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GAMMA-EXPANSION FOR A 1D CONFINED LENNARD-JONES MODEL WITH POINT DEFECT

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Abstract. We compute a rigorous asymptotic expansion of the energy of a point defect in a 1D chain of atoms with second neighbour interactions. We propose the Confined Lennard-Jones model for interatomic interactions, where it is assumed that nearest neighbour potentials are globally convex and second neighbour potentials are globally concave. We derive the Γ-limit for the energy functional as the number of atoms per period tends to infinity and derive an explicit form for the first order term in a Γ-expansion in terms of an infinite cell problem. We prove exponential decay properties for minimisers of the energy in the infinite cell problem, suggesting that the perturbation to the deformation introduced by the defect is confined to a thin boundary layer.

1. Introduction.

The analysis of discrete lattice systems and their relationship to continuum mechanics is currently a growing area of study within applied analysis. Many rigorous results have been obtained over the past ten years connecting discrete models with continuum limits, and the area was extensively surveyed in [3]. The most well-developed approaches have been either to apply Γ-convergence[1] to discrete energy functionals parametrised by the number of atoms per unit volume in the model (see [1, 7, 15]), or to apply forms of the inverse function theorem to show that for a discrete energy with the same parameter fixed, the Cauchy–Born rule holds; i.e. for a given atomistic deformation and a certain range of atomic densities there exist continuum deformations which are close in some norm, and have a similar energy (see [11, 13]).

Here, we take the former approach. We build upon recent works on surface energies in discrete systems [5, 14], which employ 'Γ-development' as first defined in [2], and extensively discussed in [8]. We define energy functionals with and without defects, and present the Confined Lennard-Jones model for interatomic interactions, which we motivate with a formal analysis. We then investigate the scaling of the perturbation to the energy which is introduced by the defect. We also provide a concrete cell problem that may be used for explicit computation of the first-order

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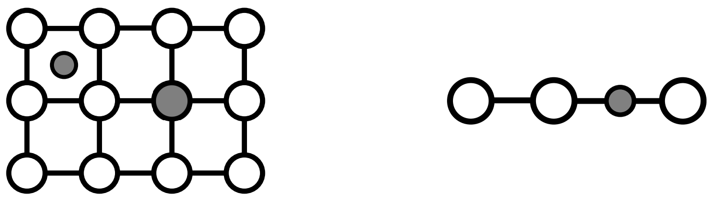
[1]For an introduction to Γ-convergence, see [4, 10].

energy, and show that a minimiser of this cell problem decays exponentially away from the defect. This allows us to conclude that minimisers of the energies with and without a defect are essentially the same except on a thin boundary layer around the defect.



(A) 2D Defects (B) 1D Defect

FIGURE 1. Impurities and Interstitials.

1.1. **Motivation.** The tools developed to study the relationship between atomistic and continuum models rely upon the high level of symmetry which is maintained after deforming a crystal. However, the pure lattice behaviour is not the only factor in determining the bulk properties of such materials. The last century saw a revolution in the materials science, as it was realised that lattice defects can change the strength of an otherwise perfect crystal by orders of magnitude. Understanding defects, how they scale and in what rigorous ways one might modify the continuum approximation of crystalline solids to take them into account is therefore key to developing our understanding of how best to model and predict their behaviour.

As a first step towards this goal, we consider arguably the simplest crystalline defect, a dilute point defect. A point defect is an interruption of the pure lattice structure caused by substituting an atom at some lattice site with an atom of a different type, (called an impurity) or by inserting an atom into the structure at a point which is not a lattice site (called an interstitial). In 1D, impurities and interstitials are essentially identical when atoms are treated as point particles with hard-core interactions, since atoms cannot move past one another, and so it is easy to modify the reference configuration to take such a defect into account. In higher dimensions, the two defects are qualitatively different (see Figure 1), with an interstitial requiring an additional point in the reference configuration which breaks the symmetry.

The model we analyse is one-dimensional, and to avoid surface effects, we use a periodic reference domain, so that in effect the atoms lie on a one-dimensional torus. The defect considered is dilute since only one atom in the chain is of a different type.

By computing the Γ-limit of the sequence of energy functionals for the model described here, we arrive at an energy which encodes some of the properties of the minimisers of the functionals along the sequence, but no quantitative information about the error made. Computing higher-order limits gives further, more quantitative control on the energy minima, and in this case will also allow us to say something more qualitative about the minimisers.

1.2. **Outline.** As discussed above, we apply Γ-convergence to a sequence of atomistic energy functionals that depend on the parameter ε, which is the inverse of the number of atoms per unit volume.

In the remainder of §1, we propose a model for interatomic interactions in a 1D chain including a point defect. We then make a formal analysis of the model to motivate this study and the Confined Lennard-Jones model which we propose, before reformulating the problem in a format amenable to analysis in the framework of the one-dimensional Calculus of Variations.

In §2, we derive the Γ-limit for the series of functionals defined in §1 as ε tends to zero, and note that the introduction of the defect does not perturb the Γ-limit at this order.

In §3, we collect and prove some results about the minimum problem for the 0^{th}-order Γ-limit of the atomistic energies, including existence, uniqueness and regularity for minimisers.

In §4, we proceed to derive a first-order Γ-limit, expressing it in terms of a minimisation problem in an infinite cell, and prove some properties of this minimum problem along the way.

1.3. **Physical model.** For now, fix $N \in \mathbb{N}$. We consider $2N$ atoms indexed by

$$i \in \{-N, \ldots, N-1\}$$

which have a spatial density of $2N/L$, where L is the total length of the deformed configuration. To make the domain periodic, we identify an atom indexed by $i = N$ with the atom $i = -N$ so that we avoid boundary effects, and defining $\varepsilon = 1/2N$, we choose to take reference positions for these atoms to be

$$x_i := i\varepsilon \in \Omega_\varepsilon := \big\{-\tfrac{1}{2}, -\tfrac{1}{2}+\varepsilon, \ldots, \tfrac{1}{2}\big\}.$$

We also define

$$\Omega := [-\tfrac{1}{2}, \tfrac{1}{2}],$$

so that $\Omega_\varepsilon = \Omega \cap \varepsilon\mathbb{Z}$. It should be noted at the outset that the choice to use $2N$ atoms will not be restrictive to our analysis but will make some of the concepts easier to elucidate, and that we will frequently write $\varepsilon \to 0$ to mean $N \to \infty$.

Fixing the coordinate system so that atom $-N$ lies at 0, any configuration can be described by a map

$$y : \Omega_\varepsilon \to [0, L] \qquad \text{such that} \qquad y(-\tfrac{1}{2}) = 0, y(\tfrac{1}{2}) = L.$$

We will use the shorthand

$$y_i := y(x_i),$$

and extend y to a map on the whole of $\varepsilon\mathbb{Z}$ by defining

$$y_{2kN+i+1} - y_{2kN+i} := y_{i+1} - y_i$$

for any $k \in \mathbb{Z}$.

The atoms in our model are assumed to interact through pair potentials which decay rapidly so that it suffices to consider an interaction between atoms and their 2 immediate neighbours on either side. As explained in §1.1, all atoms except one are of the same type, regarded as the 'pure' species. As in [6], the potential energy of a bond between atoms is assumed to be expressed as a function of the relative displacement

$$D_j y_i := \frac{y_{i+j} - y_i}{x_{i+j} - x_i} = \frac{y_{i+j} - y_i}{j\varepsilon}.$$

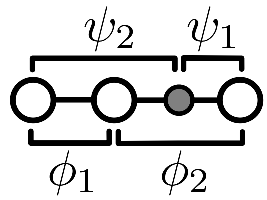


FIGURE 2. Pair Potentials

In the case where all atoms are of the pure species, a bond with relative length t has energy $\phi_1(t)$ for nearest neighbours, and $\phi_2(t)$ for second neighbours. The internal energy of the configuration arising from the interatomic forces is

$$E^\varepsilon_{\mathrm{p}}(y) := \sum_{i=-N}^{N-1} \phi_1(D_1 y_i) + \phi_2(D_2 y_i).$$

Since in each configuration we assume there is a single defect, we assume without loss of generality that the defect is at index $i = 0$. The energy of bonds of relative length t between this atom and its neighbours are $\psi_1(t)$ for the nearest neighbours and $\psi_2(t)$ for second neighbours (see Figure 2).

The introduction of the defect causes a modification of the energy which is given by the addition of the following energy term:

$$\begin{aligned} E_{\mathrm{d}}(y) := \psi_2(D_2 y_{-2}) - \phi_2(D_2 y_{-2}) + \psi_1(D_1 y_{-1}) - \phi_1(D_1 y_{-1}) \\ +\psi_1(D_1 y_0) - \phi_1(D_1 y_0) + \psi_2(D_2 y_0) - \phi_2(D_2 y_0). \end{aligned}$$

Finally, we also consider dead loads f_i acting on each atom. Taking as initial positions the points $L(x_i + \frac{1}{2})$, the work done by these forces is

$$E^\varepsilon_{\mathrm{f}}(y) := \sum_{i=-N}^{N-1} f_i\big(y_i - L(x_i + \tfrac{1}{2})\big).$$

This term can be though of as the work done by a linearisation of some external force field near the homogeneous linear state $y_i = L(x_i + \frac{1}{2})$. To keep notation concise, we will frequently write u_i to mean

$$u_i := y_i - L(x_i + \tfrac{1}{2}),$$

and we extend f by periodicity to a map over $\varepsilon\mathbb{Z}$ by defining

$$f_{2kN+i} = f_i$$

for any $k \in \mathbb{Z}$.

The total energy for the atomistic system considered is therefore

$$E^\varepsilon(y) := E^\varepsilon_{\mathrm{p}}(y) + E_{\mathrm{d}}(y) + E^\varepsilon_{\mathrm{f}}(y).$$

1.4. **Formal analysis.** We expect that atoms should minimise the energy E^ε, and we therefore seek to characterise the minimal energy and the states which attain this minimum. We will consider the situation when N is large, and when the material is behaving elastically. In this case, interatomic displacements should vary slowly over the domain, and so we assume the Cauchy–Born hypothesis holds (for more information, see [17]). This states that interatomic displacements follow linear deformations of small volumes of the solid, and so we assume that

$$D_1 y_i, D_2 y_i \simeq Dy(x_i),$$

where $y : \Omega \to [0, L]$ is some suitably smooth function describing the displacement. This means that the energy

$$\phi_1(D_1 y_i) + \phi_2(D_2 y_i) \simeq \phi_1\big(Dy(x_i)\big) + \phi_2\big(Dy(x_i)\big).$$

Motivated by this, we define W, the continuum elastic energy density to be

$$W(t) := \phi_1(t) + \phi_2(t). \tag{1}$$

The total energy is now approximately

$$E^\varepsilon(y) \simeq \sum_{i=-N}^{N-1} W(Dy(x_i)) + E_{\mathrm{d}}(y) + E^\varepsilon_{\mathrm{f}}(y).$$

We expect this energy to grow linearly as the number of atoms increases, so it makes sense to look at the mean energy per atom, $\varepsilon E^\varepsilon$, as N gets large. The size of the defect is fixed and small, so $\varepsilon E_{\mathrm{d}}(y)$ should vanish as $\varepsilon \to 0$, and

$$\begin{aligned} \varepsilon E^\varepsilon(y) &\simeq \varepsilon \sum_{i=-N}^{N-1} W\big(Dy(x_i)\big) + f_i u_i \\ &\simeq \mathcal{F}_0(y) := \int_\Omega W(Dy) + f u \,\mathrm{d}x, \end{aligned}$$

where $u(x) = y(x) - L(x + \frac{1}{2})$. The minimiser of the right hand side should satisfy the Euler–Lagrange equation for this functional,

$$\tfrac{\mathrm{d}}{\mathrm{d}x}\big(W'(Dy)\big) = f(x).$$

This equation can be integrated to give

$$W'(Dy) = \sigma(x) + \Sigma, \qquad \text{where} \qquad \sigma(x) = \int_{-1/2}^{x} f(t)\,\mathrm{d}t.$$

The defect should then contribute a further term proportional to its size, $O(\varepsilon)$, to the energy. Since the mean energy is only perturbed by a small amount, we should expect that any perturbation to the minimiser would also occur close to the defect, due to the mismatch between ϕ_i and ψ_i there. The defect always remains at $i = 0$, so when N is large, we make the ansatz that close to the defect $D_1 y_i \simeq F_0 + r_i$, where $F_0 := Dy(0)$ and r_i is a small perturbation. Defining[2]

$$\sigma^\varepsilon_{-N} := -\tfrac{1}{2}\varepsilon f_{-N} \qquad \text{and} \qquad \sigma^\varepsilon_i := \sigma^\varepsilon_{i-1} + \varepsilon f_{i-1},$$

then integrating by parts, we can rewrite the external force terms as

$$\sum_{i=-N}^{N-1} f_i u_i = -\sum_{i=-N}^{N-1} \sigma^\varepsilon_i \, D_1 u_i \quad \text{and} \quad \int_\Omega f u \,\mathrm{d}x = -\int_\Omega \sigma \, Du \,\mathrm{d}x.$$

This then means the additional contribution is

$$\begin{aligned} \frac{\varepsilon E^\varepsilon(y) - \mathcal{F}_0(y)}{\varepsilon} \simeq \tilde{E}_\infty(r) := \tilde{E}_{\mathrm{d}}(r) + \sum_{i=-\infty}^{\infty} \Big(& \phi_1\big(F_0 + r_i\big) + \phi_2\big(F_0 + \tfrac{r_i + r_{i+1}}{2}\big) - W(F_0) \\ & + \sigma(0)\big(F_0 + r_i - L\big) - \sigma(0)\big(F_0 - L\big)\Big), \end{aligned}$$

[2]The definition of σ^ε_{-N} given here is used for technical reasons during the course of §4.1; this formal analysis does not appear to require this choice.

where we have defined

$$\begin{aligned}\tilde{E}_{\mathrm{d}}(r) := \psi_2(F_0 + \tfrac{r_{-2}+r_{-1}}{2}) - \phi_2(F_0 + \tfrac{r_{-2}+r_{-1}}{2}) + \psi_1(F_0 + r_{-1}) - \phi_1(F_0 + r_{-1})\\ + \psi_1(F_0 + r_0) - \phi_1(F_0 + r_0) + \psi_2(F_0 + \tfrac{r_0+r_1}{2}) - \phi_2(F_0 + \tfrac{r_0+r_1}{2}).\end{aligned}$$

The integrated Euler–Lagrange equation for $\mathcal{F}_0$ gives

$$\tilde{E}_\infty(r) \simeq \tilde{E}_{\mathrm{d}}(r) + \sum_{i=-\infty}^{\infty} \phi_1\big(F_0 + r_i\big) + \phi_2\big(F_0 + \tfrac{r_i+r_{i+1}}{2}\big) - W(F_0) - \big(W'(F_0) - \Sigma\big) r_i.$$

The sum of the $\Sigma\, r_i$ terms should vanish due to the boundary conditions. Since we expect decaying solutions, we assign the 'core' of the defect an energy $\tilde{E}_{\mathrm{c}}(r)$, and expand in r_i outside some radius R, giving

$$\tilde{E}_\infty(r) \simeq \tilde{E}_{\mathrm{c}}(r) + \tfrac{1}{2} \sum_{|i|\geq R} \phi_1''(F_0) r_i^2 + \phi_2''(F_0)\big(\tfrac{r_i+r_{i+1}}{2}\big)^2.$$

For a minimiser of this energy, the r_i should approximately satisfy

$$\tfrac{1}{2}\phi_2''(F_0)(r_{i-1} + r_i) + \phi_1''(F_0) r_i + \tfrac{1}{2}\phi_2''(F_0)(r_i + r_{i+1}) = 0.$$

Making the usual ansatz $r_i = a\lambda^i$, a solution must satisfy

$$\tfrac{1}{2}\phi_2''(F_0) + W''(F_0)\lambda + \tfrac{1}{2}\phi_2''(F_0)\lambda^2 = 0.$$

If ϕ_1 and W are convex and ϕ_2 is concave at F_0, as is the case in Lennard-Jones type pair potentials, then a straightforward analysis of the roots of this equation implies that there are two positive real roots which multiply to give 1. These two roots correspond to an exponentially decaying solution and an exponentially growing solution.

Rigorous versions of these formal results will be the subject of this paper, and motivate the assumptions we make about the potentials and external force in the following section.

1.5. **Confined Lennard-Jones model.** Motivated by the formal analysis carried out in the previous section, this section details the assumptions that we make about the pair potentials and external force field.

We will assume that all potentials ϕ_i and ψ_i are C^2 on the interval $(0, \infty)$. Additionally, we assume the potentials and external forces satisfy the following conditions.

1. The nearest neighbour potentials are infinite for negative bond lengths and blow up as bond lengths approach zero, i.e.
$$\phi_1(t), \psi_1(t) = +\infty \text{ for } t \leq 0,$$
$$\lim_{t\searrow 0} \phi_1(t) = +\infty \quad \text{and} \quad \lim_{t\searrow 0} \psi_1(t) = +\infty.$$
2. The nearest neighbour potentials are l-convex, i.e. for any $t > 0$,
$$\phi_1''(t), \psi_1''(t) \geq l > 0.$$
3. The second neighbour potentials ϕ_2 and ψ_2 are concave.
4. The second neighbour potentials ϕ_2 and ψ_2 are 'dominated' by the nearest neighbour potentials ϕ_1 and ψ_1, i.e. there exist constants $\alpha \in (0, 1)$ and $C \in \mathbb{R}$ such that
$$\phi_2(t) \geq -\alpha\, \phi_1(t) + C, \qquad \phi_2(t) \geq -\alpha\, \psi_1(t) + C,$$
$$\psi_2(t) \geq -\alpha\, \phi_1(t) + C, \qquad \psi_2(t) \geq -\alpha\, \psi_1(t) + C.$$

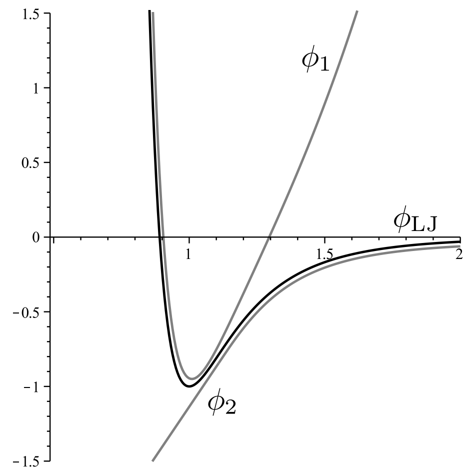


FIGURE 3. Possible choices of ϕ_1 and ϕ_2 with the assumptions prescribed which approximate a Lennard-Jones potential, ϕ_{LJ}.

5. The 'pure' potentials are such that the resulting continuum elastic potential is l-convex, i.e. defining W as in (1), for any $t > 0$,

$$W''(t) = \phi_1''(t) + \phi_2''(t) \geq l.$$

6. We assume $f_i = f(x_i)$ where $f \in \mathrm{C}^2(\Omega)$.

Remark 1. Assumption (1) prevents atoms from exchanging positions with respect to the reference configuration, and ensures that we prevent plastic deformation.

Assumptions (2) and (3) are made to simulate the behaviour of a Lennard-Jones type potential, which is convex for short bond lengths, and then concave after for any bond length past some critical length; see for example Figure 3. When under strains in the elastic regime, the nearest neighbours lie in the convex part of the potential, and all other atoms lie in the concave part.

Assumption (4) enforces the elastic behaviour of the material and prevents fracture from being favourable.

Assumption (5) prevents any form of microstructure from forming, but since the decay of Lennard-Jones potentials used in applications is always relatively rapid, this assumption is reasonable, and for the sake of clarity we avoid significant complications to our analysis.

These assumptions imply the following facts which we will use frequently throughout this paper. The fact that ϕ_2 is concave implies that

$$\tfrac{1}{2}\phi_1(a) + \tfrac{1}{2}\phi_1(b) + \phi_2\big(\tfrac{a+b}{2}\big) \geq \tfrac{1}{2}W(a) + \tfrac{1}{2}W(b). \tag{2}$$

By using the concavity of the second neighbour potentials again, we have

$$\begin{aligned}\tfrac{1}{2}\phi_1(a) &+ \psi_2\big(\tfrac{a+b}{2}\big) + \psi_1(b) + \phi_2\big(\tfrac{b+c}{2}\big) + \psi_1(c) + \psi_2\big(\tfrac{c+d}{2}\big) + \tfrac{1}{2}\phi_1(d)\\ &\geq \tfrac{1}{2}\big(\phi_1(a) + \psi_2(a)\big) + \big(\psi_1(b) + \tfrac{1}{2}\phi_2(b) + \tfrac{1}{2}\psi_2(b)\big)\\ &\qquad + \big(\psi_1(c) + \tfrac{1}{2}\psi_2(c) + \tfrac{1}{2}\phi_2(c)\big) + \tfrac{1}{2}\big(\phi_1(d) + \psi_2(d)\big).\end{aligned}$$

Assumption (4), that the behaviour of nearest neighbour potentials dominates, implies that

$$\begin{aligned}\tfrac{1}{2}\phi_1(a)+\psi_2(\tfrac{a+b}{2})+\psi_1(b)+\phi_2(\tfrac{b+c}{2})+\psi_1(c)+\psi_2(\tfrac{c+d}{2})+\tfrac{1}{2}\phi_1(d)\\ \geq(1-\alpha)\Big(\tfrac{1}{2}\phi_1(a)+\psi_1(b)+\psi_1(c)+\tfrac{1}{2}\phi_1(d)\Big)+3C,\\ \geq\tfrac{1}{2}l\left(\tfrac{1}{2}a^2+b^2+c^2+\tfrac{1}{2}d^2\right)+3C,\quad(3)\end{aligned}$$

where on the last line we have adjusted the definition of l to keep estimates concise throughout this paper. This estimate will allow us to prove coercivity results which ensure that sequences of deformations with uniformly bounded energies are compact.

1.6. **Function spaces and topologies.** In this section we define the topologies with respect to which we will carry out our analysis.

Throughout this paper, we use the usual notation for Lebesgue and Sobolev spaces, and use $\|\cdot\|_p$ and $\|\cdot\|_{1,p}$ to denote the usual norms on $\mathrm{L}^p(\Omega)$ and $\mathrm{W}^{1,p}(\Omega)$. We write $y^\varepsilon\to y$ in L^p or $y^\varepsilon\to y$ in $\mathrm{W}^{1,p}$ (or H^1) to mean

$$\|y^\varepsilon-y\|_p\to 0\quad\text{or}\quad\|y^\varepsilon-y\|_{1,p}\to 0$$

respectively. We will also refer to convergence in the weak topology on $\mathrm{H}^1(\Omega)$; we say $y_\varepsilon\rightharpoonup y$ or y_ε converges weakly to y in H^1 if for any $f\in\mathrm{H}^{-1}(\Omega)$,

$$\langle f,y^\varepsilon\rangle\to\langle f,y\rangle,$$

where $\langle\cdot,\cdot\rangle$ is the usual inner product on $\mathrm{H}^1(\Omega)$.

Since we wish to find the Γ-limit of the sequence of energy functionals $\varepsilon E^\varepsilon$ defined above, we need to ensure they are defined over the same space. Following Braides, Dal Maso and Garroni in [6], we associate any discrete deformation y^ε with a piecewise linear interpolant defined everywhere on Ω,

$$y^\varepsilon(x):=y_i^\varepsilon+D_1y_i^\varepsilon(x-x_i)\quad\text{for any}\quad x\in(x_i,x_{i+1}).$$

For each choice of ε, these linear interpolants lie in the spaces

$$\mathrm{P}^1_\varepsilon(\Omega):=\big\{y\in\mathrm{W}^{1,\infty}(\Omega):y\text{ is linear on }(x_i,x_{i+1}),\,x_i,x_{i+1}\in\Omega_\varepsilon\big\}.$$

The admissible deformations $\mathcal{A}^\varepsilon(L)$ are defined to be the set of such interpolants with the correct boundary conditions:

$$\mathcal{A}^\varepsilon(L):=\big\{y\in\mathrm{P}^1_\varepsilon(\Omega):y(-\tfrac{1}{2})=0,y(\tfrac{1}{2})=L\big\}.$$

For any ε,

$$\mathcal{A}^\varepsilon(L)\subseteq\mathcal{A}(L):=\big\{y\in\mathrm{H}^1(\Omega):y(-\tfrac{1}{2})=0,y(\tfrac{1}{2})=L\big\};$$

in fact, in the weak topology on $\mathrm{H}^1(\Omega)$, it is well-known that the sequential closure

$$\overline{\bigcup_{N=1}^{\infty}\mathcal{A}^\varepsilon(L)}=\mathcal{A}(L).$$

In §2.1, we will show that this topology arises from the assumptions made in §1.5.

Since the $\mathrm{H}^1(\Omega)$ embeds into $\mathrm{C}^0(\Omega)$, we define the projection operator $\mathcal{T}^\varepsilon:\mathcal{A}(L)\to\mathcal{A}^\varepsilon(L)$ as being

$$\big(\mathcal{T}^\varepsilon y\big)(x):=y_i+D_1y_i(x-x_i)\quad\text{for any}\quad x\in(x_i,x_{i+1}),$$

where $y_i=y(x_i)$ as before.

We are now in a position to suitably extend the functionals $\varepsilon E^\varepsilon$ so that we can take a Γ-limit. Guided by other work for similar models (amongst others, see those used in [5, 6, 7]) we define $\mathcal{F}^\varepsilon : \mathcal{A}(L) \to \mathbb{R}$ to be

$$\mathcal{F}^\varepsilon(y) := \begin{cases} \varepsilon E^\varepsilon(y) & y \in \mathcal{A}^\varepsilon(L) \\ +\infty & \text{otherwise.} \end{cases}$$

2. **The 0th-order Γ-limit.** Our first result gives the first term in the Γ-expansion of $\mathcal{F}^\varepsilon$.

Theorem 2.1 (0^{th}-order Γ-limit)**.** *With respect to convergence in* L^2,

$$\Gamma\text{-}\lim_{\varepsilon\to 0} \mathcal{F}^\varepsilon(y) = \mathcal{F}_0(y) := \int_\Omega W(Dy) + f\big(y - L(x + \tfrac{1}{2})\big)\,\mathrm{d}x.$$

The Γ-convergence of the internal energy in this result is already covered by Theorem 3.2 in [5], but we present a complete proof here in order to demonstrate the special structure of the Confined Lennard-Jones model described in §1.5. By exploiting the convexity and concavity of the potentials, we do not have to resort to a homogenisation formula to prove the liminf inequality.

As with any Γ-convergence result, we need to prove the relevant liminf and limsup inequalities. We present the proofs of these inequalities in turn.

2.1. **The liminf inequality.** The liminf inequality is the following statement:

Proposition 1. *If* $y^\varepsilon \to y$ *in* L^2 *then*

$$\liminf_{\varepsilon\to 0} \mathcal{F}^\varepsilon(y^\varepsilon) \geq \mathcal{F}_0(y).$$

To prove this, we use the fact that if

$$\sup_{\varepsilon>0} \mathcal{F}^\varepsilon(y^\varepsilon) < +\infty \qquad \text{and} \qquad y^\varepsilon \to y \text{ in } \mathrm{L}^2,$$

then $y^\varepsilon \rightharpoonup y$. This equicoercivity result is encoded in Lemma 2.2. We then prove that $\mathcal{F}^\varepsilon(y^\varepsilon)$ is approximately bounded below by $\mathcal{F}_0(y^\varepsilon)$ for any given deformation $y^\varepsilon \in \mathcal{A}^\varepsilon(L)$, and finally we can use the fact that $\mathcal{F}_0$ is lower semicontinuous with respect to weak convergence in H^1 to obtain the inequality required.

Lemma 2.2 (Weak H^1 coercivity)**.** *If* $y^\varepsilon \to y$ *in* L^2 *and* $\mathcal{F}^\varepsilon(y^\varepsilon)$ *is uniformly bounded for all* $\varepsilon > 0$*, then* $y^\varepsilon \rightharpoonup y$ *in* H^1.

The proof of this result relies upon the growth assumptions and estimates made in §1.5, and is inspired by the argument used in the proof of Theorem 4.5 in [4].

Proof. First, we estimate the energy below away from the defect. For ease of reading, let

$$P_\varepsilon := \{-N, \ldots, N-1\} \setminus \{-2, -1, 0\},$$

i.e. the set of indices which have only pure interactions with their two neighbours on the right. We now use the inequalities from the end of §1.5. The estimate made in (2), and the l-convexity of W imply that for any $y \in \mathcal{A}^\varepsilon(L)$

$$\begin{aligned}\varepsilon \sum_{i\in P_\varepsilon} \tfrac{1}{2}\phi_1(D_1 y_i) + \phi_2(D_2 y_i) + \tfrac{1}{2}\phi_1(D_1 y_{i+1}) &\geq \varepsilon \sum_{i\in P_\varepsilon} \tfrac{1}{2} W(D_1 y_i) + \tfrac{1}{2} W(D_1 y_{i+1}), \\ &\geq \varepsilon \sum_{i\in P_\varepsilon} \tfrac{1}{4} l \left(\left|D_1 y_i\right|^2 + \left|D_1 y_{i+1}\right|^2 \right) + C.\end{aligned} \tag{4}$$

The estimate made in (3) then allows us to bound the energy coming from bonds near the defect below.

$$\tfrac{1}{2}\phi_1(D_1y_{-2})+\psi_2(D_2y_{-2})+\psi_1(D_1y_{-1})+\phi_2(D_2y_{-1})+\psi_1(D_1y_0)\\ +\psi_2(D_2y_0)+\tfrac{1}{2}\phi_1(D_1y_1)\geq\sum_{i=-2}^{0}\tfrac{1}{4}l\Big(|D_1y_i|^2+|D_1y_{i+1}|^2\Big)+C. \quad (5)$$

Combining these estimates, we have that

$$\begin{aligned}\varepsilon E_{\mathrm{p}}^{\varepsilon}(y^\varepsilon)+\varepsilon E_{\mathrm{d}}(y^\varepsilon)&\geq\varepsilon\sum_{i=-N}^{N-1}\Big(\tfrac{1}{2}l\left|D_1y_i^\varepsilon\right|^2+C\Big)\\ &=\tfrac{1}{2}l\left\|Dy^\varepsilon\right\|_2^2+C. \qquad (6)\end{aligned}$$

Finally, Lemma 5.3 in [6] implies that

$$\varepsilon E_{\mathrm{f}}^{\varepsilon}(y^\varepsilon)\to\int_\Omega f\big(y-L(x+\tfrac{1}{2})\big)\,\mathrm{d}x,$$

so it follows that $\varepsilon E_{\mathrm{f}}^{\varepsilon}(y^\varepsilon)$ is uniformly bounded. Combining this fact with estimate (6), the uniform bound on $\mathcal{F}^\varepsilon$ implies

$$\sup_{\varepsilon>0}\|Dy^\varepsilon\|_2<+\infty.$$

The argument is now concluded via the standard result that $y^\varepsilon\rightharpoonup y$ in H^1 if and only if $\|y^\varepsilon\|_{1,2}$ is uniformly bounded and $y^\varepsilon\to y$ in $\mathrm{L}^2(\Omega)$. □

Remark 2. Lemma 2.2 can be interpreted as saying that if the mean energy is bounded along some sequence of atomistic deformations, then the interatomic strains do not get too large, since they are compact in the weak topology on $\mathrm{H}^1(\Omega)$. This reinforces the notion that we are in an elastic regime.

Lemma 2.2 permits us to use the fact that as W is l-convex, the map

$$y\longmapsto\int_\Omega W(Dy)\,\mathrm{d}x \qquad (7)$$

is lower semicontinuous with respect to weak convergence in $\mathrm{H}^1(\Omega)$ (see for example Corollary 2.31 in [4]). Fix $\delta>0$. The estimates made in (4) and (5) imply that

$$\varepsilon E_{\mathrm{p}}^{\varepsilon}(y^\varepsilon)+\varepsilon E_{\mathrm{d}}(y^\varepsilon)\geq\int_{\Omega\setminus(-\delta,\delta)}W(Dy^\varepsilon)\,\mathrm{d}x+C\,\delta.$$

Using Lemma 2.2 and the weak lower semicontinuity of (7), we have that

$$\begin{aligned}\liminf_{\varepsilon\to0}\big(\varepsilon E_{\mathrm{p}}^{\varepsilon}(y^\varepsilon)+\varepsilon E_{\mathrm{d}}(y^\varepsilon)\big)&\geq\liminf_{\varepsilon\to0}\int_{\Omega\setminus(-\delta,\delta)}W(Dy^\varepsilon)\,\mathrm{d}x+C\,\delta,\\ &\geq\int_{\Omega\setminus(-\delta,\delta)}W(Dy)\,\mathrm{d}x+C\,\delta.\end{aligned}$$

Since δ was arbitrary, we let $\delta\to0$, giving

$$\liminf_{\varepsilon\to0}\big(\varepsilon E_{\mathrm{p}}^{\varepsilon}(y^\varepsilon)+\varepsilon E_{\mathrm{d}}(y^\varepsilon)\big)\geq\int_\Omega W(Dy)\,\mathrm{d}x. \qquad (8)$$

Finally, convergence of the external force term is a consequence of Lemma 5.3 in [6]. This result implies that if $y^\varepsilon \to y$ in $\mathrm{L}^2(\Omega)$ and $\|Dy^\varepsilon\|_2$ is uniformly bounded, then we have that

$$\varepsilon E^\varepsilon_{\mathrm{f}}(y^\varepsilon) \to \int_\Omega f\big(y - L(x+\tfrac{1}{2})\big)\,\mathrm{d}x, \tag{9}$$

and combining (8) and (9) proves Proposition 1.

2.2. **The limsup inequality.** Now we have obtained the liminf inequality, we need to prove the limsup inequality to complete the proof of Theorem 2.1.

Proposition 2. *For any $y \in \mathcal{A}(L)$, there exists a sequence of $y^\varepsilon \in \mathcal{A}^\varepsilon(L)$ such that $y^\varepsilon \to y$ in L^2 and*

$$\limsup_{\varepsilon\to 0} \mathcal{F}^\varepsilon(y^\varepsilon) \le \mathcal{F}_0(y).$$

The construction of the sequence y^ε requires a diagonal argument which is similar in flavour to that employed in the proof of Theorem 4.5 in [4]. This argument proceeds in two steps. In the first step, the convexity of W is exploited to show that a naive approximation of $y \in \mathcal{A}(L)$ by $\mathcal{T}^\varepsilon y$ works for the 'pure' part of the energy. By linearising deformations near the defect, and therefore controlling the behaviour of the energy there, we can take a diagonal sequence to arrive at the correct inequality. Note that the inequality is trivial if $\mathcal{F}_0(y) = +\infty$, so we only need consider $y \in \mathcal{A}(L)$ such that $\mathcal{F}_0(y) < +\infty$.

Fix $y \in \mathcal{A}(L)$, and define the integrand

$$W_\varepsilon(x) := \sum_{i=-N}^{N-1} \Big(\tfrac{1}{2}\phi_2(D_2 y_{i-1}) + \phi_1(D_1 y_i) + \tfrac{1}{2}\phi_2(D_2 y_i)\Big)\cdot \chi_i(x),$$

where $\chi_i(x)$ is the indicator function for the interval (x_i, x_{i+1}). Note that by construction,

$$\int_\Omega W_\varepsilon(x)\,\mathrm{d}x = \varepsilon E^\varepsilon_{\mathrm{p}}(y).$$

We will apply Fatou's lemma to the functions W_ε.

Almost everywhere convergence of W_ε. For any $x \in \Omega$, define the sequence $i_\varepsilon := \lfloor Nx \rfloor \in \mathbb{Z}$. Then

$$x_\varepsilon := \varepsilon i_\varepsilon \to x$$

as $\varepsilon \to 0$, and applying Lebesgue's Differentiation Theorem (see for example Corollary 2 in §1.7 of [12]) gives that for almost every $x \in \Omega$,

$$D_j y_{i_\varepsilon} = \fint_{x_\varepsilon}^{x_\varepsilon + j\varepsilon} Dy(t)\,\mathrm{d}t \to Dy(x)$$

as $\varepsilon \to 0$. An immediate consequence of this and the continuity of the potentials ϕ_i is that

$$W_\varepsilon(x) \to W\big(Dy(x)\big)$$

for almost every $x \in \Omega$.

Pointwise upper bound on W_ε. Fix a point $x \in \Omega$ and the sequence i_ε as above. Dropping the subscript, we estimate

$$\begin{aligned} W_\varepsilon(x) &\le \tfrac{1}{2}\phi_2(D_2y_{i-1}) + \tfrac{1}{2}\phi_1(D_2y_{i-1}) + \phi_1(D_1y_i) + \tfrac{1}{2}\phi_1(D_2y_i) + \tfrac{1}{2}\phi_2(D_2y_i) + C, \\ &= \tfrac{1}{2}W(D_2y_{i-1}) + \phi_1(D_1y_i) + \tfrac{1}{2}W(D_2y_i) + C, \end{aligned}$$

where $-C \in \mathbb{R}$ is a lower bound for ϕ_1. Next, Assumption (4) in §1.5 implies that for some $C \in \mathbb{R}$,

$$\tfrac{1}{1-\alpha}W(t) + C \ge \phi_1(t).$$

Hence, letting $A := \max\{\frac{1}{2}, \frac{1}{1-\alpha}\}$,

$$\begin{aligned} W_\varepsilon(x) &\le A\Big(W(D_2y_{i-1}) + W(D_1y_i) + W(D_2y_i)\Big) + C, \\ &\le A\left(\fint_{x_{i-1}}^{x_{i+1}} W(Dy)\,\mathrm{d}x + \fint_{x_i}^{x_{i+1}} W(Dy)\,\mathrm{d}x + \fint_{x_i}^{x_{i+2}} W(Dy)\,\mathrm{d}x\right) + C \end{aligned}$$

by using Jensen's inequality. Since W is bounded below, we can extend the domain of integration for each integral, possibly changing the constant C, to reach the upper bound

$$W_\varepsilon(x) \le g_\varepsilon(x) := 3A\fint_{x-2\varepsilon}^{x+2\varepsilon} W(Dy)\,\mathrm{d}t + C.$$

Convergence of g_ε. As $\mathcal{F}_0(y)$ is bounded, $W(Dy)$ is integrable and so Lebesgue's Differentiation theorem implies that

$$g_\varepsilon(x) \to g(x) := 3A\,W(Dy(x)) + C$$

almost everywhere as $\varepsilon \to 0$. Furthermore, g_ε is in fact the convolution

$$g_\varepsilon = g \star \rho_\varepsilon,$$

where ρ_ε is an approximation to a Dirac mass given by

$$\rho_\varepsilon(x) := \frac{1}{4\varepsilon}\rho\left(\frac{x}{4\varepsilon}\right), \quad \text{where} \quad \rho(x) = \chi_\Omega(x).$$

The functions g_ε are in $\mathrm{L}^1(\Omega)$ because $g \in \mathrm{L}^1(\Omega)$ and $\rho_\varepsilon \in \mathrm{L}^\infty(\Omega)$, and by standard arguments

$$\int_\Omega g_\varepsilon(x)\,\mathrm{d}x \to \int_\Omega g(x)\,\mathrm{d}x$$

as $\varepsilon \to 0$. We can now apply Fatou's Lemma to $g_\varepsilon - W_\varepsilon$, which is positive, measurable, and converges almost everywhere:

$$\int_\Omega g\,\mathrm{d}x - \limsup_{\varepsilon\to 0}\int_\Omega W_\varepsilon\,\mathrm{d}x = \liminf_{\varepsilon\to 0}\int_\Omega g_\varepsilon - W_\varepsilon\,\mathrm{d}x \ge \int_\Omega g - W(Dy)\,\mathrm{d}x.$$

A rearrangement of this inequality allows us to conclude that

$$\limsup_{N\to\infty} \varepsilon E_{\mathrm{p}}^\varepsilon(y^\varepsilon) = \limsup_{N\to\infty}\int_\Omega W_\varepsilon\,\mathrm{d}x \le \int_\Omega W(Dy)\,\mathrm{d}x. \tag{10}$$

Controlling the energy near the defect. For any $y \in \mathcal{A}(L)$ and $\eta > 0$, let y^η be a linearisation close to 0 of $y \in \mathcal{A}(L)$ given by

$$y^\eta(x) := \begin{cases} y(-\eta) + \frac{y(\eta)-y(-\eta)}{2\eta}(x+\eta) & \text{when } |x| < \eta, \\ y(x) & \text{otherwise.} \end{cases}$$

Let $F^\eta := Dy^\eta(0)$. For ε sufficiently small, the defect energy for $\mathcal{T}^\varepsilon y^\eta$ is:

$$\varepsilon E_{\mathrm{d}}(\mathcal{T}^\varepsilon y^\eta) = 2\varepsilon\big(\psi_2(F^\eta) - \phi_2(F^\eta) + \psi_1(F^\eta) - \phi_1(F^\eta)\big) \leq C(\eta)\varepsilon \tag{11}$$

with η fixed. To control $\varepsilon E_{\mathrm{f}}^\varepsilon$, we can once again employ the estimate that was proven in (9), since the argument used was for a more general sequence than that chosen here. Therefore, combining (9), (10) and (11), we deduce that

$$\limsup_{\varepsilon \to 0} \mathcal{F}^\varepsilon(\mathcal{T}^\varepsilon y^\eta) \leq \mathcal{F}_0(y^\eta).$$

Since $y^\eta \to y$ in L^2 as $\eta \to 0$, we would like to show that $\mathcal{F}_0(y^\eta) \to \mathcal{F}_0(y)$ as $\eta \to 0$ in order to use a diagonalisation argument. This follows from the observation that

$$2\eta \cdot C \leq \int_{-\eta}^{\eta} W(Dy^\eta)\,\mathrm{d}x \leq \int_{-\eta}^{\eta} W(Dy)\,\mathrm{d}x,$$

since W is bounded below and convex. Both sides tend to 0 as $\eta \to 0$, so we can deduce that

$$\begin{aligned}\mathcal{F}_0(y^\eta) &= \int_\Omega W(Dy^\eta) + f\big(y^\eta - L(x+\tfrac{1}{2})\big)\,\mathrm{d}x, \\ &\leq \int_{\Omega\setminus(-\eta,\eta)} W(Dy)\,\mathrm{d}x + \int_{-\eta}^{\eta} W(Dy^\eta) + \int_\Omega f\,u\,\mathrm{d}x + \|f\|_2\|y^\eta - y\|_2, \\ &\to \mathcal{F}_0(y)\end{aligned}$$

as $\eta \to 0$, writing $u = y - L(x+\frac{1}{2})$.

Conclusion of the argument. Finally, by taking a diagonal sequence from the collection of $\mathcal{T}^\varepsilon y^\eta$, there exists $\mathcal{T}^\varepsilon y^{\eta_\varepsilon} \to y$ in L^2, along which

$$\limsup_{\varepsilon \to 0} \mathcal{F}^\varepsilon(\mathcal{T}^\varepsilon y^{\eta_\varepsilon}) \leq \mathcal{F}_0(y),$$

proving Proposition 2, and therefore concluding the proof of Theorem 2.1.

Remark 3. The defect does not introduce a perturbation to the Γ-limit at this order – see Theorem 3.2 in [5] for the Γ-limit of this problem without a defect. This is to be expected, since the 'defect set' is null in the limit as $\varepsilon \to 0$, and it therefore becomes reasonable to ask whether there is a higher order change in the energy, which is the subject of the subsequent analysis.

3. **Properties of $\mathcal{F}_0$.** The functional $\mathcal{F}_0$ is of a well-studied form, and the analysis of the minimum problem is classical. The following theorem collects relevant results regarding the functional and its minimisers which we will invoke in the following sections.

Proposition 3 (Properties of 0^{th}-order limit)**.** *The problem*

$$\operatorname{argmin}_{y \in \mathcal{A}(L)} \mathcal{F}_0(y)$$

has a unique solution $\bar{y}$, which has the following properties:

1. *$\bar{y}$ satisfies the Euler–Lagrange Equations for this problem,*
2. *$\bar{y} \in \mathrm{C}^2(\Omega)$.*

Proof. The existence part of this proof is completely classical, and can be found in [9] for example. If we suppose for the moment that minimisers are in $\mathrm{W}^{1,\infty}(\Omega)$ and satisfy the condition

$$D\bar{y}(x) \geq \delta > 0$$

for almost every $x \in \Omega$, it is also easy to show that they satisfy

$$\int_\Omega \big[W'\big(D\bar{y}\big) - \sigma\big] Dv \,\mathrm{d}x = 0 \qquad \forall\, v \in \mathrm{W}^{1,\infty}_0(\Omega), \tag{12}$$

where $\sigma(x) := \int_0^x f(t)\,\mathrm{d}t$. Since W is l-convex, $W' : \mathbb{R}^+ \to \mathbb{R}$ is strictly increasing and is a C^1 diffeomorphism. If $(W')^{-1}$ is the inverse of W', it is possible to 'explicitly' define a solution of the Euler–Lagrange equations

$$\bar{y}(x) := \int_{-\frac{1}{2}}^{x} (W')^{-1}\big(\sigma(t) + \Sigma\big)\,\mathrm{d}t,$$

where Σ is the solution of the following implicit equation:

$$\int_\Omega (W')^{-1}\big(\sigma(t) + \Sigma\big)\,\mathrm{d}t = L.$$

We can show that this equation has a solution by regarding the left hand side as a function of Σ, showing it is C^1, has a strictly positive derivative, and tends to 0 as $\Sigma \to -\infty$, so attains all possible values $L > 0$ only once. It is now simple to verify that $\bar{y}$ is C^2 and satisfies the pointwise Euler–Lagrange equation, that is

$$\tfrac{\mathrm{d}}{\mathrm{d}x} W'\big(D\bar{y}(x)\big) = f(x) \quad \Rightarrow \quad W'\big(D\bar{y}(x)\big) = \sigma(x) + \Sigma, \tag{13}$$

so all that remains to do is show that this is in fact the minimiser. Suppose that $\tilde{y} \in \mathcal{A}(L)$ minimises $\mathcal{F}_0$ and is not equal to $\bar{y}$; then

$$\begin{aligned} 0 &\geq \int_\Omega W(D\tilde{y}) - W(D\bar{y}) + f(\tilde{y} - \bar{y})\,\mathrm{d}x, \\ &= \int_\Omega W(D\tilde{y}) - W(D\bar{y}) - \sigma\big(D\tilde{y} - D\bar{y}\big)\,\mathrm{d}x, \\ &\geq \int_\Omega \big[W'(D\bar{y}) - \sigma\big] \cdot \big(D\tilde{y} - D\bar{y}\big)\,\mathrm{d}x + \tfrac{1}{2} l \|D\tilde{y} - D\bar{y}\|_2^2, \end{aligned}$$

where we have integrated by parts on the second line, and used the fact that W is l-convex on the last line. Since $\bar{y}$ has been constructed to solve the pointwise Euler–Lagrange equation (13), the integrand vanishes, and hence $\tilde{y} = \bar{y}$. This argument clearly also implies uniqueness of solutions. $\square$

4. **The 1st-order Γ-limit.** The approach taken in §2.2 gives a strong indication of the scaling of the next term in an asymptotic expansion of the energy: (11) suggests that the extra energy from the defect is only coming from a set near the defect that is of size $O(\varepsilon)$. §3 shows that we have a very clear understanding of the properties of $\bar{y}$, and thus we can reasonably hope to derive a good characterisation of the next order limit, as in [5, 14].

For this purpose, we define some additional notation. Recalling from Section 3 that

$$\bar{y} = \mathrm{argmin}_{y \in \mathcal{A}(L)} \mathcal{F}_0(y),$$

the functional from which we obtain the first-order limit is

$$\mathcal{F}_1^\varepsilon(y) := \frac{\mathcal{F}^\varepsilon(y) - \mathcal{F}_0(\bar{y})}{\varepsilon}.$$

To make the notation used in this section concise, we let $F_0 := D\bar{y}(0)$ as in §1.4, and define potentials

$$\Phi_1(t) := \phi_1(F_0 + t) - \phi_1(F_0) - \phi_1'(F_0) \cdot t,$$
$$\Phi_2(t) := \phi_2(F_0 + t) - \phi_2(F_0) - \phi_2'(F_0) \cdot t.$$

We also analogously introduce

$$\Psi_1(t) := \psi_1(F_0 + t) - \phi_1(F_0) - \phi_1'(F_0) \cdot t,$$
$$\Psi_2(t) := \psi_2(F_0 + t) - \phi_2(F_0) - \phi_2'(F_0) \cdot t,$$

although these functions will be used exclusively to write the Euler–Lagrange equations for $\tilde{E}_\infty$ (28) in a compact form.

We will show that the first-order Γ-limit can be written in terms of the infinite cell problem

$$\inf_{r \in \ell^2(\mathbb{Z})} \tilde{E}_\infty(r),$$

where $\tilde{E}_\infty : \ell^2(\mathbb{Z}) \to \mathbb{R} \cup \{+\infty\}$ is defined to be

$$\tilde{E}_\infty(r) := \begin{cases} \displaystyle\sum_{i=-\infty}^{\infty} \Phi_1(r_i) + \Phi_2\big(\tfrac{r_{i+1}+r_i}{2}\big) + \tilde{E}_{\mathrm{d}}(r), & F_0 + r_i > 0 \text{ for all } i \in \mathbb{N}, \\ +\infty & \text{otherwise,} \end{cases}$$

and we have set

$$\begin{aligned} \tilde{E}_{\mathrm{d}}(r) := {} & \psi_2\big(F_0 + \tfrac{r_{-2}+r_{-1}}{2}\big) - \phi_2\big(F_0 + \tfrac{r_{-2}+r_{-1}}{2}\big) + \psi_1\big(F_0 + r_{-1}\big) - \phi_1\big(F_0 + r_{-1}\big) \\ & + \psi_1\big(F_0 + r_0\big) - \phi_1\big(F_0 + r_0\big) + \psi_2\big(F_0 + \tfrac{r_0+r_1}{2}\big) - \phi_2\big(F_0 + \tfrac{r_0+r_1}{2}\big). \end{aligned}$$

We briefly show that $\tilde{E}_\infty$ is well-defined. It is straightforward to check that Φ_2 is concave because ϕ_2 is concave, hence

$$\tilde{E}_\infty(r) \geq \sum_{i=-\infty}^{\infty} \Phi_1(r_i) + \Phi_2(r_i) + \tilde{E}_{\mathrm{d}}(r).$$

Furthermore, the fact that W is l-convex implies

$$\Phi_1(t) + \Phi_2(t) = W(F_0 + t) - W(F_0) - W'(F_0)t \geq \tfrac{1}{2} l\, t^2, \tag{14}$$

and for $i \in \{-2, -1, 0, 1\}$, as in (5), there exists some constant $C \in \mathbb{R}$ such that

$$\sum_{i=-2}^{1} \Big(\tfrac{1}{2}\Phi_1(r_i) + \tfrac{1}{2}\Phi_1(r_{i+1}) + \Phi_2\big(\tfrac{r_i + r_{i+1}}{2}\big) \Big) + \tilde{E}_{\mathrm{d}}(r) \geq \sum_{i=-2}^{1} \tfrac{1}{2} l\, |r_i|^2 + C.$$

Hence we have that

$$\tilde{E}_\infty(r) \geq \tfrac{1}{2} l \|r\|^2_{\ell^2(\mathbb{Z})} + C, \tag{15}$$

and $\tilde{E}_\infty$ is well-defined as a function mapping $\ell^2(\mathbb{Z})$ into $\mathbb{R} \cup \{+\infty\}$.

The second main result of this paper is the following theorem.

Theorem 4.1 (1st-order Γ-limit)**.** *With respect to convergence in* L^2*, we have that*

$$\Gamma\text{-}\lim_{\varepsilon \to 0} \mathcal{F}_1^\varepsilon(y) = \mathcal{F}_1(y) := \begin{cases} \displaystyle\inf_{r \in \ell^2(\mathbb{Z})} \tilde{E}_\infty(r) & y = \bar{y}, \\ +\infty & y \neq \bar{y}. \end{cases}$$

In contrast to the results of [5, 14], we emphasise that we have an explicit representation of the 1^{st}-order limit in terms of a minimisation problem in an infinite cell. Once more, the proof of this result divides into two parts, the liminf and limsup inequalities, which we prove in the next two sections.

4.1. **The liminf inequality.** The liminf inequality is the following statement.

Proposition 4. *If $y^\varepsilon \to y$ in L^2, then*

$$\liminf_{\varepsilon\to 0} \mathcal{F}_1^\varepsilon(y^\varepsilon) \geq \mathcal{F}_1(y).$$

As in the proof of Proposition 1, we use a coercivity result which says uniform boundedness of $\mathcal{F}_1^\varepsilon(y^\varepsilon)$ implies a form of compactness for the sequence y^ε. In this proof, there are two such results, which are employed at crucial steps in the main argument. The first of these results, Lemma 4.2, states that if $\mathcal{F}_1^\varepsilon(y^\varepsilon)$ is uniformly bounded then the weak convergence of y^ε in H^1 proven in Lemma 2.2 improves to strong convergence in H^1. The second, Lemma 4.4, describes coercivity in a topology which we use to describe perturbations to the minimiser of $\mathcal{F}_0$ close to the defect. Once these results have been obtained, the main argument will follow by applying Fatou's Lemma to a suitable reinterpretation of $\mathcal{F}_1^\varepsilon(y^\varepsilon)$.

We remark at the outset that to simplify the notation, we write u, u^ε and $\bar{u}$ in place of $y - L(x+\frac{1}{2})$, $y^\varepsilon - L(x+\frac{1}{2})$ and $\bar{y} - L(x+\frac{1}{2})$ respectively.

The first key step before proving the coercivity results is to rewrite $\mathcal{F}_1^\varepsilon(y^\varepsilon)$ and $\mathcal{F}_0(\bar{y})$ by using integration by parts on the external force terms. We have that

$$\int_\Omega f\bar{u}\,\mathrm{d}x = -\int_\Omega \sigma\, D\bar{u}\,\mathrm{d}x,$$

using the boundary conditions, where $\sigma(x) := \int_{-1/2}^x f(t)\,\mathrm{d}t$ as in §1.4. Analogously, recursively define[3]

$$\begin{aligned} \sigma_{-N}^\varepsilon &:= -\tfrac{1}{2}\varepsilon f_{-N}, \\ \sigma_i^\varepsilon &:= \sigma_{i-1}^\varepsilon + \varepsilon f_{i-1}. \end{aligned}$$

This leads to the representation

$$\sum_{i=-N}^{N-1} f_i\, u_i = \sum_{i=-N}^{N-1} \frac{\sigma_{i+1}^\varepsilon - \sigma_i^\varepsilon}{\varepsilon} u_i = -\sum_{i=-N}^{N-1} \sigma_{i+1}^\varepsilon D_1 u_i.$$

We define the step function $\sigma^\varepsilon : \Omega \to \mathbb{R}$

$$\sigma^\varepsilon(x) := \sum_{i=-N}^{N-1} \sigma_{i+1}^\varepsilon\, \chi_{(x_i,x_{i+1})}(x),$$

so that if $y \in \mathcal{A}^\varepsilon(L)$,

$$\varepsilon E_{\mathrm{f}}^\varepsilon(y) = -\int_\Omega \sigma^\varepsilon\, Du\,\mathrm{d}x.$$

[3]Initially, the definition of σ_{-N}^ε can be left free; however, the particular choice of σ_{-N}^ε given here will be used to obtain (21), a pointwise estimate on $\sigma - \sigma^\varepsilon$ during the proof of Lemma 4.2.

Using these definitions, we perform careful estimates of $\mathcal{F}_1^\varepsilon(y^\varepsilon)$ by splitting the domain of integration over the intervals (x_i, x_{i+2}). For $y^\varepsilon \in \mathcal{A}^\varepsilon(L)$, define

$$s_i^\varepsilon := \phi_2(D_2 y_i^\varepsilon) + \tfrac{1}{2}\phi_1(D_1 y_i^\varepsilon) + \tfrac{1}{2}\phi_1(D_1 y_{i+1}^\varepsilon) - \tfrac{1}{2}\sigma_{i+1}^\varepsilon D_1 u_i^\varepsilon - \tfrac{1}{2}\sigma_{i+2}^\varepsilon D_1 u_{i+1}^\varepsilon \\ - \fint_{x_i}^{x_{i+2}} W(D\bar{y}) - \sigma\, D\bar{u} + \Sigma\left(Dy^\varepsilon - D\bar{y}\right) \mathrm{d}x. \quad (16)$$

if $i \in \{-N, \dots, N-1\}$, and set $s_i^\varepsilon := 0$ otherwise. Then it is easy to check that

$$\mathcal{F}_1^\varepsilon(y^\varepsilon) = \sum_{i=-\infty}^{\infty} s_i^\varepsilon + E_{\mathrm{d}}(y^\varepsilon). \quad (17)$$

We are now in a position to prove the coercivity results.

Lemma 4.2 (Strong H^1 coercivity). *If $y^\varepsilon \to y$ in L^2, and $\mathcal{F}_1^\varepsilon(y^\varepsilon)$ is uniformly bounded for all $\varepsilon > 0$, then $y^\varepsilon \to \bar{y}$ in H^1.*

Proof. Since $\mathcal{F}_1^\varepsilon(y^\varepsilon)$ is uniformly bounded, we know that for some $C \in \mathbb{R}$,

$$\left|\mathcal{F}^\varepsilon(y^\varepsilon) - \mathcal{F}_0(\bar{y})\right| \leq C\varepsilon,$$

which immediately implies that $\mathcal{F}^\varepsilon(y^\varepsilon) \to \mathcal{F}_0(\bar{y})$ as $\varepsilon \to 0$. Consequently, Lemma 2.2 applies and so $\|Dy^\varepsilon\|_2$ is uniformly bounded. Let $i \in \{-N, \dots, N-1\}$. We estimate s_i^ε below:

$$\begin{aligned} s_i^\varepsilon &\geq \fint_{x_i}^{x_{i+2}} \Big(W(Dy^\varepsilon) - W(D\bar{y}) - \sigma^\varepsilon Du^\varepsilon + \sigma D\bar{u} - \Sigma\left(Dy^\varepsilon - D\bar{y}\right)\Big) \mathrm{d}x, \\ &\geq \fint_{x_i}^{x_{i+2}} \Big(W'(D\bar{y})\big(Dy^\varepsilon - D\bar{y}\big) + \tfrac{1}{2} l\, |Dy^\varepsilon - D\bar{y}|^2 \\ &\qquad - \sigma^\varepsilon Du^\varepsilon + \sigma\, D\bar{u} - \Sigma\left(Dy^\varepsilon - D\bar{y}\right)\Big) \mathrm{d}x, \end{aligned}$$

using the concavity of ϕ_2 on the first line, and the l-convexity of W on the second. Next, as $\bar{y}$ satisfies the pointwise Euler–Lagrange equation (13),

$$\begin{aligned} s_i^\varepsilon &\geq \fint_{x_i}^{x_{i+2}} \Big(\sigma\big(Dy^\varepsilon - D\bar{y}\big) + \tfrac{1}{2} l\, |Dy^\varepsilon - D\bar{y}|^2 - \sigma^\varepsilon Du^\varepsilon + \sigma D\bar{u}\Big) \mathrm{d}x, \\ &\geq \fint_{x_i}^{x_{i+2}} \Big(\big(\sigma - \sigma^\varepsilon\big) Du^\varepsilon + \tfrac{1}{2} l\, |Dy^\varepsilon - D\bar{y}|^2 \Big) \mathrm{d}x. \end{aligned} \quad (18)$$

The latter term in the above integral is of the form we are looking for, so it now remains to show that the other term vanishes in the limit. Once this is done, we then show that the defect energy is also suitably bounded below.

Pointwise estimate on $\sigma - \sigma^\varepsilon$. Noting that Du^ε is constant on the intervals (x_i, x_{i+1}) and using the definitions of σ and σ^ε, we rewrite

$$\begin{aligned} \fint_{x_i}^{x_{i+1}} \big(\sigma - \sigma^\varepsilon\big)\, \mathrm{d}x &= \fint_{x_i}^{x_{i+1}} \left(\int_{-1/2}^{x} f(t)\, \mathrm{d}t - \varepsilon \sum_{j=-N}^{i-1} \tfrac{1}{2}\big(f_j + f_{j+1}\big) - \tfrac{1}{2}\varepsilon f_i \right) \mathrm{d}x, \\ &= \int_{-1/2}^{x_i} \Big(f(t) - (\mathcal{T}^\varepsilon f)(t) \Big)\, \mathrm{d}t + \fint_{x_i}^{x_{i+1}} \left(\int_{x_i}^{x} f(t)\, \mathrm{d}t - \tfrac{1}{2}\varepsilon f_i \right) \mathrm{d}x. \end{aligned}$$

Since we know that $f \in \mathrm{C}^2$, standard results about interpolation error (see for example [16]) imply that

$$\left| \int_{-1/2}^{x_i} \Big(f(t) - \big(\mathcal{T}^\varepsilon f\big)(t) \Big)\,\mathrm{d}t \right| \leq \tfrac{1}{12}\varepsilon^2 \|f''\|_\infty. \tag{19}$$

For the other term, we Taylor expand $f(t)$ at x_i, then evaluate integrals to show that

$$\left| \fint_{x_i}^{x_{i+1}} \int_{x_i}^{x} f(t)\,\mathrm{d}t - \tfrac{1}{2}\varepsilon f_i \,\mathrm{d}x \right| \leq \tfrac{1}{6}\varepsilon^2 \|f'\|_\infty. \tag{20}$$

Combining (19) and (20), we have

$$\begin{aligned} \left| \fint_{x_i}^{x_{i+2}} (\sigma - \sigma^\varepsilon) Du^\varepsilon \,\mathrm{d}x \right| &\leq \Big(\tfrac{1}{12}\varepsilon^2 \|f''\|_\infty + \tfrac{1}{6}\varepsilon^2 \|f'\|_\infty \Big) \frac{|D_1 u^\varepsilon_i| + |D_1 u^\varepsilon_{i+1}|}{2}, \\ &\leq C\varepsilon^2 \Big(|D_1 u^\varepsilon_i|^2 + |D_1 u^\varepsilon_{i+1}|^2 \Big)^{1/2}, \\ &\leq C\varepsilon^{3/2} \|Du^\varepsilon\|_2, \end{aligned} \tag{21}$$

where on the second line we used Jensen's inequality, and on the third line we used $\varepsilon^{1/2}$ and added further positive terms inside the brackets to get the estimate. This can be used in (18) to give

$$s^\varepsilon_i \geq -C\varepsilon^{3/2} \|Du^\varepsilon\|_2 + \tfrac{1}{2} l \fint_{x_i}^{x_{i+2}} |Dy^\varepsilon - D\bar{y}|^2 \,\mathrm{d}x. \tag{22}$$

Lower bound on defect energy. Using (5), the fact that $W(D\bar{y}) - (\sigma + \Sigma)D\bar{u}$ is finite and estimate (21),

$$\begin{aligned} \sum_{i=-2}^{0} s^\varepsilon_i + E_{\mathrm{d}}(y^\varepsilon) &\geq \sum_{i=-2}^{0} \tfrac{1}{4} l \left(\left|D_1 y^\varepsilon_i\right|^2 + \left|D_1 y^\varepsilon_{i+1}\right|^2 \right) + C \\ &\qquad - \fint_{x_i}^{x_{i+2}} \Big(\sigma^\varepsilon Du^\varepsilon + \Sigma\, Du^\varepsilon \Big)\,\mathrm{d}x, \\ &= \sum_{i=-2}^{0} \fint_{x_i}^{x_{i+2}} \Big(\tfrac{1}{2} l \,|Dy^\varepsilon|^2 - \sigma Du^\varepsilon \\ &\qquad\qquad - (\sigma^\varepsilon - \sigma) Du^\varepsilon - \Sigma\, Du^\varepsilon \Big)\,\mathrm{d}x + C, \\ &\geq \sum_{i=-2}^{0} \fint_{x_i}^{x_{i+2}} \Big(\tfrac{1}{2} l \,|Dy^\varepsilon|^2 - \|\sigma + \Sigma\|_\infty |Du^\varepsilon| + C \Big)\,\mathrm{d}x \\ &\qquad - C\varepsilon^{3/2} \|Dy^\varepsilon\|_2. \end{aligned}$$

Since $D\bar{y}$ is bounded above and below, by adjusting constants suitably we have that

$$\sum_{i=-2}^{0} s^\varepsilon_i + E_{\mathrm{d}}(y^\varepsilon) \geq \sum_{i=-2}^{0} \fint_{x_i}^{x_{i+2}} \tfrac{1}{2} l \,|Dy^\varepsilon - D\bar{y}|^2 \,\mathrm{d}x + C - C\varepsilon^{3/2} \|Dy^\varepsilon\|_2. \tag{23}$$

Conclusion of the argument. By summing over i in (22), combining with (23), and using the fact that $\|Dy^\varepsilon\|_2$ is uniformly bounded, we have shown that

$$\mathcal{F}^\varepsilon_1(y^\varepsilon) \geq -C\varepsilon^{1/2} + \tfrac{1}{2} l \sum_{i=-N}^{N-1} \fint_{x_i}^{x_{i+1}} |Dy^\varepsilon - D\bar{y}|^2 \,\mathrm{d}x + C.$$

Multiplying this inequality by ε and using the assumption that $\mathcal{F}_1^\varepsilon(y^\varepsilon)$ is uniformly bounded, we have

$$C\varepsilon \geq \tfrac{1}{2}l\|Dy^\varepsilon - D\bar{y}\|_2^2, \tag{24}$$

which proves the result. □

To prove the second coercivity result, we define the sequence of operators $\mathcal{P}_\varepsilon : \mathcal{A}^\varepsilon(L) \to \ell^2(\mathbb{Z})$ by

$$\big(\mathcal{P}_\varepsilon y\big)_i := \begin{cases} D_1 y_i - D_1\bar{y}_i & i \in \{-N, \dots, N-1\} \\ 0 & \text{otherwise.} \end{cases}$$

Clearly $\mathcal{P}_\varepsilon y$ is well-defined since this sequence is non-zero only on a finite set.

Lemma 4.3 (Weak $\ell^2(\mathbb{Z})$ coercivity)**.** *If $\mathcal{F}_1^\varepsilon(y^\varepsilon)$ is uniformly bounded, then there exists a subsequence of $\mathcal{P}_\varepsilon y^\varepsilon$ which converges weakly in $\ell^2(\mathbb{Z})$.*

Proof. By dividing (24) by ε and using Jensen's inequality, we have

$$C \geq \tfrac{1}{2}l\sum_{i=-N}^{N-1} \fint_{x_i}^{x_{i+1}} |Dy^\varepsilon - D\bar{y}|^2 \,\mathrm{d}x \geq \tfrac{1}{2}l\sum_{i=-N}^{N-1}\bigg|\fint_{x_i}^{x_{i+1}} Dy^\varepsilon - D\bar{y}\,\mathrm{d}x\bigg|^2 = \tfrac{1}{2}l\|\mathcal{P}_\varepsilon y^\varepsilon\|^2_{\ell^2(\mathbb{Z})}.$$

We have shown that the sequence $\mathcal{P}_\varepsilon y^\varepsilon$ is uniformly bounded in $\ell^2(\mathbb{Z})$, so in particular, it must have a weakly convergent subsequence. □

To conclude the argument which will prove the liminf inequality, we will use the following characterisation of weak convergence in $\ell^2(\mathbb{Z})$ which follows easily from the Riesz Representation Theorem.

Lemma 4.4. *A sequence $(r^\varepsilon) \subseteq \ell^2(\mathbb{Z})$ converges weakly to $r \in \ell^2(\mathbb{Z})$ as $\varepsilon \to 0$ if and only if the following two conditions hold:*

1. *$\|r^\varepsilon\|_{\ell^2}$ is uniformly bounded,*
2. *$r^\varepsilon \to r$ pointwise (almost everywhere in the counting measure) as $\varepsilon \to 0$.*

As indicated at the beginning of this section, we apply Fatou's Lemma to the sum (17). Suppose that $\mathcal{F}_1^\varepsilon(y^\varepsilon)$ is uniformly bounded and $y^\varepsilon \to y$. Take a subsequence y^{ε_k} such that

$$\lim_{k\to\infty} \mathcal{F}_1^{\varepsilon_k}(y^{\varepsilon_k}) = \liminf_{\varepsilon\to 0} \mathcal{F}_1^\varepsilon(y^\varepsilon),$$

and then using Lemma 4.3, a further subsequence (which we do not relabel) such that $\mathcal{P}_{\varepsilon_k} y^{\varepsilon_k}$ weakly converges to r in $\ell^2(\mathbb{Z})$. Since $\bar{y} \in \mathrm{C}^2(\Omega)$, we have that

$$D_1\bar{y}_i = \fint_{x_i}^{x_{i+1}} D\bar{y}\,\mathrm{d}x \to F_0 := D\bar{y}(0)$$

as $\varepsilon \to 0$. Fixing an index $i \in \mathbb{Z}$, Lemma 4.4 implies that

$$\begin{aligned}\big(\mathcal{P}_{\varepsilon_k} y^{\varepsilon_k}\big)_i &= D_1 y_i^{\varepsilon_k} - D_1\bar{y}_i, \\ &\to F_0 + r_i - F_0\end{aligned}$$

as $k \to \infty$, so that we may view r as a perturbation to the deformation gradient in an 'infinitesimal' neighbourhood of the defect. The 'pointwise' estimate (22) implies that for $i \in \{-N, \dots, N-1\}$

$$s_i^\varepsilon + C\varepsilon^{3/2} \geq 0,$$

so that

$$\liminf_{k\to\infty}\sum_{i=-N_k}^{N_k-1} s_i^{\varepsilon_k}+C\varepsilon_k^{3/2}\geq\sum_{i=-\infty}^{\infty}\liminf_{k\to\infty}\big(s_i^{\varepsilon_k}+C\varepsilon_k^{3/2}\big). \tag{25}$$

Since the potentials ϕ_i are continuous and $\sigma_i^\varepsilon\to\sigma(0)$ as $\varepsilon\to 0$ with i fixed, we have that

$$\liminf_{k\to\infty}\big(s_i^{\varepsilon_k}+\varepsilon_k^{3/2}\big)=\phi_2(F_0+\tfrac{r_i+r_{i+1}}{2})+\tfrac{1}{2}\phi_1(F_0+r_i)+\tfrac{1}{2}\phi_1(F_0+r_{i+1})-W(F_0)\\ -\sigma(0)(F_0+\tfrac{r_i+r_{i+1}}{2})+\sigma(0)F_0-\Sigma\,\tfrac{r_i+r_{i+1}}{2}.$$

Recalling that $\bar{y}$ satisfies the Euler–Lagrange equation pointwise, (13), we have that

$$\sigma(0)=W'(F_0)-\Sigma,$$

so that

$$\liminf_{k\to\infty}\big(s_i^{\varepsilon_k}+\varepsilon_k^{3/2}\big)=\Phi_2(r_i+r_{i+1})+\tfrac{1}{2}\Phi_1(r_i)+\tfrac{1}{2}\Phi_1(r_{i+1}). \tag{26}$$

Note that

$$\lim_{k\to\infty}\sum_{i=-N_k}^{N_k-1}C\varepsilon_k^{3/2}=\lim_{k\to\infty}C\varepsilon_k^{1/2}=0, \tag{27}$$

so then combining (25), (26) and (27), we have that

$$\liminf_{k\to\infty}\sum_{i=-\infty}^{\infty}s_i^{\varepsilon_k}\geq\sum_{i=-\infty}^{\infty}\Phi_2\big(\tfrac{r_i+r_{i+1}}{2}\big)+\tfrac{1}{2}\Phi_1(r_i)+\tfrac{1}{2}\Phi_1(r_{i+1}).$$

Finally, by possibly taking further subsequences, we can assume that $\big(\mathcal{P}_{\varepsilon_k}y^{\varepsilon_k}\big)_i$ converges uniformly for $i\in\{-2,-1,0,1\}$, and then we have

$$\begin{aligned}\liminf_{\varepsilon\to 0}\mathcal{F}_1^\varepsilon(y^\varepsilon)&=\liminf_{k\to\infty}\bigg(\sum_{i=-\infty}^{\infty}s_i^{\varepsilon_k}+\tilde{E}_{\mathrm{d}}(\mathcal{P}_\varepsilon y^{\varepsilon_k})\bigg),\\ &\geq\tilde{E}_\infty(r),\\ &\geq\inf_{r\in\ell^2(\mathbb{Z})}\tilde{E}_\infty(r),\end{aligned}$$

proving Proposition 4.

Remark 4. By definition, we have

$$\sum_{i=-N}^{N-1}\big(\mathcal{P}_\varepsilon y^\varepsilon\big)_i=0$$

for any $y^\varepsilon\in\mathcal{A}^\varepsilon(L)$. If $\mathcal{P}_\varepsilon y^\varepsilon\rightharpoonup r$ in $\ell^1(\mathbb{Z})$, we could conclude that

$$\sum_{i=-\infty}^{\infty}r_i=0;$$

however, since we have convergence only in $\ell^2(\mathbb{Z})$, this is false in general. It is therefore clear that the set of compactly supported mean zero sequences is dense in the weak topology on $\ell^2(\mathbb{Z})$.

4.2. **The limsup inequality.** The limsup inequality is the following statement.

Proposition 5. *For every $y \in \mathcal{A}(L)$, there exists a sequence $y^\varepsilon \to y$ in L^2 such that*

$$\limsup_{\varepsilon\to 0} \mathcal{F}_1^\varepsilon(y^\varepsilon) \leq \mathcal{F}_1(y).$$

This statement is trivial in the case where $y \neq \bar{y}$, so we only need to construct the sequence for $y = \bar{y}$. In order to construct the limsup sequence, we will show that there exists a minimiser of $\tilde{E}_\infty$, and then combine a suitable truncation of this minimiser with $\mathcal{T}^\varepsilon \bar{y}$ to get the result.

Proposition 6 (Properties of 1st-order limit)**.** *Let $\tilde{E}_\infty : \ell^2(\mathbb{Z}) \to \mathbb{R} \cup \{+\infty\}$ be defined as in §4. Then there exist minimisers of $\tilde{E}_\infty$ which satisfy an infinite system of nonlinear algebraic Euler–Lagrange equations, given in (28).*

Proof. Since $\tilde{E}_\infty(r) < +\infty$ for the constant sequence $r = 0$, the infimum is less than $+\infty$. Recall from (15) that

$$\tilde{E}_\infty(r) \geq \tfrac{1}{2} l \, \|r\|^2_{\ell^2(\mathbb{Z})} + C.$$

This bound implies that $\tilde{E}_\infty$ is coercive, and applying Fatou's lemma as above with the pointwise lower bound (14) implies that $\tilde{E}_\infty$ is weakly lower semicontinuous. A standard application of the Direct Method of the Calculus of Variations now yields existence.

To obtain the Euler–Lagrange equations, suppose r is a minimiser of $\tilde{E}_\infty$. Let $e^i \in \ell^2(\mathbb{Z})$ be the sequence which has

$$e^i_j = \begin{cases} 1 & j = i, \\ 0 & \text{otherwise}. \end{cases}$$

Let $i \notin \{-2, -1, 0, 1\}$; for small enough $t > 0$, $\tilde{E}_\infty(r + te^i) < +\infty$, and

$$\begin{aligned} 0 &\leq \frac{\tilde{E}_\infty(r + te^i) - \tilde{E}_\infty(r)}{t}, \\ &= \int_0^1 \tfrac{1}{2}\Phi_2'\big(\tfrac{r_{i-1}+r_i+st}{2}\big) + \Phi_1'(r_i + st) + \tfrac{1}{2}\Phi_2'\big(\tfrac{r_i+st+r_{i+1}}{2}\big)\,\mathrm{d}s. \end{aligned}$$

Applying the Dominated Convergence Theorem and repeating the argument for $t < 0$ now implies that

$$\tfrac{1}{2}\Phi_2'\big(\tfrac{r_{i-1}+r_i}{2}\big) + \Phi_1'(r_i) + \tfrac{1}{2}\Phi_2'\big(\tfrac{r_i+r_{i+1}}{2}\big) = 0. \tag{28a}$$

By the same argument, we also have that

$$\tfrac{1}{2}\Phi_2'\big(\tfrac{r_{-3}+r_{-2}}{2}\big) + \Phi_1'(r_{-2}) + \tfrac{1}{2}\Psi_2'\big(\tfrac{r_{-2}+r_{-1}}{2}\big) = 0, \tag{28b}$$

$$\tfrac{1}{2}\Psi_2'\big(\tfrac{r_{-2}+r_{-1}}{2}\big) + \Psi_1'(r_{-1}) + \tfrac{1}{2}\Phi_2'\big(\tfrac{r_{-1}+r_0}{2}\big) = 0, \tag{28c}$$

$$\tfrac{1}{2}\Phi_2'\big(\tfrac{r_{-1}+r_0}{2}\big) + \Psi_1'(r_0) + \tfrac{1}{2}\Psi_2'\big(\tfrac{r_0+r_1}{2}\big) = 0, \tag{28d}$$

$$\tfrac{1}{2}\Psi_2'\big(\tfrac{r_0+r_1}{2}\big) + \Phi_1'(r_1) + \tfrac{1}{2}\Phi_2'\big(\tfrac{r_1+r_2}{2}\big) = 0, \tag{28e}$$

completing the proof. □

In order to complete the proof of the limsup inequality, we will require a better understanding of minimisers of $\tilde{E}_\infty$, and so we prove the following sequence of results, which amount to regularity results for solutions of the Euler–Lagrange equations (28). From now on, we fix $r \in \ell^2(\mathbb{Z})$ as being one particular minimiser of $\tilde{E}_\infty$.

Lemma 4.5. *Suppose that $r \in \ell^2(\mathbb{N})$ solves (28a) for all $i \geq 2$. Then*

$$r_1 \geq 0 \quad \Rightarrow \quad r_1 = \max_{j\in\mathbb{N}}\{r_j\};$$
$$r_1 \leq 0 \quad \Rightarrow \quad r_1 = \min_{j\in\mathbb{N}}\{r_j\}.$$

Proof. We prove only the first conclusion, the proof of the second being similar. Suppose for contradiction that $r \in \ell^2(\mathbb{N})$ solves (28a) and $r_1 \neq \max_{j\in\mathbb{N}}\{r_j\}$. Since $r_j \to 0$ as $j \to \infty$, it follows that r must have an interior maximum, i.e. there exists r_M with $M > 1$ such that

$$r_M = \max_{j\in\mathbb{N}}\{r_j\} > r_1 \geq 0.$$

Then because Φ_2 is concave, we have that Φ_2' is monotone decreasing, and hence

$$\begin{aligned} 0 &= \tfrac{1}{2}\Phi_2'\big(\tfrac{r_{M-1}+r_M}{2}\big) + \Phi_1'(r_M) + \tfrac{1}{2}\Phi_2'\big(\tfrac{r_M+r_{M+1}}{2}\big), \\ &\geq \Phi_2'(r_M) + \Phi_1'(r_M), \\ &= W'(F_0 + r_M) - W'(F_0), \\ &= \int_0^{r_M} W''(F_0 + s)\,\mathrm{d}s, \\ &\geq l\, r_M, \end{aligned} \tag{29}$$

in contradiction to the statement that $r_M > 0$. □

Corollary 1. *Suppose that $r \in \ell^2(\mathbb{N})$ solves (28a) for all $i \geq 2$. Then*

$$r_1 \geq 0 \quad \Rightarrow \quad r_i \geq r_{i+1} \geq 0 \text{ for all } i \in \mathbb{N};$$
$$r_1 \leq 0 \quad \Rightarrow \quad r_i \leq r_{i+1} \leq 0 \text{ for all } i \in \mathbb{N}.$$

Proof. Estimate (29) states that if

$$r_i = \max\{r_{i-1}, r_i, r_{i+1}\}, \quad \text{then} \quad r_i \leq 0.$$

Similarly, it is possible to show that if

$$r_i = \min\{r_{i-1}, r_i, r_{i+1}\}, \quad \text{then} \quad r_i \geq 0.$$

Suppose that r has a local maximum $r_M < 0$ with $M > 1$. Then $r_{M+1} \leq r_M < 0$. Since local minima can only occur when $r_i \geq 0$, r_{M+1} cannot be a local minimum, and so $r_{M+2} \leq r_{M+1} < 0$. Proceeding by induction, $r_i \leq r_M < 0$ for all $i \geq M$, which contradicts the fact that $r \in \ell^2(\mathbb{N})$. A similar argument prevents the existence of local minima r_M with $r_M > 0$.

Next suppose that $r_M = 0$ is a local maximum for $M > 1$. If $r_{M+1} < 0$, then the previous argument applies. If $r_{M+1} = 0$, then it too must be a local maximum or minimum, depending on the sign of r_{M+2}. If $r_{M+2} \neq 0$, then we can apply the previous arguments again to arrive at a contradiction, so by induction we have that $r_i = 0$ for all $i \geq M$.

We have therefore shown that there can be no internal maxima, unless they are degenerate in the sense that r is identically 0 after the maximum, and by a similar argument, we can show that there can be no internal minima except if they are degenerate in the same sense. We can now conclude that any solution of (28a) must be decreasing if $r_1 \geq 0$, or increasing if $r_1 \leq 0$, which concludes the proof. □

Finally, we prove that minimisers have exponentially small 'tails'.

Proposition 7 (Exponential decay)**.** *Suppose that $r \in \ell^2(\mathbb{N})$ solves (28a) for all $i \geq 2$. If $C \geq 0$ is a constant such that*

$$0 \geq \Phi_2''(t) \geq -C,$$

for all $t \in \big[\inf r_j, \sup r_j\big]$ then setting $\lambda := \frac{C}{l+C}$, we have that

$$|r_i| \leq \lambda^{i-1} |r_1|$$

for all $i \geq 2$.

Proof. We will only prove the result for $r_1 \geq 0$, since the other case is similar. Corollary 1 implies that $\sup r_j = r_1$ and $\inf r_j = 0$. By using the definitions of Φ_1 and Φ_2 and the Fundamental Theorem of Calculus, we may rewrite (28a) as

$$\begin{aligned} 0 &= \tfrac{1}{2}\Phi_2'\big(\tfrac{r_{i-1}+r_i}{2}\big) + \Phi_1'(r_i) + \tfrac{1}{2}\Phi_2'\big(\tfrac{r_i+r_{i+1}}{2}\big), \\ &= \tfrac{1}{2}\phi_2'\big(F_0 + \tfrac{r_{i-1}+r_i}{2}\big) + \phi_1'(F_0+r_i) + \tfrac{1}{2}\phi_2'\big(F_0 + \tfrac{r_i+r_{i+1}}{2}\big) - W'(F_0), \\ &= \tfrac{1}{2}\Big(\phi_2'\big(F_0 + \tfrac{r_{i-1}+r_i}{2}\big) - \phi_2'(F_0+r_i)\Big) + \tfrac{1}{2}\Big(\phi_2'\big(F_0 + \tfrac{r_i+r_{i+1}}{2}\big) - \phi_2'(F_0+r_i)\Big) \\ &\qquad + W'(F_0+r_i) - W'(F_0), \\ &= \int_{r_i}^{r_{i-1}} \Phi_2''\big(\tfrac{r_i+t}{2}\big)\,\mathrm{d}t + \int_{r_i}^{r_{i+1}} \Phi_2''\big(\tfrac{r_i+t}{2}\big)\,\mathrm{d}t + \int_0^{r_i} W''\big(F_0+t\big)\,\mathrm{d}t. \end{aligned}$$

Using the conclusion of Corollary 1 once more, $r_{i-1} \geq r_i \geq r_{i+1}$, so we have

$$\begin{aligned} 0 &= \int_{r_i}^{r_{i-1}} \Phi_2''\big(\tfrac{r_i+t}{2}\big)\,\mathrm{d}t - \int_{r_{i+1}}^{r_i} \Phi_2''\big(\tfrac{r_i+t}{2}\big)\,\mathrm{d}t + \int_0^{r_i} W''\big(F_0+t\big)\,\mathrm{d}t, \\ &\geq -\int_{r_i}^{r_{i-1}} C\;\mathrm{d}t + \int_0^{r_i} l\;\mathrm{d}t, \end{aligned}$$

which following from the assumed bound on the second derivative of Φ_2, and the l-convexity of W. Evaluating the integrals and rearranging gives

$$\lambda\, r_{i-1} \geq r_i,$$

which holds for any $i \geq 2$, and the decay estimate now follows by induction. □

Remark 5. It should immediately be noted that since r_i converges to zero exponentially as $i \to \pm\infty$, $r \in \ell^1(\mathbb{Z})$. This will be crucial in what follows.

We can now apply this characterisation of minimisers of $\tilde{E}_\infty$ to complete the proof of Proposition 5. Let the sequence of functions $y^{\varepsilon,\delta}$ be given by

$$y^{\varepsilon,\delta}(x) := \int_{-1/2}^{x} Dy^{\varepsilon,\delta}(t)\,\mathrm{d}t,$$

where we have set

$$\begin{aligned} Dy^{\varepsilon,\delta}(x) &:= \begin{cases} D_1\bar{y}_i + r_i - \bar{r}^\delta & x \in (x_i, x_{i+1}),\ i \in \{-K,\dots,K-1\}, \\ D_1\bar{y}_i & x \in (x_i, x_{i+1}),\ i \notin \{-K,\dots,K-1\}, \end{cases} \\ \bar{r}^\delta &:= \delta \sum_{i=-K}^{K-1} r_i, \end{aligned}$$

and $\delta := 1/(2K)$. We will prove estimates for $y^{\varepsilon,\delta}$, and then set δ as a function of ε in order to obtain the recovery sequence. Since $r \in \ell^1(\mathbb{Z})$, we have that

$$|\bar{r}^\delta| \leq \delta \sum_{i=-K}^{K-1} |r_i| \leq \delta \|r\|_{\ell^1(\mathbb{Z})}. \tag{30}$$

By construction, $y^{\varepsilon,\delta} \in \mathcal{A}^\varepsilon(L)$ as long as $\delta \geq \varepsilon$, i.e. $K \leq N$.

Ensuring $W(Dy^{\varepsilon,\delta})$ is well-defined. We now wish to check that $W(D_1 y_i^{\varepsilon,\delta})$ is well-defined. Since $\tilde{E}_\infty(r) < +\infty$, we have that for all $i \in \mathbb{Z}$,

$$W(F_0 + r_i) < +\infty \quad \Rightarrow \quad F_0 + r_i > 0.$$

Recalling from §3 that $F_0 = D\bar{y}(0) > 0$, and as $r \in \ell^2$, $r_i \to 0$ as $i \to \infty$, it follows that $F_0 + r_i$ is uniformly bounded away from 0. Next, by using the Mean Value Theorem and (30), we estimate for $i \in \{-K, \dots, K-1\}$ that

$$\begin{aligned}
|D_1 y_i^{\varepsilon,\delta} - F_0 - r_i| &= \left| \fint_{x_i}^{x_{i+1}} D\bar{y}\,\mathrm{d}x - \bar{r}^\delta - D\bar{y}(0) \right|, \\
&= |D\bar{y}(\xi) - \bar{r}^\delta - D\bar{y}(0)|, \\
&\leq \left| \int_0^\xi D^2\bar{y}(x)\,\mathrm{d}x \right| + \delta\|r\|_{\ell^1(\mathbb{Z})}, \\
&\leq |x_{i+1}| \|D^2\bar{y}\|_\infty + \delta\|r\|_{\ell^1(\mathbb{Z})}, \\
&\leq \frac{\varepsilon}{2\delta}\|D^2\bar{y}\|_\infty + \delta\|r\|_{\ell^1(\mathbb{Z})}.
\end{aligned}$$

On the second line, ξ is some point in (x_i, x_{i+1}), and on the final line we have used $|x_{i+1}| \leq K\varepsilon = \frac{\varepsilon}{2\delta}$. For fixed i, it is now clear that since $W(t)$ is Lipschitz for $t > 0$,

$$\left|W\big(D_1 y_i^{\varepsilon,\delta}\big) - W(F_0 + r_i)\right| \leq C\big(\tfrac{\varepsilon}{\delta} + \delta\big),$$

therefore $W(D_1 y_i^{\varepsilon,\delta})$ is finite when $\varepsilon \ll \delta \ll 1$. We can additionally estimate

$$\begin{aligned}
|D_1 y_i^{\varepsilon,\delta} - D\bar{y}(x)| &= \left| \fint_{x_i}^{x_{i+1}} \Big(D\bar{y}\,\mathrm{d}x - \bar{r}^\delta - D\bar{y}(x) \Big)\,\mathrm{d}x \right|, \\
&\leq \varepsilon\|D^2\bar{y}\|_\infty + \delta\|r\|_{\ell^2(\mathbb{Z})}.
\end{aligned} \tag{31}$$

Pointwise upper bounds on $s_i^{\varepsilon,\delta}$. Next, we define $s_i^{\varepsilon,\delta}$ in a similar fashion to (16), but adding and subtracting an extra $\phi_1(D_2 y_i^{\varepsilon,\delta})$ term, we have

$$\begin{aligned}
s_i^{\varepsilon,\delta} = \bigg(W(D_2 y_i^{\varepsilon,\delta}) - \fint_{x_i}^{x_{i+2}} W(D\bar{y})\,\mathrm{d}x \bigg) \\
+ \Big(\tfrac{1}{2}\phi_1(D_1 y_i^{\varepsilon,\delta}) + \tfrac{1}{2}\phi_1(D_1 y_{i+1}^{\varepsilon,\delta}) - \phi_1(D_2 y_i^{\varepsilon,\delta}) \Big) \\
+ \fint_{x_i}^{x_{i+2}} \Big(\sigma D\bar{u} - \sigma^\varepsilon D u^{\varepsilon,\delta} - \Sigma\left(Dy^{\varepsilon,\delta} - D\bar{y}\right) \Big)\,\mathrm{d}x, \\
=: T_1 + T_2 + T_3.
\end{aligned}$$

T_1 can be treated using Jensen's inequality and the convexity of W:

$$\begin{aligned}
T_1 &= W(D_2 y_i^{\varepsilon,\delta}) - \fint_{x_i}^{x_{i+2}} W(D\bar{y})\,\mathrm{d}x \\
&\le \tfrac{1}{2} W(D_1 y_i^{\varepsilon,\delta}) + \tfrac{1}{2} W(D_1 y_{i+1}^{\varepsilon,\delta}) - \fint_{x_i}^{x_{i+1}} W(D\bar{y})\,\mathrm{d}x, \\
&\le \fint_{x_i}^{x_{i+2}} W(Dy^{\varepsilon,\delta}) - W(D\bar{y})\,\mathrm{d}x, \\
&\le \fint_{x_i}^{x_{i+1}} W'(Dy^{\varepsilon,\delta})\big(Dy^{\varepsilon,\delta} - D\bar{y}\big)\,\mathrm{d}x. \qquad (32)
\end{aligned}$$

The final integral term, T_3, is bounded by

$$\begin{aligned}
T_3 &= \fint_{x_i}^{x_{i+2}} \sigma D\bar{u} - \sigma^{\varepsilon} Du^{\varepsilon,\delta} - \Sigma\left(Du^{\varepsilon,\delta} - D\bar{u}\right)\mathrm{d}x \\
&= \fint_{x_i}^{x_{i+2}} (\sigma + \Sigma)\big(D\bar{u} - Du^{\varepsilon,\delta}\big) + (\sigma - \sigma^{\varepsilon}) Du^{\varepsilon,\delta}\,\mathrm{d}x, \\
&\le \fint_{x_i}^{x_{i+2}} W'(D\bar{y})\big(D\bar{y} - Dy^{\varepsilon,\delta}\big)\,\mathrm{d}x + C\varepsilon^{3/2}\|Du^{\varepsilon,\delta}\|_2, \qquad (33)
\end{aligned}$$

using the Euler–Lagrange equations and the estimate proved in (21). The remaining part of the expression, T_2, can then be estimated as follows:

$$\begin{aligned}
T_2 &= \tfrac{1}{2}\phi_1(D_1 y_i^{\varepsilon,\delta}) + \tfrac{1}{2}\phi_1(D_1 y_{i+1}^{\varepsilon,\delta}) - \phi_1\big(D_2 y_i^{\varepsilon,\delta}\big) \\
&= \frac{1}{4}\int_{D_1 y_i^{\varepsilon,\delta}}^{D_1 y_{i+1}^{\varepsilon,\delta}} \int_{D_1 y_i^{\varepsilon,\delta}}^{D_1 y_{i+1}^{\varepsilon,\delta}} \phi_1''\big(\tfrac{s+t}{2}\big)\,\mathrm{d}s\,\mathrm{d}t, \\
&\le C\left|D_1 y_{i+1}^{\varepsilon,\delta} - D_1 y_i^{\varepsilon,\delta}\right|^2,
\end{aligned}$$

where we have used the fact that ϕ_1'' is bounded on the domain of integration for sufficiently small ε and δ, and $\phi_1 \in \mathrm{C}^2$. If $i \in \{-K, \dots, K-1\}$, then applying the Mean Value Theorem with $\xi \in (x_i, x_{i+1})$ and $\zeta \in (x_{i+1}, x_{i+2})$ gives

$$\begin{aligned}
\tfrac{1}{2}\phi_1(D_1 y_i^{\varepsilon,\delta}) + \tfrac{1}{2}\phi_1(D_1 y_{i+1}^{\varepsilon,\delta}) - \phi_1\big(D_2 y_i^{\varepsilon,\delta}\big) &\le C|D\bar{y}(\xi) - D\bar{y}(\zeta) + r_{i+1} - r_i|^2, \\
&\le C\Big(\|D^2\bar{y}\|_\infty \varepsilon + |r_i| + |r_{i+1}|\Big)^2, \\
&\le C\Big(\|D^2\bar{y}\|_\infty^2 \varepsilon^2 + |r_i|^2 + |r_{i+1}|^2\Big). \qquad (34)
\end{aligned}$$

In the case where $i \notin \{-K, \dots, K-1\}$, we obtain

$$\tfrac{1}{2}\phi_1(D_1 y_i^{\varepsilon,\delta}) + \tfrac{1}{2}\phi_1(D_1 y_{i+1}^{\varepsilon,\delta}) - \phi_1\big(D_2 y_i^{\varepsilon,\delta}\big) \le C\varepsilon^2\|D^2\bar{y}\|_\infty.$$

Adding together (32), (33) and (34), for $i \in \{-K-1, \dots, K-1\}$ we have

$$\begin{aligned} s_i^{\varepsilon,\delta} &\leq \fint_{x_i}^{x_{i+2}} \Big(W'(Dy^{\varepsilon,\delta}) - W'(D\bar{y})\Big)\big(Dy^{\varepsilon,\delta} - D\bar{y}\big)\,\mathrm{d}x + C\varepsilon^{3/2}\|Du^{\varepsilon,\delta}\|_2 \\ &\qquad + C\varepsilon^2 + C\big(|r_i|^2 + |r_{i+1}|^2\big), \\ &\leq C\fint_{x_i}^{x_{i+2}} |Dy^{\varepsilon,\delta} - D\bar{y}|^2\,\mathrm{d}x + C\Big(\varepsilon^{3/2} + \varepsilon^2 + |r_i|^2 + |r_{i+1}|^2\Big), \\ &\leq C\left(\big(\varepsilon+\delta\big)^2 + \varepsilon^{3/2} + \varepsilon^2 + |r_i|^2 + |r_{i+1}|^2\right), \\ &\leq C\left(\delta^2 + \varepsilon^{3/2} + \varepsilon^2 + |r_i|^2 + |r_{i+1}|^2\right), \end{aligned}$$

using $W' \in \mathrm{C}^1$, estimate (31) and Jensen's inequality. For the other indices, we obtain

$$\begin{aligned} s_i^{\varepsilon,\delta} &\leq \fint_{x_i}^{x_{i+2}} \Big(W'(Dy^{\varepsilon,\delta}) - W'(D\bar{y})\Big)\big(Dy^{\varepsilon,\delta} - D\bar{y}\big)\,\mathrm{d}x + C\varepsilon^{3/2}\|Du^{\varepsilon,\delta}\|_2, \\ &\leq C\left(\varepsilon^2 + \varepsilon^{3/2}\right). \end{aligned}$$

Conclusion of the argument. The two pointwise estimates just obtained imply

$$\begin{aligned} \sum_{i=-\infty}^{\infty} s_i^{\varepsilon,\delta} &\leq C\sum_{i=-N}^{N-1} \varepsilon^{3/2} + C\sum_{i=-K}^{K}\big(|r_i|^2 + \delta^2\big), \\ &\leq C\Big(\varepsilon^{1/2} + \|r\|^2_{\ell^2(\mathbb{Z})} + \delta\Big). \end{aligned}$$

By choosing $K = \lfloor\sqrt{N}\rfloor$, we have that $\delta \leq C\varepsilon^{1/2}$, and so an application of Fatou's Lemma with the pointwise upper bound we have just proven implies that

$$\begin{aligned} \limsup_{\varepsilon\to 0}\left(\sum_{i=-\infty}^{\infty} s_i^{\varepsilon,\delta} + \tilde{E}_{\mathrm{d}}\big(\mathcal{P}_\varepsilon y^{\varepsilon,\delta}\big)\right) &\leq \sum_{i=-\infty}^{\infty}\limsup_{\varepsilon\to 0} s_i^{\varepsilon,\delta} + \lim_{\varepsilon\to 0}\tilde{E}_{\mathrm{d}}\big(\mathcal{P}_\varepsilon y^{\varepsilon,\delta}\big), \\ &= \tilde{E}_\infty(r). \end{aligned}$$

This now proves Proposition 5, and concludes the proof of Theorem 4.1.

Remark 6. This result shows that the perturbation to the minimiser from the continuum model is confined to an exponentially thin boundary layer. Note that the linearisation of the functional $\tilde{E}_\infty$ in §1.4 yielded a similar solution structure; this exponential decay suggests that any interaction between defects of the type described here is likely to 'decouple' if one were to study a situation in which there were multiple defects of a fixed and finite number which are well-separated in the limit $\varepsilon \to 0$.

Conclusion. We have presented an analysis of a model for a point defect in a 1D chain of atoms interacting under assumptions which attempt to replicate a Lennard-Jones type interactions in an elastic regime. We have derived the 0^{th}-order Γ-limit, given in Theorem 2.1, which is identical to the limit when there is no defect.

In Theorem 4.1, we proved that the 1^{st}-order Γ-limit exists and gave an explicit characterisation of the limit as a discrete variational problem, the solution of which can be seen as the corrector to the elastic field predicted by the 0^{th}-order Γ-limit. In so doing, we proved Propositions 6 and 7, which show that solutions $r \in \ell^2(\mathbb{Z})$ exists, and have exponential decay — that is, they satisfy the bound $|r_i| \leq C\lambda^{|i|}$ with $0 \leq \lambda < 1$.

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