$$(A.2) \quad A' := \begin{pmatrix} c + c_d & c_d \\ c_d & c + c_d \end{pmatrix}.$$

The general case of a lattice Λ can be dealt with a change of variable obtaining

$$(A.3) \quad A_\Lambda := \det \bar{L}_\Lambda \bar{L}_\Lambda^{-1} A' (\bar{L}_\Lambda^{-1})^T.$$

Then, by the very definition of A_Λ , we have

$$(A.4) \quad \lambda_{\text{self}} = \frac{\sqrt{\det A_\Lambda}}{2\pi} = \frac{\sqrt{c^2 + 2cc_d}}{2\pi}.$$

Now we specialize the formula of the renormalized energy in (3.4) to each of our lattices. For every $\mathbf{d} = (d_1, \dots, d_M) \in \{+1, -1\}^M$ and $x_1, \dots, x_M \in \Omega$, we have

$$\begin{aligned} W_{\Lambda_B, \mathbf{d}}(x_1, \dots, x_M) &:= -\frac{\sqrt{3}c}{2\pi} \left(\sum_{i \neq j} d_i d_j \log |x_i - x_j| + \sum_i d_i R_{\Lambda_B}(x_i) \right) \\ W_{\Lambda_F, \mathbf{d}}(x_1, \dots, x_M) &:= -\frac{c}{2\pi} \left(\sum_{i \neq j} d_i d_j \log |\sqrt{B_{\Lambda_F}}(x_i - x_j)| + \sum_i d_i R_{\Lambda_F}(x_i) \right), \\ W_{\Lambda_H, \mathbf{d}}(x_1, \dots, x_M) &:= -\frac{c}{2\pi} \left(\sum_{i \neq j} d_i d_j \log |\sqrt{B_{\Lambda_H}}(x_i - x_j)| + \sum_i d_i R_{\Lambda_H}(x_i) \right), \end{aligned}$$

where B_{Λ_F} , B_{Λ_H} and $R(x)$ are defined according to (3.2), and (3.3). Specifically, we have

$$B_{\Lambda_F} := \begin{pmatrix} 1/\sqrt[4]{2} & 0 \\ 0 & \sqrt[4]{2} \end{pmatrix} \quad \text{and} \quad B_{\Lambda_H} := \begin{pmatrix} \sqrt[4]{8/9} & 0 \\ 0 & \sqrt[4]{9/8} \end{pmatrix}.$$

Finally, we consider the case of nearest and next-to-nearest neighbor interactions in the SC crystal. This corresponds to considering interactions along the directions $e_1, e_2, e_1 + e_2, e_1 - e_2$ on the two dimensional lattice $\Lambda_S = \mathbb{Z}^2$. In [19] it is proven that the Γ -convergence expansion in (3.1) holds true if the potentials $f_{i,j}$ depend only on $i - j$ and there exist constants $c', c'_d > 0$ such that

$$\begin{aligned} f_{i, i+\xi}(t) &\geq \frac{c'}{4\pi^2} (1 - \cos(2\pi t)), \quad f_{i, i+\xi}(t) = c't^2 + o(t^2) \quad \text{if } \xi \in \{e_1, e_2\} \\ f_{i, i+\zeta}(t) &\geq \frac{c'_d}{4\pi^2} (1 - \cos(2\pi t)), \quad f_{i, i+\zeta}(t) = c'_d t^2 + o(t^2) \quad \text{if } \zeta \in \{e_1 + e_2, e_1 - e_2\}. \end{aligned}$$

The conditions above mean in particular that the energy functional is isotropic. In this case it is easy to see (see [19] for more details) that $A_{\Lambda_S} := (c' + 2c'_d)I$ and

$$W_{\Lambda_S, \mathbf{d}}(x_1, \dots, x_M) := -\frac{c' + 2c'_d}{2\pi} \left(\sum_{i \neq j} d_i d_j \log |x_i - x_j| + \sum_i d_i R_{\Lambda_S}(x_i) \right).$$

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(Roberto Alicandro) DIEI, UNIVERSITÀ DI CASSINO E DEL LAZIO MERIDIONALE, VIA DI BIASIO 43, 03043 CASSINO (FR), ITALY

E-mail address, R. Alicandro: alicandr@unicas.it

(Lucia De Luca) ZENTRUM MATHEMATIK - M7, TECHNISCHE UNIVERSITÄT MÜNCHEN, BOLTZMANNSTRASSE 3, 85748 GARCHING, GERMANY

E-mail address, L. De Luca: deluca@ma.tum.de

(Adriana Garroni) DIPARTIMENTO DI MATEMATICA “GUIDO CASTELNUOVO”, SAPIENZA UNIVERSITÀ DI ROMA, P.LE ALDO MORO 5, I-00185 ROMA, ITALY

E-mail address, A. Garroni: garroni@mat.uniroma1.it

(Marcello Ponsiglione) DIPARTIMENTO DI MATEMATICA “GUIDO CASTELNUOVO”, SAPIENZA UNIVERSITÀ DI ROMA, P.LE ALDO MORO 5, I-00185 ROMA, ITALY

E-mail address, M. Ponsiglione: ponsigli@mat.uniroma1.it