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► **To cite this version:**

Thomas Hudson. Upscaling a model for the thermally-driven motion of screw dislocations. 2015. hal-01236494v1

**HAL Id: hal-01236494**

**<https://hal.science/hal-01236494v1>**

Preprint submitted on 1 Dec 2015 (v1), last revised 19 Jul 2016 (v2)

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# UPSCALING A MODEL FOR THE THERMALLY-DRIVEN MOTION OF SCREW DISLOCATIONS

T. HUDSON

ABSTRACT. We formulate and study a Markovian model for the thermally-driven motion of screw dislocations. Waiting times for transitions from state to state are assumed to be exponentially distributed with rates expressed in terms of the energy barrier between the states. By using a form of duality, asymptotic descriptions of the energy barriers are computed, and two dimensionless parameters are identified. In a certain parameter regime, the process satisfies a Large Deviations Principle. This gives a description of the most probable path as a gradient flow with non-quadratic dissipation: by then considering a further parameter regime, we recover the usual quadratic dissipation used in discrete dislocation dynamics simulations.

## 1. INTRODUCTION

Dislocations are topological line defects whose motion is a key factor in the plastic behaviour of crystalline solids. Originally hypothesised in order to explain a discrepancy between predicted and observed yield stress in metals [32, 33, 37], they were subsequently experimentally identified in the 1950s via electron microscopy [22, 7]. Although the discovery of dislocations is now more than 80 years distant, the study of these objects remains of significant interest to Materials Scientists and Engineers today. In particular, a cubic centimetre of a metallic solid may contain between  $10^5$  and  $10^9$ m of dislocation lines [26], leading to a dense networked geometry and inducing complex stress fields in the material which are relatively poorly understood. Accurately modelling the behaviour of dislocations therefore remains a major hurdle to obtaining predictive models of plasticity on a single crystal scale.

In this work, we propose and study a discrete stochastic model for the thermally-driven motion of straight screw dislocations in a cylindrical crystal. The basic thermodynamic assumption of the model is that the motion of dislocations proceeds by random jumps between “adjacent” equilibria, with the rate of jumps being governed by the temperature and the energy barrier between states, i.e. the minimal additional energy the configuration must gain in order to pass to from one state to another. The energy we prescribe to describe the system is a discrete anti-plane lattice model, variants of which have been extensively studied in recent literature [34, 25, 2, 24, 1].

By rescaling the model in space and time, we identify two dimensionless parameters. With a specific family of scalings corresponding to the regime where dislocations are well-spaced relative to the lattice spacing, the time over which the system is observed is long and the system temperature is low, we find we may apply the theory of Large Deviations in the spirit of [8] to obtain a mesoscopic evolution law for the most probable trajectory of a configuration of discrete dislocations.

The major contribution of this work is to demonstrate that in the regime we consider, the correct mobility for dislocations is non-linear, and exhibits anisotropy depending upon the underlying lattice, contrary to the linear isotropic mobility often assumed in discrete dislocation dynamics simulations [3, 11, 10].

**1.1. Kinetic Monte Carlo models.** We consider a model for dislocation motion which is based on the observation that at low temperatures, thermally-driven systems spend long periods of time close to local equilibria, before transitioning to an adjacent state. It is a classical assertion that such transitions are approximately exponentially distributed, with a rate which depends upon the

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*Date:* October 10, 2015.

*Key words and phrases.* Screw dislocations, anti-plane shear, lattice models, Kinetic Monte Carlo, Large Deviations.

temperature and energy barrier which must be overcome to pass into a new state [27]. The rate of transition from state  $\mu$  to state  $\nu$  is approximately

$$\mathcal{R}(\mu \rightarrow \nu) := \mathcal{S}(\mu \rightarrow \nu)e^{-\beta\mathcal{B}(\mu \rightarrow \nu)}, \quad (1.1)$$

where

- $\beta := (k_B T)^{-1}$  is the inverse of the thermodynamic temperature of the system, with  $k_B$  being Boltzmann's constant and  $T$  is the absolute temperature;
- $\mathcal{B}(\mu \rightarrow \nu)$  is the additional energy relative to the energy at state  $\mu$  that the system must acquire in order to pass to the state  $\nu$ ; and
- $\mathcal{S}(\mu \rightarrow \nu)$  is an entropic term corresponding to the “size” of the pathway by which  $\mu$  may pass to  $\nu$  with close to minimal additional energy.

We may generate a simple random model of such a system by listing the local equilibria  $\mu$ , and prescribing a set of equilibria  $\mathcal{N}_\mu$  which may be accessed from  $\mu$ , as well as the rates  $\mathcal{B}(\mu \rightarrow \nu)$ . Given that the system is in a state  $\mu$  at time 0, it jumps at a time  $t = \tau$  to a state  $\nu' \in \mathcal{N}_\mu$ , where

$$\tau \sim \text{Exp} \left( \sum_{\nu \in \mathcal{N}_\mu} \mathcal{R}(\mu \rightarrow \nu) \right) \quad \text{and} \quad \mathbb{P}[\mu \rightarrow \nu' | t = \tau] = \frac{\mathcal{R}(\mu \rightarrow \nu')}{\sum_{\nu \in \mathcal{N}_\mu} \mathcal{R}(\mu \rightarrow \nu)}.$$

This defines a Markov process: such processes are sometimes called Kinetic Monte Carlo (KMC) models, and are highly computationally efficient [38]. KMC models have recently been particularly successful in the study of pattern formation during epitaxial growth [6, 36].

A major hurdle to the study of a KMC model is the prescription of the rates  $\mathcal{R}(\mu \rightarrow \nu)$ . In practice, these must be derived or precomputed by some means, normally from a more costly *ab initio* or molecular dynamics computation. Likewise, the majority of the analysis below is devoted to rigorously deriving an asymptotic expression for energy barrier  $\mathcal{B}(\mu \rightarrow \nu)$ , which then informs our choice of  $\mathcal{R}(\mu \rightarrow \nu)$  using (1.1).

**1.2. Modeling screw dislocations.** To define  $\mathcal{B}(\mu \rightarrow \nu)$ , we must prescribe an energy for a configuration of dislocations. In several recent works, variants of an anti-plane lattice model have been studied in which the notion of the energy per unit length of a configuration of straight screw dislocations can be made mathematically precise using the topological framework described in [4]. We follow [25, 24] in considering the energy difference

$$E_n(y; \tilde{y}) := \sum_{e \in n\mathcal{D}_1} [\psi(\mathbf{d}y(e)) - \psi(\mathbf{d}\tilde{y}(e))],$$

where  $n\mathcal{D} \subset \mathbb{R}^2$  is a scaled convex lattice polygon in either the square, triangular or hexagonal lattice,  $n\mathcal{D}_1$  denotes a set of pairs of interacting lines of atoms,  $\mathbf{d}$  is a finite difference operator,  $y$  and  $\tilde{y}$  are anti-plane displacement fields, and  $\psi(s) := \frac{1}{2}\lambda \text{dist}(s, \mathbb{Z})^2$ . A *locally stable equilibrium* is then a displacement  $y$  such that  $u = 0$  minimises  $E_n(y + u; y)$  among all perturbations which are sufficiently small in the energy norm.

Configurations containing dislocations are identified by considering *bond-length 1-forms* associated with  $\mathbf{d}y$ , which we define in §2.5. In analogy with the procedure described in §1.3 of [23], we then define the Burgers vector in a region of the crystal as the integral of the bond-length 1-form around the boundary of the region. This defines a field  $\mu$ , which is the *dislocation configuration*, and we say that the displacement field  $y$  *contains the dislocations*  $\mu$ .

The results of [24], [2] and [1] demonstrate that there are many locally stable equilibria of this energy containing dislocations for a variety of lattice structures. In Theorem 3.1 we give a precise construction of these equilibria with the particular choice of  $\psi$  we study here in the particular cases where . For two dislocation densities  $\mu$  and  $\nu$ , we define the energy barrier from  $\mu$  to  $\nu$  as

$$\mathcal{B}(\mu \rightarrow \nu) := \min_{\gamma \in \Gamma_n(\mu \rightarrow \nu)} \max_{t \in [0,1]} E(\gamma(t); u^\mu),$$

where  $u^\mu, u^\nu$  are locally stable equilibria containing dislocation configurations  $\mu$  and  $\nu$  respectively and  $\Gamma_n(\mu \rightarrow \nu)$  is the space of continuous paths connecting these equilibria.

Theorem 3.2 gives an asymptotic expansion of the energy barrier between adjacent configurations of dislocations, which we use to define  $\mathcal{R}(\mu \rightarrow \nu)$ .

**1.3. Upscaling via a Large Deviations Principle.** The theory of Large Deviations has been developed in order to derive asymptotics for the probability of rare events in random processes; major treatises on the subject include [16, 14, 12, 15].

A sequence of random variables  $X^n$  taking values on a metric space  $M$  is said to satisfy a Large Deviations Principle if there exists a lower semicontinuous functional  $I : M \rightarrow [0, +\infty]$  such that for any open set  $A \subseteq M$ ,

$$\liminf_{n \rightarrow \infty} \frac{1}{n} \mathbb{P}[X^n \in A] \geq - \inf_{x \in A} I(x),$$

and for any closed set  $B \subseteq M$ , we have that

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \mathbb{P}[X^n \in B] \leq - \inf_{x \in B} I(x).$$

The function  $I$  is called the *rate function* of the Large Deviations Principle, and is called *good* if each of the sets

$$\{x \mid I(x) \leq a\} \quad \text{with } a \in \mathbb{R}$$

is compact in  $M$ . The existence of a Large Deviations Principle may be interpreted as saying that

$$\mathbb{P}[X^n \in A] \simeq \exp\left(-n \inf_{x \in A} I(x)\right), \quad \text{as } n \rightarrow \infty,$$

i.e. sets which do not contain  $I^{-1}(0)$  have exponentially small probability as  $n \rightarrow \infty$ .

In our case, the random variables  $X^n$  will correspond to trajectories of the dislocation configuration through space. In §6.1, we rescale these trajectories in time and space, and identify two dimensionless parameters governing the behaviour of the system. Passing to a limit in which these parameters remain fixed allows us to state Theorem 6.1, which asserts that a Large Deviations principle holds for the processes in the cases where the underlying lattice is either the square or hexagonal lattice, and to conjecture such a principle in the case of the triangular lattice.

In each case, we may identify an explicit rate functional, as in [8]: this demonstrates that the “most probable” trajectory of the dislocation configuration is the solution of a nonlinear gradient flow.

In §6.3, we discuss the interpretation of this result, and show that the additional regimes identified in [8] also apply here: in particular, we recover the linear gradient flow structure normally used in Discrete Dislocation Dynamics simulations [3, 11, 10].

**1.4. Notation.** Since we use a significant amount of notation throughout this paper, Table 1 is provided for the reader’s convenience below.

## 2. PRELIMINARIES

**2.1. Lattice complex.** We begin by recalling some facts about lattice complexes, which provide the correct tools to study dislocations in the model we consider. The basic definitions and results given in this section are those of [4]; for further details on the definition of a CW complex, we refer the reader to Section 2 of [4], and for more background on the topology of such constructions in a general setting, either the Appendix of [21], or [31].

**2.1.1. Construction of a lattice complex.** Given a Hausdorff topological space  $S$ , a 0-cell is simply a member of some subset of points in  $S$ . Higher-dimensional cells are then defined iteratively with increasing dimension: for  $p \geq 1$ , a  $p$ -dimensional cell (or  $p$ -cell) is  $e \subset S$  for which there exists a homeomorphism mapping the interior of the  $p$ -dimensional closed ball in  $\mathbb{R}^p$  for some  $p \in \mathbb{N}$  onto  $e$ , and mapping the boundary of the ball onto a finite union of cells with dimension less than  $p$ .

A CW complex is a Hausdorff topological space along with a collection of cells as defined above, such that  $S$  is the disjoint union of all cells, and having the property that  $A \subseteq S$  is closed if and only if  $A \cap e$  is open in  $e$  for every cell  $e$  in the CW complex.

The CW complex is *m-dimensional* if the maximum dimension of any cell is  $m$ , and  $S$  is referred to as the *underlying space* of the complex. The set of all  $p$ -cells is denoted  $S_p$ .

| Symbol   | Description  |
|--|--|
| $\Lambda$  | An $m$ -dimensional multilattice identified with a lattice complex                                 |
| Tr, Sq, Hx   | The triangular, square and hexagonal lattices in $\mathbb{R}^2$                                    |
| $K, N, N^*$  | Constants depending on $\Lambda$ .   |
| $\mathcal{D}$  | A convex lattice polygon   |
| $\Lambda_p, \Lambda_p^*$                             | The set of $p$ -cells in the primal and dual lattice complexes induced by $\Lambda$                |
| $\mathcal{D}_p, \mathcal{D}_p^*$                     | The set of $p$ -cells in the primal and dual lattice subcomplexes induced by $\mathcal{D}$         |
| $\text{Ext}(\mathcal{D}_p)$                          | The set of $p$ -cells in $\mathcal{D}_p$ at the ‘‘edge’’ of the complex induced by $\mathcal{D}$ . |
| $\text{Int}(\mathcal{D}_p)$                          | The set of $p$ -cells in $\mathcal{D}_p$ which lie ‘‘away from the edge of $\mathcal{D}$ ’’.       |
| $\partial, \delta$                                   | The boundary and coboundary operators  |
| $\mathbf{d}, \delta$                                 | The differential and codifferential on forms defined on the lattice complex                        |
| $\Delta$   | The Hodge Laplacian on forms   |
| $\mathcal{W}(\Lambda_p), \mathcal{W}(\mathcal{D}_p)$ | The set of $p$ -forms on $\Lambda$ and $\mathcal{D}$   |
| $\mathcal{L}^2(\Lambda_p)$                           | The Hilbert space of square-integrable $p$ -forms on $\Lambda$                                     |
| $\mathcal{W}_0(\mathcal{D}_p)$                       | The set of $p$ -forms on $\mathcal{D}$ which vanish on $\text{Ext}(\mathcal{D}_p)$ .               |
| $(\cdot)^*$  | The duality mapping on $p$ -cells and $p$ -forms   |
| $E_n(y; \tilde{y})$                                  | Energy difference between deformations $y$ and $\tilde{y}$   |
| $\psi$   | Potential giving energy per unit length of interaction between columns of atoms                    |
| $[\mathbf{d}u]$                                      | The set of bond-length 1-forms corresponding to $\mathbf{d}u$                                      |
| $u^\mu$  | A locally stable equilibrium containing dislocations $\mu$   |
| $\mathcal{B}_n(\mu \rightarrow \nu)$                 | Energy barrier to pass from $u^\mu$ to $u^\nu$   |
| $\Gamma_n(\mu \rightarrow \nu)$                      | The space of paths in deformation space connecting $u^\mu$ and $u^\nu$ .                           |
| $\mathbb{1}_e$                                       | The $p$ -form which is $\pm 1$ on $\pm e$ and 0 otherwise  |
| $G_\Lambda$  | The Green’s function for the full lattice $\Lambda$  |
| $Q_r^\Lambda$  | A polygonal set of radius $r$ in the lattice $\Lambda$   |
| $\omega_e^r$   | The harmonic measure for $Q_r^\Lambda$ evaluated at $e \in \text{Ext}(Q_{\Lambda,0}^r)$            |
| $G^{\mu^*}$  | Solution to $\Delta^* G^{\mu^*} = \mu^*$ in $\mathcal{W}_0(n\mathcal{D}_0^*)$                      |
| $\mathcal{M}_{\epsilon,n}(b_1, \dots, b_m)$          | A set of ‘‘well-separated’’ dislocation positions  |
| $\mathcal{M}_{\epsilon,\infty}(b_1, \dots, b_m)$     | A set of macroscale ‘‘well-separated’’ dislocation positions                                       |
| $\mathcal{R}_n(\mu \rightarrow \nu)$                 | The rate of transitions from $\mu \rightarrow \nu$   |
| $\mathcal{I}_n(\mu \rightarrow \nu)$                 | Entropic contribution to rate of transition  |
| $\beta$  | Inverse thermodynamic temperature per unit area  |
| $\mathcal{T}$  | Characteristic timescale of observation  |
| $D([0, T]; M)$                                       | The Skorokhod space of càdlàg functions from $[0, T]$ to a metric space $M$                        |
| $\Omega_n, H_n$                                      | The infinitesimal and nonlinear generators of the KMC process                                      |
| $\mathcal{H}^\Lambda, \mathcal{L}^\Lambda$           | Hamiltonian and Lagrangian for KMC process.  |
| $\Psi_{A,B}^\Lambda$                                 | Dissipation potential  |
| $\mathcal{I}_{A,B}^\Lambda$                          | Rate functional  |

TABLE 1. Notation conventions used throughout the paper.

$p$ -cells may be assigned an orientation consistent with the usual notion, and we write  $-e$  to mean the  $p$ -cell with opposite orientation to that of  $e$ .

We may define an operator  $\partial$ , called the boundary operator, which maps oriented  $p$ -cells to consistently oriented  $(p-1)$ -cells, which intuitively are ‘‘the boundary’’ of the original cell. Similarly, a coboundary operator,  $\delta$  may be defined, which maps an oriented  $p$ -cell,  $e$ , to all consistently oriented  $p+1$ -cells in the boundary of which  $e$  lies.

We now recall from [4] that a lattice complex is a CW complex such that:

- the underlying space is all of  $\mathbb{R}^m$ ,

- the set of 0-cells forms an  $m$ -dimensional lattice, and
- the cell set is translation and symmetry invariant.

Throughout, we will denote such a lattice complex  $\Lambda$ , and the set of  $p$ -cells of the corresponding complex will be  $\Lambda_p$ .

Later, it will be particularly convenient to consider translations of lattice  $p$ -cells, so for  $e \in \Lambda_p$  and  $\mathbf{a} \in \mathbb{R}^m$ , we define

$$e + \mathbf{a} := \{x \in \mathbb{R}^m \mid x = y + \mathbf{a}, y \in e\}.$$

It will also frequently be convenient later to represent a 1-cell by identifying it through its boundary. We write

$$e = [a, b] \quad \text{to mean} \quad e \in \Lambda_1 \quad \text{such that} \quad \partial e = a \cup -b.$$

2.1.2. *Spaces of  $p$ -forms and calculus on lattices.*  $\mathscr{W}(\Lambda_p)$  denotes the space of real-valued  $p$ -forms, that is

$$\mathscr{W}(\Lambda_p) := \{f : \Lambda_p \rightarrow \mathbb{R} \mid f(e) = -f(-e), \text{ for any } e \in \Lambda_p\}.$$

It is straightforward to see that this is a vector space under pointwise addition. We also define the set of *compactly-supported*  $p$ -forms,

$$\mathscr{W}_c(\Lambda_p) := \{f \in \mathscr{W}(\Lambda_p) \mid \bigcup\{e \mid f(e) \neq 0\} \text{ is compact in } \mathbb{R}^m\}.$$

Let  $A \subset \Lambda_p$  be finite; then for  $f \in \mathscr{W}(\Lambda_p)$ , we define the integral

$$\int_A f := \sum_{e \in A} f(e).$$

The differential and codifferential are respectively defined to be the linear operators  $\mathbf{d} : \mathscr{W}(\Lambda_p) \rightarrow \mathscr{W}(\Lambda_{p-1})$  and  $\delta : \mathscr{W}(\Lambda_p) \rightarrow \mathscr{W}(\Lambda_{p+1})$ , where

$$\mathbf{d}f(e) := \int_{\partial e} f \quad \text{and} \quad \delta f(e) := \int_{\delta e} f.$$

The bilinear form

$$(f, g) := \int_{\Lambda_p} fg$$

is well-defined whenever  $f \in \mathscr{W}_c(\Lambda_p)$  or  $g \in \mathscr{W}_c(\Lambda_p)$ . Moreover, if  $f \in \mathscr{W}_c(\Lambda_p)$  and  $g \in \mathscr{W}_c(\Lambda_{p+1})$ , we have the integration by parts formula

$$(\mathbf{d}f, g) = (f, \delta g). \tag{2.1}$$

Furthermore, by defining

$$\mathscr{L}^2(\Lambda_p) := \left\{ f \in \mathscr{W}(\Lambda_p) \mid \sum_{e \in \Lambda_p} |f(e)|^2 < +\infty \right\},$$

this bilinear form defines an inner product on this  $\mathscr{L}^2(\Lambda_p)$ : it is straightforward to show that this is then a Hilbert space with the induced norm, which we denote  $\|u\|_2 := (u, u)^{1/2}$ .

We also recall the definition of the Hodge Laplacian as the operator

$$\Delta : \mathscr{W}(\Lambda_p) \rightarrow \mathscr{W}(\Lambda_p) \quad \text{with} \quad \Delta f := (\delta \mathbf{d} + \mathbf{d} \delta)f. \tag{2.2}$$

when  $p \neq 0$  and  $p \neq m$ , and in the cases where  $p = 0$  and  $p = m$ ,  $\Delta = \delta \mathbf{d}$  and  $\Delta = \mathbf{d} \delta$  respectively. Any function satisfying  $\Delta f = 0$  on  $A \subset \Lambda_p$  is said to be *harmonic on  $A$* .

Throughout the paper,  $\mathbb{1}_e$  will always denote the  $p$ -form

$$\mathbb{1}_e(a) := \begin{cases} \pm 1 & a = \pm e, \\ 0 & \text{otherwise.} \end{cases}$$

**2.2. Dual complex.** The common notion of duality which occurs in algebraic topology is that of the cohomology. This is usually presented as an abstract algebraic structure, since the algebraic structure is usually all which is needed to deduce topological information about a CW complex. In some cases it may also be given a more concrete identification; this identification will be particularly important for the subsequent analysis.

Given an  $m$ -dimensional lattice complex, when possible, we define the dual complex as follows:

- For any  $e \in \Lambda_m$ , let  $e^* := \int_e x dx$ , the barycentre of set  $e$  in  $\mathbb{R}^m$ , and let

$$\Lambda_0^* := \{e^* \mid e \in \Lambda_m\}.$$

- For a collection of elementary  $m$ -cells  $A \in \Lambda_m$ , let

$$A^* := \bigcup_{e \in A} e^*. \quad (2.3)$$

- Now, iterate over  $p = m - 1, m - 2, \dots, 0$ : for each  $p$ , let  $e \in \Lambda_{p+1}$ , and identify  $\partial e \in \Lambda_p$  as a sum of elementary  $p$ -cells. Find the corresponding cells in  $\Lambda_{p+1}^*$ . Define  $e^* \in \Lambda_{m-p}^*$  to be the convex hull of  $(\partial e)^*$  with  $(\partial e)^*$  removed, assigning  $e^*$  the same orientation as  $e$ . For  $A$ , a sum of elementary  $p$ -cells, we again define  $A^*$  via (2.3).

We now define boundary and coboundary operators on the dual lattice complex,  $\partial^*$  and  $\delta^*$ , so that

$$\partial^* e^* = (\delta e)^*, \quad \text{and} \quad \delta^* e^* = (\partial e)^*. \quad (2.4)$$

By construction,  $*$  :  $\Lambda_p \rightarrow \Lambda_{m-p}^*$  defines an isomorphism of the additive group structure usually defined on lattice complexes (see §2.2 of [4]). (2.4) may then be interpreted as the statement of the Poincaré duality theorem (see for example Section 3.3 of [21]).

The construction described above, is succinctly represented in the following commutation diagram.

$$\begin{array}{ccccccc} \cdots & \Lambda_{p+1} & \xleftarrow{\partial} & \Lambda_p & \xleftarrow{\partial} & \Lambda_{p-1} & \cdots \\ & \uparrow * & & \uparrow * & & \uparrow * & \\ \cdots & \Lambda_{m-p-1}^* & \xleftarrow{\delta^*} & \Lambda_{m-p}^* & \xleftarrow{\delta^*} & \Lambda_{m-p+1}^* & \cdots \\ & \downarrow * & & \downarrow * & & \downarrow * & \end{array}$$

Since the differential and codifferential inherit features from the structure of the CW complex on  $p$ -forms are defined, we now show that similar duality properties hold for the differential complexes on  $\Lambda$  and  $\Lambda^*$ . For any  $f \in \mathcal{W}(\Lambda_p)$ , we define  $f^* \in \mathcal{W}(\Lambda_{m-p}^*)$  via

$$f^*(e^*) := f(e).$$

Again, it may be checked that  $*$  :  $\mathcal{W}(\Lambda_p) \rightarrow \mathcal{W}(\Lambda_{m-p}^*)$  is an isomorphism; in fact,  $*$  defines an isometry of the spaces  $\mathcal{L}^2(\Lambda_p)$  and  $\mathcal{L}^2(\Lambda_{m-p}^*)$ . The differential, denoted  $\mathbf{d}^* : \mathcal{W}(\Lambda_p^*) \rightarrow \mathcal{W}(\Lambda_{p-1}^*)$ , and codifferential, denoted  $\delta^* : \mathcal{W}(\Lambda_{p-1}^*) \rightarrow \mathcal{W}(\Lambda_p^*)$ , are then

$$\mathbf{d}^* f^*(e^*) := \int_{\partial^* e^*} f^* = \int_{\delta e} f = \delta f(e), \quad \text{and} \quad \delta^* f^*(e^*) := \int_{\delta^* e^*} f^* = \int_{\partial e} f = \mathbf{d} f(e).$$

Again, this relationship is concisely expressed in the following diagram.

$$\begin{array}{ccccccc} \cdots & \mathcal{W}(\Lambda_{p+1}) & \xleftarrow{\mathbf{d}} & \mathcal{W}(\Lambda_p) & \xleftarrow{\mathbf{d}} & \mathcal{W}(\Lambda_{p-1}) & \cdots \\ & \uparrow * & & \uparrow * & & \uparrow * & \\ \cdots & \mathcal{W}(\Lambda_{m-p-1}^*) & \xleftarrow{\delta^*} & \mathcal{W}(\Lambda_{m-p}^*) & \xleftarrow{\delta^*} & \mathcal{W}(\Lambda_{m-p+1}^*) & \cdots \\ & \downarrow * & & \downarrow * & & \downarrow * & \end{array}$$

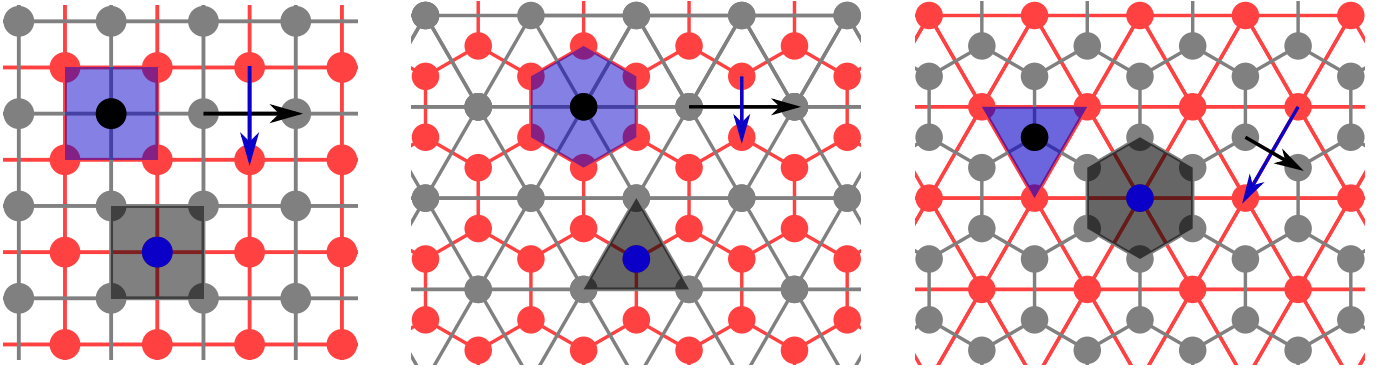


FIGURE 1. The square, triangular and hexagonal lattices respectively, and their duals. Primal lattices are shown in grey, dual lattices in red; 2-cells are left uncoloured. Particular primal cells are highlighted in black, and their respective dual cells are given in blue.

**2.3. Examples: the square, triangular and hexagonal lattices.** In the analysis which follows, we focus exclusively on 2-dimensional lattice complexes, and in particular the triangular, square and hexagonal lattices denoted  $\text{Tr}$ ,  $\text{Sq}$  and  $\text{Hx}$  respectively. Let  $R_4$  and  $R_6$  be the rotation matrices

$$R_4 := \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \quad \text{and} \quad R_6 := \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}.$$

For convenience, we define  $\mathbf{e}_1 := (1, 0)^T$ ,  $\mathbf{a}_1 := (1, 0)^T$ , and

$$\mathbf{e}_i := R_4^{i-1} \mathbf{e}_1 \quad \text{and} \quad \mathbf{a}_j := R_6^{j-1} \mathbf{a}_1$$

for  $i = 1, \dots, 4$  and  $j = 1, \dots, 6$ . The triangular, square and hexagonal lattices are then defined to be

$$\text{Tr} := [\mathbf{a}_1, \mathbf{a}_2] \cdot \mathbb{Z}^2, \quad \text{Sq} := \mathbb{Z}^2, \quad \text{and} \quad \text{Hx} := \sqrt{3}\text{Tr} \cup [\sqrt{3}\text{Tr} + \mathbf{e}_2].$$

The nearest neighbour directions in  $\text{Sq}$  are then  $\mathbf{e}_i$ , and  $\mathbf{a}_i$  in  $\text{Tr}$  or  $\text{Hx}$ . We may define lattice complexes based on these sets (see §2.3.2 and §2.3.3 of [4] and [5]), and moreover

$$\text{Sq}^* = \text{Sq} + \frac{1}{2}(\mathbf{e}_1 + \mathbf{e}_2), \quad \text{Tr}^* = \frac{1}{3}\text{Hx} + \frac{1}{3}(\mathbf{a}_2 + \mathbf{a}_3), \quad \text{and} \quad \text{Hx}^* = \sqrt{3}\text{Tr} + \frac{\sqrt{3}}{3}(\mathbf{a}_1 + \mathbf{a}_2).$$

Figure 2.3 illustrate the three lattices and the duality mapping between  $\Lambda$  and  $\Lambda^*$ .

Throughout the paper,  $K$ ,  $N$  and  $N^*$  will denote constants which depends upon the lattice considered:

$$K = \begin{cases} 2 & \text{if } \Lambda = \text{Hx}, \\ 4 & \text{if } \Lambda = \text{Sq}, \\ 6 & \text{if } \Lambda = \text{Tr}, \end{cases} \quad N = \begin{cases} 3 & \text{if } \Lambda = \text{Hx}, \\ 4 & \text{if } \Lambda = \text{Sq}, \\ 6 & \text{if } \Lambda = \text{Tr}, \end{cases} \quad \text{and} \quad N^* = \begin{cases} 6 & \text{if } \Lambda = \text{Hx}, \\ 4 & \text{if } \Lambda = \text{Sq}, \\ 3 & \text{if } \Lambda = \text{Tr}. \end{cases}$$

We remark that  $N$  and  $N^*$  are the number of nearest neighbours in the primal and dual lattice respectively.

**2.4. Finite lattice subcomplexes.** For the particular application we will consider, we will make use of finite subcomplexes of the full lattice complex, and so we now make precise the notation we use as well as the particular assumptions made throughout our analysis.

**2.4.1. Induced subcomplexes.** Given a finite subset  $\mathcal{A}_0 \subset \Lambda_0$ , we define the *induced lattice subcomplex* by inductively defining

$$\mathcal{A}_p := \{e \in \Lambda_p \mid \partial e \subset \mathcal{A}_{p-1}\}.$$

This is a well-defined CW complex when the corresponding boundary  $\partial^A$  and coboundary  $\delta^A$  operators are defined by restriction, i.e.

$$\partial^A e := \partial e \cap \mathcal{A}_{p-1}, \quad \text{and} \quad \delta^A e = (\delta e) \cap \mathcal{A}_{p+1} \quad \text{for all } e \in \mathcal{A}_p.$$



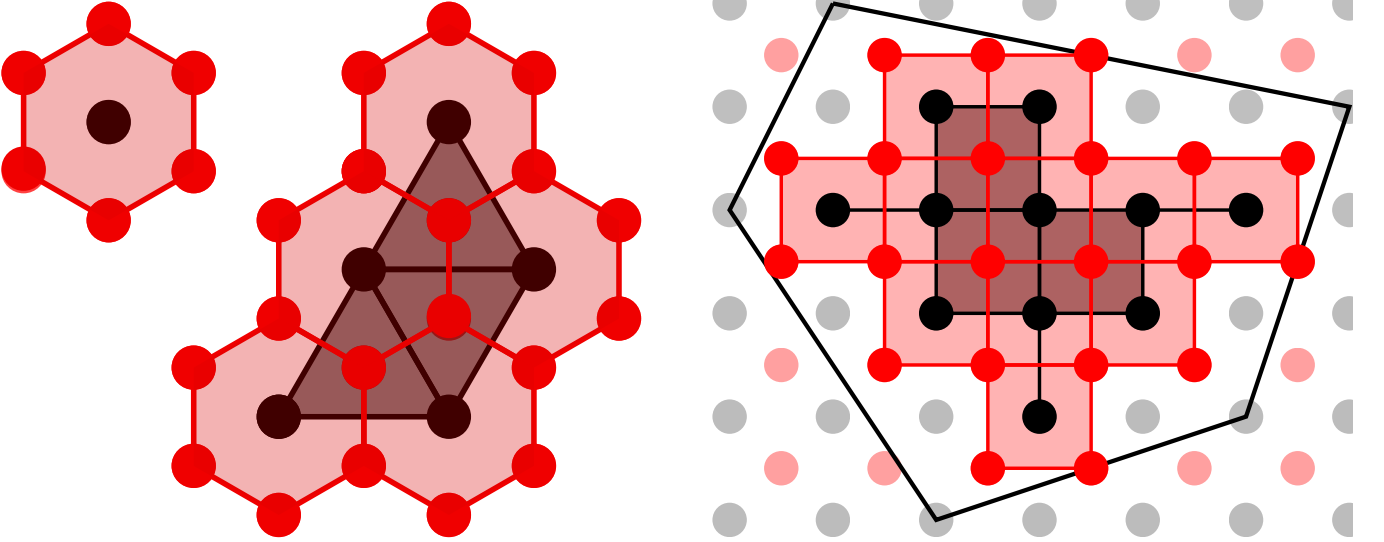


FIGURE 2. On the left, an example of primal (in black) and dual (in red) induced subcomplexes for a general subset of the triangular lattice:  $\mathcal{A}_0$  is the set of black points. On the right, a lattice polygon  $\mathcal{D}$ , and the corresponding primal and dual subcomplexes, which are both path- and simply-connected .

The induced differential and codifferential operators  $\mathbf{d}^{\mathcal{A}}$  and  $\delta^{\mathcal{A}}$  are then defined in the same way as  $\mathbf{d}$  and  $\delta$ , using  $\partial^{\mathcal{A}}$  and  $\delta^{\mathcal{A}}$  in place of  $\partial$  and  $\delta$ , and we may define the spaces  $\mathcal{W}(\mathcal{A}_p)$  and  $\mathcal{L}^2(\mathcal{A}_p)$ .

It will be convenient to distinguish what we term the *exterior* and *interior*  $p$ -cells of the CW complex  $\mathcal{A}$ , respectively defined to be

$$\text{Ext}(\mathcal{A}_p) := \{e \in \mathcal{A}_p \mid \delta e \neq \delta^{\mathcal{A}} e\}, \quad \text{and} \quad \text{Int}(\mathcal{A}_p) := \mathcal{A}_p \setminus \text{Ext}(\mathcal{A}_p).$$

The former set may be thought of as the ‘edge’ of the lattice subcomplex, and the latter as the ‘interior’ of the lattice subcomplex.

We now define a subcomplex of the dual lattice complex which we call the *dual subcomplex induced by  $\mathcal{A}_0$* . Let  $\mathcal{A}_m^* := \{e^* \in \Lambda_m^* \mid e \in \mathcal{A}_0\}$ , and inductively define

$$\mathcal{A}_{m-p}^* := \{e^* \in \Lambda_{m-p}^* \mid e^* \in \partial^* a^* \text{ for some } a^* \in \mathcal{A}_{m-p+1}^*\}$$

for  $p \geq 1$ . We remark that this definition is *not* equivalent to defining sets of sets of dual  $p$ -cells by directly taking the dual of the primal  $p$ -cells; however, we do have the inclusion

$$[\mathcal{A}_p]^* \subseteq \mathcal{A}_{m-p}^* \quad \text{for each } p,$$

where equality always holds when  $p = m$  by definition. The other inclusions follow by induction on  $p$ : note that  $e \in \mathcal{A}_p$  with  $p \geq 1$  implies that  $e \in \delta^{\mathcal{A}} a$  for some  $a \in \mathcal{A}_{p-1}$ ,  $\delta^{\mathcal{A}} a \subseteq \delta a$ , and hence  $e^* \in \partial^* a^*$  for some  $a^* \in \mathcal{A}_{m-p+1}^*$ . As before, we may define  $\partial^{\mathcal{A}^*}$  and  $\delta^{\mathcal{A}^*}$  by restriction, which in turn leads us to define operators  $\mathbf{d}^{\mathcal{A}^*}$  and  $\delta^{\mathcal{A}^*}$  analogously.

Similarly, let

$$\text{Ext}(\mathcal{A}_p^*) := \{e^* \in \mathcal{A}_p^* \mid \delta^* e^* \neq \delta^{\mathcal{D}^*} e^*\}, \quad \text{and} \quad \text{Int}(\mathcal{A}_p^*) := \mathcal{A}_p^* \setminus \text{Ext}(\mathcal{A}_p^*).$$

By construction,  $\text{Ext}(\mathcal{A}_2^*) = \emptyset$ , and  $e \in \text{Ext}(\mathcal{A}_{n-p}^*)$  if and only if there exists no  $a \in \mathcal{A}_p$  with  $e = a^*$  (see Figure 2.4.1 for an illustration).

From now on, it will always be clear from the context whether we are referring to the relevant operators on  $\Lambda$  and  $\Lambda^*$ , or on  $\mathcal{A}$  and  $\mathcal{A}^*$ , so for the sake of concision, we will suppress  $\mathcal{A}$  from our notation.

**2.4.2. Subcomplexes induced by a domain.** We will say that an induced lattice subcomplex is path-connected if for any  $e, e' \in \mathcal{A}_0$ , there exists  $\gamma \subset \mathcal{A}_1$  such that

$$\partial \gamma = e \cup -e',$$

and call such  $\gamma \subset \mathcal{A}_1$  a *path* which connects  $e$  and  $e'$ . We will say a lattice subcomplex is *simply-connected* if for any  $\gamma' \subset \mathcal{A}_1$  such that  $\partial\gamma' = \emptyset$ ,  $\gamma' = \partial A$  for some  $A \in \mathcal{A}_2$ .

Throughout our analysis,  $\mathcal{D}$  will always denote a closed convex lattice polygon, i.e. a non-empty compact convex subset of  $\mathbb{R}^2$  which has corners  $c_l \in \Lambda$ , and internal angles  $\omega_l$  where  $l = 1, \dots, L$ , ordered with clockwise orientation as in [19]. We will later consider the scaled domain  $n\mathcal{D}$ ,  $n \in \mathbb{N}$ ; note that  $n\mathcal{D}$  remains a lattice polygon.

We then denote  $n\mathcal{D}$  to be the largest induced lattice subcomplex with respect to inclusion such that

- $n\mathcal{D}_p \subset n\overline{\mathcal{D}}$  for all  $p$ ,
- $n\mathcal{D}_p^* \subset n\overline{\mathcal{D}}$  for all  $p$ ,
- $n\mathcal{D}$  and  $n\mathcal{D}^*$  are both path connected and simply connected.

It can be shown that such a complex always exists as long as  $n$  is sufficiently large, since  $\mathcal{D}$  is convex: we give one example in Figure 2.4.1.

2.4.3. *Counting and distances.* For a collection of  $p$ -cells  $C \subset \mathcal{D}_p$ , we write  $\#C$  to designate the smallest number of elementary  $p$ -cells  $e_i$  such that  $C = \bigcup_{i=1}^{\#C} e_i$ .

We define  $\text{diam}(\mathcal{D})$  to be

$$\text{diam}(\mathcal{D}) := \max \{|x - y| \mid x, y \in \mathcal{D}\},$$

and we note that there exists a constant  $C_\Lambda > 0$  which depends only on the underlying lattice  $\Lambda$  such that

$$\max \left\{ \min \{ \# \gamma \mid \gamma \subset n\mathcal{D}_1, \partial\gamma = e - e' \} \mid e', e \in \text{Ext}(n\mathcal{D}_0) \right\} \leq C_\Lambda n \text{diam}(\mathcal{D}).$$

We write  $\text{dist}(A, B)$  to mean the shortest distance between two sets  $A, B \subset \mathbb{R}^m$ , i.e.

$$\text{dist}(A, B) := \inf \{|x - y| \mid x \in A, y \in B\}.$$

2.4.4. *Spaces of  $p$ -forms on lattice subcomplexes.* The space of  $p$ -forms on the lattice subcomplex induced by  $\mathcal{A}_0 \subset \Lambda_0$  is denoted

$$\mathscr{W}(\mathcal{A}_p) := \{u : \mathcal{A}_p \rightarrow \mathbb{R} \mid u(e) = -u(-e)\}.$$

As for  $\Lambda$ , we define the inner product

$$(u, v) := \int_{\mathcal{A}_p} uv,$$

denoting the induced norm  $\|u\|_2 := (u, u)^{1/2}$ ; since  $\mathcal{A}_p$  is finite, this is always well-defined. We will also occasionally make use of the norm

$$\|u\|_\infty := \max_{e \in \mathcal{A}_p} |u(e)|.$$

We denote the subspace of  $p$ -forms vanishing on  $\text{Ext}(\mathcal{A}_p)$

$$\mathscr{W}_0(\mathcal{A}_p) := \{u \in \mathscr{W}(\mathcal{A}_p) \mid u = 0 \text{ on } \text{Ext}(\mathcal{A}_p)\},$$

which is clearly a vector space, and the bilinear form

$$((u, v)) := \int_{n\mathcal{D}_1} \mathbf{d}u \mathbf{d}v$$

is a well-defined inner product on  $\mathscr{W}_0(\mathcal{A}_0)$ .  $\mathscr{W}_0(\mathcal{A}_0)$  is thus a Hilbert space with the corresponding norm, denoted  $\|u\|_{1,2} := ((u, u))^{1/2}$ . We now demonstrate positive-definiteness of the inner product, since we will use the resulting version of Poincaré inequality below.

Since  $n\mathcal{D}$  is path-connected, for any  $e \in \text{Int}(n\mathcal{D}_0)$ , there exists  $\gamma \subset \mathcal{D}_1$  such that  $\partial\gamma = e \cup -e'$ , with  $e' \in \text{Ext}(n\mathcal{D}_0)$  and  $\#\gamma \leq C_\Lambda n \text{diam}(\mathcal{D})$ . For any  $u \in \mathscr{W}_0(\mathcal{D}_0)$ , we then have  $u(e) = \int_\gamma \mathbf{d}u$ , so applying the Cauchy-Schwarz inequality, we have

$$|u(e)|^2 = \left| \int_\gamma \mathbf{d}u \right|^2 \leq \#\gamma \int_\gamma |\mathbf{d}u|^2 \leq \#\gamma \int_{n\mathcal{D}_1} |\mathbf{d}u|^2.$$

Integrating over  $n\mathcal{D}_0$ , and noting that there exists a constant  $C'_\Lambda > 0$  which depends only on the underlying lattice  $\Lambda$  such that  $\#n\mathcal{D}_0 \leq C'_\Lambda n^2 \text{diam}(\mathcal{D})^2$ , we have

$$\int_{n\mathcal{D}_0} |u|^2 \leq C''_\Lambda n^3 \text{diam}(\mathcal{D})^3 \int_{n\mathcal{D}_1} |\mathbf{d}u|^2, \quad (2.5)$$

where  $C''_\Lambda = C_\Lambda C'_\Lambda$ . We note that the same inequality also holds for  $u \in \mathscr{W}_0(n\mathcal{D}_0^*)$  by a similar argument.

**2.4.5. Duality for  $p$ -forms on lattice subcomplexes.** We define the duality mapping  $*$  :  $\mathscr{W}(n\mathcal{D}_p) \rightarrow \mathscr{W}_0(n\mathcal{D}_{2-p}^*)$  as follows:

$$u^*(a) = \begin{cases} u(e) & a = e^* \in \text{Int}(n\mathcal{D}_{2-p}^*), \\ 0 & a \in \text{Ext}(n\mathcal{D}_{2-p}^*). \end{cases}$$

We note that this mapping is well-defined since as noted in §2.4.1,  $a \in \text{Ext}(n\mathcal{D}_{2-p}^*)$  if and only if there exists no  $e \in n\mathcal{D}_p$  with  $a = e^*$ . This duality mapping defines an isomorphism from  $\mathscr{W}(\mathcal{D}_p)$  to  $\mathscr{W}_0(\mathcal{D}_{n-p}^*)$  as vector spaces; since in addition

$$(u, u) = \int_{n\mathcal{D}_p} |u|^2 = \int_{\text{Int}(n\mathcal{D}_p^*)} |u^*|^2 = \int_{n\mathcal{D}_p^*} |u^*|^2 = (u^*, u^*),$$

it follows that  $*$  defines an isometry of the spaces  $\mathscr{L}^2(n\mathcal{D}_p)$  to  $\mathscr{L}^2(n\mathcal{D}_{2-p}^*)$ .

Moreover, for any  $e \in n\mathcal{D}_p$ , by using this definition, we verify that

$$\mathbf{d}u(e) = \int_{\partial e} u = \int_{(\partial e)^*} u^* = \int_{\delta^* e^*} u^* = \delta^* u^*(e^*), \quad \text{and} \quad \delta u(e) = \int_{\delta e} u = \int_{(\delta e)^*} u^* = \int_{\partial^* e^*} u^* = \mathbf{d}^* u^*(e^*). \quad (2.6)$$

**2.5. Dislocation configurations.** We now recall some definitions from [24]. Given  $u \in \mathscr{W}(n\mathcal{D}_0)$ , we define the associated set of *bond-length 1-forms*

$$[\mathbf{d}u] := \left\{ \alpha \in \mathscr{W}(n\mathcal{D}_1) \mid \|\alpha\|_\infty \leq \frac{1}{2}, \alpha - \mathbf{d}u \in \mathbb{Z} \right\}.$$

A *dislocation core* is any positively-oriented 2-cell  $e \in n\mathcal{D}_2$  such that

$$\mathbf{d}\alpha(e) = \int_{\partial e} \alpha \neq 0.$$

Let  $\mu \in \mathscr{W}(n\mathcal{D}_2)$ , with  $\mu : n\mathcal{D}_2 \rightarrow \{-1, 0, +1\}$ . We will say that  $u$  is a deformation *containing the dislocation configuration*  $\mu$  if

$$\exists \alpha \in [\mathbf{d}u] \quad \text{such that} \quad \mathbf{d}\alpha = \mu.$$

For the purposes of our analysis, we define sets of admissible dislocation configurations. For  $\epsilon > 0$ ,  $n \in \mathbb{N}$ , and  $b_i \in \{\pm 1\}$  for  $i = 1, \dots, m$ , we define the set  $\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  of 2-forms

$$\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m) := \left\{ \mu = \sum_{i=1}^m b_i \mathbb{1}_{e_i} \mid e_i \in n\mathcal{D}_2 \text{ positively oriented, } \text{dist}(e_i, \text{Ext}(n\mathcal{D}_0)) \geq n\epsilon, \right. \\ \left. \text{dist}(e_i, e_j) \geq \epsilon n, \text{ for all } i, j \in \{1, \dots, m\}, i \neq j \right\}.$$

Each 2-form in this set represents a collection of  $m$  dislocations with respective Burgers vectors  $b_1, \dots, b_m$  and cores  $e_1, \dots, e_m$ . These dislocations are separated from each other and from the boundary by a distance of at least  $\epsilon n$ .

## 3. MAIN RESULTS: ENERGY BARRIERS

**3.1. Energy difference functional and equilibria.** As in [25] and [24], we consider a nearest-neighbour anti-plane lattice model for a crystal. Let  $\psi : \mathbb{R} \rightarrow \mathbb{R}$  be given by  $\psi(x) := \frac{1}{2}\lambda \text{dist}(x, \mathbb{Z})^2$ . We consider the energy difference functional

$$E_n(y; \tilde{y}) := \int_{n\mathcal{D}_1} [\psi(\mathbf{d}y) - \psi(\mathbf{d}\tilde{y})].$$

This functional is a model for potential energy per unit height of a long cylindrical crystal, and points  $n\mathcal{D}_0$  correspond to columns of atoms which are assumed to be periodic in the direction perpendicular to the plane considered. For further motivation of this model, we refer the reader to §1 of [1].

We briefly remark that in general  $\psi$  should be expected to be smooth; however, our results here rely heavily on the definition of  $\psi$ , which permits us to give precise analytical results.

Following Definition 1 of [24], we will say that  $y \in \mathcal{W}(n\mathcal{D}_0)$  is a *locally stable equilibrium* if there exists  $\epsilon > 0$  such that

$$E_n(y + u; y) \geq 0 \quad \text{whenever } \|u\|_{1,2} \leq \epsilon.$$

Due to the periodicity of  $\psi$ , we note that any locally stable equilibrium generates an entire family of equilibria: letting  $z \in \mathcal{W}(n\mathcal{D}_0)$  taking values in  $H + \mathbb{Z}$  for some  $H \in \mathbb{R}$ , if  $y$  is a locally stable equilibrium, then so is  $y + z$ . These equilibria are physically indistinguishable, since they correspond to a vertical ‘shifts’ of columns by an integer number of lattice spacings, and a rigid vertical translation of the entire crystal by  $H$ . We therefore define the equivalence relation

$$u \sim v \quad \text{if and only if } u = v + z, \quad \text{where } z : n\mathcal{D}_0 \rightarrow \mathbb{Z} + H \quad \text{for some } H \in \mathbb{R}, \quad (3.1)$$

and denote the equivalence classes of this relation as  $\llbracket y \rrbracket$ .

We recall that Theorem 3.3 in [24] gives sufficient conditions such that locally stable equilibria containing dislocations exist in the case of a more general choice of  $\psi$  than we choose here. Our first main result is similar, but gives a very precise representation of the corresponding bond-length 1-form in this case.

**Theorem 3.1.** *Fix  $\epsilon > 0$  and  $\mathcal{D}$  to be a convex lattice polygon. If  $n$  is sufficiently large, then for each  $\mu \in \mathcal{M}_{\epsilon,n}(b_1, \dots, b_m)$  there exists a corresponding locally stable equilibrium  $u^\mu$  which contains the dislocation configuration  $\mu$ . Moreover, this set is unique up to the equivalence relation defined in (3.1), and for any  $u \in \llbracket u^\mu \rrbracket$ ,  $\alpha \in [\mathbf{d}u]$  satisfies  $\alpha^* = \mathbf{d}^*G^{\mu^*}$ , where  $G^{\mu^*} \in \mathcal{W}_0(\mathcal{D}_0)$  is the solution to*

$$\Delta^*G^{\mu^*} = \mu^* \text{ in } \text{Int}(n\mathcal{D}_0^*), \quad \text{with } G^{\mu^*} = 0 \text{ on } \text{Ext}(n\mathcal{D}_0^*). \quad (3.2)$$

*Strategy of proof.* To prove this result, we begin by showing that if  $u$  is a locally stable equilibrium containing dislocations  $\mu$ , then  $\alpha \in [\mathbf{d}u]$  must satisfy

$$\|\alpha\|_\infty < \frac{1}{2}, \quad \mathbf{d}\alpha = \mu \text{ on } n\mathcal{D}_2, \quad \text{and} \quad \delta\alpha = 0 \text{ on } n\mathcal{D}_0. \quad (3.3)$$

We show that these conditions are satisfied by at most one  $\alpha \in \mathcal{W}(n\mathcal{D}_1)$ , and using the duality transformation described in §2.2, we verify that  $\alpha \in \mathcal{W}(n\mathcal{D}_1)$  satisfying  $\alpha^* = \mathbf{d}^*G^{\mu^*}$  verifies the latter two conditions. Showing that  $\|\alpha\|_\infty = \|\mathbf{d}^*G^{\mu^*}\|_\infty < \frac{1}{2}$  is the most technical aspect, and requires us to develop a theory which is analogous to interior estimates for continuum elliptic problems. To conclude, we obtain the class  $\llbracket u^\mu \rrbracket$  by ‘integrating’  $\alpha$ . The development of these tools and the proof of this theorem is the main focus of §4.

**3.2. Energy barriers.** Let  $C([0, 1]; \mathcal{W}(n\mathcal{D}_0))$  denote the space of continuous paths from  $[0, 1]$  to  $\mathcal{W}(n\mathcal{D}_0)$ . For  $\mu$  and  $\nu \in \mathcal{M}_{\epsilon,n}(b_1, \dots, b_m)$ , we define the set of continuous paths which move any local equilibrium in  $\llbracket u^\mu \rrbracket$  to any other local equilibrium in  $\llbracket u^\nu \rrbracket$  to be

$$\Gamma_n(\mu \rightarrow \nu) := \{ \gamma \in C([0, 1]; \mathcal{W}(n\mathcal{D}_0)) \mid \gamma(0) \in \llbracket u^\mu \rrbracket, \gamma(1) \in \llbracket u^\nu \rrbracket, \alpha \in [\mathbf{d}\gamma(t)] \Rightarrow \mathbf{d}\alpha = \mu \text{ or } \nu \}.$$

We define the *energy barrier for the transition from  $\mu$  to  $\nu$*  for  $\mu, \nu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  to be

$$\mathcal{B}_n(\mu \rightarrow \nu) := \min_{\gamma \in \Gamma_n(\mu \rightarrow \nu)} \max_{t \in [0, 1]} E_n(\gamma(t); u^\mu). \quad (3.4)$$

Our second result concerns an asymptotic representation of this quantity.

**Theorem 3.2.** *Suppose that  $\mu, \nu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  such that  $\mu - \nu = b_i[\mathbb{1}_p - \mathbb{1}_q]$  for some  $i$ , where  $q^* = p^* + \mathbf{a}$ . For  $i = 1, \dots, m$ , let  $\bar{x}_i \in \mathcal{D}$  be such that  $\text{dist}(\bar{x}_i, \frac{1}{n}e_i^*) \leq \frac{1}{n}$ . Then there exist constants  $c_0$  and  $c_1$  which depends only on the underlying lattice  $\Lambda$  such that*

$$\mathcal{B}_n(\mu \rightarrow \nu) = \lambda c_0 + \lambda c_1 n^{-1} \left[ \nabla \bar{y}_j(\bar{x}_j) \cdot \mathbf{a} + \sum_{i | i \neq j} b_j b_i \nabla \mathcal{G}_{\bar{x}_i}(\bar{x}_j) \cdot \mathbf{a} \right] + o(n^{-1}),$$

where

- (1)  $\lambda$  is given in the definition of  $\psi$ ,
- (2)  $\bar{y}_j$  solves the boundary value problem

$$-\Delta \bar{y}_j = 0 \text{ in } \mathcal{D}, \quad \bar{y}_j(\cdot) = \frac{1}{\kappa\pi} \log(|\cdot - \bar{x}_j|) \text{ on } \partial\mathcal{D},$$

- (3)  $\mathcal{G}_y$  is the solution to

$$-\Delta \mathcal{G}_y = \frac{\kappa}{2} \delta_y \text{ in } \mathcal{D}, \quad \text{with } \mathcal{G} = 0 \text{ on } \partial\mathcal{D}.$$

- (4)  $o(n^{-1})$  satisfies  $o(n^{-1}) \rightarrow 0$  as  $n \rightarrow \infty$ , uniformly for all  $\mu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$ .

*Strategy of proof.* The proof of this result is the main focus of §5. Our main task is the explicit construction of a *transition state*, i.e.  $u \in \mathcal{W}(n\mathcal{D}_0)$  such that

$$E_n(u; u^\mu) = \min_{\gamma \in \Gamma_n(\mu \rightarrow \nu)} \max_{t \in [0, 1]} E_n(\gamma(t); u^\mu).$$

This may be seen as a generalisation of the notion of a critical point, but is not a true critical point, since  $E_n$  is not smooth at  $u$ . Nevertheless, we show that  $\alpha \in [\mathbf{d}u]$  has a dual which is closely related to the interpolation of  $\mathbf{d}^*G^{\mu^*}$  and  $\mathbf{d}^*G^{\nu^*}$  which arise from (3.2). This dual representation, combined with the precise asymptotics obtained for  $\mathbf{d}^*G^{\mu^*}$  in order to prove Theorem 3.1, allow us to derive the expression of  $\mathcal{B}(\mu \rightarrow \nu)$ .

#### 4. PROOF OF THEOREM 3.1: DISCRETE ELLIPTIC REGULARITY

In this section, we develop discrete elliptic estimates which will allow us to prove Theorem 3.1: many the tools used are analogous to those used in the regularity theory of scalar elliptic partial differential equations (see for example [18]).

**4.1. Existence of solution to the Poisson problem.** We begin by proving existence of solutions to the Poisson boundary value problem in a general path-connected subcomplex  $\mathcal{A}$ .

**Lemma 4.1.** *Suppose  $\mathcal{A}$  is a path-connected lattice subcomplex; Let  $g : \text{Ext}(\mathcal{D}_0) \rightarrow \mathbb{R}$ , and  $f : \text{Int}(\mathcal{D}_0) \rightarrow \mathbb{R}$ : then there exists a unique solution  $u \in \mathcal{W}(\mathcal{D}_0)$  to the problem*

$$\Delta u = f \text{ in } \text{Int}(\mathcal{D}_0) \quad \text{with } u = g \text{ on } \text{Ext}(\mathcal{D}_0).$$

*Proof.* We employ a discrete version of the Dirichlet principle: extend  $g$  to a 0-form by defining  $g(e) := 0$  for all  $e \in \text{Int}(\mathcal{D}_0)$ , and let  $I : \mathcal{W}_0(\mathcal{D}_0) \rightarrow \mathbb{R}$  be given by

$$I(v) := \frac{1}{2}(\mathbf{d}(v + g), \mathbf{d}(v + g)) - \int_{\text{Int}(\mathcal{D}_0)} f v.$$

It is straightforward to verify that this functional is twice Gateau-differentiable, with

$$\langle DI(v), u \rangle = (\mathbf{d}(v + g), \mathbf{d}u) - \int_{\text{Int}(\mathcal{D}_0)} f u, \quad \text{and} \quad \langle D^2 I(v)u, u \rangle = ((u, u)).$$

It follows that  $I$  is strictly convex, so has a unique minimiser. By setting  $u = \mathbb{1}_e$  for any  $e \in \text{Int}(\mathcal{D}_0)$ , this minimiser  $v$  satisfies

$$\Delta(v + g) = f \text{ in } \text{Int}(\mathcal{D}_0),$$

and  $v + g = g$  on  $\text{Ext}(\mathcal{D}_0)$  by definition.  $\square$

**4.2. Maximum principle for harmonic 0-forms.** Our next auxiliary result is to prove the following discrete maximum principle.

**Lemma 4.2.** *Suppose that  $u \in \mathcal{W}(n\mathcal{D}_0)$ . Then*

$$\begin{aligned} \Delta u \geq 0 \text{ on } \text{Int}(n\mathcal{D}_0) & \text{ implies } \min_{e \in n\mathcal{D}_0} u(e) = \min_{e \in \text{Ext}(n\mathcal{D}_0)} u(e), \quad \text{and} \\ \Delta u \leq 0 \text{ on } \text{Int}(n\mathcal{D}_0) & \text{ implies } \max_{e \in n\mathcal{D}_0} u(e) = \max_{e \in \text{Ext}(n\mathcal{D}_0)} u(e). \end{aligned}$$

*Proof.* We prove only the former statement, the proof of the latter being almost identical. Suppose that  $u$  satisfies  $\Delta u \geq 0$  on  $\text{Int}(n\mathcal{D}_0)$ . Suppose that there exists  $e \in \text{Int}(n\mathcal{D}_0)$  such that

$$u(e) = \min_{e' \in n\mathcal{D}_0} u(e').$$

Either  $e \in \text{Ext}(n\mathcal{D}_0)$ , so there is nothing to prove, or else  $e \in \text{Int}(n\mathcal{D}_0)$ . Since

$$\Delta u(e) = \sum_{\substack{e' \in n\mathcal{D}_0 \\ \text{dist}(e', e) = 1}} [u(e) - u(e')] \geq 0,$$

it follows that  $u(e) = u(e')$  for all  $e'$  with  $\text{dist}(e, e') = 1$ . Iterating, and using the fact that  $n\mathcal{D}$  is compact, we find that  $\min_{e \in n\mathcal{D}_0} u(e) = \min_{e \in \text{Ext}(n\mathcal{D}_0)} u(e)$ , as required.  $\square$

**4.3. Lattice Green's functions.** We next assert the following lemma, concerning the existence of a full lattice Green's function  $G$ .

**Lemma 4.3.** *Suppose that  $\Lambda = \text{Sq}$ ,  $\text{Tr}$ , or  $\text{Hx}$ . Then there exists a lattice Green's function  $G_\Lambda \in \mathcal{W}(\Lambda_0)$  such that*

$$G_\Lambda(0) = 0, \quad \Delta G_\Lambda = \mathbb{1}_0.$$

*In addition:*

- (1)  $G_\Lambda$  is invariant under the group of lattice point symmetries, i.e. if  $\mathbf{R} : \mathbb{R}^2 \rightarrow \mathbb{R}^2$  is a linear transformation such that  $\mathbf{R}(\Lambda_0) = \Lambda_0$ , then

$$G_\Lambda(\mathbf{R}(e)) = G_\Lambda(e).$$

- (2)  $\sup_{e \in \Lambda_1} |\mathbf{d}G_\Lambda(e)| = \mathbf{N}^{-1}$ , where  $\mathbf{N}$  is the connectivity of the lattice  $\Lambda$ .
- (3) There exists a constant  $C_\Lambda \in \mathbb{R}$  such that if  $u(e) := G_\Lambda(e) + C_\Lambda + \frac{1}{\kappa\pi} \log(\text{dist}(0, \xi))$ , then

$$|u(e)| \lesssim |\text{dist}(e, 0)|^{-1} \log |\text{dist}(e, 0)| \tag{4.1}$$

$$\text{and } |\mathbf{d}u(e)| \lesssim |\text{dist}(e, 0)|^{-2} \log |\text{dist}(e, 0)|. \tag{4.2}$$

The usual way to construct  $G_\Lambda$  is via the Fourier transform, and the existence of such a Green's function in the case of Bravais lattices is a classical assertion, as is the symmetry (1). The bounds (4.1) and (4.2) are proved in Theorem 3.5 of [13] for Bravais lattices, covering the cases where  $\Lambda = \text{Sq}$  and  $\Lambda = \text{Tr}$ . It therefore remains to prove (2), and the other results in the  $\Lambda = \text{Hx}$  case; we postpone these proofs until §A.1. The main fact used in proving the results for  $\text{Hx}$  is that  $\text{Hx}$  may be viewed as a subset of  $\text{Tr}$ .

**4.4. The harmonic measure and interior differential estimates.** We now assert the existence of the harmonic measure, which allows us to express functions which are harmonic in a region in terms of their boundary values. In order to do so, we introduce

$$Q_\Lambda^r := \begin{cases} [-r, r]^2 \cap \Lambda & \Lambda = \text{Sq}, \\ \{x \in \mathbb{R}^2 \mid |x \cdot (\frac{\sqrt{3}}{2}, \frac{1}{2})^T|, |x \cdot (-\frac{\sqrt{3}}{2}, \frac{1}{2})^T|, |x \cdot (0, -1)^T| \leq \frac{\sqrt{3}}{2}r\} \cap \Lambda & \Lambda = \text{Tr, Hx}. \end{cases} \quad (4.3)$$

**Lemma 4.4.** *Let  $Q_\Lambda^r$  be as defined in (4.3). Then for each  $e \in \text{Ext}(Q_{\Lambda,0}^r)$ , there exists  $\omega_e^r \in \mathscr{W}(Q_{\Lambda,0}^r)$  satisfying*

$$\Delta \omega_e^r = 0 \text{ in } \text{Int}(Q_{\Lambda,0}^r), \quad \text{with } \omega_e^r = \frac{\mathbb{1}_e}{\#\text{Ext}(Q_{\Lambda,0}^r)} \text{ on } \text{Ext}(Q_{\Lambda,0}^r).$$

$\omega_e^r$  additionally satisfies the following properties:

(1) *If  $u \in \mathscr{W}(Q_{\Lambda,0}^r)$  is harmonic in  $Q_{\Lambda,0}^r$ , then for any  $e \in \mathcal{D}_0$ ,*

$$u(a) = \sum_{e \in \text{Ext}(Q_{\Lambda,0}^r)} \omega_e^r(a) u(e).$$

(2) *There exists a constant  $C_\Lambda > 0$  depending only on  $\Lambda$  such that*

$$|\mathbf{d}\omega_e^r(b)| \leq C_\Lambda \log(r) r^{-2} \quad \text{where } b = [0, a]. \quad (4.4)$$

*for any nearest-neighbour direction  $a$ .*

The function  $\omega_e^r$  is called the harmonic measure, and enjoys a variety of interpretations, both probabilistic and analytic: for further detail, we refer the reader to [17]. The existence of  $\omega_e^r$  and statement (1) follow directly from Lemma 4.1. In the case where  $\Lambda = \text{Sq}$ , a proof of (4.4) with the improved upper bound  $C_\Lambda r^{-2}$  is given in Lemma 3 of [20] using an explicit construction of  $\omega_e^r$ . Further results on the harmonic measure in the square lattice may also be found in Chapter 8 of [28].

*Proof.* To prove this result, we use the discrete analogue of Green's formula:

$$\int_{\text{Int}(Q_{r,0}^\Lambda)} u \Delta v - v \Delta u = \int_{\text{Ext}(Q_{r,0}^\Lambda)} u \Delta v - v \Delta u = \sum_{e \in \text{Ext}(Q_{r,0}^\Lambda)} \left[ u(e) \left( \int_{\delta_e} \mathbf{d}v \right) - v(e) \left( \int_{\delta_e} \mathbf{d}u \right) \right],$$

which follows by applying (2.1) to the extension of  $u, v, \mathbf{d}u$  and  $\mathbf{d}v$  by 0 to the full lattice complex. Consider  $v$  which is the solution to

$$\Delta v = 0, \quad v(e) = G_\Lambda(e + \mathbf{a}) - G_\Lambda(e) \text{ on } \text{Ext}(Q_{r,0}^\Lambda).$$

Such  $v$  clearly exists by Theorem 4.1, and by applying Lemma 4.2 and then Lemma 4.3, we obtain that

$$\sup_{e' \in Q_{r,1}^\Lambda} |\mathbf{d}v(e')| \leq 2 \sup_{e' \in Q_{r,0}^\Lambda} |v(e')| \leq 2 \sup_{e' \in \text{Ext}(Q_{r,0}^\Lambda)} |v(e')| \leq C_\Lambda r^{-1} \log(r). \quad (4.5)$$

Defining  $u \in \mathscr{W}(Q_{r,0}^\Lambda)$  by  $u(e) := G_\Lambda(e + \mathbf{a}) - G_\Lambda(e) - v(e)$ , we have that  $\Delta u = \mathbb{1}_{e+\mathbf{a}} - \mathbb{1}_e$ , and hence

$$\mathbf{d}\omega_e^r([0, 0 + \mathbf{a}]) = \int_{\text{Int}(Q_{r,0}^\Lambda)} \omega_e^r \Delta u - u \Delta \omega_e^r = \int_{\text{Ext}(Q_{r,0}^\Lambda)} \omega_e^r \Delta u - u \Delta \omega_e^r = \frac{\Delta u(e)}{\#\text{Ext}(Q_{r,0}^\Lambda)}.$$

Now, applying Lemma 4.3 and (4.5), we obtain

$$|\Delta u(e)| \leq C_\Lambda r^{-2} \log(r)$$

which completes the proof.  $\square$

**Lemma 4.5.** *Suppose that  $u \in \mathscr{W}(n\mathcal{D}_0)$  satisfies  $\Delta u = 0$  and  $u = g$  on  $\text{Ext}(n\mathcal{D}_0)$  with  $g : \text{Ext}(n\mathcal{D}_0) \rightarrow \mathbb{R}$ . Then there exists a constant  $C_\Lambda > 0$  depending only on  $\Lambda$  such that*

$$|\mathbf{d}u(e)| \leq C_\Lambda \frac{\log(\text{dist}(e, \text{Ext}(n\mathcal{D}_0)))}{\text{dist}(e, \text{Ext}(n\mathcal{D}_0))} \sup_{e' \in \text{Ext}(n\mathcal{D}_0)} |g(e')| \quad \text{for any } e \in \mathcal{D}_1.$$

*Proof.* Suppose that  $e = [\mathbf{a}, \mathbf{b}] \in n\mathcal{D}_1$ . Let  $Q_\Lambda^r$  be as defined in (4.3), where  $r = \lfloor \text{dist}(a, \text{Ext}(n\mathcal{D}_0)) \rfloor$ ; then  $\mathbf{a} + Q_\Lambda^r \subset n\mathcal{D}_0$ , and statement (1) in Lemma 4.4 implies that

$$w(e) = \sum_{e' \in \text{Ext}(\mathbf{a} + Q_{\Lambda,0}^r)} \omega_{e'}^r(e) w(e'), \quad \text{so} \quad \mathbf{d}w(e) = \sum_{e' \in \text{Ext}(\mathbf{a} + Q_{\Lambda,0}^r)} \mathbf{d}\omega_{e'}^r(e) w(e').$$

Applying statement (2) of Lemma 4.4 and Lemma 4.2, it follows that

$$|\mathbf{d}w(e)| \leq \sup_{e' \in \text{Ext}(\mathbf{a} + Q_{\Lambda,0}^r)} |w(e')| \sum_{e' \in \text{Ext}(\mathbf{a} + Q_{\Lambda,0}^r)} |\mathbf{d}\omega_{e'}^r(e)| \leq C_\Lambda \frac{\log(r)}{r} \sup_{e' \in \text{Ext}(n\mathcal{D}_0)} |g(e')|. \quad \square$$

**4.5. Green's functions on finite subcomplexes.** We have now collected the necessary tools with which we will prove Theorem 3.1. The final auxiliary result which we require is the following precise description of the differential of solutions to (3.2).

**Theorem 4.6.** *Suppose that  $\mu = \sum_{i=1}^m b_i \mathbb{1}_{e_i} \in \mathcal{M}_{\epsilon,n}(b_1, \dots, b_m)$ . Then let  $G^{\mu^*} \in \mathcal{W}(n\mathcal{D}_0^*)$  be the solution to (3.2). Letting  $x \in n\mathcal{D}_0$  with  $[x, x + \mathbf{a}] \in n\mathcal{D}_1^*$ , we have*

$$\begin{aligned} \mathbf{d}^* G^{\mu^*}([x, x + \mathbf{a}]) &= b_i \mathbf{d}^* G_{\Lambda^*}([x - e_i^*, x + a - e_i^*]) + n^{-1} \left[ b_i \nabla \bar{y}_i(\tfrac{1}{n}x) \cdot a + \sum_{j \neq i} b_j \nabla \mathcal{G}_{\bar{x}_j}(\tfrac{1}{n}x) \cdot a \right] \\ &\quad + O(n^{-1-\delta} \log(n)), \end{aligned}$$

where:

- (1)  $G_{\Lambda^*}$  is the full lattice Green's function for  $\Lambda^*$ , whose existence was asserted in Theorem 4.3,
- (2)  $e_i^*$  minimises  $\text{dist}(x, e_i^*)$  over all  $i = 1, \dots, m$ ,
- (3) for each  $i$ ,  $\bar{x}_i \in \mathcal{D}$  satisfies  $\text{dist}(\bar{x}_i, \frac{1}{n}e_i^*) \leq \frac{1}{n}$ ,
- (4)  $\mathcal{G}_y$  is the continuum Dirichlet Green's function on  $\mathcal{D}$  corresponding to the point  $y$ , i.e. the solution to

$$\Delta \mathcal{G}_y(\cdot) = \frac{\kappa}{2} \delta(\cdot - y) \text{ in } \mathcal{D}, \quad \text{with } \mathcal{G}_y = 0 \text{ on } \partial\mathcal{D},$$

- (5)  $\bar{y}_i$  solves

$$\Delta \bar{y}_i = 0 \text{ in } \mathcal{D}, \quad \text{with } \bar{y}_i(s) = \frac{1}{\kappa\pi} \log(|s - \bar{x}_i|) \text{ on } \partial\mathcal{D},$$

- (6)  $\delta > 0$  is an exponent which depends only on  $\omega_l$ , the interior angles at the corners of  $\mathcal{D}$ , and
- (7)  $O(n^{-1-\delta} \log(n))$  denotes an error term which is uniform for all  $\mu \in \mathcal{M}_{\epsilon,n}(b_1, \dots, b_m)$ .

*Strategy of the proof* The proof of this result is technical, so we postpone it to §A.2. The main strategy is similar in spirit to that taken in the proof of Theorem 3.3 in [24]: we decompose  $G^{\mu^*}$  as a sum of full lattice Green's functions restricted to  $n\mathcal{D}_0^*$ , continuum boundary correctors  $\bar{y}_i$  and discrete correctors. We then treat each of these components separately, applying Lemma 4.3, the regularity theory of [19], the maximum principle proved in Lemma 4.2 and the interior estimates Lemma 4.5 to analyse each piece in turn.

Theorem 4.6 now implies the following corollary.

**Corollary 4.7.** *Given  $\epsilon > 0$  and a convex lattice polygon  $\mathcal{D} \subset \mathbb{R}^2$ , for all  $n$  sufficiently large,*

$$\sup_{e \in n\mathcal{D}_1} |\mathbf{d}^* G^{\mu^*}(e)| < \frac{1}{2} \quad \text{for any } \mu \in \mathcal{M}_{\epsilon,n}(b_1, \dots, b_m).$$

*Proof.* Let  $e \in n\mathcal{D}_1$ , and let  $e_i^* \in \text{argmin} \{ \text{dist}(e, e_i^*) \mid e_i^* \in \text{supp}\{\mu\} \}$ . Applying Theorem 4.6, and splitting  $\mathcal{G}_{\bar{x}_i}(x) = \frac{1}{\kappa\pi} \log(|x - \bar{x}_i|) + \bar{y}_i(x)$ , we obtain the estimate

$$|\mathbf{d}G^{\mu^*}(e)| \leq \sup_{e \in \Lambda_1^*} |\mathbf{d}^* G_{\Lambda^*}(e)| + n^{-1} \left[ \frac{(m-1)\epsilon}{\kappa\pi} + \sum_{i=1}^m \|\bar{y}_i\|_{\mathcal{X}} \right] + O(n^{-1-\delta} \log(n)),$$

where we recall the definition of the norm  $\|\cdot\|_{\mathcal{X}}$  from (A.3). Further, from §A.2.2 we have that  $\|\bar{y}_i\|_{\mathcal{X}}$  is uniformly bounded for  $\bar{x}_i \in \{x \in \mathcal{D} \mid \text{dist}(x, \partial\mathcal{D}) \geq \epsilon\}$ , and so applying statement (2) of Theorem 4.3, we have the result.  $\square$



**4.6. Proof of Theorem 3.1.** We now complete the proof of Theorem 3.1. First, we prove the necessity of the equilibrium conditions given in (3.3).

Let  $u$  be a locally stable equilibrium containing the dislocation configuration  $\mu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$ . By inspecting the proof of Lemma 5.1 in [2], it follows that if  $\mathbf{d}u(e) \in \frac{1}{2} + \mathbb{Z}$  for some  $e \in n\mathcal{D}_1$ , then there exist lower energy states arbitrarily close to  $u$ , and so any  $\alpha \in [\mathbf{d}u]$  has  $\|\alpha\|_\infty < \frac{1}{2}$ . By definition, we have that  $\mathbf{d}\alpha = \mu$ . Finally, let  $v \in \mathcal{W}(n\mathcal{D}_0)$  be arbitrary; then for  $t$  sufficiently small,  $\|\alpha + t\mathbf{d}v\|_\infty < \frac{1}{2}$ , hence

$$E_n(u + tv; u) = \int_{n\mathcal{D}_1} \psi(\alpha + t\mathbf{d}v) - \psi(\alpha) = \int_{n\mathcal{D}_1} \lambda t \alpha \mathbf{d}v + \frac{1}{2} \lambda t^2 |\mathbf{d}v|^2.$$

It follows that  $(\alpha, \mathbf{d}v) = 0$  for any  $v \in \mathcal{W}(n\mathcal{D}_0)$ , hence  $\delta\alpha = 0$ .

Next, we show that if  $\alpha$  satisfies the equilibrium conditions (3.3), then it is unique. Suppose that  $\alpha$  and  $\alpha'$  satisfy (3.3). We define  $\beta = \alpha - \alpha'$ , and note that  $\beta^* \in \mathcal{W}_0(n\mathcal{D}_1^*)$  satisfies  $\mathbf{d}^*\beta^* = 0$  and  $\delta^*\beta^* = 0$ . Since  $n\mathcal{D}^*$  is simply connected, the former condition implies that  $\beta^* = \mathbf{d}^*w$  for some  $w \in \mathcal{W}_0(n\mathcal{D}_0^*)$ , which must satisfy  $\Delta^*w = 0$ : by Lemma 4.1, it follows that  $w = 0$ , hence  $\beta = 0$ , and thus  $\alpha = \alpha'$ .

Since  $*$  is a bijection between  $\mathcal{W}(n\mathcal{D}_1)$  and  $\mathcal{W}_0(n\mathcal{D}_1^*)$ , there exists  $\alpha \in \mathcal{W}(n\mathcal{D}_1)$  such that  $\alpha^* = \mathbf{d}^*G^{\mu^*}$ . Furthermore, by using (2.6), we have that

$$\begin{aligned} \mathbf{d}\alpha(e) &= \delta^*\mathbf{d}^*G^{\mu^*}(e^*) = \mu^*(e^*) = \mu(e), \quad \text{for } e \in n\mathcal{D}_2, \\ \text{and } \delta\alpha(e) &= (\mathbf{d}^*)^2G^{\mu^*}(e^*) = 0 \quad \text{for } e \in n\mathcal{D}_0. \end{aligned}$$

Finally, we note that  $\|\alpha\|_\infty = \|\mathbf{d}G^{\mu^*}\|_\infty$ , hence applying Corollary 4.7, it follows that  $\alpha$  satisfies (3.3).

To demonstrate that  $\alpha \in [\mathbf{d}u^\mu]$  for some  $u^\mu \in \mathcal{W}(n\mathcal{D}_0)$ , fix  $e' \in n\mathcal{D}_0$ , and define  $u(e') = 0$ . Using the fact that  $n\mathcal{D}$  is path-connected, let  $\gamma^e$  be the path such that  $\partial\gamma^e = e' \cup -e$ , and define

$$u^\mu(e) := \int_{\gamma^e} \alpha.$$

Letting  $b = [c, d] \in n\mathcal{D}_1$ , we find that

$$\mathbf{d}u(b) = \int_{\gamma^d} \alpha - \int_{\gamma^c} \alpha = \int_{\gamma^d \cup -\gamma^c \cup -b} \alpha + \int_b \alpha.$$

Noting that  $\partial(\gamma^d \cup -\gamma^c \cup -b) = \emptyset$ , we apply the fact that  $n\mathcal{D}$  is simply connected to assert that  $\gamma^d - \gamma^c - b = \partial A$ , for some  $A \in n\mathcal{D}_2$ , hence

$$\mathbf{d}u(b) = \alpha(b) + \int_{\partial A} \alpha = \alpha(b) + \int_A \mu \in \alpha(b) + \mathbb{Z}.$$

It follows that  $\alpha \in [\mathbf{d}u^\mu]$ . To prove that  $u^\mu$  is unique up to the equivalence (3.1), we note that if  $\alpha \in [\mathbf{d}u]$  and  $\alpha \in [\mathbf{d}v]$ , then by the definition of a bond-length 1-form (see §2.5), it follows that

$$\mathbf{d}u(e) = \mathbf{d}v(e) + Z(e) \quad \text{for all } e \in n\mathcal{D}_1, \quad \text{with } Z : n\mathcal{D}_1 \rightarrow \mathbb{Z}.$$

Moreover,  $\mathbf{d}Z = 0$ , so  $Z = \mathbf{d}z$ , and it is straightforward to check that  $z : n\mathcal{D}_0 \rightarrow H + \mathbb{Z}$  for some  $H \in \mathbb{R}$ , completing the proof of Theorem 3.1.

## 5. COMPUTING THE ENERGY BARRIERS TO DISLOCATION MOTION

This section is devoted to the proof of Theorem 3.2. We proceed in several steps. We first demonstrate that there exists  $u$  “solving” the min-max problem used to define  $\mathcal{B}(\mu \rightarrow \nu)$ . We then identify necessary conditions for such a solution, and show that these necessary conditions identify a pair of bond-length 1-forms. We then construct bond-length 1-forms corresponding to the transition state via duality using an interpolation of dual Green’s functions, and verify that the necessary conditions are satisfied.

**5.1. Solving the min-max problem.** We will prove existence by using an equivalent formulation of the problem, which we describe here.

5.1.1. *Quotient space.* Recall that in (3.1) we defined  $\sim$  be an equivalence relation on  $u \in \mathscr{W}(n\mathcal{D}_0)$  given by

$$u \sim v \quad \text{whenever} \quad u = v + z + C \quad \text{for some } z : n\mathcal{D}_0 \rightarrow \mathbb{Z} \text{ and some } C \in \mathbb{R}.$$

We define the quotient space  $\mathcal{Q} := \mathscr{W}(n\mathcal{D}_0)/\sim$  of equivalence classes  $\llbracket u \rrbracket$ . We claim that this is a metric space when endowed with the metric

$$d_{\mathcal{Q}}(\llbracket u \rrbracket, \llbracket v \rrbracket) = \|\alpha\|_2, \quad \text{where } \alpha \in [\mathbf{d}u - \mathbf{d}v], \quad \text{for any } u \in \llbracket u \rrbracket \text{ and } v \in \llbracket v \rrbracket.$$

If  $u \sim v$ , then  $\mathbf{d}u \in \mathbf{d}v + \mathbb{Z}$ , and hence  $[\mathbf{d}u] = [\mathbf{d}v]$ . Symmetry is immediate, and  $0 \in [\mathbf{d}u - \mathbf{d}v]$  implies that  $u - v \sim 0$ , hence  $d_{\mathcal{Q}}(u, v) = 0$  implies that  $u \sim v$ . Finally, for the triangle inequality, by checking cases it may be shown that

$$\beta \in [\mathbf{d}u], \beta' \in [\mathbf{d}v] \text{ and } \alpha \in [\mathbf{d}u + \mathbf{d}v] \quad \text{imply that} \quad |\alpha(e)| \leq |\beta(e)| + |\beta'(e)| \text{ for all } e \in n\mathcal{D}_1,$$

and the triangle inequality follows, so the metric is well-defined. Moreover, the space is complete and totally bounded, hence the Heine–Borel theorem applies, and  $\mathcal{Q}$  is compact. We recall that the mapping  $u \mapsto \llbracket u \rrbracket$  is the natural embedding of  $\mathscr{W}(n\mathcal{D}_0)$  in  $\mathcal{Q}$ .

5.1.2. *Redefining the energy.* As remarked in §3.1, if  $u, u', v \in \mathscr{W}(n\mathcal{D}_0)$  with  $u \sim u'$ , then  $E(u, v) = E(u', v)$ . It follows that the mapping

$$\mathcal{E}(\llbracket u \rrbracket) := E(u, v) \quad \text{where } u \in \llbracket u \rrbracket \text{ is well-defined.}$$

Suppose that  $u \in \llbracket u \rrbracket$ , and  $u' \in \llbracket u' \rrbracket$ , and that  $\alpha \in [\mathbf{d}u - \mathbf{d}u']$ . Then

$$|\mathcal{E}(\llbracket u \rrbracket) - \mathcal{E}(\llbracket u' \rrbracket)| = \left| \int_{n\mathcal{D}_1} \psi(\mathbf{d}u' + \alpha) - \psi(\mathbf{d}u') \right| \lesssim C \int_{n\mathcal{D}_1} |\alpha| \lesssim \|\alpha\|_2 = d_{\mathcal{Q}}(\llbracket u \rrbracket, \llbracket v \rrbracket),$$

where we use the fact that  $\psi$  is uniformly Lipschitz, and then apply the Cauchy–Schwarz inequality. It follows that  $\mathcal{E}$  is uniformly Lipschitz on  $\mathcal{Q}$ .

5.1.3. *Path space.* Next define the metric space  $C([0, 1]; \mathcal{Q})$  of continuous functions from  $[0, 1]$  to  $\mathcal{Q}$ , with the usual metric

$$d_{\mathcal{Q}}^{\infty}(\gamma, \gamma') := \sup_{t \in [0, 1]} d_{\mathcal{Q}}(\gamma(t), \gamma'(t)).$$

The mapping  $\gamma \mapsto \max_{t \in [0, 1]} \mathcal{E}(\gamma(t))$  is continuous with respect to this metric, since  $\mathcal{E}$  is uniformly continuous on  $\mathcal{Q}$ .

We suppose that  $n$  is large enough for the conclusion of Theorem 3.1 to hold, and write  $\llbracket u^{\mu} \rrbracket$  to mean the equivalence class containing  $u^{\mu}$ , the locally stable equilibria corresponding to the dislocation positions  $\mu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$ . This permits us to define the sets of paths

$$\tilde{\Gamma}_n(\mu \rightarrow \nu) := \{ \gamma \in C([0, 1]; \mathcal{Q}) \mid \gamma(0) = \llbracket u^{\mu} \rrbracket, \gamma(1) = \llbracket u^{\nu} \rrbracket, \alpha \in [\mathbf{d}\gamma(t)] \text{ has } \mathbf{d}\alpha \in \{\mu, \nu\}, \forall t \in [0, 1] \}.$$

This should be thought of as the set of paths through phase space which move dislocations from  $\mu$  to  $\nu$  without visiting any intermediate states.

5.1.4. *Existence.* We recall that the energy barrier was defined to be

$$\mathcal{B}_n(\mu \rightarrow \nu) = \inf_{\gamma \in \tilde{\Gamma}_n(\mu, \nu)} \sup_{t \in [0, 1]} E_n(\gamma(t); u^{\mu}).$$

The following lemma now demonstrates the existence of a transition state.

**Lemma 5.1.** *If  $n$  is sufficiently large, for any  $\mu, \nu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  such that  $\tilde{\Gamma}_n(\mu \rightarrow \nu)$  is non-empty, there exists  $u \in \mathscr{W}(n\mathcal{D}_0)$  such that*

$$E_n(u; u^{\mu}) = \mathcal{B}_n(\mu \rightarrow \nu).$$

We will call such  $u$  a *transition state* for the transition from  $\mu$  to  $\nu$ .

*Proof.* We first note that since  $\mathcal{Q}$  is compact,  $C([0, 1]; \mathcal{Q})$  is compact. By assumption,  $\Gamma_n(\mu \rightarrow \nu)$  is non-empty, and so the space  $\tilde{\Gamma}_n(\mu \rightarrow \nu)$  is non-empty by applying the natural embedding  $\gamma(t) \mapsto \llbracket \gamma(t) \rrbracket$ : by definition, this is surjective. Moreover, we have that

$$\max_{t \in [0, 1]} E(\gamma(t); u^\mu) = \max_{t \in [0, 1]} \mathcal{E}(\llbracket \gamma(t) \rrbracket).$$

Since  $\tilde{\gamma} \mapsto \max_{t \in [0, 1]} \mathcal{E}(\tilde{\gamma}(t))$  is continuous, there exists a minimiser

$$\tilde{\gamma} \in \operatorname{argmin} \left\{ \max_{t \in [0, 1]} \mathcal{E}(\tilde{\gamma}(t)) \mid \tilde{\gamma} \in \overline{\tilde{\Gamma}_n(\mu \rightarrow \nu)} \right\},$$

where  $\overline{\tilde{\Gamma}_n(\mu \rightarrow \nu)}$  denotes the closure of  $\tilde{\Gamma}_n(\mu \rightarrow \nu)$  in  $\mathcal{Q}$ . As  $t \mapsto \mathcal{E}(\tilde{\gamma}(t))$  is also continuous, it follows that there exists  $u \in \llbracket u \rrbracket$  with  $\llbracket u \rrbracket = \gamma(t^*) \in \overline{\Gamma_n(\mu \rightarrow \nu)}$  for some  $t^* \in [0, 1]$  realising

$$E(u; u^\mu) = \min_{\tilde{\gamma} \in \overline{\tilde{\Gamma}_n(\mu \rightarrow \nu)}} \max_{t \in [0, 1]} \mathcal{E}(\tilde{\gamma}(t)) = \min_{\gamma \in \overline{\Gamma_n(\mu \rightarrow \nu)}} \max_{t \in [0, 1]} E(\gamma(t); u^\mu). \quad \square$$

**5.2. Necessary conditions.** We now identify necessary conditions on the transition state  $u$  identified in Lemma 5.1.

**Lemma 5.2.** *Suppose that  $u \in \mathcal{W}(n\mathcal{D}_0)$  is a transition state for the transition from  $\mu$  to  $\nu$ , where  $\mu - \nu = b_i[\mathbb{1}_p - \mathbb{1}_q]$  and  $p$  and  $q$  are adjacent. Then  $u \in \{u \in \mathcal{W}(n\mathcal{D}_0) \mid \alpha \in [\mathbf{d}u] \text{ has } \alpha(l) = \pm \frac{1}{2}\}$ , where  $\delta l = q \cup -p$ , and moreover there exist exactly two  $\alpha_\uparrow, \alpha_\downarrow \in [\mathbf{d}u]$ , with*

- (1)  $\mathbf{d}\alpha_\uparrow = \mu, \mathbf{d}\alpha_\downarrow = \nu$ ,
- (2)  $\delta\alpha_\uparrow(a) = \delta\alpha_\downarrow(a) = 0$  for all  $a \pm \notin \partial l$ ,
- (3)  $\delta\alpha_\uparrow(b) + \delta\alpha_\uparrow(c) = 0$  and  $\delta\alpha_\downarrow(b) + \delta\alpha_\downarrow(c) = 0$  for  $b - c = \partial l$ , and
- (4)  $-\alpha_\uparrow(l) = \alpha_\downarrow(l) = \frac{1}{2}b_i$ .

*Proof.* We begin by proving that there exist transition states in the set

$$B := \{u \in \mathcal{W}(n\mathcal{D}_0) \mid \alpha \in [\mathbf{d}u] \text{ has } \alpha(b) = \pm \frac{1}{2} \text{ for some } b \in n\mathcal{D}_1\}.$$

We remark that any  $\gamma \in \Gamma_n(\mu \rightarrow \nu)$  must pass through  $B$ , since it is only on this set that we may have  $\alpha, \alpha' \in [\mathbf{d}\gamma(t)]$  with

$$\mathbf{d}\alpha(p) = b_i, \quad \mathbf{d}\alpha(q) = 0, \quad \text{and} \quad \mathbf{d}\alpha'(p) = 0, \quad \mathbf{d}\alpha'(q) = b_j.$$

Suppose that  $\gamma \in \overline{\Gamma_n(\mu \rightarrow \nu)}$  solves the minimisation problem (3.4), and attains a transition state  $u = \gamma(t^*)$  at  $t = t^*$ . Suppose further that  $u \notin B$ .

Taking an interval with  $t^* \in [t_1, t_2]$  such that  $\gamma(t) \notin B$  for all  $t \in [t_1, t_2]$ , and  $\gamma(t_1), \gamma(t_2) \neq \gamma(t^*)$ , we define

$$\beta(t) := \begin{cases} \gamma(t) & t \notin [t_1, t_2], \\ \frac{t_2-t}{t_2-t_1}\gamma(t_1) + \frac{t-t_1}{t_2-t_1}\gamma(t_2) & t \in [t_1, t_2]. \end{cases}$$

This is a valid competitor for the minimum problem, and moreover by using strict convexity of  $\psi(x)$  for  $x \in [n - \frac{1}{2}+, n + \frac{1}{2}]$  for any  $n \in \mathbb{Z}$ , we obtain

$$E(\gamma(t^*); u^\mu) \leq \sup_{t \in (t_1, t_2)} E(\beta(t); u^\mu) < \max \{E(\gamma(t_1); u^\mu), E(\gamma(t_2); u^\mu)\} \leq E(\gamma(t^*); u^\mu),$$

which is a contradiction.

Suppose once more that  $\gamma$  is a minimal path, and  $\max_{t \in [0, 1]} E[\gamma(t); u^\mu]$  attaining a transition state at  $t = t^*$ . Suppose also that  $\alpha \in [\mathbf{d}\gamma(t^*)]$  has  $\alpha(e) = \pm \frac{1}{2}$  for some  $e \neq \pm l$ . Let  $a \in \partial e$  such that  $e \notin \pm \partial l$ . Then by considering  $\gamma(t^*) + s\mathbb{1}_a$ , and following the strategy of proof of Lemma 5.1 in [2], it may be checked that there exists  $\delta > 0$  such that for all  $s \in [0, \delta)$  or for all  $s \in (-\delta, 0]$ ,

- (1)  $\alpha \in [\mathbf{d}(\gamma(t^*) + s\mathbb{1}_a)]$  satisfies  $\mathbf{d}\alpha \in \{\mu, \nu\}$ , and
- (2)  $E[\gamma(t^*) + s\mathbb{1}_a; \gamma(t^*)] < 0$  if  $s \neq 0$ .

By redefining  $\gamma$  to pass through  $\gamma(t^*) + s\mathbb{1}_a$  in a neighbourhood of  $t^*$ , it follows that  $\gamma(t^*)$  cannot be a transition state, and hence if  $u$  is a transition state with  $\alpha \in [\mathbf{d}u]$ ,  $\alpha(e) = \pm\frac{1}{2}$  if and only if  $e = \pm l$ .

By considering paths  $\beta$  which have  $\beta(t^*) = \gamma(t^*) + s\mathbb{1}_a$  with  $a \notin \partial l$ , we obtain that

$$E(\gamma(t^*); u^\mu) \leq E(\gamma(t^*) + s\mathbb{1}_a; u^\mu)$$

for all  $s$  sufficiently small. If  $\alpha \in [\mathbf{d}\gamma(t^*)]$ , we have that

$$\int_{n\mathcal{D}_1} \alpha \mathbf{d}\mathbb{1}_a = \delta\alpha(a) = 0.$$

By considering  $\gamma(t^*) + s[\mathbb{1}_b + \mathbb{1}_c]$ , where  $\partial l = b - c$ , we obtain that

$$\delta\alpha(b) + \delta\alpha(c) = 0,$$

hence we have proved that a transition state must satisfy conditions (1)–(4).

Next, we prove that  $\mathbf{d}\alpha_\uparrow = \mu$ ,  $\alpha_\uparrow(l) = \frac{1}{2}$  and conditions (2) and (3) define a unique 1-form, which is an elastic strain at the transition state. Suppose that  $\alpha_\uparrow$  and  $\alpha'_\uparrow$  satisfy these conditions. Defining  $\theta := \alpha_\uparrow - \alpha'_\uparrow$ , we have that  $\mathbf{d}\theta = 0$ , hence  $\theta = \mathbf{d}v$  for some 0-form  $v$  since  $n\mathcal{D}$  is simply connected. Furthermore,  $\mathbf{d}v(l) = 0$ ,  $\Delta v(b) = s$  and  $\Delta v(c) = -s$  for some  $s \in \mathbb{R}$ . Then we have

$$(\theta, \theta) = (\mathbf{d}v, \mathbf{d}v) = (\Delta v, v) = s \mathbf{d}v(l) = 0,$$

implying that  $\theta = 0$ , and hence  $\alpha_\uparrow$  is unique. It may be similarly verified that  $\alpha_\downarrow$  exists and is unique, completing the proof.  $\square$

**5.3. Construction of the transition state.** In Theorem 3.1, we found that the bond length 1-forms corresponding to local equilibria containing dislocations are related to dual Green's functions. By considering this relationship, it is natural to consider strains dual to interpolations of these Green's functions as possible candidates for the transition state  $u$ . We therefore define  $G^t := (1-t)G^{\mu^*} + tG^{\nu^*}$ , where  $t \in [0, 1]$ ,  $G^{\mu^*}$  and  $G^{\nu^*}$  solve (3.2). We note that

$$\Delta^* G^t(p) = b_j(1-t) \quad \text{and} \quad \Delta^* G^t(q) = b_j t.$$

We also expect that the transition state should occur when the 1-cell between the 2-cells  $p$  and  $q$  is 'twisted' the most. As in Lemma 5.2, set  $l \in n\mathcal{D}_1$  with  $\partial^* l^* = q^* - p^*$ . We will choose  $t \in [0, 1]$  such that

$$\begin{aligned} \Delta^* G^t(p^*) + \mathbf{d}^* G^t(l^*) &= \frac{1}{2} b_j, & \Leftrightarrow & \quad (1-t)b_j + \mathbf{d}^* G^t(l^*) = \frac{1}{2} b_j, \\ \text{and } \Delta^* G^t(q^*) - \mathbf{d}^* G^t(l^*) &= \frac{1}{2} b_j, & \Leftrightarrow & \quad t b_j - \mathbf{d}^* G^t(l^*) = \frac{1}{2} b_j. \end{aligned}$$

Solving, we find that

$$t = \frac{\frac{1}{2} b_j + \mathbf{d}^* G^{\mu^*}(l^*)}{b_j + \mathbf{d}^* G^{\mu^*}(l^*) - \mathbf{d}^* G^{\nu^*}(l^*)}. \quad (5.1)$$

Noting that  $\mathbf{d}^* G^{\mu^*}(l^*) = \frac{1}{m} b_j + o(1)$  and  $\mathbf{d}^* G^{\nu^*}(l^*) = -\frac{1}{m} b_j + o(1)$  as  $n \rightarrow \infty$  by Theorem 4.6, we see that  $t \in [0, 1]$ .

We now define  $\alpha_\uparrow$  and  $\alpha_\downarrow$  via

$$\alpha_\uparrow^*(e^*) := \begin{cases} \mathbf{d}^* G^t(e^*) & e^* \neq \pm l^*, \\ \mp \frac{1}{2} b_j & e^* = \pm l^*, \end{cases} \quad \text{and} \quad \alpha_\downarrow^*(e^*) := \begin{cases} \mathbf{d}^* G^t(e^*) & e^* \neq \pm l^*, \\ \mp \frac{1}{2} b_j & e^* = \pm l^*, \end{cases}$$

where  $t$  is given by (5.1). Letting  $\alpha^\mu \in [\mathbf{d}u^\mu]$ , for any  $e \in n\mathcal{D}_2$  with  $e \neq p, q$ , by duality we have

$$\mathbf{d}[\alpha_\uparrow - \alpha^\mu](e) = \Delta^* G^t(e^*) - \Delta^* G^{\mu^*}(e^*) = t[\Delta^* G^{\nu^*}(e^*) - \Delta^* G^{\mu^*}(e^*)] = 0.$$

Again, by duality we also have

$$\begin{aligned} \mathbf{d}[\alpha_\uparrow - \alpha^\mu](p) &= \Delta^* G^t(p^*) + \mathbf{d}^* G^t(l^*) + \frac{1}{2} b_j - \Delta^* G^{\mu^*}(p^*) = 0, \\ \mathbf{d}[\alpha_\uparrow - \alpha^\mu](q) &= \Delta^* G^t(q^*) - \mathbf{d}^* G^t(l^*) - \frac{1}{2} b_j - \Delta^* G^{\mu^*}(p^*) = 0. \end{aligned}$$

Similarly,  $\mathbf{d}[\alpha_\downarrow - \alpha^\nu] = 0$ . It follows therefore that there exist  $v_\uparrow$  and  $v_\downarrow$  such that  $\alpha_\uparrow \in [\mathbf{d}u^\mu + \mathbf{d}v_\uparrow]$ , and  $\alpha_\downarrow \in [\mathbf{d}u^\nu + \mathbf{d}v_\downarrow]$ .

We also note that if  $a \notin \pm \partial l$  and  $\partial l = b - c$ , then

$$\begin{aligned} \delta[\alpha_\uparrow - \alpha^\mu](a) &= (\mathbf{d}^*)^2(G^t - G^{\mu^*})(a^*) = 0, \\ \delta[\alpha_\uparrow - \alpha^\mu](b) + \delta[\alpha_\uparrow - \alpha^\mu](c) &= (\mathbf{d}^*)^2[G^t - G^{\mu^*}](b^*) + (\mathbf{d}^*)^2[G^t - G^{\mu^*}](c^*) = 0. \end{aligned}$$

It follows that  $\alpha_\uparrow$  and  $\alpha_\downarrow$  satisfy conditions (1)–(4) of Lemma 5.2, and hence we have constructed the bond-length one forms corresponding to the transition state.

Finally, we define  $\gamma \in \Gamma_n(\mu \rightarrow \nu)$  via

$$\gamma(t) := \begin{cases} u^\mu + 2tv_\uparrow & t \in [0, \frac{1}{2}], \\ u^\mu + v_\uparrow + (2t - 1)v_\downarrow & t \in (\frac{1}{2}, 1], \end{cases}$$

which demonstrates that  $\Gamma_n(\mu \rightarrow \nu)$  is non-empty, and hence  $\mathcal{B}_n(\mu \rightarrow \nu)$  exists.

**5.4. Conclusion of the proof of Theorem 3.2.** We now use the dual representation of  $\alpha_\uparrow$ ,  $\alpha^\mu$  and  $\alpha^\nu$  to give an asymptotic expression for  $\mathcal{B}(\mu \rightarrow \nu)$  as  $n \rightarrow \infty$ . We use duality to compute

$$\begin{aligned} \mathcal{B}(\mu \rightarrow \nu) &= E(u^\mu + u_\uparrow; u^\mu), \\ &= \frac{1}{2}\lambda[(\alpha_\uparrow, \alpha_\uparrow) - (\alpha^\mu, \alpha^\mu)], \\ &= \frac{1}{2}\lambda[(\mathbf{d}^*G^{\mu^*} + t(\mathbf{d}^*G^{\nu^*} - \mathbf{d}^*G^{\mu^*}), \mathbf{d}^*G^{\mu^*} + t(\mathbf{d}^*G^{\nu^*} - \mathbf{d}^*G^{\mu^*})) - (\mathbf{d}^*G^{\mu^*}, \mathbf{d}^*G^{\mu^*})], \\ &= \lambda t(\mathbf{d}^*G^{\nu^*} - \mathbf{d}^*G^{\mu^*}, \mathbf{d}^*G^{\mu^*}) + \frac{1}{2}\lambda t^2(\mathbf{d}^*G^{\nu^*} - \mathbf{d}^*G^{\mu^*}, \mathbf{d}^*G^{\nu^*} - \mathbf{d}^*G^{\mu^*}), \\ &= \lambda t(\Delta^*G^{\nu^*} - \Delta^*G^{\mu^*}, G^{\mu^*}) + \frac{1}{2}\lambda t^2(\Delta^*G^{\nu^*} - \Delta^*G^{\mu^*}, G^{\nu^*} - G^{\mu^*}), \\ &= \lambda t b_j[G^{\mu^*}(q^*) - G^{\mu^*}(p^*)] + \frac{1}{2}\lambda t^2 b_j([G^{\nu^*}(q^*) - G^{\nu^*}(p^*)] - [G^{\mu^*}(q^*) - G^{\mu^*}(p^*)]) \\ &= \lambda t b_j \mathbf{d}^*G^{\mu^*}(l^*) + \frac{1}{2}\lambda t^2 b_j[\mathbf{d}^*G^{\mu^*}(l^*) - \mathbf{d}G^{\nu^*}(l^*)]. \end{aligned} \tag{5.2}$$

We now use the result of Theorem 4.6 to derive an asymptotic description of the above quantity. Suppose that  $q^* - p^* = a$  for some nearest neighbour lattice direction  $a$ , then

$$b_j \mathbf{d}^*G^{\mu^*}(l^*) = \mathbf{d}G_{\Lambda^*}(0, a) + n^{-1} \left[ \nabla \bar{y}_j(\bar{x}_j) \cdot a + \sum_{i \neq j} b_j b_i \nabla \mathcal{G}_{\bar{x}_j}(\bar{x}_i) \cdot a \right] + O(n^{-1-\delta} \log(n)) \tag{5.3}$$

$$\text{and} \quad b_j [\mathbf{d}^*G^{\mu^*}(l^*) - \mathbf{d}G^{\nu^*}(l^*)] = 2\mathbf{d}G_{\Lambda^*}(0, a) + O(n^{-1-\delta} \log(n)). \tag{5.4}$$

It follows that

$$\begin{aligned} t &= \frac{\frac{1}{2}b_j + b_j \mathbf{d}G_{\Lambda^*}(0, a) + n^{-1} \left[ b_j \nabla \bar{y}_j(\bar{x}_j) \cdot a + \sum_{i \neq j} b_i \nabla \mathcal{G}_{\bar{x}_j}(\bar{x}_i) \cdot a \right] + O(n^{-1-\delta} \log(n))}{b_j + 2b_j \mathbf{d}G_{\Lambda^*}(0, a) + O(n^{-1-\delta} \log(n))}, \\ &= \frac{1}{2} + n^{-1} \frac{\nabla \bar{y}_j(\bar{x}_j) \cdot a + \sum_{i \neq j} b_i b_j \nabla \mathcal{G}_{\bar{x}_j}(\bar{x}_i) \cdot a}{1 + 2\mathbf{d}G_{\Lambda^*}(0, a)} + O(n^{-1-\delta} \log(n)), \end{aligned} \tag{5.5}$$

where we use that  $b_j = 1/b_j$  since  $b_j = \pm 1$ . Substituting (5.3), (5.4) and (5.5) into (5.2), we obtain

$$\begin{aligned} \mathcal{B}_n(\mu \rightarrow \nu) &= \frac{3}{4}\lambda \mathbf{d}G_{\Lambda^*}(0, a) + n^{-1}\lambda \frac{\frac{1}{2} + 3\mathbf{d}G_{\Lambda^*}(0, a)}{1 + 2\mathbf{d}G_{\Lambda^*}(0, a)} \left[ \nabla \bar{y}_j(\bar{x}_j) \cdot a + \sum_{i \neq j} b_j b_i \nabla \mathcal{G}_{\bar{x}_j}(\bar{x}_i) \cdot a \right] \\ &\quad + O(n^{-1-\delta} \log(n)), \end{aligned}$$

completing the proof of Theorem 3.2.

## 6. KMC MODEL AND LARGE DEVIATIONS PRINCIPLE

**6.1. Modeling.** We now formulate the KMC model for dislocation motion which we consider, as well as the spatial and temporal scaling regime which we consider. We make several modeling assumptions, which we discuss in detail here.

First, we make the assumption that the only possible transitions are from  $\mu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  to  $\nu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  with

$$\mu - \nu = b_i[\mathbb{1}_{e_i} - \mathbb{1}_{e'_i}] \quad \text{for some } i \in \{1, \dots, m\}, \quad \text{where } e'_i = (e_i')^* + \mathbf{n},$$

where  $\mathbf{n}$  is a dual lattice direction. This assumption is made since the coherent movement of multiple dislocations at the same time is likely to be an event with very small probability in a large system, and we expect dislocations to only move to “adjacent” core positions.

As explained in the introduction, we then assume that the transition time for a dislocation  $\mu$  to  $\nu$  is exponentially distributed with rate

$$\mathcal{R}_n(\mu \rightarrow \nu) := [\mathcal{S}_n(\mu \rightarrow \nu)]^{-1} \exp(-\beta \mathcal{B}_n(\mu \rightarrow \nu)), \quad (6.1)$$

where:

- (1)  $\mathcal{B}_n(\mu \rightarrow \nu)$  is the energy barrier for the transition from  $\mu$  to  $\nu$  defined by (3.4),
- (2)  $\beta = (k_B T)^{-1}$  is the inverse thermodynamic temperature, and
- (3)  $\mathcal{S}_n(\mu \rightarrow \nu)$  is the pre-exponential rate factor which is related to the entropic “width” of the pathways connecting  $\mu$  and  $\nu$ , and hence also depends on the inverse temperature  $\beta$ .

In common with many KMC models for crystalline materials, we make the assumption that  $\mathcal{S}_n(\mu \rightarrow \nu) = \mathcal{S}_0 + o(1)$  as  $\beta \rightarrow \infty$ , uniformly in  $n$ . Here, we justify this assumption by noting that Lemma 5.2 shows that there is essentially only one path which realises the optimal transition path to move from  $\mu$  to  $\nu$ , and moreover the width of this path in phase space should be approximately the same for each transition as dislocations become very far apart.

6.1.1. *Setup.* We now make a choice of rescaling. Since we are interested in the physically interesting case of observing a large system over a long timescale, we let  $\mathcal{T}_n > 1$  be the timescale of observation, which will be taken relative to the typical timescale on which a dislocation configuration changes.

First, we denote what we term the *boundary of*  $\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$

$$\partial \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m) := \left\{ \mu = \sum_{i=1}^m b_i \mathbb{1}_{e_i} \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m) \mid \mu + b_i [\mathbb{1}_{e_i + \mathbf{n}} - \mathbb{1}_{e_i}] \notin \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m) \text{ for some } i \right\}.$$

Since we expect our modelling assumptions to break down as dislocations approach one another and the boundary, we will stop the evolution if it reaches this set.

Now define the set of admissible (macroscale) dislocation positions to be

$$\mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m) := \left\{ (\bar{x}_1, \dots, \bar{x}_m) \in \mathcal{D}^m \mid \bar{x}_i \in \mathcal{D}, |\bar{x}_i - \bar{x}_j| \geq \epsilon, \text{dist}(\bar{x}_i, \partial \mathcal{D}) \geq \epsilon, \forall i, j \text{ with } i \neq j \right\},$$

and identify  $\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  with a subset of this space by the mapping

$$\iota_n : \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m) \rightarrow \mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m), \quad \text{where } \iota \left( \sum_{i=1}^m b_i \mathbb{1}_{e_i} \right) = \left( \frac{1}{n} e_1^*, \dots, \frac{1}{n} e_m^* \right).$$

It is clear that this map is well-defined, and by endowing  $\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  with the metric

$$r_n(\mu, \nu) = \sum_{i=1}^m \frac{1}{n} \text{dist}(e_i^*, (e'_i)^*) \quad \text{where } \mu = \sum_{i=1}^m b_i \mathbb{1}_{e_i} \text{ and } \nu = \sum_{i=1}^m b_i \mathbb{1}_{e'_i},$$

and  $\mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m)$  with the metric

$$r_\infty(\mu, \nu) = \sum_{i=1}^m \text{dist}(\bar{x}_i, \bar{x}'_i) \quad \text{where } \mu = (\bar{x}_1, \dots, \bar{x}_m) \text{ and } \nu = (\bar{x}'_1, \dots, \bar{x}'_m),$$

$\iota_n$  is an isometric embedding. Moreover, the spaces are compact.

Let  $D([0, T]; \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m))$  denote the Skorokhod space of càdlàg maps from  $[0, T] \subset \mathbb{R}$  with values in  $\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$ , and denote the space of continuous bounded real-valued functions from  $\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  to be  $C_b(\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m))$ : this is in fact the space of all real-valued functions on  $\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$ , since the metric  $r_n$  induces the discrete topology.

Now consider the sequence of Markov processes  $Y^n \in D([0, T]; \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m))$  which is killed on the boundary  $\partial \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$ , and has the infinitesimal generator  $\Omega_n : C_b(\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)) \rightarrow C_b(\mathcal{M}_{\epsilon, n}(b_1, \dots, b_m))$  defined via

$$[\Omega_n f](\mu) = \sum_{\nu | r_n(\nu, \mu) = n^{-1}} \mathcal{T}_n \mathcal{R}_n(\mu \rightarrow \nu) [f(\nu) - f(\mu)],$$

where  $\mathcal{R}_n(\mu \rightarrow \nu)$  is defined in (6.1).

We note that since  $\mathcal{R}_n(\mu \rightarrow \nu)$  is positive and bounded away from 0 and  $+\infty$  uniformly in  $\mu, \nu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  and  $n \in \mathbb{N}$ , we have that  $\Omega_n$  is a bounded linear operator. Defining  $X_t^n := \iota_n(Y_t^n)$ , we have that  $X_t^n$  is a Markov process on the space  $\mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m)$ .

6.1.2. *The nonlinear generator and choice of scaling.* As in Lemma 5.8 of [15], the nonlinear generator  $H_n$  is defined to be

$$H_n f := \frac{1}{n} e^{-nf} [\Omega_n e^{nf}].$$

Suppose that  $f \in C^2(\mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m))$ , and let  $x^n = (\frac{1}{n} e_1^*, \dots, \frac{1}{n} e_m^*)$ . Then asymptotically, we have that

$$H_n(f \circ \iota_n)(x^n) = \sum_{i=1}^m \sum_{j=1}^{\mathbf{N}^*} \frac{\mathcal{T}_n \mathcal{R}_n(\mu \rightarrow \nu)}{n} (\exp [\partial_i f(x^n) \cdot \mathbf{n}_{i,j} + o(n^{-1})] - 1) \quad \text{as } n \rightarrow \infty,$$

where  $\mathbf{n}_{i,j}$  are the nearest neighbour directions in  $\Lambda^*$  at  $e_i^*$ , and  $\mathbf{N}^*$  is the number of nearest neighbours in  $\Lambda^*$ . Now, by applying Theorem 3.2 and the assumption that  $\mathcal{S}_n(\mu \rightarrow \nu) = \mathcal{S}_0 + o(1)$ , we have that

$$\frac{\mathcal{T}_n \mathcal{R}_n(\mu \rightarrow \nu)}{n} = \frac{\mathcal{T}_n e^{-\beta \lambda c_0}}{n \mathcal{S}_0} \exp \left( - \frac{\beta \lambda c_1}{n} \left[ \nabla \bar{y}_j(x_j^n) \cdot \mathbf{n}_{i,j} + \sum_{i | i \neq j} b_j b_i \nabla \mathcal{G}_{x_i^n}(x_j^n) \cdot \mathbf{n}_{i,j} \right] \right) + o(1),$$

We identify two parameters in this expression, which we now argue should be seen as dimensionless:

$$A := \frac{\mathcal{T}_n e^{-\beta \lambda c_0}}{n \mathcal{S}_0} \quad \text{and} \quad B := \beta \lambda n^{-1}.$$

Since our domain is viewed as a cross-section of a long cylinder of material, we have that

- (1)  $\mathcal{T}_n$  has units of time,
- (2)  $n$  is a measure of the diameter of the domain relative to the interatomic spacing, and hence has units of length,
- (3)  $\beta = (k_B T)^{-1}$  is the inverse thermodynamic temperature of the system per unit area with units of [energy per unit area] $^{-1}$ , and
- (4)  $\lambda$  has units of energy per unit height of the cylinder.

Dimensionally, we expect  $\mathcal{S}_0$  to be the ‘number’ of exits from  $\mu$  to the state  $\nu$ , i.e. the amount of surface ‘area’ in phase space through which states pass from  $\mu$  to  $\nu$ , divided by the volume in the state. Since the dividing surface between states is an  $(\#n\mathcal{D}_0 - 1)$ -dimensional set in phase space, it follows that  $\mathcal{S}_0$  should have units which are the inverse of those for a single degree of freedom, i.e. here, length $^{-1}$ .

Additionally, we note that  $e^{\beta \lambda c_0}$  can be seen as the mean time for a single dislocation to jump in the full lattice, and hence is interpreted as having units of time.

We may think of  $\mathcal{T}_n e^{-\beta \lambda c_0}$  as being the mean number of times at which sufficient potential energy is attained to cause a jump of one lattice spacing in unit ‘observed’ time,  $\mathcal{T}_n e^{-\beta \lambda c_0} / \mathcal{S}_0$  the number of *successful* jumps of one lattice spacing, and hence the total lattice distance travelled: when divided by the macroscopic lengthscale  $n$ ,  $A$  therefore become the proportion of the body crossed during the time which the system is observed.

To interpret  $B$ , we think of  $\lambda$  as being a measure of the energy per unit length required to move the system from one state to another, and  $n\beta^{-1}$  as being the thermal energy per unit length available to the system in order to achieve such movement.  $B$  is therefore viewed as comparing the energy required for dislocation motion and the thermal energy available.

In the following, we will consider a scaling regime where  $n \rightarrow \infty$  with  $A$  and  $B$  are held constant: assuming that  $\lambda$  and  $\mathcal{S}_0$  remain constant, this is the regime in which a large system is observed at low temperature for a long time.

**6.2. Large Deviations Principle.** We now follow the method summarised in [8] and exposed in detail in [15] to formally derive a rate functional for a Large Deviations principle.

6.2.1. *The cases  $\Lambda = \text{Hx}$  and  $\Lambda = \text{Sq}$ .* When  $\Lambda = \text{Hx}$  or  $\Lambda = \text{Sq}$ , the dual lattice is isomorphic to  $\text{Tr}$  or  $\text{Sq}$  respectively, and hence the set of nearest neighbour directions in the dual lattice is always the same.

As  $n \rightarrow \infty$  in the parameter regime we have prescribed above and  $\text{dist}(x^n, \bar{x}) = O(n^{-1})$  as  $n \rightarrow \infty$ , we have

$$H_n(f \circ \iota_n)(x^n) \rightarrow Hf(\bar{x}) := \sum_{i=1}^m \sum_{j=1}^{N^*} A(e^{\partial_j f(x) \cdot \mathbf{n}_j} - 1) \exp\left(-B\left[\nabla \bar{y}_i(\bar{x}_i) + \sum_{k \neq j} b_i b_k \nabla \mathcal{G}_{\bar{x}_j}(\bar{x}_i)\right] \cdot \mathbf{n}_j\right),$$

where  $\mathbf{n}_j$  are the nearest neighbour directions in  $\Lambda^*$ . Note that the operator  $H$  is well-defined for any  $f \in C^1(\mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m))$ .

Recall the definition of  $\bar{y}_i$  as the solution to

$$-\Delta \bar{y}_i = 0 \text{ in } \mathcal{D}, \quad \text{and} \quad \bar{y}_i(s) = \frac{1}{K\pi} \log(|s - \bar{x}_i|) \text{ on } \partial \mathcal{D}.$$

Following the approach of [2] and [1], we define the renormalised energy for  $\bar{x} \in \mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m)$  to be

$$\mathcal{W}(\bar{x}) := - \sum_{\substack{i, j=1 \\ i \neq j}}^m \frac{b_i b_j}{2K\pi} \log(|\bar{x}_i - \bar{x}_j|) + \sum_{i, j=1}^m b_i b_j \bar{y}_i(\bar{x}_j).$$

Recalling the definition of  $\mathcal{G}$  from Theorem 3.2, we have that

$$\partial_i \mathcal{W}(\bar{x}) = \nabla \bar{y}_i(\bar{x}_i) + \sum_{j \neq i} b_i b_j \nabla \mathcal{G}_{\bar{x}_j}(\bar{x}_i).$$

This allows us to express

$$Hf(\bar{x}) = \sum_{i=1}^m \sum_{j=1}^{N^*} A\left(\cosh\left[(\partial_i f(\bar{x}) - B\partial_i \mathcal{W}(\bar{x})) \cdot \mathbf{n}_j\right] - \cosh\left[-B\partial_i \mathcal{W}(\bar{x}) \cdot \mathbf{n}_j\right]\right).$$

This leads us to define the *Hamiltonian*,  $\mathcal{H}^\Lambda : \mathcal{D}^m \times (\mathbb{R}^2)^m$ , as

$$\mathcal{H}^\Lambda(\bar{x}, p) := \sum_{i=1}^m \sum_{j=1}^{N^*/2} 2A\left(\cosh\left[(p_i - B\partial_i \mathcal{W}(\bar{x})) \cdot \mathbf{n}_j\right] - \cosh\left[-B\partial_i \mathcal{W}(\bar{x}) \cdot \mathbf{n}_j\right]\right),$$

where  $p = (p_1, \dots, p_m)$  with  $p_i \in \mathbb{R}^2$  for each  $i$ . The *Lagrangian* is the Legendre–Fenchel transform (for further details on this topic, see §8.10 in [35]) of the Hamiltonian of  $\mathcal{H}^\Lambda$ , i.e.

$$\mathcal{L}^\Lambda(\bar{x}, \xi) := \sup_{p \in (\mathbb{R}^2)^m} \{\langle \xi, p \rangle - \mathcal{H}(\bar{x}, p)\},$$

where  $\langle \cdot, \cdot \rangle$  is the inner product on  $(\mathbb{R}^2)^m$  given by  $\langle \xi, p \rangle := \sum_{i=1}^m \xi_i \cdot p_i$ . We now follow [8] in defining  $\Psi_{A,B}^{\text{Hx}}, \Psi_{A,B}^{\text{Sq}} : (\mathbb{R}^2)^m \rightarrow \mathbb{R}$  via

$$\begin{aligned} \Psi_{A,B}^{\text{Hx}}(f) &:= \sum_{i=1}^m \sum_{j=1}^6 \frac{A}{B} [\cosh(Bf_i \cdot \mathbf{a}_j) - 1], \\ \Psi_{A,B}^{\text{Sq}}(f) &:= \sum_{i=1}^m \sum_{j=1}^4 \frac{A}{B} [\cosh(Bf_i \cdot \mathbf{e}_j) - 1], \end{aligned}$$

which permits us to write

$$\mathcal{H}^\Lambda(\bar{x}, p) = B[\Psi_{A,B}^\Lambda(\frac{1}{B}p - \nabla \mathcal{W}(\bar{x})) - \Psi_{A,B}^\Lambda(-\nabla \mathcal{W}(\bar{x}))].$$



$\Psi_{A,B}^\Lambda$  is (strictly) convex, and hence has a convex dual, given by its Legendre–Fenchel transform, denoted  $\Phi_{A,B}^\Lambda$ . Moreover, by properties of the Legendre–Fenchel transform, we have that

$$\begin{aligned} \nabla\Phi_{A,B}^\Lambda(\xi) = \frac{1}{B}p - \nabla\mathcal{W}(\bar{x}) &\Leftrightarrow \xi = \nabla\Psi_{A,B}^\Lambda\left(\frac{1}{B}p - \nabla\mathcal{W}(\bar{x})\right) \\ &\Leftrightarrow p \in \operatorname{argmax}_{p'}\{\langle \xi, p' \rangle - \mathcal{H}^\Lambda(\bar{x}, p')\}. \end{aligned}$$

Using this fact, we have that

$$\begin{aligned} \mathcal{L}^\Lambda(\bar{x}, \xi) &= \langle B\nabla\Phi_{A,B}^\Lambda(\xi) + B\nabla\mathcal{W}(\bar{x}), \xi \rangle - \mathcal{H}^\Lambda(\bar{x}, B\nabla\Phi_{A,B}^\Lambda(\xi) + B\nabla\mathcal{W}(\bar{x})) \\ &= \langle B\nabla\Phi_{A,B}^\Lambda(\xi) + B\nabla\mathcal{W}(\bar{x}), \xi \rangle - B\Psi_{A,B}^\Lambda(\nabla\Phi_{A,B}^\Lambda(\xi)) + B\Psi_{A,B}^\Lambda(-\nabla\mathcal{W}(\bar{x})) \end{aligned}$$

Using the property that  $\langle u, v \rangle = \Psi_{A,B}^\Lambda(u) + \Phi_{A,B}^\Lambda(v)$ , we then have

$$\mathcal{L}^\Lambda(\bar{x}, \xi) = B\Phi_{A,B}^\Lambda(\xi) + B\Psi_{A,B}^\Lambda(-\nabla\mathcal{W}(\bar{x})) + B\langle \nabla\mathcal{W}(\bar{x}), \xi \rangle,$$

which leads us to define the rate functional  $\mathcal{J}_{A,B}^\Lambda : D([0, T]) \rightarrow \mathbb{R}$  with

$$\mathcal{J}_{A,B}^\Lambda(\bar{x}) := \begin{cases} B \int_0^T \Phi_{A,B}^\Lambda(\dot{\bar{x}}) + \Psi_{A,B}^\Lambda(-\nabla\mathcal{W}(\bar{x})) + \langle \nabla\mathcal{W}(\bar{x}), \dot{\bar{x}} \rangle dt & \bar{x} \in AC([0, T]; \mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m)), \\ +\infty & \text{otherwise;} \end{cases}$$

here  $AC([0, T]; \mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m))$  denotes the set of absolutely continuous functions from  $[0, T]$  taking values in  $\mathcal{D}^m$ .

We may now state the following theorem, the proof of which is given in Chapter 5, §2 of [16], or §10.3 of [15]; see [9] for related results concerning a discrete–time model on a lattice.

**Theorem 6.1.** *Suppose that  $\Lambda = \text{Hx}$  or  $\Lambda = \text{Sq}$ , and that  $X_0^n = \iota_n(x^n)$  where  $x^n \rightarrow \bar{x}_0 \in \mathcal{M}_{\delta, \infty}(b_1, \dots, b_m)$  as  $n \rightarrow \infty$  with  $\delta > \epsilon$ . Then for  $T = T(\delta)$  small enough, the processes  $X_t^n$  satisfy a Large Deviations principle with good rate function  $\mathcal{J}_{A,B}^\Lambda$ .*

The requirement that the initial condition lies in  $\mathcal{M}_{\delta, \infty}$  prevents the process from immediately hitting the boundary  $\partial\mathcal{M}(b_1, \dots, b_m)$ .

6.2.2. *The case  $\Lambda = \text{Tr}$ .* Here the situation is more complicated. Since  $\text{Tr}^*$  is isomorphic to  $\text{Hx}$ , which not a Bravais lattice, the value of  $\Omega_n f(x^n)$  depends strongly upon the specific sublattice on which each of the dislocations lies. This suggest more sophisticated averaging techniques beyond the scope of this paper would need to be developed in order to demonstrate a Large Deviations Principle for the motion of dislocations on  $\text{Tr}^*$ .

However, since  $H_n f$  converges uniformly to a well–defined limit if we fix  $x_i^n$  to be on a specific sublattice, it seems natural to conjecture that the Hamiltonian converges “weakly–\*” to the average of these limits, i.e.

$$\mathcal{H}^{\text{Tr}}(\bar{x}, p) := \sum_{i=1}^m \sum_{j=1}^6 \frac{1}{2} A \left( \cosh \left[ (p_i - B\partial_i \mathcal{W}(\bar{x})) \cdot \mathbf{a}_j \right] - \cosh \left[ -B\partial_i \mathcal{W}(\bar{x}) \cdot \mathbf{a}_j \right] \right).$$

Defining  $\Psi_{A,B}^{\text{Tr}}$  in a similar way as

$$\Psi_{A,B}^{\text{Tr}}(f) := \sum_{i=1}^m \sum_{j=1}^6 \frac{A}{2B} [\cosh(Bf_i \cdot \mathbf{a}_j) - 1],$$

we may define the action functional  $\mathcal{J}_{A,B}^{\text{Tr}} : D([0, T]; \mathcal{M}_{\epsilon, \infty}(b_1, \dots, b_m)) \rightarrow \mathbb{R}$  with

$$\mathcal{J}_{A,B}^{\text{Tr}}(\bar{x}) := \begin{cases} B \int_0^T [\Psi_{A,B}^{\text{Tr}}]^*(\dot{\bar{x}}) + \Psi_{A,B}^{\text{Tr}}(-\nabla\mathcal{W}(\bar{x})) + \langle \nabla\mathcal{W}(\bar{x}), \dot{\bar{x}} \rangle dt & \bar{x} \in AC([0, T]; \mathcal{D}^m), \\ +\infty & \text{otherwise.} \end{cases}$$

We therefore propose the following conjecture for the processes  $X^n$  when  $\Lambda = \text{Tr}$ .

**Conjecture 6.2.** *Suppose that  $\Lambda = \text{Tr}$ , and that  $X_0^n = \iota_n(x^n)$  where  $x^n \rightarrow \bar{x}_0 \in \mathcal{M}_{\delta, \infty}(b_1, \dots, b_m)$  as  $n \rightarrow \infty$  with  $\delta > \epsilon$ . Then for  $T = T(\delta)$  small enough, the processes  $X_t^n$  satisfy a Large Deviations principle with good rate function  $\mathcal{J}_{A,B}^{\text{Tr}}$ .*

**6.3. Interpretation.** The Large Deviations Principles discussed above entail that, for large  $n$ , the most probable trajectory of the system is the minimiser of  $\mathcal{J}_{A,B}^\Lambda$ . As has been noted in [29, 8], there is a close link between minimisers of Large Deviations rate functionals and gradient flows: we also observe this phenomenon here.

Using properties of the Legendre–Fenchel transform, we see that the integrand of the rate functional is postive, and is zero if and only if  $x$  satisfies (see [35] or [30])

$$\dot{\bar{x}} = \nabla \Psi_{A,B}^\Lambda(-\nabla \mathcal{W}(\bar{x})) \quad \text{with} \quad \bar{x}(0) = \bar{x}_0.$$

The latter expression can be expressed analytically as a combination of sinh functions, and could easily be implemented in currently available discrete dislocation dynamics codes.

Furthermore, as in Theorem 3.1 of [8], we may recover a quadratic dissipation in the limit where  $A \rightarrow \infty$  and  $B \rightarrow 0$ .

**Theorem 6.3.** *Suppose that  $A \rightarrow \infty$  and  $B \rightarrow 0$  with  $AB \rightarrow \omega$ . Then*

$$\Gamma\text{-}\lim_{B \rightarrow 0} \frac{1}{B} \mathcal{J}_{\omega/B,B}^\Lambda(x) = \begin{cases} \int_0^T \frac{1}{2\omega \mathbf{N}^*} |\dot{x}|^2 + \frac{\omega \mathbf{N}^*}{2} |\nabla \mathcal{W}(x)|^2 + \langle \nabla \mathcal{W}(x), \dot{x} \rangle dt & x \in \text{H}^1([0, T]; \mathcal{D}^m), \\ +\infty & \text{otherwise.} \end{cases}$$

The proof of this result is essentially identical to that given in [8], upon noting that

$$\begin{aligned} \Psi_{\omega/B,B}^\Lambda(f) &\rightarrow \sum_{i=1}^m \sum_{j=1}^{\mathbf{N}^*} (f_i \cdot \mathbf{n}_j)^2 = \sum_{i=1}^m \frac{\mathbf{N}^*}{2} |f_i|^2 & \text{if } \Lambda = \text{Hx or Sq}, \\ \Psi_{\omega/B,B}^{\text{Tr}}(f) &\rightarrow \sum_{i=1}^m \sum_{j=1}^6 \frac{1}{2} (f_i \cdot \mathbf{n}_j)^2 = \sum_{i=1}^m \frac{\mathbf{N}^*}{2} |f_i|^2 & \text{if } \Lambda = \text{Tr}, \end{aligned}$$

uniformly on compact sets, and monotonically everywhere. This convergence then entails the convergence of  $\Phi_{\omega/B,B}^\Lambda(\xi) \rightarrow \frac{1}{2\omega \mathbf{N}^*} |\xi|^2$  by properties of the Legendre–Fenchel transform.

Recalling the interpretation of  $A$  and  $B$  given in §6.1.2, this could be viewed as corresponding to passing to the regime where the thermal energy is much larger than the energy barrier to dislocation motion, but where the proportion of the cylinder crossed by a dislocation during the observed time is small. However, raising the temperature inevitably has an effect upon the entropy which is unaccounted for in this model: moreover, the rate functional degenerates as  $B \rightarrow 0$ , so the physical interpretation of this limit is unclear.

Finally, we remark that is also possible to consider the other scaling regime analysed in [8], in which  $B \rightarrow \infty$  with

$$\log(A) = -c_2 B \quad \text{for some } c_2.$$

In terms of the dimensional parameters described in §6.1, this becomes

$$\log\left(\frac{\mathcal{I}_n}{\mathcal{I}_0 n}\right) - c_0 \lambda \beta = -c_2 \frac{\lambda \beta}{n}.$$

Assuming that  $\lambda$  and  $\mathcal{I}_0$  remain fixed, the only way in which this scaling regime can be attained is if  $n$  remains fixed, with  $\beta \rightarrow \infty$  and  $\mathcal{I}_n \rightarrow \infty$ . However, since our analysis relied upon the fact that  $n \rightarrow \infty$  to ensure that lower-order terms vanish in  $\mathcal{R}_n(\mu \rightarrow \nu)$ , we cannot be certain that this limit corresponds to a physically-relevant limit, and so we do not study it here.

## APPENDIX A. GREEN'S FUNCTIONS: PROOFS

**A.1. Proof of Lemma 4.3 (2) and the case  $\Lambda = \text{Hx}$ .** We first prove (2) for  $\Lambda = \text{Sq}$  and  $\Lambda = \text{Tr}$ . Let  $\mathbf{a}$  be a nearest neighbour direction in the lattice, and by the symmetry of  $G_\Lambda$  from (1), for any  $b = [0, \mathbf{a}]$  we have

$$1 = \Delta G_\Lambda(0) = \mathbf{N}G_\Lambda(0) - \mathbf{N}G_\Lambda(\mathbf{a}) = -\mathbf{N}G_\Lambda(\mathbf{a}).$$

Hence  $\mathbf{d}G_\Lambda(b) = \mathbf{N}^{-1}$ . Consider  $v \in \mathscr{W}(\Lambda_0)$  defined to be

$$v(e) := G_\Lambda(e + \mathbf{a}) - G_\Lambda(e).$$

It follows that  $\Delta v = \mathbb{1}_{-\mathbf{a}} - \mathbb{1}_0$ . Applying the maximum principle on the set

$$\mathcal{B}_r := \{e \in \Lambda_0 \mid \text{dist}(e, 0) \leq r, e \neq 0, -\mathbf{a}\},$$

we note that the maximum and minimum of  $v$  are attained on  $\text{Ext}(B'_{r,0})$ , since  $G_\Lambda$  is harmonic on  $\text{Int}(B'_{r,0})$ . Now, applying (3) and letting  $r$  tend to infinity implies the desired result, noting that  $v(0) = -v(-\mathbf{a}) = \mathbf{N}^{-1}$ .

We next prove the theorem for the case where  $\Lambda = \text{Hx}$ . Recall that  $\text{Hx}$  is a multilattice, and may be written as

$$\text{Hx} = \sqrt{3}\text{Tr} \cup (\sqrt{3}\text{Tr} + \mathbf{e}_2).$$

We define  $G_{\text{Hx}} \in \mathscr{W}(\text{Hx}_0)$  to be

$$G_{\text{Hx}}(e) := \begin{cases} 3G_{\text{Tr}}(e/\sqrt{3}) & e \in \sqrt{3}\text{Tr}, \\ \sum_{e' \mid \text{dist}(e', e)=1} G_{\text{Tr}}(e'/\sqrt{3}) & e \in \sqrt{3}(\text{Tr} + \mathbf{e}_2), \end{cases}$$

where  $G_{\text{Tr}}$  is the lattice Green's function for  $\Lambda = \text{Tr}$ . We note that  $\Delta G_{\text{Hx}}(e) = 0$  by definition for  $e \in \sqrt{3}\text{Tr} + \mathbf{e}_2$ , and for  $e \in \sqrt{3}\text{Tr}$ , we have that

$$\begin{aligned} \Delta G_{\text{Hx}}(e) &= 9G_{\text{Tr}}(e/\sqrt{3}) - \sum_{a \mid \text{dist}(a, e)=1} \left( \sum_{b \mid \text{dist}(b, a)=1} G_{\text{Tr}}(b/\sqrt{3}) \right), \\ &= 6G_{\text{Tr}}(e/\sqrt{3}) - \sum_{a \mid \text{dist}(a, e)=\sqrt{3}} G_{\text{Tr}}(a/\sqrt{3}), \\ &= \mathbb{1}_0(e). \end{aligned}$$

Moreover  $G_{\text{Hx}}(0) = G_{\text{Tr}}(0) = 0$ . The symmetry of  $G_{\text{Tr}}$  also implies (1) for  $G_{\text{Hx}}$ .

Furthermore, let  $C_{\text{Tr}}$  be the constant in statement (3) for the case where  $\Lambda = \text{Tr}$ , and define

$$u_{\text{Hx}}(e) := G_{\text{Hx}}(e) + \frac{1}{2\pi} \log |\text{dist}(e/\sqrt{3}, 0)| + 3C_{\text{Tr}} = G_{\text{Hx}}(e) + \frac{1}{2\pi} \log |\text{dist}(e, 0)| + 3C_{\text{Tr}} - \frac{1}{4\pi} \log(3).$$

we see that for  $e \in \sqrt{3}\text{Tr}$ ,  $u_{\text{Hx}}$  satisfies (4.1) by the assertion for the case where  $\Lambda = \text{Tr}$ . For  $e \in \sqrt{3}\text{Tr}$ , define  $v_{\text{Tr}}(e) := G_{\text{Tr}}(e/\sqrt{3}) + \frac{1}{6\pi} \log |\text{dist}(e/\sqrt{3}, 0)|$ ; then for  $e \in \sqrt{3}\text{Tr} + \mathbf{e}_2$ , we have

$$u_{\text{Hx}}(e) = \frac{1}{2\pi} \log |\text{dist}(e/\sqrt{3}, 0)| + \sum_{e' \mid \text{dist}(e, e')=1} \left( v_{\text{Tr}}(e') - \frac{1}{6\pi} \log |\text{dist}(e'/\sqrt{3}, 0)| \right).$$

Since  $\log |x|$  is harmonic away from 0, Taylor expanding to third-order about  $e$  and using the symmetry of  $\text{Hx}$  implies that

$$\frac{1}{2\pi} \log |\text{dist}(e/\sqrt{3}, 0)| - \sum_{e' \mid \text{dist}(e, e')=1} \frac{1}{6\pi} \log |\text{dist}(e'/\sqrt{3}, 0)| \lesssim |\text{dist}(e, 0)|^{-3}. \quad (\text{A.1})$$

Applying this estimate and (4.1) for  $\Lambda = \text{Tr}$ , we obtain that

$$|u(e)| \lesssim |\text{dist}(e, 0)|^{-1} \log |\text{dist}(e, 0)|$$

for all  $e \in \text{Hx}$ .

To demonstrate (4.2), we suppose that  $b = [e, e + \mathbf{a}]$ , where without loss of generality, we take  $e \in \sqrt{3}\text{Tr}$  and  $e + \mathbf{a} \in \sqrt{3}\text{Tr} + \mathbf{e}_2$ . Then

$$|\mathbf{d}u_{\text{Hx}}(b)| = |v_{\text{Tr}}(e + \sqrt{3}\mathbf{a}_{i+1}) + v_{\text{Tr}}(e + \sqrt{3}\mathbf{a}_i) - 2v_{\text{Tr}}(e)| \\ + \frac{1}{2\pi} \log |\text{dist}([e + \mathbf{a}]/\sqrt{3}, 0)| - \sum_{e' | \text{dist}(e+\mathbf{a}, e')=1} \frac{1}{6\pi} \log |\text{dist}(e'/\sqrt{3}, 0)|$$

for some  $i$ . Now using the definition of  $v_{\text{Tr}}$ , then applying statement (3) in the case  $\Lambda = \text{Tr}$  and (A.1) gives the result.

**A.2. Proof of Theorem 4.6.** We will prove this in several steps: we first decompose  $G^{\mu*}$ , then obtain estimates on the differential of each component of the decomposition in turn. Since the entire proof takes place in the  $n\mathcal{D}^*$ , for conciseness we drop  $*$  from our notation throughout.

**A.2.1. Decomposition of  $G^\mu$ .** We begin by decomposing

$$G^\mu(e) = \sum_{i=1}^m b_i G_\Lambda(e - e_i) + \sum_{i=1}^m \bar{y}_i^n(e) + u(e) + v(e), \quad (\text{A.2})$$

where:

- (1)  $G_\Lambda$  is the full (dual) lattice Green's function,
- (2)  $\bar{y}_i^n(x) := \bar{y}_i(\frac{1}{n}x)$ , where  $\bar{y}_i$  solves  $\Delta \bar{y}_i = 0$  on  $\mathcal{D}$  with boundary values

$$\bar{y}_i(x) = \frac{1}{\kappa\pi} b_i \log(|x - \bar{x}_i|),$$

- (3)  $u$  is the solution to the discrete Poisson problem

$$\Delta u = 0 \quad \text{with} \quad u(e) = - \sum_{i=1}^m [b_i G_\Lambda(e - e_i) + \bar{y}_i^n(e)] \quad \text{on} \quad \text{Ext}(n\mathcal{D}_0), \quad \text{and}$$

- (4)  $v$  is the solution to the discrete Poisson problem

$$\Delta v = - \sum_{i=1}^m \Delta \bar{y}_i^n \quad \text{with} \quad v(e) = 0 \quad \text{on} \quad \text{Ext}(n\mathcal{D}_0).$$

In combination, Lemma 4.3, the theory of boundary value problems on polygons in [19], and Lemma 4.1 allow us to conclude that each of the terms in this decomposition is well-defined. Furthermore, equality follows since solutions to the Poisson problem are unique by Lemma 4.1.

**A.2.2. Regularity of  $\bar{y}_i$ .** We now recall some facts concerning the regularity of  $\bar{y}_j$  from [19]. There exists  $\sigma \in (0, 1)$  such that, applying Theorem 6.4.2.6 in [19],  $\bar{y}_i$  lies in the space

$$\mathcal{X} := C^{4,\sigma}(\bar{\mathcal{D}}) + \text{span}\{\mathfrak{S}_{l,m} \mid m \in \mathbb{N}, 0 < m < (4 + \sigma)\omega_l/\pi\},$$

where  $\mathfrak{S}_{l,m}$  is given in polar coordinates  $(r_l, \theta_l)$  about the  $c_l$ , the  $l$ th corner of  $\mathcal{D}$  as

$$\mathfrak{S}_{l,m}(r_l, \theta_l) := \begin{cases} r_l^{m\pi/\omega_l} \sin(\frac{m\pi}{\omega_l}\theta_l) \eta(r_l), & m\pi/\omega_l \notin \mathbb{N}, \\ r_l^{m\pi/\omega_l} \log(r_l) [\sin(\frac{m\pi}{\omega_l}\theta_l) + \theta_l \cos(\frac{m\pi}{\omega_l}\theta_l)] \eta(r_l), & m\pi/\omega_l \in \mathbb{N}. \end{cases}$$

where we recall that  $\omega_l$  is the interior angle at  $c_l$  and we set  $\eta \in C_0^\infty(\mathbb{R})$  to be a cutoff function so that  $\eta(x) = 1$  for  $|x|$  sufficiently small, and  $\text{supp}\{\mathfrak{S}_{l,m}\} \cap \text{supp}\{\mathfrak{S}_{l',n}\} = \emptyset$  for any  $n, m \in \mathbb{N}$  and any  $l \neq l'$ .

We note that  $\bar{y}_i$  only fails to be  $C^{4,\sigma}$  at the corners of the domain  $\mathcal{D}$ , and since  $\mathcal{D}$  is convex,  $\pi/\omega_l > 1$ , which implies that  $\mathfrak{S}_{l,m} \in C^{1,\delta}(\bar{\mathcal{D}})$ : hence  $\bar{y}_i \in C^{1,\delta}(\bar{\mathcal{D}})$  with  $\delta := \min_l \{\pi/\omega_l - 1\} \in (0, \frac{1}{2}]$ .  $\mathcal{X}$  is a Banach space when endowed with the norm

$$\left\| v + \sum_{0 < m < (4+\sigma)\omega_l/\pi} C_{l,m} \mathfrak{S}_{l,m} \right\|_{\mathcal{X}} := \|v\|_{C^{4,\sigma}(\bar{\mathcal{D}})} + \sum_{0 < m < (4+\sigma)\omega_l/\pi} |C_{l,m}|. \quad (\text{A.3})$$

Furthermore, it can be checked that the mapping

$$\mathcal{S} : \{x \in \mathcal{D} \mid \text{dist}(x, \partial\mathcal{D}) \geq \epsilon/2\} \rightarrow \mathcal{X} \quad \text{where} \quad \mathcal{S}(\bar{x}_i) := \bar{y}_i$$

is continuous, and is hence bounded, since the domain of  $\mathcal{S}$  is compact.

A.2.3. *Estimating  $\mathbf{d}G_\Lambda$  and  $\mathbf{d}\bar{y}_j^n$ .* Applying (4.2) for any  $e_j$  which is not the closest point to  $e$  in the support of  $\mu$ , we have that

$$\left| \mathbf{d}G_\Lambda(e - e_j, e + a - e_j) - \int_0^1 \frac{1}{\mathbf{K}\pi} \frac{e + ta - e_j}{|e + ta - e_j|^2} \cdot a \, dt \right| \lesssim \frac{\log|e - e_j|}{|e - e_j|^2} = O(n^{-2} \log(n)),$$

which holds uniformly for  $\mu \in \mathcal{M}_{\epsilon, n}(b_1, \dots, b_m)$  since  $\text{dist}(e, e_j) \geq \frac{1}{2} \text{dist}(e_i, e_j) \geq \frac{1}{2} \epsilon n$ . Furthermore, using the homogeneity and regularity of  $(x, y) \mapsto \frac{x-y}{|x-y|^2}$  to Taylor expand under the integral, we have

$$\mathbf{d}G_\Lambda(e - e_j, e + a - e_j) = n^{-1} \frac{1}{m\pi} \frac{\frac{1}{n}e - \bar{x}_j}{|\frac{1}{n}e - \bar{x}_j|^2} \cdot a + O(n^{-2} \log(n)). \quad (\text{A.4})$$

Using the representation of  $\bar{y}_j \in \mathcal{X}$  and Taylor expanding, we have

$$|\mathbf{d}\bar{y}_j^n(e, e + a) - n^{-1} \nabla \bar{y}_j(\frac{1}{n}e) \cdot a| \leq n^{-2} \sum_{l=1}^L |\text{dist}(\frac{1}{n}e, c_l)|^{\pi/\omega_l - 2} \|\bar{y}_j\|_{\mathcal{X}}. \quad (\text{A.5})$$

A.2.4. *Estimating  $\mathbf{d}u$ .* We now use Lemma 4.5 to estimate  $\mathbf{d}u$ . Defining  $g : \text{Ext}(n\mathcal{D}_0) \rightarrow \mathbb{R}$  to be

$$g(e) := \sum_{j=1}^m b_j G_\Lambda(e - x_j^n) + \bar{y}_j^n(e). \quad (\text{A.6})$$

By applying (4.1) and again invoking the definition and regularity of  $\bar{y}_j^n$  to Taylor expand near the boundary, we have that

$$\|g\|_{\ell^\infty(\text{Ext}(\mathcal{D}_0))} \lesssim n^{-1} \|\bar{y}\|_{\mathcal{X}} + O(n^{-1} \log(n)),$$

where the latter term is uniform in  $n$  for fixed  $\epsilon$ . Lemma 4.5 now implies that

$$|\mathbf{d}u(e)| \lesssim n^{-1} \log(n) |\text{dist}(e, \text{Ext}(n\mathcal{D}_0))|^{-1}. \quad (\text{A.7})$$

A.2.5. *Estimating  $\Delta \bar{y}_j^n$ .* For the purpose of estimating  $\mathbf{d}v$ , we now obtain bounds on  $\Delta \bar{y}_j^n$ . For any  $e \in n\mathcal{D}_0 \setminus \text{Ext}(n\mathcal{D}_0)$ , we use the regularity of  $\bar{y}_j$  to Taylor expand, obtaining

$$\begin{aligned} \Delta \bar{y}_j^n(e) &= \sum_{j=1}^N \int_0^1 \nabla \bar{y}_j(\frac{1}{n}(e + ta_i)) \cdot \frac{1}{n} \mathbf{a}_i \, dt, \\ &= \sum_{j=1}^N \int_0^1 \frac{1}{2} n^{-3} \nabla^3 \bar{y}_j(\frac{1}{n}e) [\mathbf{a}_i, \mathbf{a}_i, \mathbf{a}_i] + \frac{1}{6} n^{-4} (1-t)^3 \nabla^4 \bar{y}_j(\frac{1}{n}(e + ta_i)) [\mathbf{a}_i, \mathbf{a}_i, \mathbf{a}_i, \mathbf{a}_i] \, dt, \end{aligned} \quad (\text{A.8})$$

where  $\mathbf{a}_i$  are nearest neighbour directions in the dual lattice, and the terms involving  $\nabla \bar{y}_j$  and  $\nabla^2 \bar{y}_j$  cancel respectively by lattice symmetry and the fact that  $\bar{y}_j$  is harmonic. If the dual lattice is Sq or Tr, then the terms involving  $\nabla^3 \bar{y}_j$  also cancel, which entails that

$$|\Delta \bar{y}_j^n(e)| \leq \frac{1}{6} n^{-4} \sum_{i=1}^N \int_0^1 (1-t)^3 |\nabla^4 \bar{y}_j(\frac{1}{n}(e + ta_i))| \, dt.$$

By using the description of  $\bar{y}_j$  as a sum of  $v \in C^{4, \sigma}(\bar{\mathcal{D}})$  and  $\mathfrak{S}_{j, m}$ , it can be seen that each of the integrands in the estimate above is bounded any  $e \in n\mathcal{D}$  and  $\mathbf{a}_i$ , and moreover

$$|\Delta \bar{y}_j^n(e)| \leq \frac{1}{6} N n^{-4} \|\bar{y}\|_{\mathcal{X}} \sum_l |\text{dist}(\frac{1}{n}e, c_l)|^{\pi/\omega_l - 4}. \quad (\text{A.9})$$

Returning to the case where the dual lattice is  $\text{Hx}$ , we first Taylor expand to third-order to obtain that

$$|\Delta \bar{y}_j^n(e)| \leq \frac{1}{2} n^{-3} \sum_l \text{dist}(\frac{1}{n}e, c_l)^{\pi/\omega_l-3} \|\bar{y}\|_{\mathcal{X}}. \quad (\text{A.10})$$

Taylor expanding to fourth-order, we may apply an identical analysis to that made when  $\Lambda = \text{Tr}$  or  $\Lambda = \text{Sq}$  to estimate those terms involving  $\nabla^4 \bar{y}_i$  in (A.8). Define

$$A := \{e \in \text{Int}(n\mathcal{D}_0) \mid e, e + \mathbf{e}_2 \in \text{Int}(n\mathcal{D}_0)\}. \quad (\text{A.11})$$

For all  $e \in A$ , we have

$$\begin{aligned} & \left| \frac{1}{2} n^{-3} \sum_{i=1}^3 \left( \nabla^3 \bar{y}_j(\frac{1}{n}e) [\mathbf{a}_{2i}, \mathbf{a}_{2i}, \mathbf{a}_{2i}] - \nabla^3 \bar{y}_j(\frac{1}{n}(e + \mathbf{e}_2)) [\mathbf{a}_i, \mathbf{a}_i, \mathbf{a}_i] \right) \right| \\ &= \left| \frac{1}{2} n^{-4} \sum_{i=1}^3 \int_0^1 \nabla^4 \bar{y}_j(\frac{1}{n}(e + t\mathbf{e}_2)) [\mathbf{e}_2, \mathbf{a}_i, \mathbf{a}_i, \mathbf{a}_i] \right|, \\ & \leq \frac{3}{2} n^{-4} \sum_l \text{dist}(\frac{1}{n}e, c_l)^{\pi/\omega_l-4} \|\bar{y}\|_{\mathcal{X}}. \end{aligned}$$

Using this estimate, and the argument used above in the case where the dual lattice was  $\text{Tr}$ , for any  $e \in A$ , we deduce that

$$|\Delta \bar{y}_j^n(e) + \Delta \bar{y}_j^n(e + \mathbf{e}_2)| \leq 2n^{-4} \sum_l \text{dist}(\frac{1}{n}e, c_l)^{\pi/\omega_l-4} \|\bar{y}\|_{\mathcal{X}}. \quad (\text{A.12})$$

**A.2.6. Estimating  $\mathbf{d}v$ .** It remains to bound  $\mathbf{d}v$ . We proceed by constructing upper and lower bounds on  $v$  by using estimates (A.9), (A.10) and (A.12) and the full lattice Green's function. Recalling the result of Lemma 4.3, for any  $e \in \mathcal{D}$ , we note that

$$\begin{aligned} \Delta [G_\Lambda(\cdot - e) + \frac{1}{K\pi} \log |n \text{diam}(\mathcal{D})|] &= \mathbb{1}_e \quad \text{in } \text{Int}(n\mathcal{D}_0), \text{ and} \\ G_\Lambda(\cdot - e) + \frac{1}{K\pi} \log |n \text{diam}(\mathcal{D})| &\geq 0 \quad \text{on } \text{Ext}(n\mathcal{D}_0). \end{aligned}$$

Next, we define neighbourhoods of each corner of the domain

$$B_{l,\epsilon} := \{e \in \text{Int}(n\mathcal{D}_0) \mid \text{dist}(\frac{1}{n}e, c_l) \leq \epsilon\}.$$

Recalling that  $\delta := \min\{\frac{\pi}{\omega_l} - 1\} \in (0, \frac{1}{2}]$ , estimate (A.9) implies that

$$|\Delta \bar{y}_j^n(e)| \lesssim n^{-4} \epsilon^{\delta-3} \|\bar{y}_j\|_{\mathcal{X}} \quad \text{on } \text{Int}(n\mathcal{D}_0) \setminus \bigcup_l B_{l,\epsilon}. \quad (\text{A.13})$$

We now define

$$v^\pm(e) := - \left[ \sum_{e' \in n\mathcal{D}_0} \Delta \bar{y}_j^n(e') G_\Lambda(e - e') \right] \pm c_n,$$

where  $c_n$  is a small constant depending upon  $n$  that we will choose later. We note that  $\Delta[v - v^\pm] = 0$ , so choosing  $c_n$  such that  $v^+ \geq 0$  and  $v^- \leq 0$  on  $\text{Ext}(n\mathcal{D}_0)$ , Lemma 4.2 would imply that

$$v^-(e) \leq v(e) \leq v^+(e) \quad \text{for all } e \in \text{Int}(n\mathcal{D}_0).$$

When the dual lattice is either  $\text{Tr}$  or  $\text{Sq}$ , applying estimate (A.13), and summing,

$$|v^\pm(e)| \lesssim \|\bar{y}\|_{\mathcal{X}} \left[ \sum_{\substack{e' \in \text{Int}(n\mathcal{D}_0) \\ e' \notin \bigcup_l B_{l,\epsilon}}} n^{-4} \epsilon^{\delta-3} |G_\Lambda(e - e')| + n^{-1-\delta} \sum_{e \in \bigcup_l B_{l,\epsilon}} \text{dist}(e', nc_l)^{\delta-3} |G_\Lambda(e - e')| \right] + c_n n^2.$$

Treating each sum separately, we see that

$$\begin{aligned} \sum_{\substack{e' \in \text{Int}(n\mathcal{D}_0) \\ e' \notin \bigcup_l B_{l,\epsilon}}} |G_\Lambda(e - e')| &\lesssim \left[ \sum_{\substack{e' \in \text{Int}(n\mathcal{D}_0) \\ e' \notin \bigcup_l B_{l,\epsilon}}} \log |\text{dist}(e, e') + 1| \right] \lesssim n^2 \log(n), \\ \sum_{e' \in \bigcup_l B_{l,\epsilon}} |\text{dist}(e', nc_l)|^{\delta-3} |G_\Lambda(e - e')| &\lesssim \log(n) \sum_{e \in \bigcup_l B_{l,r}} |\text{dist}(e', nc_l)|^{\delta-3} \lesssim \log(n), \end{aligned}$$

recalling that statement (3) of Theorem 4.3 implies that  $|G_\Lambda(e)| \lesssim \log |\text{dist}(e, 0)|$ ,  $\text{diam}(n\mathcal{D}) = O(n)$ , and the sum on the second line converges since  $\delta \leq \frac{1}{2} < 1$ .

These estimates imply that

$$|v^\pm(e)| \lesssim \|\bar{y}\|_{\mathcal{X}} n^{-1-\delta} \log(n) + c_n n^2,$$

so choosing  $c_n = O(n^{-3-\delta} \log(n))$  gives

$$|v(e)| = O(n^{-1-\delta} \log(n)), \quad \text{and hence} \quad |\mathbf{d}v(e)| = O(n^{-1-\delta} \log(n)) \quad (\text{A.14})$$

for all  $e \in C_1(n\mathcal{D})$ .

When the dual lattice is  $\text{Hx}$ , recall the definition of  $A$  from (A.11), and set

$$A' := \{e \in \text{Int}(n\mathcal{D}_0) \mid e - \mathbf{e}_2 \notin \text{Int}(n\mathcal{D}_0)\}.$$

For any  $e' \in A$ , we apply (A.10), (A.12), and the conclusions of Theorem 4.3 to deduce that

$$\begin{aligned} &|G_{\text{Hx}}(e - e') \Delta \bar{y}_j^n(e) + G_{\text{Hx}}(e + \mathbf{e}_2 - e') \Delta \bar{y}_j^n(e + \mathbf{e}_2)| \\ &\leq |G_{\text{Hx}}(e - e')| n^{-4} |\text{dist}(\frac{1}{n}e, c_l)|^{\pi/\omega_l-4} + |\mathbf{d}G_{\text{Hx}}(e - e', e + \mathbf{e}_2 - e')| n^{-3} |\text{dist}(\frac{1}{n}e, c_l)|^{\pi/\omega_l-3} \\ &\leq \log |\text{dist}(e, e')| n^{-4} |\text{dist}(\frac{1}{n}e, c_l)|^{\pi/\omega_l-4} + \frac{\log |\text{dist}(e, e')|}{\text{dist}(e, e')} n^{-3} |\text{dist}(\frac{1}{n}e, c_l)|^{\pi/\omega_l-3}. \end{aligned}$$

By summing over  $e' \in A$ , we obtain

$$\sum_{e' \in A} |G_{\text{Hx}}(e - e') \Delta \bar{y}_j^n(e') + G_{\text{Hx}}(e + \mathbf{e}_2 - e') \Delta \bar{y}_j^n(e' + \mathbf{e}_2)| \lesssim \|\bar{y}_j\|_{\mathcal{X}} [\log(n) n^{-2} \epsilon^{\delta-3} + n^{-1-\delta} \log(n)]. \quad (\text{A.15})$$

Next, we sum (A.10) over  $A'$ , noting that  $\#A' = O(n)$ , to obtain

$$\begin{aligned} \sum_{e' \in A'} |G_\Lambda(e - e')| |\Delta \bar{y}_j^n(e')| &\lesssim \|\bar{y}_j\|_{\mathcal{X}} \log(n) \left[ \sum_{\substack{e' \in A' \\ e' \notin \bigcup_l B_{l,\epsilon}}} n^{-3} \epsilon^{\delta-2} + n^{-1-\delta} \sum_{\substack{e' \in A' \\ e' \in \bigcup_l B_{l,\epsilon}}} \text{dist}(e', nc_l)^{\delta-2} \right], \\ &\lesssim \|\bar{y}_j\|_{\mathcal{X}} [\epsilon^{\delta-2} \log(n) n^{-2} + n^{-1-\delta} \log(n)]. \end{aligned} \quad (\text{A.16})$$

Putting (A.15) and (A.16) together, and applying similar arguments to that made for the other cases above, we deduce that (A.14) also holds in the case where the dual lattice is  $\text{Hx}$ .

**A.2.7. Conclusion.** Combining (A.4), (A.5), (A.7) and (A.14) and noting that

$$\nabla \bar{y}_j(x) + \frac{1}{m\pi} \frac{x - \bar{x}_j}{|x - \bar{x}_j|^2} = \nabla \mathcal{G}_{\bar{x}_j}(x),$$

we now obtain the desired result.

#### ACKNOWLEDGEMENTS

**Thanks:** The author would like to thank Giovanni Bonaschi and Giacomo Di Gesú for informative discussions on Large Deviations Principles while carrying out this work.

**Funding:** This study was funded by a public grant overseen by the French National Research Agency (ANR) as part of the ‘‘Investissements d’Avenir’’ program (reference: ANR-10-LABX-0098).

**Conflict of interest:** The author declares that there is no conflict of interest regarding this work.

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