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ANALYSIS OF A PROTOTYPICAL MULTISCALE METHOD COUPLING ATOMISTIC AND CONTINUUM MECHANICS

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Abstract. In order to describe a solid which deforms smoothly in some region, but non smoothly in some other region, many multiscale methods have recently been proposed. They aim at coupling an atomistic model (discrete mechanics) with a macroscopic model (continuum mechanics). We provide here a theoretical ground for such a coupling in a one-dimensional setting. We briefly study the general case of a convex energy, and next concentrate on a specific example of a nonconvex energy, the Lennard-Jones case. In the latter situation, we prove that the discretization needs to account in an adequate way for the coexistence of a discrete model and a continuous one. Otherwise, spurious discretization effects may appear. We provide a numerical analysis of the approach.

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1. Introduction

Traditionally, mechanics makes use of a continuum description of matter [9, 15]. However, when nanoscale phenomena arise, the atomistic nature of material cannot be ignored: for instance, to understand how dislocations appear and propagate under a nanoindenter, one has to describe the deformed atomistic lattice. The situation is the same when the material is subjected to singular body forces, or is likely to break because of extensional forces. In all these examples, an appropriate model to describe the localized phenomena is the atomistic model, in which the solid is considered as a set of discrete particles interacting through given interatomic potentials.

Nevertheless, the size of the materials that can be simulated by only resorting to an atomistic description is very small in comparison with the size of the materials one is interested in. Indeed, for some phenomena we have mentioned above, it is not possible to make accurate computations by just considering a small piece of material, because large scale or bulk effects have to be accounted for. For instance, crack propagation depends on the far stress field (so there is an influence of the coarse scale onto the fine scale), and, at the same time, when crack propagates, it creates stress waves that modify the far stress field (so there is also a feedback influence of the fine scale onto the coarse scale).

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Fortunately, in the situations we have considered above, the deformation is smooth in the major part of the solid. Hence, a natural idea is to try to take advantage of both models, the continuous one and the atomistic one, by coupling them. The atomistic model is used in the zone where the deformation is expected to be non smooth, while the continuum description is used everywhere else. Many methods following this paradigm have been proposed and employed on realistic and complex situations: see [18, 25, 26] for some variational approaches (based on global minimizers), and [7] for time-dependent methods based on hybrid Hamiltonians. Notice that alternative ways, consisting in the approximation of the variational problems with a Γ-limit approach [5], or considering local minimizers instead of global ones [11], have also been considered.

We consider here a prototypical example of a variational method that couples a fine scale model in one zone with a coarse-grained model in another zone. This example is a toy-model for more advanced methods such as the Quasi-Continuum Method [12, 16, 18–22]. At least from the theoretical standpoint, a first key issue in the method is the *consistency* of the two models. Indeed, if the solution to be determined is smooth, then the solution given by the coarse-grained model should be the same as that given by the fine scale model, within an error controlled by the discretization parameters. A second issue is the *adaptivity* in the determination of the zones: we need to know where to use one model rather than the other one. Several multiscale methods that we have mentioned above include such an adaptation procedure, that seems however to lack from a rigorous basis.

The present work aims at giving such a theoretical basis for the micro-macro variational approach under study. The setting is one-dimensional. It is a clear limitation of the work. We have not been able to extend our analysis to the three-dimensional mechanically relevant case and it is not clear to us, even at the formal level, which of the results contained here may survive in the three-dimensional setting. We however hope that the present study will contribute to a better understanding of the fundamental issues.

1.1. **The atomistic and continuum problems**

Let us consider a one dimensional material, occupying in the reference configuration the domain $\Omega = (0, L)$. Let u be the deformation, *i.e.* the map defined on Ω such that $u(x)$ is the position, in the current configuration, of a material point that is at x in the reference configuration. This material is subjected to body forces f and to Dirichlet boundary conditions $u(0) = 0$ and $u(L) = a > 0$.

The solid will be described at two different space scales:

- the fine scale, at which the atomistic nature of the matter is taken into account;
- the coarse scale, which corresponds to a continuum description.

At the fine scale, the solid is considered as a set of $N+1$ atoms, whose current positions are $(u^i)_{i=0}^N$. The energy of the system is modelled by nearest-neighbour interactions:

$$E_\mu(u^0, \dots, u^N) = h \sum_{i=0}^{N-1} W\left(\frac{u^{i+1} - u^i}{h}\right) - h \sum_{i=0}^{N} u^i\, f(i\, h). \tag{1}$$

In this equation, W is the interaction potential between atoms and h is the atomic lattice parameter, which is linked to the number of atoms and the size of the solid by $L = Nh$. The potential W is normalized so that its minimum is attained at 1. The atomistic equilibrium configuration, denoted by $u_\mu = (u_\mu^0, \dots, u_\mu^N)$, is the solution[1] of the variational problem

$$I_\mu = \inf\left\{E_\mu(u^0, \dots, u^N),\ (u^0, \dots, u^N) \in X_\mu(a)\right\}, \tag{2}$$

where the minimizing space is

$$X_\mu(a) = \left\{(u^0, \dots, u^N),\ u^0 = 0,\ u^N = a,\ \forall i,\ u^{i+1} > u^i\right\}. \tag{3}$$

[1] Existence and uniqueness of solutions will be discussed in the next sections.

Recall that a deformation u of the solid is mechanically admissible only if it is an injective function. As we work in a one-dimensional setting and impose $u^N = a > 0 = u^0$, a necessary and sufficient condition for injectivity is that u is increasing, thus the constraint $u^{i+1} > u^i$ in (3).

On the other hand, at the coarse scale, the solid deformation is described by a map $u : \Omega \to \mathbb{R}$ chosen in the variational space

$$X_M(a) = \left\{u \in H^1(\Omega),\ u(0) = 0,\ u(L) = a,\ u \text{ is increasing on } \Omega\right\}. \tag{4}$$

The energy of the system reads

$$E_M(u) = \int_\Omega W(u'(x))\, \mathrm{d}x - \int_\Omega f(x)\, u(x)\, \mathrm{d}x. \tag{5}$$

We will give below (see Sect. 1.4.1) more precise assumptions to ensure that the energy is well-defined as soon as $u \in H^1(\Omega)$. The equilibrium configuration, denoted by $u_M(x)$, is a solution of the variational problem

$$I_M = \inf\left\{E_M(u),\ u \in X_M(a)\right\}. \tag{6}$$

Remark 1.1. In a two- or three-dimensional setting, some sufficient conditions for the injectivity of a map are given in [9], pp. 222–231.

The question we address in the present work concerns the approximation of problem (2). Indeed, for any deformation u of the material, the energy is given by (1), but the number of atoms to be considered in the sum, typically of the order 10^{23} in a macroscopic sample of material, makes the computation of (1) untractable in practice.

When the deformation u is regular and fixed independently of h, it has been shown in [4] that the atomistic energy $E_\mu(u(0), u(h), \ldots, u(Nh))$ converges to $E_M(u)$ when the atomic lattice parameter h goes to 0 and the number of atoms goes to infinity such that Nh remains constant, $Nh = L$. This result ensures the above mentioned *consistency* of the two descriptions, (1) on the one hand and (5) on the other hand, and also provides with an economical way to compute the sum (1), namely by approximating the integral (5). It remains that, when deformations that are expected to play a role are not regular enough to allow for the above convergence, the only way to compute the energy seems to be resorting to the atomistic expression (1). An economical approach is the coupled approach we consider in the present work.

1.2. **A coupled problem**

Let $\Omega_M \subset \Omega$ be an open subset of the solid in which the deformation u is supposed to be smooth enough so that the atomistic expression of the energy may be replaced by the continuum one. Throughout this article, we suppose that Ω_M satisfies the following property:

Property 1.1. For simplicity, we suppose

$$\Omega_M = \bigcup_{j=1}^{J} (a_j h, b_j h)\ \subset \Omega, \tag{7}$$

with $a_j, b_j \in \{0, \ldots, N\}$, $a_j < b_j < a_{j+1}$, and where the number J of connected components of Ω_M is bounded by $\mathcal{N}_{cc}$, where $\mathcal{N}_{cc}$ is a given fixed parameter (see Fig. 1).

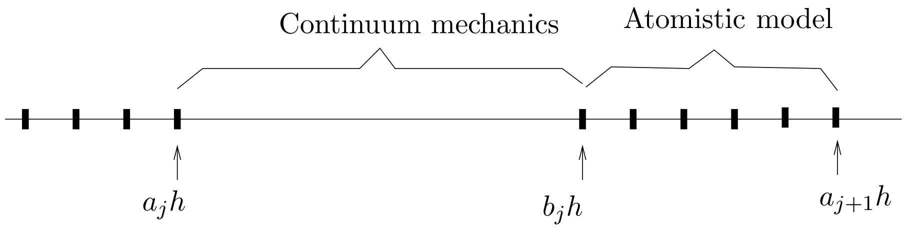

FIGURE 1. Partition of Ω into a regular zone Ω_M where the continuum mechanics model is used, and a singular zone Ω_μ where the atomistic model is used. By definition, we have $a_j h \in \Omega_\mu$ and $b_j h \in \Omega_\mu$.

Definition 1.1. Let us denote by

$$\mathbb{N}_\mu = \left\{ i \in \{0, \ldots, N-1\};\ ih \in \Omega_\mu \text{ and } ih + h \in \Omega_\mu \right\} \tag{8}$$

the set of indices i such that both atoms i and $i+1$ are contained in Ω_μ.

With (7), we can see that $\mathbb{N}_\mu = \cup_{j=1}^{J-1} \{b_j, \ldots, a_{j+1} - 1\}$.

For any partition $\Omega = \Omega_M \cup \Omega_\mu$, the solid deformation can be described by an element of the hybrid (atomistic/continuum) space

$$X_c(a, \Omega_M) = \left\{ \begin{array}{c} u;\ u_{|\Omega_M} \in X_W(\Omega_M), u_{|\Omega_\mu} \text{is the discrete set of variables} \, (u^i)_{ih \in \Omega_\mu}, \\ u\left((a_j h)^+\right) = u^{a_j},\ u\left((b_j h)^-\right) = u^{b_j}, \\ u \text{ is increasing on } \Omega \end{array} \right\}, \tag{9}$$

where $X_W(\Omega_M)$ is some functional space that depends on the potential W and that will be made precise below. We have written down the boundary conditions supposing that 0 and L are in $\overline{\Omega_M}$ (otherwise, adequate and simple modifications are in order). The last line in (9) is equivalent to the injectivity of u.

A natural idea is to first fix Ω_M, next, for each $u \in X_c(a, \Omega_M)$, to define the energy of the deformed system by

$$E_c(u) = h \sum_{i \in \mathbb{N}_\mu} W\left(\frac{u^{i+1} - u^i}{h}\right) - h \sum_{i, ih \in \Omega_\mu} u^i f(ih) + \int_{\Omega_M} W(u') - uf, \tag{10}$$

and finally to state a minimization problem at Ω_M fixed,

$$I_c(\Omega_M) = \inf \left\{ E_c(u),\ u \in X_c(a, \Omega_M) \right\}. \tag{11}$$

The point is unfortunately that Ω_M is difficult, or even impossible, to determine in advance. In fact, it depends on the minimizer u_μ of (2) as it should, vaguely stated, consist of all the zones of regularity of u_μ (in order to allow for both an economical and correct evaluation of the energy), and u_μ, which is the reference (ideal) solution, cannot be computed. In the case of a *convex* interaction potential W, it is possible to explicitly determine the zone Ω_M of regularity of u_μ. Consequently:

(1) when the atomistic solution u_μ is smooth in some region of Ω, the set Ω_M is a domain embedding this region;
(2) the minimization problem (11) is theoretically well posed;
(3) an algorithm can be proposed to compute a solution of (11);
(4) the error between the computed solution and the reference solution u_μ may be estimated.

Section 1.4 briefly presents the main mathematical statements corresponding to the above claims. On the other hand, we deal in Section 2 with a *nonconvex* interaction potential W, which is the mechanically relevant case.

The examination is performed on a special case of a nonconvex elastic energy density W, that is the Lennard-Jones case. Then, the minimization problem set with energy (10) is ill-posed. Both the continuum model and the atomistic model are unable to sustain traction (see Sects. 2.1 and 2.2), and a fracture appears for any extensional load. With the coupled model, a spurious effect appears in the energy functional (10): the comparison of the energy of a fracture in the zone Ω_μ with that of the same fracture in the zone Ω_M shows that the energetically most favorable situation is the latter (see Sect. 2.3). This rules out the possibility of ever self-consistently adapting the partition to the singularities of the deformation and leads us to a modification of the coupled energy: instead of defining it by (10), we define it by

$$E_{\rm mod}(u) = h \sum_{i\in\mathbb{N}_\mu} W\left(\frac{u^{i+1}-u^i}{h}\right) - h \sum_{i,ih\in\Omega_\mu} u^i f(ih) + \int_{\Omega_M} W^h(u') - uf\,, \tag{12}$$

with

$$W^h(r) = W(r) + \sqrt{h}\,\tau(r-r_0).$$

In the latter relation, r_0 is some threshold parameter (to be made precise below) and the function τ, which does not depend on h, is a regularization of the function $t \in \mathbb{R} \mapsto t_+ = \max(0,t)$. The minimization problem associated to the energy (12) reads

$$I_{\rm mod}(\Omega_M) = \inf\left\{E_{\rm mod}(u),\ u \in X_c(a,\Omega_M)\right\}. \tag{13}$$

This modification remedies to the above obstruction, and is also consistent both with the atomistic model energy (1) and the continuum mechanics model energy (5). Again, as in the convex case, Ω_M should consist of all the zones of regularity of the reference solution u_μ. In Sections 2.4 and 2.5, we show that this set can be approximated by a set (again denoted by Ω_M) that can be computed. We then show that the solution of the so-obtained problem (13) is a converging approximation of the reference solution u_μ, and that, when the solid is subjected to an extensional load, the atomistic domain $\Omega_\mu = \Omega \setminus \Omega_M$ contains the fracture.

1.3. **Outline of the article**

We wish to point out that the main purpose of the present work is to study the coupled (atomistic/continuum) models (11) and (13), in the nonconvex case, because this is the mechanically relevant case and the most interesting case from numerical analysis standpoint. But before going to this, we need to lay some groundwork. First, for the sake of comparison, we study in Section 1.4 the continuum, the atomistic and the coupled problems in the convex case. Next, in the nonconvex case, we need to study the continuum and the atomistic problems separately (this is performed in Sects. 2.1 and 2.2).

All these problems of Sections 1.4, 2.1, 2.2 have been addressed before in the literature (see [9,13,15,23,24]). But in the absence of a systematic mathematical study and with a view to self-consistency, we have chosen to still present them in the following way. For the case of a convex energy (Sect. 1.4), since the analysis is quite simple, the main results will be stated without any proofs. The detailed arguments and some additional comments can be found in [3,14]. In the nonconvex case, for the continuum and atomistic problems, we again state the main results, but postpone the proofs until appendices A, B and C. The reader, either familiar with such studies, or not mathematically oriented, may directly proceed to the heart of the matter, namely Sections 2.3, 2.4 and 2.5, where the most original results are discussed.

We collect now the main results of our work. At this stage, they are somewhat vaguely stated, but they will be made precise below.

(1) The atomistic problem (2) and the continuum problem (6) are well posed in the convex case (see *Lem.* 1.1) and in the Lennard-Jones case (see *Thms.* 2.1 and 2.3).

(2) In the convex case,
  - for any $\Omega_M \subset \Omega$, the coupled problem (11) is well posed (see *Lem.* 1.1);
  - it is possible to define Ω_M in such a way that the solution of the coupled problem (11) is a converging approximation of the solution of the atomistic problem (2) (see Def. 1.3 and *Thm.* 1.1).

(3) In the Lennard-Jones case,
  - for any $\Omega_M \subset \Omega$, the coupled problem (13) is well posed (see *Thm.* 2.5) and if a fracture appears, it is located in Ω_μ;
  - it is possible to define Ω_M in such a way that the solution of the modified coupled problem (13) is a converging approximation of the solution of the atomistic problem (2) (see *Thm.* 2.6 and Def. 2.1).

1.4. **The case of a convex elastic energy density** W

Let us first make precise the space $X_c(a, \Omega_M)$ defined in (9). In this section, we set $X_W(\Omega_M) = H^1(\Omega_M)$.

1.4.1. *Properties of the variational problems*

In this subsection, we provide conditions ensuring that the variational problems we consider are well-posed. Let us begin with a definition

Definition 1.2. We suppose that the body forces f satisfy

$$f \in \mathcal{C}^0\left(\overline{\Omega}\right). \tag{14}$$

Let us define F_M and F_μ by

$$\forall x \in \Omega,\ F_M(x) = \int_0^x f(s)\,\mathrm{d}s, \tag{15}$$

$$F_\mu^0 = 0 \quad \text{and} \quad \forall i \in \{1, \ldots, N\},\ F_\mu^i = h\sum_{j=1}^{i} f(jh). \tag{16}$$

For any Ω_M, we also define a function F_c as follows: on Ω_M, we set, for all $x \in (a_jh, b_jh)$, $j \in \{1, \ldots, J\}$,

$$F_c(x) = \int_{\Omega_M \cap (0,x)} f(s)\,\mathrm{d}s + h\sum_{k=1}^{j-1}\left(f(b_kh) + f(b_kh + h) + \ldots + f(a_{k+1}h)\right), \tag{17}$$

whereas, on Ω_μ, for all $j \in \{1, \ldots, J-1\}$, we set, for all $i \in \{b_j, \ldots, a_{j+1}\}$,

$$F_c^i = \int_{\Omega_M \cap (0,ih)} f(s)\,\mathrm{d}s + h\sum_{k=1}^{j-1}\left(f(b_kh) + \ldots + f(a_{k+1}h)\right) + h\sum_{q=b_j}^{i} f(qh). \tag{18}$$

We note that F_c is continuous on Ω_M, continuous at a_jh, but not continuous at b_jh. In the sequel of this section, we assume that the elastic energy density W satisfies

$$\begin{cases} W \in \mathcal{C}^2(\mathbb{R}), \\ \exists \alpha > 0,\ \forall x \in \mathbb{R}, \quad \alpha \le W''(x), \\ \exists \beta > 0, \forall x \in \mathbb{R}, \quad |W'(x)| \le \beta\,|x-1|. \end{cases} \tag{19}$$

Although W is defined on $\mathbb{R}$, we need in fact to know $W(x)$ only for $x > 0$, due to the injectivity constraint that is included in the variational spaces (3), (4) and (9). Let us set

$$a_M^* = \int_\Omega (W')^{-1} \Big(W'(0) + \sup_\Omega F_M - F_M(x) \Big) \,\mathrm{d}x, \tag{20}$$

$$a_\mu^* = h \sum_{i=0}^{N-1} (W')^{-1} \Big(W'(0) + \Big(\sup_{0\le i\le N-1} F_\mu^i \Big) - F_\mu^i \Big), \tag{21}$$

$$a_c^* = \int_{\Omega_M} (W')^{-1} \left(W'(0) + \overline{F_c} - F_c(x) \right) \mathrm{d}x + h \sum_{i\in\mathbb{N}_\mu} (W')^{-1} \left(W'(0) + \overline{F_c} - F_c^i \right), \tag{22}$$

where $\overline{F_c} = \sup(\sup_{x\in\Omega_M} F_c(x), \sup_{i\in\mathbb{N}_\mu} F_c^i)$. Then, we have:

Lemma 1.1 (existence and uniqueness of solutions)**.** *Let Ω_M be a fixed subdomain of Ω. We assume that the elastic energy density W satisfies* (19) *and that the body forces f satisfy* (14)*.*

If $a > a_M^*$, then the continuum problem (6) *has a unique minimizer u_M, which is in addition in $H^2(\Omega)$. If $a < a_M^*$, the problem* (6) *is not attained.*

If $a > a_\mu^*$, then the atomistic problem (2) *has a unique minimizer u_μ. If $a \le a_\mu^*$, then the problem* (2) *is not attained.*

If $a > a_c^*$, then the coupled problem (11) *has a unique minimizer u_c. If $a < a_c^*$, the problem* (11) *is not attained.*

Before proceeding further, let us recall the Euler-Lagrange equation for (2). Under the assumption $a > a_\mu^*$, the constraint $u^{i+1} > u^i$ is not active, thus

$$\forall i \in \{1,\ldots,N-1\}, \quad W'\left(\frac{u_\mu^i - u_\mu^{i-1}}{h}\right) - W'\left(\frac{u_\mu^{i+1} - u_\mu^i}{h}\right) - hf(ih) = 0. \tag{23}$$

An equivalent formulation is easily obtained:

$$\forall i \in \{0,\ldots,N-1\}, \quad \frac{u_\mu^{i+1} - u_\mu^i}{h} = (W')^{-1}\left(\lambda_\mu - F_\mu^i\right), \tag{24}$$

where $\lambda_\mu = W'\left((u_\mu^1 - u_\mu^0)/h\right)$ and F_μ is defined by (16). With similar arguments, it can be shown that the minimizer u_c of (11) satisfies

$$\begin{aligned} &\forall x \in \Omega_M, \ u_c'(x) = (W')^{-1}\left(\lambda_c - F_c(x)\right), \\ &\forall i \in \mathbb{N}_\mu, \quad \frac{u_c^{i+1} - u_c^i}{h} = (W')^{-1}\left(\lambda_c - F_c^i\right), \end{aligned} \tag{25}$$

where $\lambda_c = W'(u_c'(0))$ (recall we have assumed $0 \in \overline{\Omega_M}$), the set $\mathbb{N}_\mu$ is defined by (8) and F_c is defined by (17) and (18).

1.4.2. *Definition of the partition*

We now introduce a criterion in order to define the subdomain Ω_M. Actually, due to the convexity of W, which allows for elliptic regularity results on the Euler-Lagrange equation (23), the singularities of the solution u_μ are solely linked to the singularities of the body forces f. So the subdomain Ω_M is simply the zone of regularity of f. The situation will be radically different in the Lennard-Jones case (see Def. 2.1).

Definition 1.3 (partition in the convex case)**.** We assume that (14) is satisfied. Let $\kappa_f > 0$. We say that the interval $(ih, ih+h)$ is a *regular interval* if $f \in W^{1,1}(ih, ih+h)$ with

$$\forall x \in (ih, ih+h), \ |f(x)| \le \kappa_f \quad \text{and} \quad \int_{ih}^{ih+h} |f'(x)| \,\mathrm{d}x \le h\frac{\kappa_f}{L}\cdot$$

We define

$$\Omega_M = \bigcup^{*}_{(ih,ih+h)\ \text{regular}} (ih, ih+h) \quad \text{and} \quad \Omega_\mu = \Omega \setminus \Omega_M,$$

where $\bigcup^{*}$ means that the point $\{ih\}$ is also included in Ω_M if both $(ih-h, ih)$ and $(ih, ih+h)$ are regular intervals.

By construction, f and f' are bounded on Ω_M:

$$\|f\|_{L^\infty(\Omega_M)} \le \kappa_f \quad \text{and} \quad \|f'\|_{L^1(\Omega_M)} \le \kappa_f. \tag{26}$$

In Definition 1.2, we have introduced the functions F_M, F_μ and F_c (see (15), (16), (17) and (18)). An estimate of their difference is provided by the following lemma.

Lemma 1.2. *We assume that the body forces satisfy* (14) *and* (26). *Then*

$$\lim_{h\to 0} \sup_k \left|F_M(kh) - F_\mu^k\right| = 0, \tag{27}$$

and, for all h,

$$\begin{aligned} &\forall k \ s.t.\ kh \in \Omega_M,\ |F_c(kh) - F_\mu^k| \le h\kappa_f(\mathcal{N}_{cc}+1),\\ &\forall k \ s.t.\ kh \in \Omega_\mu,\ |F_c^k - F_\mu^k| \le h\kappa_f(\mathcal{N}_{cc}+1). \end{aligned} \tag{28}$$

1.4.3. *Comparison of the atomistic problem and the coupled problem*

In this subsection, we assume that the partition is defined according to Definition 1.3. We introduce:

Definition 1.4. The operator $\Pi_c : v_\mu \in X_\mu(a) \mapsto \Pi_c v_\mu \in X_c(a, \Omega_M)$ is the interpolation-on-Ω_M operator defined by

$$\forall x \in \Omega_M,\ (\Pi_c v_\mu)(x) = v_r(x), \quad \text{and} \quad \forall ih \in \Omega_\mu,\ (\Pi_c v_\mu)^i = v_\mu^i,$$

where v_r is the piecewise linear interpolate of v_μ, at points ih, in Ω_M.

The operator $\Pi_\mu : v_c \in X_c(a, \Omega_M) \mapsto \Pi_\mu v_c \in X_\mu(a)$ is the evaluation operator defined by

$$\forall ih \in \Omega_M,\ (\Pi_\mu v_c)^i = v_c(ih), \quad \text{and} \quad \forall ih \in \Omega_\mu,\ (\Pi_\mu v_c)^i = v_c^i.$$

Next, for any $u \in X_c$, we define

$$\|u\|_{L^\infty(X_c)} = \max\left(\|u\|_{L^\infty(\Omega_M)}, \max_{i, ih\in\Omega_\mu} |u^i|\right), \tag{29}$$

$$|u|_{W^{1,\infty}(X_c)} = \max\left(\|u'\|_{L^\infty(\Omega_M)}, \max_{i\in\mathbb{N}_\mu} \left|\frac{u^{i+1}-u^i}{h}\right|\right), \tag{30}$$

and for any $u \in X_\mu$,

$$\|u\|_{L^\infty(X_\mu)} = \max_{i\in[0,N]} |u^i| \quad \text{and} \quad |u|_{W^{1,\infty}(X_\mu)} = \max_{i\in[0,N-1]} \left|\frac{u^{i+1}-u^i}{h}\right|. \tag{31}$$

The main result for the comparison of the atomistic and the coupled problems in this convex case is the following:

Theorem 1.1. *We assume* (14), (19) *and*

$$a > a_M^*, \tag{32}$$

where a_M^* is defined by (20). *We also assume that the partition $\Omega = \Omega_M \cup \Omega_\mu$ is defined according to Definition 1.3 for some $\kappa_f > 0$. Let Π_c and Π_μ be the operators defined in Definition 1.4.*

Then there exist $h_0 \le 1$ (which depends on κ_f) and constants C_1 and $C_i(\kappa_f)$, $i = 2, \ldots, 5$, such that, for all $h \le h_0$, problems (2) *and* (11) *have unique minimizers, respectively denoted by u_μ and u_c. In addition these minimizers satisfy*

$$|u_c|_{W^{1,\infty}(X_c)} \le C_1 \quad \text{and} \quad |u_\mu|_{W^{1,\infty}(X_\mu)} \le C_1,$$

and are at a distance of order h from one another in the sense that

$$|(\Pi_\mu u_c) - u_\mu|_{W^{1,\infty}(X_\mu)} \le C_2(\kappa_f) h \kappa_f, \tag{33}$$

$$|u_c - (\Pi_c u_\mu)|_{W^{1,\infty}(X_c)} \le C_2(\kappa_f) h \kappa_f, \tag{34}$$

$$\|(\Pi_\mu u_c) - u_\mu\|_{L^\infty(X_\mu)} \le C_3(\kappa_f) h \kappa_f, \tag{35}$$

$$\|u_c - (\Pi_c u_\mu)\|_{L^\infty(X_c)} \le C_4(\kappa_f) h \kappa_f, \tag{36}$$

while the energy infima also differ of an order h:

$$|I_c(\Omega_M) - I_\mu| \le C_5(\kappa_f) h \kappa_f. \tag{37}$$

The constant C_1 does not depend on κ_f, and the functions $\kappa_f \mapsto C_i(\kappa_f)$, $i = 2, \ldots, 5$, are bounded on any compact set.

Remark 1.2. The proof (not included herein for the sake of brevity) yields the following explicit expressions for the constants C_i, $i = 1, \ldots, 5$:

$$C_1 = \frac{L}{4\alpha}\|f\|_{L^\infty(\Omega)} + 4\frac{a}{L}, \qquad C_2(\kappa_f) = \frac{2 + \mathcal{N}_{cc}}{\alpha}\left(1 + \frac{\beta_K(\kappa_f)}{\alpha}\right),$$
$$C_3(\kappa_f) = L\, C_2(\kappa_f), \quad C_4(\kappa_f) = C_2(\kappa_f)\, h + C_3(\kappa_f),$$
$$C_5(\kappa_f) = 2a + L\left(\beta\, C_2(\kappa_f)(C_1 + 1) + C_3(\kappa_f)\|f\|_{L^\infty(\Omega)}\right),$$

where $\beta_K(\kappa_f) = \max_K W''\left(W'(\cdot)\right)$.
Here, K is the closed interval of center 0 and of radius $h_0\kappa_f(1 + \mathcal{N}_{cc}) + \beta\,(C_1 + 1)$.

Remark 1.3. An alternative method to evaluate $u_\mu - u_c$ is based on the observation that minimizing E_μ over $X_\mu(a)$ is equivalent to minimizing E_c over a finite element space $X_c^h(a, \Omega_M) \subset X_c(a, \Omega_M)$ of mesh size h, where the body force integral term is now computed by a numerical integration formula (namely, a Riemann sum). So standard results of FEM theory can be applied in order to obtain an H^1 estimate on $u_\mu - u_c$. However, obtaining L^∞ estimates from such an argument is more tricky (see [6, 8, 10, 17]).

Remark 1.4. In view of Remark 1.3, the atomistic problem can be seen as a continuum problem posed on a finite element space of mesh size h. Therefore the convergence of order h for the "first derivative" of $u_c - u_\mu$ is sharp (see (33) and (34)). Using an argument *à la Aubin-Nitsche*, and assuming additionally that $W \in \mathcal{C}^3(\mathbb{R})$ and $f \in H^2(\Omega_M)$, one can improve (35) and (36) and show that, for h small enough,

$$\|(\Pi_\mu u_c) - u_\mu\|_{L^\infty(X_\mu)} + \|u_c - \Pi_c u_\mu\|_{L^\infty(X_c)} \le Ch^2$$

for some constant C that does not depend on h.

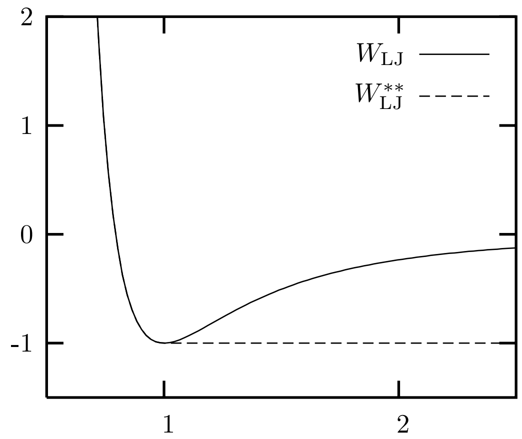

FIGURE 2. The Lennard-Jones potential (solid line) and its convex envelop (dashed line).

2. The Lennard-Jones case

In this section, the interaction potential is the Lennard-Jones potential

$$W_{\rm LJ}(r) = \frac{1}{r^{12}} - \frac{2}{r^6}, \tag{38}$$

which attains its minimum at 1: $W_{\rm LJ}(1) = \inf W_{\rm LJ} = -1$.

Let $W_{\rm LJ}^{**}$ be the convex envelop of $W_{\rm LJ}$, and let us set

$$r_c = \left(\frac{13}{7}\right)^{1/6} \approx 1.11,$$

such that $W_{\rm LJ}$ is convex on the interval $(0, r_c)$ and concave on $(r_c, +\infty)$. We also define the functions

$$\psi \ : \ (-\infty, W_{\rm LJ}'(r_c)) \to (0, r_c) \quad \text{such that} \quad \psi \circ W_{\rm LJ}' = \mathrm{Id}, \tag{39}$$

$$\varphi \ : \ (0, W_{\rm LJ}'(r_c)) \to (r_c, +\infty) \quad \text{such that} \quad \varphi \circ W_{\rm LJ}' = \mathrm{Id}. \tag{40}$$

For $x \leq 0$, we will also make use of the notation $\left(W_{\rm LJ}'\right)^{-1}(x) = \psi(x)$, as there is in such a case no ambiguity. We denote by $H(t)$ the Heaviside function ($H(t) = 0$ if $t < 0$, $H(t) = 1$ otherwise).

We use the Lennard-Jones potential as a prototype for a nonconvex interaction potential. One important feature allowing for the appearance of fracture is that $\lim\limits_{r\to\infty} W_{\rm LJ}(r)/r = 0$.

In Section 2.1, we study the continuum mechanics problem (6), and show that a fracture (a Dirac mass in the derivative of the deformation) appears for any extensional load. The atomistic model (2), studied in Section 2.2, exhibits the same behavior. For the sake of conciseness, and in order to concentrate on the coupled problem that will be dealt with in the subsequent sections, we have postponed the somewhat lengthy proofs of the main results of Sections 2.1 and 2.2 (namely *Thms.* 2.1, 2.2 and 2.3) to Appendices A–C. In Section 2.3, we study the coupled problem (11) where the energy is defined by (10). In Section 2.4, we study the modified coupled problem (13) with the energy (12). We then propose a way to build the atomistic-continuum partition (see Def. 2.1 below) such that the solution of the modified coupled problem approaches the solution of the atomistic problem. To build the partition, we will make use of a preliminary step: the determination of the solution of the continuum problem, a task which is assumed to be little demanding computationally in comparison with the resolution of a problem with a discrete component. The situation is thus different from the convex case in which we only use the given body forces f, and not the solution of the continuum problem, to define the partition.

Before entering the details, let us point out that the analysis below is highly dependent on the one-dimensional setting we chose here. However, the fact that the most natural way to couple the atomistic and the continuum models creates some difficulties (see Sect. 2.3) is more general, and occurs also in higher dimensions.

Remark 2.1. The results of this section do not depend on the particular choice of the exponents that we have made in (38). One would obtain the same results with the potential $W(r) = \frac{q}{r^p} - \frac{p}{r^q}$ with $p > q > 0$.

2.1. The continuum problem

We study in this subsection the continuum problem (6) for the Lennard-Jones potential, with $f \in L^1(\Omega)$. The natural variational space is

$$X_M(a) = \left\{ u \in W^{1,1}(\Omega), \quad \frac{1}{u'} \in L^{12}(\Omega), \quad u' > 0 \ a.e., \quad u(0) = 0, \quad u(L) = a \right\}, \tag{41}$$

which will possibly need to be enlarged in order for the energy (5) to have a minimizer, as will be seen below. Let us set

$$\theta_M = \int_\Omega \left(W'_{\mathrm{LJ}}\right)^{-1} (\inf F_M - F_M(x)) \, \mathrm{d}x, \tag{42}$$

$$v_1(x) = \left(W'_{\mathrm{LJ}}\right)^{-1} (\inf F_M - F_M(x)), \tag{43}$$

where F_M is defined by (15). We also recall (see [1,2]) the definition of the set

$$SBV(\Omega) = \left\{ u \in \mathcal{D}'(\Omega), \quad u' = D_a u + \sum_{i \in \mathbb{N}} v_i \delta_{x_i}, \quad D_a u \in L^1(\Omega), \quad x_i \in \Omega, \quad \sum_{i \in \mathbb{N}} |v_i| < +\infty \right\}.$$

We now state the main result of the present subsection. Its proof is contained in Appendix A.

Theorem 2.1 (minimizers of the continuum LJ model)**.** *If $\theta_M \geq a$, where θ_M is defined by* (42)*, then the problem*

$$I_M^1 = \inf \{ E_M(u), \ u \in X_M(a) \}, \tag{44}$$

where $X_M(a)$ is defined by (41) *and E_M is defined by* (5)*, has a unique minimizer.*

If $\theta_M < a$, then the problem (44) *is not attained, but the problem*

$$I_M^{BV} = \inf \left\{ E_M(u), \ u \in SBV(\Omega), \ \frac{1}{u'} \in L^{12}(\Omega), \ u' > 0, \ u(0) = 0, \ u(L) = a \right\} \tag{45}$$

has at least one minimizer. Moreover, $I_M^{BV} = I_M^1$ and the minimizers of the problem (45) *are the functions*

$$u(x) = \int_0^x v_1(t) \, \mathrm{d}t + \sum_{i \in \mathbb{I}} \tilde{v}_i H(x - x_i),$$

where $v_1 \in L^1(\Omega)$ is defined by (43)*, $\mathbb{I}$ is any countable set, and $\tilde{v}_i$ and x_i are any real numbers such that*

$$\sum_{i \in \mathbb{I}} \tilde{v}_i = a - \theta_M \quad \text{and} \quad \forall i \in \mathbb{I}, \ \tilde{v}_i > 0, \ x_i \in \arg\inf F_M.$$

Remark 2.2. Let $u \in SBV(\Omega)$: its derivative reads $u' = D_a u + \sum_i \tilde{v}_i \delta_{x_i}$ with $D_a u \in L^1(\Omega)$. The notation $u' > 0$ means $D_a u > 0$ *a.e.* on Ω and $\tilde{v}_i > 0$. When $u' > 0$, we also use the convention $\frac{1}{u'} = \frac{1}{D_a u}$. The reason is that the inverse of a regularization of u' converges to the inverse of $D_a u$ in the sense of distribution. Since $W_{\rm LJ}(+\infty) = 0$, we will also use the convention $W_{\rm LJ}(u') = W_{\rm LJ}(D_a u)$.

2.2. **The atomistic problem**

In this subsection, we study the atomistic problem (2), where the energy E_μ is given by (1) with $W \equiv W_{\rm LJ}$. In particular, we show that, for some particular choices of boundary conditions, a fracture appears. This means that the distance between a pair (and actually only one) of consecutive atoms is outstretched. The ideas of the proof are first explained on the simple case $f \equiv 0$. Next we deal with the general case, which is more technical. The main result of this subsection is Theorem 2.3, which is a generalization of some results given in [24].

2.2.1. *The case of no body force*

To study problem (2), we need the following lemma.

Lemma 2.1. *If $a > L$, there exists h_0 such that, for all $h \le h_0$, there exists a unique pair $(s(h), s_f(h)) \in \mathbb{R}^2$ such that*

$$1 \le s(h) \le 1 + h,\ W'_{\rm LJ}(s(h)) = W'_{\rm LJ}(s_f(h)) \text{ and } (L-h)s(h) + h s_f(h) = a. \tag{46}$$

In addition, we have the estimates

$$s_f(h) \sim_{h\to 0} \frac{a-L}{h} \quad \text{and} \quad s(h) - 1 \sim_{h \to 0} C_0 h^7,$$

for some C_0 that does not depend on h.

We skip the proof of Lemma 2.1, since it proceeds from an elementary study of the variations of the function $g(s) = W'_{\rm LJ}(s) - W'_{\rm LJ}\left(\frac{a-(L-h)s}{h}\right)$.

We now state

Theorem 2.2. *We suppose that there are no body force: $f \equiv 0$.*
If $a \le L$, then (2) has a unique minimizer, defined by $u_\mu^i = ih\, a/L$, $i = 0, \dots, N$.
If $a > L$, then there exists h_0 such that, for all $h \le h_0$, the minimizers of (2) are exactly the N discrete functions defined for $i_\mu \in \{0, \dots, N-1\}$ by

$$\frac{u_\mu^{i_\mu+1} - u_\mu^{i_\mu}}{h} = s_f(h) \quad \text{and} \quad \forall i \ne i_\mu,\ \frac{u_\mu^{i+1} - u_\mu^i}{h} = s(h), \tag{47}$$

where $s(h)$ and $s_f(h)$ are defined by Lemma 2.1.

The proof is contained in Appendix B.

2.2.2. *The general case*

We now assume that the body forces f are in $\mathcal{C}^0\left(\overline{\Omega}\right)$, and are not necessarily zero. This regularity assumption is needed for E_μ to be well-defined. For any configuration $u \in X_\mu(a)$, we define a partition of the set of indices $\{0, \dots, N-1\}$ in 3 different subsets:

$$G_1(u) = \left\{ i \in [0, N-1];\ 0 < \tfrac{u^{i+1} - u^i}{h} \le 1 \right\}, \quad G_2(u) = \left\{ i \in [0, N-1];\ 1 < \tfrac{u^{i+1} - u^i}{h} < r_c \right\},$$
$$G_3(u) = \left\{ i \in [0, N-1];\ r_c \le \tfrac{u^{i+1} - u^i}{h} \right\}.$$

Let us set

$$\underline{F_\mu} = \inf_{i=0,\dots,N-1} F_\mu^i, \tag{48}$$

$$\theta_\mu = h \sum_{i=0}^{N-1} (W'_{\rm LJ})^{-1}(\underline{F_\mu} - F_\mu^i), \tag{49}$$

where F_μ is defined by (16). In view of (27), we have $\lim_{h\to 0} \theta_\mu = \theta_M$, where θ_M, given by (42), is the threshold for appearance of a fracture in the continuum model (see *Thm.* 2.1). We note that, if $f \equiv 0$, $\theta_\mu = \theta_M = L$. To study problem (2), we need the following lemma:

Lemma 2.2 (estimate on the Lagrange multiplier for the atomistic problem (2))**.** *Let i_μ be an index such that $F_\mu^{i_\mu} = \underline{F_\mu}$, and let us assume that $a > \theta_M$.*

There exists h_0 such that, for all $h \le h_0$, there exists a unique λ_μ such that

$$0 < \lambda_\mu \le h \quad \textit{and} \quad h \sum_{i\in\{0,\dots,N-1\}, i\neq i_\mu} \psi\left(\underline{F_\mu} - F_\mu^i + \lambda_\mu\right) + h\varphi(\lambda_\mu) = a, \tag{50}$$

where ψ and φ are defined by (39) *and* (40)*.*

In addition, λ_μ does not depend on i_μ and satisfies $\lambda_\mu \sim_{h\to 0} C_0 h^7$, for some C_0 that does not depend on h.

The proof of Lemma 2.2 is rather simple and based on the study of the variations on $[0, h]$ of the function g_μ defined by $g_\mu(\lambda) = \lambda - W'_{\rm LJ}\left(\frac{a - h\sum_{i\neq i_\mu} \psi\left(\underline{F_\mu} - F_\mu^i + \lambda\right)}{h}\right)$. We now turn to Theorem 2.3 that is the main result of this section. Its proof is contained in Appendix C.

Theorem 2.3 (minimizers of the atomistic problem (2))**.** *We assume that $f \in \mathcal{C}^0\left(\overline{\Omega}\right)$. Let θ_μ be defined by* (49)*.*

If $a \le \theta_\mu$, then (2) *has a unique minimizer.*

If $a > \theta_M$, there exists h_0 such that, for all $h \le h_0$, the minimizers of (2) *are exactly the discrete functions defined for $i_\mu \in \{0, \dots, N-1\}$ such that $F_\mu^{i_\mu} = \underline{F_\mu}$ by $u_\mu^0 = 0$ and*

$$\frac{u_\mu^{i_\mu+1} - u_\mu^{i_\mu}}{h} = \varphi(\lambda_\mu) \quad \textit{and} \quad \forall i \neq i_\mu,\ \frac{u_\mu^{i+1} - u_\mu^i}{h} = \psi(\underline{F_\mu} - F_\mu^i + \lambda_\mu), \tag{51}$$

where λ_μ is defined by Lemma 2.2 and ψ and φ are defined by (39) *and* (40)*. In addition, $G_3(u_\mu) = \{i_\mu\}$ and*

$$\frac{u_\mu^{i_\mu+1} - u_\mu^{i_\mu}}{h} \sim_{h\to 0} \frac{a - \theta_M}{h}. \tag{52}$$

Remark 2.3. If $\theta_\mu < \theta_M$, Theorem 2.3 does not apply to $a \in (\theta_\mu, \theta_M]$. Note however that $\lim_{h\to 0} \theta_\mu = \theta_M$, thus all boundary conditions a are asymptotically covered.

2.3. **The natural coupled approach**

We study in this subsection the problem (11). We will see that this coupled problem, though natural, has a flaw. In order to illustrate this fact, we restrict ourselves to the case $f \equiv 0$ (see Rem. 2.6 below for the case $f \neq 0$). We also assume that

$$a > L,$$

so that a fracture must appear when minimizing (11). Note that if $a \le L$, the minimizers of the continuum and atomistic problems are equal and no singularity appears, and it is therefore not interesting to use a coupled method. We assume that $\Omega = (0, L)$ is partitioned into two subsets Ω_M and $\Omega_\mu = \Omega \setminus \Omega_M$, and that, for

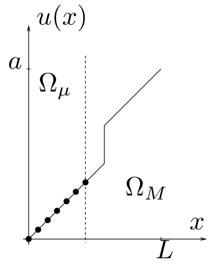

FIGURE 3. A minimizer of problem (11).

simplicity, $\Omega_\mu = (0, Kh], \quad \Omega_M = (Kh, L)$. We will see in Remark 2.4 below that the treatment of the general case follows exactly the same lines. Our aim is to study the minimization problem (11), where the variational space $X_c(a, \Omega_M)$ is defined by (9), with $X_W(\Omega_M) = SBV(\Omega_M)$, and where the corresponding energy E_c is given by (10), with $W \equiv W_{\rm LJ}$. The key ingredient of the mathematical analysis is the following observation. Let us choose $x_0 \in \Omega_M$ and let us consider the configurations $u_1 \in X_c(a, \Omega_M)$ and $u_2 \in X_c(a, \Omega_M)$ defined by

$$\begin{array}{ll} \forall i \in \{0, 1, \ldots, K\},\ u_1^i = ih, & \forall x \in \Omega_M,\ u_1(x) = x + (a - L) H(x - x_0), \\ \forall i \in \{1, \ldots, K\},\ u_2^i = ih + (a - L), & \forall x \in \Omega_M,\ u_2(x) = x + (a - L) \end{array} \tag{53}$$

and $u_2^0 = 0$. Within the configuration u_1 (resp. u_2), a fracture appears in Ω_M (resp. in Ω_μ). We have $E_c(u_1) = E_c(F \in \Omega_M) = L\, W_{\rm LJ}(1)$ and $E_c(u_2) = E_c(F \in \Omega_\mu) = L\, W_{\rm LJ}(1) + h + O(h^7)$, so

$$E_c(F \in \Omega_\mu) > E_c(F \in \Omega_M). \tag{54}$$

So, if the energy is defined by (10), a fracture costs less energy when it lies in Ω_M ($F \in \Omega_M$) than when it lies in Ω_μ ($F \in \Omega_\mu$). Hence, the fracture of the minimizers of (11) appears in Ω_M, as stated by the following lemma.

Lemma 2.3. *For h small enough, the minimizers of problem* (11) *are of the form*

$$u^i = ih \quad \forall i \in \{0, 1, \ldots, K\}, \tag{55}$$

$$u(x) = x + \sum_{i \in \mathbb{I}} \tilde{v}_i H(x - x_i), \quad \forall i,\ x_i \in (Kh, L),\ \tilde{v}_i > 0, \tag{56}$$

with $\mathbb{I} \subset \mathbb{N}$ and $\sum_{i \in \mathbb{I}} \tilde{v}_i = a - L$.

Proof. Since the minimum of $W_{\rm LJ}$ is attained at 1, we have $E_c(u) \geq Kh W_{\rm LJ}(1) + (L - Kh) W_{\rm LJ}(1)$, with a strict inequality if for some $i \in \{0, 1, \ldots K-1\}$, $\dfrac{u^{i+1} - u^i}{h} \neq 1$. Moreover, this value is attained when u is of the form (56). Conversely, if u is a minimizer, we necessarily have (55), and the restriction of u to Ω_M is thus a minimizer of

$$I_M^{Kh,L}(a - Kh) = \inf \left\{ \int_{Kh}^L W_{\rm LJ}(u'),\ u \in SBV(Kh, L),\ u' > 0, \frac{1}{u'} \in L^{12}(Kh, L), \quad u(Kh) = Kh,\ u(L) = a \right\}.$$

Now, Theorem 2.1 implies that a minimizer of this problem satisfies (56). $\square$

Remark 2.4. The case of a general set Ω_μ may be treated likewise. Then, any minimizer of problem (11) satisfies:

$$\begin{aligned} u^{i+1} - u^i &= h \quad \forall i \text{ s.t. } ih \in \Omega_\mu \text{ and } ih + h \in \Omega_\mu, \\ u' &= 1 + \sum_{i \in \mathbb{I}} \tilde{v}_i \delta_{x_i} \text{ in } \Omega_M, \quad \forall i,\ x_i \in \Omega_M, \quad \tilde{v}_i > 0, \quad \text{and } \sum_{i \in \mathbb{I}} \tilde{v}_i = a - L. \end{aligned}$$

The above argument shows that, in the simplest case where we expect a fracture of the material, for any partition of the domain Ω into a regular domain Ω_M and a singular one Ω_μ, the fracture naturally appears in the regular one.

Hence, if the following algorithm is used to compute an approximation of u_μ: initialize Ω_μ to $\emptyset$,

(1) solve (11) for $\Omega_M = \Omega \setminus \Omega_\mu$;
(2) find the set where the solution u_c of (11) has a large derivative, enlarge Ω_μ correspondingly if necessary and go back to 1,

then Ω_μ converges to Ω, because, at each step, the above algorithm computes a solution having a singularity in the set Ω_M. The latest iterations are therefore as costly as the determination of the atomistic solution.

Remark 2.5. A way around the above difficulty might be to allow the set Ω_μ to shrink back if the computed minimizer happens to be regular enough (in some sense) in Ω_μ. However, we have not been able to solve the difficulty with this alternative strategy.

Remark 2.6. The preceding analysis can be carried out in the case of a force $f \neq 0$ satisfying $f \in \mathcal{C}^0(\overline{\Omega})$. Let us assume that $a > \theta_M$, where θ_M is defined by (42), and that $\inf_{x \in \Omega_M} F_c(x) = \inf_{i \in \mathbb{N}_\mu} F_c^i$, where F_c is defined by (17) and (18). Let $E_c(F \in \Omega_M)$ (resp. $E_c(F \in \Omega_\mu)$) be the energy of a configuration with a fracture in Ω_M (resp. Ω_μ). Then the inequality (54) holds.

2.4. **A modified coupled approach**

In this subsection, we propose a way to build a coupled problem that remedies to the difficulties observed in the previous subsection.

We again assume, for the time being, that the partition $\Omega = \Omega_M \cup \Omega_\mu$ is given. We show in Theorem 2.5 that the modified coupled variational problem (13) is well-posed. In Theorem 2.6, we show that its solution is a converging approximation of the solution to the atomistic problem (2), and in Section 2.5, we will propose a definition of the partition (see Def. 2.1 below).

The variational space we work with is $X_c(a, \Omega_M)$ defined by (9) with

$$X_W(\Omega_M) = \left\{ u;\ u \in W^{1,1}(\Omega_M),\ \frac{1}{u'} \in L^{12}(\Omega_M) \right\}.$$

As announced in the Introduction, the modified coupled energy is given by

$$E_{\text{mod}}(u) = h \sum_{i \in \mathbb{N}_\mu} W_{\text{LJ}} \left(\frac{u^{i+1} - u^i}{h} \right) - h \sum_{i, ih \in \Omega_\mu} u^i f(ih) + \int_{\Omega_M} W_{\text{LJ}}^h(u') - uf\,,$$

with

$$W_{\text{LJ}}^h(r) = W_{\text{LJ}}(r) + \sqrt{h}\ \tau(r - r_0).$$

Here, r_0 is any real number in $(1, r_c)$ and the function τ is a regularization of the function $t \in \mathbb{R} \mapsto t_+ = \max(0, t)$ (in particular, it does not depend on h).

The energy E_{mod} differs from the natural coupled energy E_c given by (10) by the use of the energy density W_{LJ}^h instead of W_{LJ} on the continuum domain Ω_M. Let us explain this choice, assuming that there are no body forces. According to the definition (12), the energy of the fractured configurations (53) reads $E_{\rm mod}(F \in \Omega_\mu) = LW_{\rm LJ}(1) + h + O(h^7)$ and $E_{\rm mod}(F \in \Omega_M) = LW_{\rm LJ}(1) + (a-L)\sqrt{h}$, so

$$E_{\rm mod}(F \in \Omega_\mu) < E_{\rm mod}(F \in \Omega_M). \tag{57}$$

If we compare (54) and (57), we see that, with the modified definition of the coupled energy, a fracture costs now less energy when it lies in Ω_μ than when it lies in Ω_M.

Remark 2.7. It is worth emphasizing that the additional term $\sqrt{h}\tau(r-r_0)$ inserted in $W^h_{\rm LJ}$ is by no means the only manner to successfully modify the interaction potential. We only use the fact that $\sqrt{h} \longrightarrow 0$ and $h \ll \sqrt{h}$.

Let us now assume that the solution u_μ of the atomistic problem (2) shows a fracture (on the atom i_μ), and that we want to use a coupled model to compute an approximation of u_μ. At this point, the domain Ω_M is unknown. In order to determine both Ω_M and an approximation of u_μ, a possible algorithm is the one already given in the previous subsection, which consists in iterating over two steps, first solve a coupled problem with Ω_M fixed, second modify the partition according to the computed solution. Assume now that, at some moment, a "correct" partition has been found, in the sense that the atom i_μ (where we expect the fracture to take place) belongs to Ω_μ. At that moment, we want the algorithm to stop, because the zone Ω_μ is satisfactory. Let us consider the minimization problem of the first step of the algorithm. The position of the fracture is such that its energy cost is minimal. If one works with the coupled energy (10), then, as explained in the previous subsection, the fracture is located in Ω_M, which is not satisfactory. If one works with the modified coupled energy (12), then, in view of (57), the fracture is located in Ω_μ and the computed solution is smooth in Ω_M, so the partition is not updated and the algorithm stops.

The difference between E_c defined by (10) and $E_{\rm mod}$ defined by (12) is of order $\sqrt{h}$, that is a small quantity (recall that h is the atomic lattice parameter). However, even if it is small, this correction has an influence on the choices of the zones, since it allows for the zone Ω_μ to contain the fracture.

Before studying the modified coupled problem (13), we study the continuum problem with energy density $W^h_{\rm LJ}$. The following Theorem (which is to be compared with Theorem 2.1) will be needed in the sequel.

Theorem 2.4. *Consider the energy E^h_M defined by*

$$E^h_M(u) = \int_\Omega W^h_{\rm LJ}(u'(x)) - f(x)u(x)\,{\rm d}x.$$

Let us set $\beta^h(x) \in (0, r_c)$ such that $W'_{\rm LJ}(\beta^h(x)) = \sqrt{h} + \inf F_M - F_M(x)$ and $\theta^h_M = \int_\Omega \beta^h(x)\,{\rm d}x$.

If $\theta^h_M \geq a$, then the problem

$$\inf\left\{E^h_M(u), \quad u \in W^{1,1}(\Omega), \quad \frac{1}{u'} \in L^{12}(\Omega), \quad u' > 0 \text{ a.e.}, \quad u(0) = 0, \quad u(L) = a\right\} \tag{58}$$

has a unique minimizer which reads $u(x) = \int_0^x \psi\left(-\lambda + \inf F_M - F_M(s)\right){\rm d}s$ for some $\lambda \geq -\sqrt{h}$ and where ψ is defined by (39)*.*

If $\theta^h_M < a$, then (58) *is not attained, but the problem*

$$\inf\left\{E^h_M(u), \quad u \in SBV(\Omega), \quad \frac{1}{u'} \in L^{12}(\Omega), \quad u' > 0, \quad u(0) = 0, \quad u(L) = a\right\} \tag{59}$$

has at least one minimizer.
Moreover, the minimizers of (59) *are exactly the functions $u(x) = \int_0^x \beta^h(t)\,{\rm d}t + \sum_{i\in\mathbb{I}} \tilde v_i H(x - x_i)$, where $\mathbb{I}$ is any countable set, and $\tilde v_i$ and x_i are any real numbers such that*

$$\sum_{i\in\mathbb{I}} \tilde v_i = a - \theta^h_M \quad \text{and} \quad \forall i \in \mathbb{I},\ \tilde v_i > 0,\ x_i \in \arg\inf F_M.$$

We skip the proof of Theorem 2.4, which is an easy adaptation of the proof of Theorem 2.1.

We now study the existence and the uniqueness of solutions of the modified coupled problem (13). Let F_c be defined by (17) and (18), and let us set

$$\underline{F_c} = \inf\left(\inf_{\Omega_M} F_c, \inf_{i\in\mathbb{N}_\mu} F_c^i\right).$$

The threshold for the appearance of a fracture will be shown to be

$$\theta_{\text{mod}} = \int_{\Omega_M} (W'_{\text{LJ}})^{-1}\left(\underline{F_c} - F_c(x)\right)\,\mathrm{d}x + h\sum_{i\in\mathbb{N}_\mu} (W'_{\text{LJ}})^{-1}\left(\underline{F_c} - F_c^i\right).$$

Remark 2.8. The modified coupled problem (13) could have been introduced in the convex case, although it was not needed (the coupled problem (11) leads to satisfactory results). In this case, one would have proved results similar to those given in Lemma 1.1 and Theorem 1.1.

To study the problem (13), we need the following lemma:

Lemma 2.4. *Let us assume that $a > \theta_M$, where θ_M is defined by* (42)*, and that the partition is such that, for any h small enough, there exists $i_{mod} \in \mathbb{N}_\mu$ such that*

$$\underline{F_c} \le F_c^{i_{mod}} \le \underline{F_c} + Ch \tag{60}$$

for some constant C that does not depend on h.

Then there exists h_0 such that, for all $h \le h_0$, there exists a unique λ_{mod} such that $0 \le \lambda_{mod} \le Ch$ and

$$h\sum_{i\in\mathbb{N}_\mu, i\neq i_{mod}} \psi\left(\underline{F_c} - F_c^i + \lambda_{mod}\right) + h\varphi(\underline{F_c} - F_c^{i_{mod}} + \lambda_{mod}) + \int_{\Omega_M} \psi\left(\underline{F_c} - F_c(x) + \lambda_{mod}\right)\,\mathrm{d}x = a \tag{61}$$

where ψ and φ are defined by (39) *and* (40)*.*

Proof. Let us define $g_{\text{mod}}(\lambda) = \lambda + \underline{F_c} - F_c^{i_{\text{mod}}} - W'_{\text{LJ}}\left(\frac{p_{\text{mod}}(\lambda)}{h}\right)$ on $[0, 2Ch]$, where

$$p_{\text{mod}}(\lambda) = a - h\sum_{i\in\mathbb{N}_\mu, i\neq i_{\text{mod}}} \psi\left(\underline{F_c} - F_c^i + \lambda\right) - \int_{\Omega_M} \psi\left(\underline{F_c} - F_c(x) + \lambda\right)\,\mathrm{d}x.$$

For h small enough, g_{mod} is an increasing function and $g_{\text{mod}}(2Ch) \ge Ch - W'_{\text{LJ}}\left(\frac{a-\theta_M}{2h}\right) > 0$. Moreover, $g_{\text{mod}}(0) < 0$. Hence there exists a unique $\lambda_{\text{mod}} \in [0, 2Ch]$ such that $g_{\text{mod}}(\lambda_{\text{mod}}) = 0$. □

Theorem 2.5 (minimizers of the modified coupled problem)**.** *We assume that $f \in \mathcal{C}^0(\overline{\Omega})$ and that there exists $\varepsilon_f > 0$ such that* (26) *is satisfied.*

If $a \le \theta_{mod}$, then problem (13) *has a unique minimizer u_{mod}, which is smooth: there exists C_0 independent of h such that*

$$|u_{mod}|_{W^{1,\infty}(X_c)} \le C_0, \tag{62}$$

where $|\cdot|_{W^{1,\infty}(X_c)}$ is defined by (30)*.*

If $a > \theta_M$, and if

$$\exists i_0 \in \mathbb{N}_\mu \text{ such that } \underline{F_\mu} \le F_\mu^{i_0} \le \underline{F_\mu} + C_1 h, \tag{63}$$

for some constant $C_1 \ge 0$ independent of h (recall $\underline{F_\mu}$ is defined by (48)*), then there exists $h_0 > 0$ such that, for all $h \le h_0$, the minimizers of* (13) *are exactly the functions defined, for $i_{mod} \in \mathbb{N}_\mu$ such that $F_c^{i_{mod}} = \inf_{i\in\mathbb{N}_\mu} F_c^i$,* *by* $u_{mod}(0) = 0$ *and*

$$\begin{cases} u'_{mod}(x) = \psi\left(\lambda_{mod} + \underline{F_c} - F_c(x)\right) \ \textit{on } \Omega_M, \\ \dfrac{u_{mod}^{i+1} - u_{mod}^{i}}{h} = \psi\left(\lambda_{mod} + \underline{F_c} - F_c^i\right) \ \textit{for all } i \in \mathbb{N}_\mu, i \neq i_{mod}, \\ \dfrac{u_{mod}^{i_{mod}+1} - u_{mod}^{i_{mod}}}{h} = \varphi\left(\lambda_{mod} + \underline{F_c} - F_c^{i_{mod}}\right), \end{cases} \tag{64}$$

where λ_{mod} *is defined by Lemma 2.4.*

Remark 2.9. If $\theta_{\rm mod} < \theta_M$, Theorem 2.5 does not apply to $a \in (\theta_{\rm mod}, \theta_M]$. Note however that $\lim_{h\to 0} \theta_{\rm mod} = \theta_M$, thus all boundary conditions a are asymptotically covered.

Proof of Theorem 2.5. The proof in the case $\theta_{\rm mod} \geq a$ follows the same pattern as the proof of Theorem 2.1 (in the case $\theta_M \geq a$). We concentrate on the case $a > \theta_M$. Let us set

$$P_x^c(t) = W_{\rm LJ}^h(t) + \left(F_c(x) - \underline{F_c}\right)t, \tag{65}$$

$$P_i^c(t) = W_{\rm LJ}(t) + (F_c^i - \underline{F_c})t, \tag{66}$$

and, for $i \in \mathbb{N}_\mu$,

$$v_{1,c}^i = (W'_{\rm LJ})^{-1}\left(\underline{F_c} - F_c^i\right). \tag{67}$$

For $x \in \Omega_M$, we also define $\beta_x^c \in (0, r_c)$ such that

$$W'_{\rm LJ}(\beta_x^c) = \sqrt{h} + \underline{F_c} - F_c(x). \tag{68}$$

We first reformulate the energy $E_{\rm mod}$, which reads
$E_{\rm mod}(u) = \int_{\Omega_M} P_x^c(u'(x))\,{\rm d}x + h\sum_{i\in\mathbb{N}_\mu} P_i^c\left(\frac{u^{i+1}-u^i}{h}\right) + a\left(\underline{F_c} - F_c(L)\right).$
Let us consider the problem

$$\overline{I}_{\rm mod} = \inf\left\{\overline{E}_{\rm mod}(v),\ v \in Y_c(a, \Omega_M)\right\}, \tag{69}$$

where $\overline{E}_{\rm mod}$ is given by

$$\overline{E}_{\rm mod}(v) = \int_{\Omega_M} P_x^c(v(x))\,{\rm d}x + h\sum_{i\in\mathbb{N}_\mu} P_i^c(v^i), \tag{70}$$

and where $Y_c(a, \Omega_M)$ is given by

$$Y_c(a, \Omega_M) = \left\{ \begin{array}{c} v;\ v \in L^1(\Omega_M),\ \dfrac{1}{v} \in L^{12}(\Omega_M),\ v_{|\mathbb{N}_\mu} \text{ is the discrete set} \\ \text{of variables } (v^i)_{i\in\mathbb{N}_\mu},\ v > 0,\ \displaystyle\int_{\Omega_M} v + h\sum_{i\in\mathbb{N}_\mu} v^i = a \end{array} \right\}. \tag{71}$$

Clearly, $I_{\rm mod} = \overline{I}_{\rm mod} + a\left(\underline{F_c} - F_c(L)\right)$ and u is a minimizer of (13) if and only if v, defined by $\forall x \in \Omega_M$, $v(x) = u'(x)$ and $\forall i \in \mathbb{N}_\mu,\ v^i = \frac{u^{i+1}-u^i}{h}$, is a minimizer of (69).

Step 1 (a lower bound on the atomistic deformation)**.** Let u_n be a minimizing sequence of problem (13) and let v_n be the associated minimizing sequence of problem (69). Since u_n is an increasing function, we have $0 \leq v_n^i \leq a/h$ for all i in $\mathbb{N}_\mu$. So, up to a subsequence extraction, we can assume that the sequence $\left(v_n^i\right)_n$ converges. Let us set

$$a_\mu^\infty = \lim_{n\to+\infty} h\sum_{i\in\mathbb{N}_\mu} v_n^i. \tag{72}$$

As $\int_{\Omega_M} v_n + h \sum_{i\in\mathbb{N}_\mu} v_n^i = a$, we can also define $a_M^\infty = \lim_{n\to+\infty} \int_{\Omega_M} v_n(x)\,\mathrm{d}x = a - a_\mu^\infty$. Let us establish a lower bound on a_μ^∞. For all $t > 0$, we have

$$P_x^c(t) \geq P_x^c(\beta_x^c) + \sqrt{h}\,(t - \beta_x^c), \tag{73}$$

$$P_i^c(t) \geq P_i^c(v_{1,c}^i), \tag{74}$$

where P_x^c, P_i^c, β_x^c and $v_{1,c}$ are defined by (65), (66), (68) and (67). We now consider (70) with $v \equiv v_n$. With (73) and (74), we obtain

$$\overline{I}_{\mathrm{mod}} \geq \int_{\Omega_M} P_x^c(\beta_x^c)\,\mathrm{d}x + \sqrt{h}\left(a_M^\infty - \int_{\Omega_M} \beta_x^c\,\mathrm{d}x\right) + h \sum_{i\in\mathbb{N}_\mu} P_i^c(v_{1,c}^i). \tag{75}$$

Let us now choose $i_{\mathrm{mod}} \in \mathbb{N}_\mu$ such that $F_c^{i_{\mathrm{mod}}} = \inf_{i\in\mathbb{N}_\mu} F_c^i$. With (63) and (28), we see that

$$\underline{F_c} \leq F_c^{i_{\mathrm{mod}}} \leq \underline{F_c} + Ch \tag{76}$$

for some constant C that does not depend on h. Let us consider the test function v_b defined by $v_b(x) = \beta_x^c$ in Ω_M, $v_b^i = v_{1,c}^i$ for all $i \in \mathbb{N}_\mu$, $i \neq i_{\mathrm{mod}}$, and $v_b^{i_{\mathrm{mod}}}$ such that $\int_{\Omega_M} v_b + h \sum_{i\in\mathbb{N}_\mu} v_b^i = a$. By construction, we have

$$v_b^{i_{\mathrm{mod}}} \sim_{h\to 0} (a - \theta_M)/h. \tag{77}$$

The function β_x^c is continuous and positive, and $v_b^i > 0$ for all $i \in \mathbb{N}_\mu$. So v_b is a test function for (69), and we have

$$\overline{I}_{\mathrm{mod}} \leq \overline{E}_{\mathrm{mod}}(v_b) = \int_{\Omega_M} P_x^c(\beta_x^c)\,\mathrm{d}x + h \sum_{i\in\mathbb{N}_\mu} P_i^c(v_{1,c}^i) + hP_{i_{\mathrm{mod}}}^c(v_b^{i_{\mathrm{mod}}}) - hP_{i_{\mathrm{mod}}}^c(v_{1,c}^{i_{\mathrm{mod}}}). \tag{78}$$

The last two terms of (78) satisfy

$$hP_{i_{\mathrm{mod}}}^c(v_b^{i_{\mathrm{mod}}}) - hP_{i_{\mathrm{mod}}}^c(v_{1,c}^{i_{\mathrm{mod}}}) = h\left(W_{\mathrm{LJ}}(v_b^{i_{\mathrm{mod}}}) - W_{\mathrm{LJ}}(v_{1,c}^{i_{\mathrm{mod}}})\right) + h(F_c^{i_{\mathrm{mod}}} - \underline{F_c})(v_b^{i_{\mathrm{mod}}} - v_{1,c}^{i_{\mathrm{mod}}}). \tag{79}$$

We now bound this quantity. From (67), we have $0 < v_{1,c}^{i_{\mathrm{mod}}} \leq 1$, thus $W_{\mathrm{LJ}}(v_{1,c}^{i_{\mathrm{mod}}}) \geq W_{\mathrm{LJ}}(1)$. With this inequality and (77), we obtain

$$h\left(W_{\mathrm{LJ}}(v_b^{i_{\mathrm{mod}}}) - W_{\mathrm{LJ}}(v_{1,c}^{i_{\mathrm{mod}}})\right) \leq Ch \tag{80}$$

for some C that does not depend on h. Since $\lim_{h\to 0} h(v_b^{i_{\mathrm{mod}}} - v_{1,c}^{i_{\mathrm{mod}}}) = a - \theta_M$, we infer from (76) that

$$h(F_c^{i_{\mathrm{mod}}} - \underline{F_c})(v_b^{i_{\mathrm{mod}}} - v_{1,c}^{i_{\mathrm{mod}}}) \leq Ch \tag{81}$$

for some C that does not depend on h. Collecting (80) and (81), we obtain $hP_{i_{\mathrm{mod}}}^c(v_b^{i_{\mathrm{mod}}}) - hP_{i_{\mathrm{mod}}}^c(v_{1,c}^{i_{\mathrm{mod}}}) \leq Ch$. Inserting this inequality in (78) and making use of (75), we see that $a_M^\infty - \int_{\Omega_M} \beta_x^c\,\mathrm{d}x \leq C\sqrt{h}$. Since $\theta_M = \lim_{h\to 0}\left(\int_{\Omega_M} \beta_x^c\,\mathrm{d}x + \int_{\Omega_\mu} (W_{\mathrm{LJ}}')^{-1}(\inf F_M - F_M(x))\,\mathrm{d}x\right)$, we obtain, for h small enough, the following lower bound on a_μ^∞:

$$\frac{a - \theta_M}{2} + \int_{\Omega_\mu} (W_{\mathrm{LJ}}')^{-1}(\inf F_M - F_M(x))\,\mathrm{d}x \leq a_\mu^\infty. \tag{82}$$

Step 2 (an auxiliary problem)**.** For any positive real numbers a_M and a_μ, let us define

$$I_M(a_M) = \inf\left\{\int_{\Omega_M} P_x^c(v(x))\,\mathrm{d}x,\ v \in L^1(\Omega_M),\ \frac{1}{v} \in L^{12}(\Omega_M), v > 0\ a.e.\ \text{on}\ \Omega_M,\ \int_{\Omega_M} v = a_M\right\} \tag{83}$$

and

$$I_\mu(a_\mu) = \inf\left\{h\sum_{i\in\mathbb{N}_\mu} P_i^c(v^i),\ v^i > 0,\ h\sum_{i\in\mathbb{N}_\mu} v^i = a_\mu\right\}. \tag{84}$$

Problem (83) (resp. (84)) can be studied with arguments similar to the ones used to prove Theorem 2.4 (resp. *Thm.* 2.3). The conclusion is the following: let

$$a_M^{th} = \int_{\Omega_M} \psi\left(\sqrt{h} + \inf_{\Omega_M} F_c - F_c(x)\right) \mathrm{d}x, \tag{85}$$

and

$$a_\mu^{th} = \int_{\Omega_\mu} (W'_{\mathrm{LJ}})^{-1}\left(\inf_{\Omega} F_M - F_M(x)\right) \mathrm{d}x. \tag{86}$$

If $a_M \leq a_M^{th}$, then problem (83) has a unique minimizer which is continuous, and if $a_M > a_M^{th}$, then problem (83) has no minimizer (any minimizing sequence converges to some measure which includes Dirac masses). If $a_\mu > a_\mu^{th}$, then a fracture appears in the minimizer(s) of (84).

With (69), (70) and (71), we see that $\overline{I}_{\mathrm{mod}} = \inf\left\{I_M(a-\overline{a}) + I_\mu(\overline{a}),\ \overline{a}\in[0,a]\right\}$. Let us define g by

$$g(\overline{a}) = I_M(a-\overline{a}) + I_\mu(\overline{a}), \tag{87}$$

and let $\overline{a}^*$ be any real number in $[0,a]$ such that $\overline{I}_{\mathrm{mod}} = \inf g = g(\overline{a}^*)$. One can consider a minimizing sequence of problem (84) with $a_\mu = \overline{a}^*$, and one can also consider a minimizing sequence of problem (83) with $a_M = a - \overline{a}^*$. So we can build a minimizing sequence v_n of problem (69) and apply results of Step 1 to this sequence. By construction, $h\sum_{i\in\mathbb{N}_\mu} v_n^i = \overline{a}^*$, so the real number a_μ^∞ defined by (72) reads $a_\mu^\infty = \overline{a}^*$. Hence, with (82) and (86), we see that $\overline{a}^* \in I_g$, where we set $I_g = \left[\frac{a-\theta_M}{2} + a_\mu^{th}\ ,\ a\right]$. So $\overline{I}_{\mathrm{mod}} = \inf\left\{g(\overline{a}),\ \overline{a}\in I_g\right\}$. In the sequel of this Step, we study the variations of the function g to show that, on the interval I_g, g has a unique minimizer.

Let us choose $\overline{a}\in I_g$, let us set $a_\mu = \overline{a}$ and $a_M = a - \overline{a}$ and let us consider problems (83) and (84). Since $\overline{a} > a_\mu^{th}$, problem (84) is an atomistic problem with boundary conditions so that a fracture appears. With results of Section 2.2, one can show that there exists $\lambda_\mu \in [0,h]$ such that the minimizers v of (84) read $v^{i_{\mathrm{mod}}} = \varphi(\lambda_\mu)$ and $\forall i \neq i_{\mathrm{mod}},\ v^i = \psi(\inf_{i\in\mathbb{N}_\mu} F_c^i - F_c^i + \lambda_\mu)$, where i_{mod} is any index such that $F_c^{i_{\mathrm{mod}}} = \inf_{i\in\mathbb{N}_\mu} F_c^i$. We have also shown that λ_μ depends on a_μ but not on i_{mod}. As a consequence, we can compute $I_\mu(a_\mu)$ and show that

$$\frac{\mathrm{d}I_\mu(a_\mu)}{\mathrm{d}a_\mu} = \lambda_\mu + \inf_{i\in\mathbb{N}_\mu} F_c^i - \underline{F_c}. \tag{88}$$

In addition,

$$\frac{\mathrm{d}\lambda_\mu}{\mathrm{d}a_\mu} \sim_{h\to 0} -Ch^7 \tag{89}$$

for some constant $C > 0$. We now study problem (83). If $a_M \leq a_M^{th}$ defined by (85), then problem (83) has a unique minimizer v which reads $v(x) = \psi\left(-\lambda_M + \inf_{\Omega_M} F_c - F_c(x)\right)$ for some $\lambda_M \geq -\sqrt{h}$. If $a_M > a_M^{th}$, then problem (83) has one or many minimizers v which read $v(x) = \psi\left(\sqrt{h} + \inf_{\Omega_M} F_c - F_c(x)\right) +$ Dirac masses . So we can compute $I_M(a_M)$ and show that

$$\frac{\mathrm{d}I_M(a_M)}{\mathrm{d}a_M} = -\lambda_M + \inf_{\Omega_M} F_c - \underline{F_c}, \tag{90}$$

where $\lambda_M \in [-\sqrt{h}, +\infty)$. If $a_M \geq a_M^{th}$, then $\lambda_M = -\sqrt{h}$, and if $a_M \leq a_M^{th}$, then

$$\frac{\mathrm{d}\lambda_M}{\mathrm{d}a_M} \leq -\frac{W''_{\mathrm{LJ}}(1)}{2\,|\Omega_M|}\cdot \tag{91}$$

We now study the variations of the function g defined by (87). In view of (88) and (90), it satisfies

$$g'(\overline{a}) = \lambda_M - \inf_{\Omega_M} F_c + \lambda_\mu + \inf_{i\in\mathbb{N}_\mu} F_c^i. \tag{92}$$

If $\inf_{i\in\mathbb{N}_\mu} F_c^i \geq \inf_{\Omega_M} F_c$, then $\underline{F_c} = \inf_{\Omega_M} F_c$, and with (76), we obtain

$$\inf_{i\in\mathbb{N}_\mu} F_c^i - \inf_{\Omega_M} F_c \leq Ch. \tag{93}$$

The above inequality also holds if $\inf_{i\in\mathbb{N}_\mu} F_c^i < \inf_{\Omega_M} F_c$. Inserting (93) in (92), and since $\lambda_\mu \leq h$, we obtain $g'(\overline{a}) \leq \lambda_M + Ch$ for some constant C that does not depend on h.

If $a_M = a - \overline{a} \geq a_M^{th}$ then $\lambda_M = -\sqrt{h}$, so $g'(\overline{a}) < 0$. If $a - \overline{a} \leq a_M^{th}$, we differentiate (92) with respect to $\overline{a}$, and with (89) and (91), one can show that $g''(\overline{a}) > 0$. Since $g'(a) = +\infty$, there exists a unique $\overline{a}^*$ which minimizes g on I_g, and $\overline{a}^* \in (a - a_M^{th}, a)$.

Step 3 (conclusion)**.** We know that $\overline{I}_{\mathrm{mod}} = \inf g = g(\overline{a}^*)$ with $\overline{a}^* \in I_g \cap (a - a_M^{th}, a)$. There exist minimizers for problem (83) with $a_M = a - \overline{a}^* < a_M^{th}$ and for problem (84) with $a_\mu = \overline{a}^*$. So problems (69) and (13) have a minimizer. Let now u_{mod} be a minimizer of problem (13) and let v_{mod} be its first derivative, which is a minimizer of (69). As g has a unique minimizer $\overline{a}^*$, we see that $\int_{\Omega_M} v_{\mathrm{mod}}(x)\,\mathrm{d}x = a - \overline{a}^* < a_M^{th}$, so that u_{mod} has no fracture on Ω_M. We also see that $h\sum_{i\in\mathbb{N}_\mu} v_{\mathrm{mod}}^i = \overline{a}^* \geq \frac{a-\theta_M}{2} + a_\mu^{th}$, so u_{mod} has a unique fracture on Ω_μ. We apply Theorem 2.3 on problem (84) and Theorem 2.4 on problem (83), and we obtain (64) for some Lagrange multiplier $\lambda_{\mathrm{mod}}^* \in (0, Ch)$.

We now identify λ_{mod}^*. We know that $\lambda_{\mathrm{mod}}^* \in (0, Ch)$, and we see from (64) that λ_{mod}^* satisfies (61). In addition, we see that (63) implies (60). Since $a > \theta_M$, we can apply Lemma 2.4, that defines λ_{mod}, and we have $\lambda_{\mathrm{mod}}^* = \lambda_{\mathrm{mod}}$. □

We now estimate the difference between a minimizer u_{mod} of the modified coupled problem (13) and a minimizer u_μ of the atomistic problem (2).

Theorem 2.6 (estimate on the minimizers)**.** *We assume that $f \in \mathcal{C}^0(\overline{\Omega})$ and that there exists $\kappa_f > 0$ such that* (26) *is satisfied. Let u_μ be a minimizer of problem* (2) *and u_{mod} be a minimizer of problem* (13).

If $a < \theta_M$, then there exist $h_0 \leq 1$ and $C(\kappa_f)$, that both depend on κ_f, such that, for all $h \leq h_0$, the minimizers u_μ and u_{mod}, as well as their respective energies, are at distance of order h in the sense that

$$|(\Pi_\mu u_{mod}) - u_\mu|_{W^{1,\infty}(X_\mu)} + |u_{mod} - (\Pi_c u_\mu)|_{W^{1,\infty}(X_c)} \leq C(\kappa_f) h \kappa_f, \tag{94}$$

$$\|(\Pi_\mu u_{mod}) - u_\mu\|_{L^\infty(X_\mu)} + \|u_{mod} - (\Pi_c u_\mu)\|_{L^\infty(X_c)} \leq C(\kappa_f) h \kappa_f, \tag{95}$$

$$|I_{mod} - I_\mu| \leq C(\kappa_f) h \kappa_f, \tag{96}$$

where Π_c and Π_μ are the operators defined in Definition 1.4, and $\|\cdot\|_{L^\infty(X_c)}$, $|\cdot|_{W^{1,\infty}(X_c)}$, $\|\cdot\|_{L^\infty(X_\mu)}$ and $|\cdot|_{W^{1,\infty}(X_\mu)}$ are the norms defined by (29), (30) *and* (31)*. In addition, the function $\kappa_f \mapsto C(\kappa_f)$ is bounded on any compact set.*

If $a > \theta_M$, and if the partition $\Omega = \Omega_M \cup \Omega_\mu$ satisfies (63)*, then there exist $h_0 \leq 1$ and a constant C (that both depend on κ_f) such that, for all $h \leq h_0$, there exist $i_\mu \in \{0, \dots, N-1\}$ and $i_{mod} \in \mathbb{N}_\mu$ so that*

$$\|u'_{mod} - (\Pi_c u_\mu)'\|_{L^\infty(\Omega_M \setminus [i_\mu h, i_\mu h + h])} \leq Ch, \tag{97}$$

$$\sup_{i \in \mathbb{N}_\mu, i \neq i_\mu, i \neq i_{mod}} \left| \frac{u^{i+1}_{mod} - u^i_{mod}}{h} - \frac{u^{i+1}_\mu - u^i_\mu}{h} \right| \leq Ch, \tag{98}$$

$$\left| (u^{i_{mod}+1}_{mod} - u^{i_{mod}}_{mod}) - (u^{i_\mu+1}_\mu - u^{i_\mu}_\mu) \right| \leq Ch, \tag{99}$$

$$u^{i_{mod}+1}_{mod} - u^{i_{mod}}_{mod} \sim_{h \to 0} a - \theta_M, \qquad u^{i_\mu+1}_\mu - u^{i_\mu}_\mu \sim_{h \to 0} a - \theta_M, \tag{100}$$

$$|I_{mod} - I_\mu| \leq Ch. \tag{101}$$

In the case $a > \theta_M$, we see that both u_μ and u_{mod} have a singularity, that is localized on a unique atom pair (see (100)). With (99), we can see that the difference between the discontinuity of u_{mod} and of u_μ converges to 0 when h goes to zero.

Proof. We first treat the case $a < \theta_M$. Then, for h small enough, the atomistic problem (2) and the modified coupled problem (13) are well-posed (see *Thms.* 2.3 and 2.5), and the analysis can be conducted in exactly the same way as in the convex case (see *Thm.* 1.1). We thus obtain estimates (94), (95) and (96), which are similar to (33), (34), (35), (36) and (37).

We now treat the case $a > \theta_M$. Then, for h small enough, the configuration u_μ, which is a minimizer of the atomistic problem (2), is given by (51) for some $i_\mu \in \{0, \dots, N-1\}$ and some $\lambda_\mu \in (0, h]$ (see *Thm.* 2.3). The configuration u_{mod}, which is a minimizer of problem (13), is given by (64) for some $i_{\text{mod}} \in \mathbb{N}_\mu$ and some $\lambda_{\text{mod}} \in (0, Ch]$ (see *Thm.* 2.5). Hence, we obtain

$$|\lambda_\mu - \lambda_{\text{mod}}| \leq Ch, \tag{102}$$

for some constant C that does not depend on h. Collecting (51), (64) and (102), we obtain estimates (97) and (98). Using boundary conditions, one can prove (99). The estimate (52) implies the estimate (100) on u_μ, and we infer from the latter and (99) the estimate (100) on u_{mod}. Collecting (97), (98) and (99), we obtain the energy estimate (101). □

2.5. Definition of the partition

In the statement of Theorem 2.6, we have supposed that we were given some body forces f and a partition $\Omega = \Omega_M \cup \Omega_\mu$ satisfying (26) and (63). In the sequel, we describe a strategy to find such a partition without resorting to the computation of F_μ, an object which is expensive to compute.

Definition 2.1 (partition in the Lennard-Jones case)**.** We assume that $f \in W^{1,1}(\Omega)$. Let us fix $\kappa_f > 0$, and let $u_M \in SBV(\Omega)$ be a minimizer of the continuum problem (45).

The interval $(ih, ih+h)$ is said to be a *regular interval* if f satisfies

$$\forall x \in (ih, ih+h), \ |f(x)| \leq \kappa_f \quad \text{and} \quad \int_{ih}^{ih+h} |f'(x)| \, \mathrm{d}x \leq h \frac{\kappa_f}{L},$$

and if u_M is continuous on $[ih, ih+h]$.

We define Ω_M by

$$\Omega_M = \overset{*}{\bigcup_{(ih,ih+h)\ \text{regular}}} (ih, ih+h) \text{ and } \Omega_\mu = \Omega \setminus \Omega_M,$$

where $\overset{*}{\bigcup}$ means that the point $\{ih\}$ is also included in Ω_M if both $(ih-h, ih)$ and $(ih, ih+h)$ are regular intervals.

Note that we make a stronger assumption on f than before (until now, we have only assumed $f \in \mathcal{C}^0(\overline{\Omega})$).

Remark 2.10. In the case $a \leq \theta_M$, one can show that problem (45) has a unique minimizer u_M, which is the minimizer of (44). So u_M is continuous on Ω and the last condition for an interval to be regular is always satisfied.

Theorem 2.7. *Let us consider a partition $\Omega = \Omega_M \cup \Omega_\mu$ as defined by Definition 2.1. Then the body forces f satisfy* (26)*. If $a > \theta_M$, then the function F_μ defined by* (16) *satisfies* (63)*.*

Proof. Estimates (26) are a direct consequence of the definition of Ω_M. We now assume $a > \theta_M$ and prove (63). Let us first note that the assumption $f \in W^{1,1}(\Omega)$ implies that

$$\forall k \in \{0, \ldots, N\}, \quad \left|F_M(kh) - F_\mu^k\right| \leq h \|f'\|_{L^1(\Omega)}, \tag{103}$$

which is a better estimate than (27).

Theorem 2.1 shows that the minimizers u_M of (45) read $u_M(x) = \int_0^x v_1(t)\,\mathrm{d}t + \sum_{i\in\mathbb{I}} \tilde{v}_i H(x - x_i)$, where $v_1 \in L^1(\Omega)$ is defined by (43), $\mathbb{I}$ is any countable set, and $\tilde{v}_i$ and x_i are such that, for all $i \in \mathbb{I}$, $\tilde{v}_i > 0$ and $x_i \in \arg\inf F_M$. So u_M is not continuous at x_1. Let σ_1 be such that $x_1 \in [\sigma_1 h, \sigma_1 h + h)$. So the interval $(\sigma_1 h, \sigma_1 h + h)$ is not regular, thus $[\sigma_1 h, \sigma_1 h + h] \subset \Omega_\mu$, *i.e.* $\sigma_1 \in \mathbb{N}_\mu$. With (103), we see that

$$|F_M(\sigma_1 h) - F_\mu^{\sigma_1}| \leq h \|f'\|_{L^1(\Omega)}. \tag{104}$$

We also have

$$|F_M(x_1) - F_M(\sigma_1 h)| \leq \int_{\sigma_1 h}^{x_1} |f(s)| \mathrm{d}s \leq h \|f\|_{L^\infty(\Omega)}. \tag{105}$$

We also infer from (103) that

$$|\inf F_M - \underline{F_\mu}| \leq Ch \tag{106}$$

for some C that does not depend on h, and where $\underline{F_\mu} = \inf_{0\leq i\leq N-1} F_\mu^i$. As $F_M(x_1) = \inf F_M$, we infer from (104), (105) and (106) that $|F_\mu^{\sigma_1} - \underline{F_\mu}| \leq Ch$. As $\sigma_1 \in \mathbb{N}_\mu$, we obtain (63). □

Appendix A

Proof of Theorem 2.1. The energy (5) can also be written

$$E_M(u) = \int_\Omega \left(W_{\rm LJ}(u'(x)) + (F_M(x) - \inf F_M)\, u'(x)\right) {\rm d}x + a\left(\inf F_M - F_M(L)\right). \tag{107}$$

We first treat the case $\theta_M \geq a$. Consider the following minimization problem:

$$\overline{I}_M = \inf\left\{\overline{E}_M(v), \quad v \in L^1(\Omega), \quad v > 0 \ a.e., \quad \frac{1}{v} \in L^{12}(\Omega), \quad \int_\Omega v = a\right\},$$

where $\overline{E}_M(v) = \int_\Omega W_{\rm LJ}(v) + (F_M - \inf F_M)\, v$. Clearly, $I^1_M = \overline{I}_M + a\left(\inf F_M - F_M(L)\right)$ and u is a minimizer of I^1_M if and only if u' is a minimizer of $\overline{I}_M$. Let us define

$$v_0(x) = \left(W'_{\rm LJ}\right)^{-1}\left(\inf F_M - F_M(x) - \lambda\right), \tag{108}$$

where $\lambda \geq 0$ is chosen such that $\int_\Omega v_0 = a$. This is possible because $\int_\Omega \left(W'_{\rm LJ}\right)^{-1}\left(\inf F_M - F_M(x)\right) {\rm d}x = \theta_M \geq a$ and $\lim_{\lambda\to+\infty} \int_\Omega \left(W'_{\rm LJ}\right)^{-1}\left(\inf F_M - F_M(x) - \lambda\right) {\rm d}x = L\left(W'_{\rm LJ}\right)^{-1}(-\infty) = 0$. We see that $v_0(x)$ is a continuous function which satisfies $v_0(x) \geq \left(W'_{\rm LJ}\right)^{-1}\left(\inf F_M - \sup F_M - \lambda\right) > 0$. Thus it is a test function for $\overline{I}_M$. Consider now $v \in L^1(\Omega)$ satisfying $v > 0$, $1/v \in L^{12}(\Omega)$ and $\int_\Omega v = a$. The function $\underline{v} = \inf\{v, 1\}$ satisfies $\overline{E}_M(v) \geq \overline{E}_M(\underline{v})$. Define now for $\alpha \in [0,1]$ the function $p(\alpha) = \overline{E}_M\left((1-\alpha)v_0 + \alpha\underline{v}\right)$. We have that p is convex, because both v_0 and $\underline{v}$ ly in $(0,1]$ where $W_{\rm LJ}$ is convex, and that $p'(0) = -\lambda\int_\Omega\left(\underline{v} - v_0\right) \geq 0$, hence p is nondecreasing. Therefore $p(0) = \overline{E}_M\left(v_0\right) \leq p(1) = \overline{E}_M\left(\underline{v}\right) \leq \overline{E}_M(v)$. Hence, v_0 is a minimizer of $\overline{I}_M$. On the other hand, if for some v as above, $\overline{E}_M\left(v_0\right) = \overline{E}_M\left(v\right)$, then $p(\alpha)$ must be constant on $\alpha \in [0,1]$ and $\overline{E}_M\left(v\right) = \overline{E}_M\left(\underline{v}\right)$. As the minimum of $W_{\rm LJ}$ is attained at 1, the latter implies that $v = \underline{v}$, while p constant implies that $p'' = 0$, thus $v_0 = \underline{v}$ (because $W_{\rm LJ}$ is strictly convex on $(0,1]$). This shows that v_0 is the unique minimizer of $\overline{I}_M$, and that $u_0(x) = \int_0^x v_0(t)\,{\rm d}t$ is the unique minimizer of (44).

We now turn to the case $\theta_M < a$ and show that (45) has at least a minimizer. Consider $u \in SBV(\Omega)$ such that $1/u' \in L^{12}(\Omega)$, $u' > 0$, $u(0) = 0$ and $u(L) = a$. We use the notation $u' = D_a u + \sum_{i\in\mathbb{I}} \tilde{v}_i \delta_{x_i}$ with $D_a u \in L^1(\Omega)$, $D_a u > 0$ and $\tilde{v}_i > 0$. Recall that we use the convention that $W_{\rm LJ}(u') = W_{\rm LJ}(D_a u)$. Thus

$$E_M(u) = \int_\Omega P_x(D_a u(x))\,{\rm d}x + \sum_{i\in\mathbb{I}} \tilde{v}_i\left(F_M(x_i) - \inf F_M\right) + a\left(\inf F_M - F_M(L)\right), \tag{109}$$

where $P_x(t)$ is the function

$$P_x(t) = W_{\rm LJ}(t) + (F_M(x) - \inf F_M)\, t. \tag{110}$$

On $(0,+\infty)$, this function has a unique minimizer which is the function $v_1(x)$ defined by (43). So $P_x(D_a u(x)) \geq P_x(v_1(x))$ on Ω and we infer from (109) that

$$E_M(u) \geq \int_\Omega P_x(v_1(x))\,\mathrm{d}x + \sum_{i\in\mathbb{I}} \tilde{v}_i \left(F_M(x_i) - \inf F_M\right) + a\left(\inf F_M - F_M(L)\right). \tag{111}$$

Consider now a point $x_0 \in \arg\inf F_M$, and define

$$u_0(x) = \int_0^x v_1(t)\,\mathrm{d}t + (a-\theta_M)H(x-x_0). \tag{112}$$

We have $D_a u_0 = v_1 \in L^1(\Omega)$. Since v_1 is a continuous function which satisfies $v_1(x) \geq \inf v_1 > 0$, we see that $1/v_1 \in L^{12}(\Omega)$, thus u_0 is an admissible function of (45) and, making use of (109) with $u \equiv u_0$, we obtain

$$E_M(u_0) = \int_\Omega P_x(v_1(x))\,\mathrm{d}x + a\left(\inf F_M - F_M(L)\right). \tag{113}$$

Collecting (111) and (113), we obtain

$$E_M(u) \geq E_M(u_0) + \sum_{i\in\mathbb{I}} \tilde{v}_i \left(F_M(x_i) - \inf F_M\right) \tag{114}$$

for all test functions u of problem (45) such that $u' = D_a u + \sum_{i\in\mathbb{I}} \tilde{v}_i \delta_{x_i}$. Since $\tilde{v}_i > 0$, we have $E_M(u) \geq E_M(u_0)$ and the function u_0 is a minimizer of problem (45).

We now look for all the minimizers of problem (45). Let u be any test function. From (114), we see that $E_M(u) > E_M(u_0)$ if there exists $i \in \mathbb{I}$ such that $x_i \notin \arg\inf F_M$ and $\tilde{v}_i > 0$. In addition, in view of (109) and (113), we infer from $E_M(u) = E_M(u_0)$ that $\int_\Omega P_x(D_a u(x))\,\mathrm{d}x = \int_\Omega P_x(v_1(x))\,\mathrm{d}x$. As $v_1(x)$ is the unique minimizer of $t \in (0,+\infty) \mapsto P_x(t)$, we obtain that $v_1 = D_a u$ *a.e.* on Ω. Hence, any minimizer of (45) may be written $u(x) = \int_0^x \left(W'_{\mathrm{LJ}}\right)^{-1}\left(\inf F_M - F_M(t)\right)\,\mathrm{d}t + \sum_{i\in\mathbb{I}} \tilde{v}_i H(x-x_i)$, where $\mathbb{I}$ is any countable set, $x_i \in \arg\inf F_M$ and $\tilde{v}_i > 0$ for all $i \in \mathbb{I}$, and $\sum_{i\in\mathbb{I}} \tilde{v}_i = a - \theta_M$.

Let us now show that $I_M^{BV} = I_M^1$. We already have $I_M^{BV} \leq I_M^1$ and we have shown that $I_M^{BV} = E_M(u_0)$, where u_0 is defined by (112). Let u_0^ε be a regularization of u_0: then u_0^ε is a test function for (44) and $I_M^{BV} = E_M(u_0) = \lim_{\varepsilon\to 0} E_M(u_0^\varepsilon) \geq I_M^1$. Thus $I_M^{BV} = I_M^1$. To prove that problem (44) is not attained, we argue by contradiction. Let us assume that problem (44) is attained and let $\underline{u}$ be a minimizer. With (107), we see that

$$E_M(\underline{u}) = \int_\Omega P_x(\underline{u}'(x))\,\mathrm{d}x + a\left(\inf F_M - F_M(L)\right), \tag{115}$$

where $P_x(t)$ is defined by (110). We have $E_M(\underline{u}) = I_M^1 = I_M^{BV} = E_M(u_0)$, thus, in view of (113) and (115), we obtain $\int_\Omega P_x(v_1(x))\,\mathrm{d}x = \int_\Omega P_x(\underline{u}'(x))\,\mathrm{d}x$, which implies that $v_1(x) = \underline{u}'(x)$ *a.e.* on Ω. But this is impossible since $\int_\Omega v_1 = \theta_M < a = \int_\Omega \underline{u}'$. □

Appendix B

Proof of Theorem 2.2. As we impose the increasing condition $u^{i+1} > u^i$, any minimizing sequence u_n^i satisfies $0 \leq u_n^i \leq a$ for all i, hence is compact in $\mathbb{R}^{N+1}$. Thus, one can extract a subsequence that converges to a configuration (denoted by u_μ) which is a minimizer of the energy. This configuration satisfies the constraint $u_\mu^{i+1} > u_\mu^i$ for all i. Otherwise, there exists i such that $\lim\limits_{n\to+\infty} u_n^{i+1} - u_n^i = 0$, which implies, as $W_{\mathrm{LJ}}(0) = +\infty$, that the infimum (2) is $+\infty$, which is a contradiction. Hence, (2) has at least one minimizer.

Choosing $u^i = ih\ a/L$ as a test function, we show that $L\, W_{\mathrm{LJ}}\,(a/L) \geq I_\mu$. Bounding W_{LJ} from below by W_{LJ}^{**}, and utilizing the convexity of W_{LJ}^{**}, we show that $I_\mu \geq L W_{\mathrm{LJ}}^{**}\,(a/L)$. Thus $L\, W_{\mathrm{LJ}}\left(\frac{a}{L}\right) \geq I_\mu \geq L\, W_{\mathrm{LJ}}^{**}\left(\frac{a}{L}\right)$.

We first treat the case $a \leq L$, where $W_{\mathrm{LJ}}\,(a/L) = W_{\mathrm{LJ}}^{**}\,(a/L)$, thus $I_\mu = L\, W_{\mathrm{LJ}}\,(a/L)$. The configuration $u_\mu^i = ih\ a/L$ is thus a minimizer. Let us now consider a configuration u for which the quantities $\frac{u^{i+1}-u^i}{h}, i = 0, \ldots, N-1$, are not all equal to a/L. Then

$$E_\mu(u) = h\sum_{i=0}^{N-1} W_{\mathrm{LJ}}\left(\frac{u^{i+1}-u^i}{h}\right) \geq h\sum_{i=0}^{N-1} W_{\mathrm{LJ}}^{**}\left(\frac{u^{i+1}-u^i}{h}\right) > L\, W_{\mathrm{LJ}}^{**}\left(\frac{h}{L}\sum_{i=0}^{N-1}\frac{u^{i+1}-u^i}{h}\right),$$

where we have made use of the strict case of the convexity inequality. Thus we have $E_\mu(u) > L\, W_{\mathrm{LJ}}^{**}(a/L) = I_\mu$, and u is not a minimizer. This shows the uniqueness claimed in the theorem.

We now turn to the case $a > L$. Let us consider a minimizer u_μ of problem (2). As $W_{\mathrm{LJ}}(0) = +\infty$, the constraint $u^{i+1} > u^i$ is not active, so the Euler-Lagrange equation of (2) reads as (23):

$$\forall i \in \{1, \ldots, N-1\}, \quad W_{\mathrm{LJ}}'\left(\frac{u_\mu^i - u_\mu^{i-1}}{h}\right) = W_{\mathrm{LJ}}'\left(\frac{u_\mu^{i+1} - u_\mu^i}{h}\right).$$

If one slope $\frac{u_\mu^{i+1}-u_\mu^i}{h}$ is equal to or smaller than 1, then the same holds for the other slopes, and this is in contradiction with the fact that $a > L$. So all the slopes are strictly larger than 1. In addition, due to the variations of W_{LJ}, there are two values $s^*(h)$ and $s_f^*(h)$, with $1 < s^*(h) \leq r_c \leq s_f^*(h)$, $W_{\mathrm{LJ}}'(s^*(h)) = W_{\mathrm{LJ}}'(s_f^*(h))$, such that each of the slopes is either $s^*(h)$ or $s_f^*(h)$. Let $k = \mathrm{Card}\left\{i \in \{0, \ldots, N-1\} \text{ such that } \frac{u_\mu^{i+1}-u_\mu^i}{h} = s_f^*(h)\right\}$. We have $(L-kh)s^*(h) + khs_f^*(h) = a$ and $I_\mu = (L-kh)W_{\mathrm{LJ}}(s^*(h)) + khW_{\mathrm{LJ}}(s_f^*(h))$.

We claim that $k = 1$. For this purpose, we consider the discrete function u_b defined by $u_b^i = ih$ for $i = 0, \ldots, N-1$, and $u_b^N = a$. Its energy is $E_\mu(u_b) = (L-h)\, W_{\mathrm{LJ}}(1) + hW_{\mathrm{LJ}}\left(\frac{a-L}{h}+1\right)$, and satisfies $\lim\limits_{h\to 0} E_\mu(u_b) = L\, W_{\mathrm{LJ}}(1)$. We first show that $k \neq 0$. Otherwise, all slopes $\left(u_\mu^{i+1} - u_\mu^i\right)/h$ are equal to the same value $s^*(h)$, which thus needs to be a/L. As u_μ is a minimizer, $I_\mu = L\, W_{\mathrm{LJ}}(a/L)$. However, we also have $I_\mu \leq E_\mu(u_b)$. Letting h go to zero, we obtain $W_{\mathrm{LJ}}(a/L) \leq W_{\mathrm{LJ}}(1)$, which is a contradiction as $a > L$.

We now show that $k \leq 1$. As $I_\mu \leq E_\mu(u_b)$, one obtains

$$L\left(W_{\mathrm{LJ}}(s^*(h)) - W_{\mathrm{LJ}}(1)\right) + kh\left(W_{\mathrm{LJ}}(s_f^*(h)) - W_{\mathrm{LJ}}(s^*(h))\right) \leq -hW_{\mathrm{LJ}}(1). \tag{116}$$

The left hand side is a sum of two nonnegative terms, for $1 < s^*(h) \leq s_f^*(h)$ and W_{LJ} is an increasing function on $[1, +\infty)$. So we have $\lim\limits_{h\to 0} W_{\mathrm{LJ}}(s^*(h)) = W_{\mathrm{LJ}}(1)$, hence $\lim\limits_{h\to 0} s^*(h) = 1$, which in turn implies that $\lim\limits_{h\to 0} s_f^*(h) = +\infty$. Inserting this information in (116), we obtain $k \leq 3/2$, thus $k = 1$ for h small enough.

We finally identify $(s^*(h), s_f^*(h))$ for h small enough. We have $(L-h)s^*(h) + hs_f^*(h) = a$. So, using $\lim\limits_{h\to 0} s^*(h) = 1$, we see that $s_f^*(h) \sim_{h\to 0} (a-L)/h$. So $W_{\mathrm{LJ}}'(s^*(h)) = W_{\mathrm{LJ}}'(s_f^*(h)) \sim Ch^7$, and $s^*(h) = 1 + O(h^7)$. As a consequence, $s^*(h) \in [1, 1+h]$. By uniqueness of the pair $(s(h), s_f(h))$ satisfying (46) (see Lemma 2.1 above), one has $s^*(h) = s(h)$ and $s_f^*(h) = s_f(h)$. So u_μ satisfies (47) for some integer i_μ. □

Appendix C

Proof of Theorem 2.3. If $f \equiv 0$, then Theorem 2.3 is identical to Theorem 2.2. We now concentrate on the case $f \neq 0$. As in the proof of Theorem 2.1 (Appendix A), we first reformulate the energy, here in term of the slopes

$$v^i = \frac{u^{i+1} - u^i}{h}, \quad 0 \le i \le N-1. \tag{117}$$

The energy (1) can be written $E_\mu(u) = a\left(\underline{F_\mu} - F_\mu^N\right) + h\sum_{i=0}^{N-1}\left(W_{\rm LJ}\left(\frac{u^{i+1}-u^i}{h}\right) + \left(F_\mu^i - \underline{F_\mu}\right)\frac{u^{i+1}-u^i}{h}\right)$. Then we consider

$$\overline{I}_\mu = \inf\left\{\overline{E}_\mu(v);\ v \in Y_\mu(a)\right\}, \tag{118}$$

where the space $Y_\mu(a)$ is defined by $Y_\mu(a) = \left\{v = (v^0, \dots, v^{N-1}) \in \mathbb{R}^N,\ h\sum_{i=0}^{N-1} v^i = a,\ v^i > 0\right\}$, and the energy $\overline{E}_\mu$ by $\overline{E}_\mu(v) = h\sum_{i=0}^{N-1}\left(W_{\rm LJ}(v^i) + \left(F_\mu^i - \underline{F_\mu}\right)v^i\right)$. Clearly, $I_\mu = \overline{I}_\mu + a\left(\underline{F_\mu} - F_\mu^N\right)$. If u is a minimizer of (2), then the discrete function v defined from u by (117) is a minimizer of (118). On the other hand, if v is a minimizer of (118), then u defined by $u^i = h\sum_{j=0}^{i-1} v^j$ for $i \ge 1$ and $u^0 = 0$ is a minimizer of (2).

Let v_n be a minimizing sequence of $\overline{I}_\mu$. Since $0 < v_n^i \le a/h$ for all $0 \le i \le N-1$ and all n, one can extract a subsequence that converges to the configuration v_μ. Again, since $W_{\rm LJ}(0) = +\infty$ and the infimum (118) is not equal to $+\infty$, we have $v_\mu^i > 0$ for all $0 \le i \le N-1$ and v_μ is a minimizer of (118). Hence (118), and therefore (2), have at least one minimizer, we denote by v_μ and u_μ two corresponding minimizers of (118) and (2).

In the case $a \le \theta_\mu$, the proof of uniqueness follows the same lines as the proof of Theorem 2.1, in the case $a \le \theta_M$.

We now turn to the case $a > \theta_M$. As $\lim\limits_{h\to 0} \theta_\mu = \theta_M$, we choose h small enough such that $a > \theta_\mu$. We introduce the function $P_i(t) = W_{\rm LJ}(t) + (F_\mu^i - \underline{F_\mu})t$, which attains its minimum with respect to $t \in [0, +\infty)$ at $t = v_1^i$ defined by

$$v_1^i = (W_{\rm LJ}')^{-1}(\underline{F_\mu} - F_\mu^i), \quad i = 0, \dots, N-1. \tag{119}$$

We notice that

$$\forall v \in Y_\mu(a), \quad \overline{E}_\mu(v) = h\sum_{i=0}^{N-1} P_i(v^i) \ge \overline{E}_\mu(v_1). \tag{120}$$

As $W_{\rm LJ}(0) = +\infty$, the constraint $v^i > 0$ is not active in (118), so the Euler-Lagrange equation of (118) reads

$$W_{\rm LJ}'(v_\mu^i) + F_\mu^i - \underline{F_\mu} = \lambda_\mu^*, \tag{121}$$

where λ_μ^* is the Lagrange multiplier associated to the constraint $h\sum\limits_{i=0}^{N-1} v_\mu^i = a$. Since $a > \theta_\mu$, one can show that $\lambda_\mu^* > 0$ (otherwise, (121) leads to $v_\mu^i \le v_1^i$, and summing these inequalities leads to $a \le \theta_\mu$). It holds that

$$\forall i \in G_1(u_\mu) \cup G_2(u_\mu), \quad v_\mu^i = \psi(\underline{F_\mu} - F_\mu^i + \lambda_\mu^*). \tag{122}$$

Step 1 ($\liminf\ h\,\mathrm{Card}(G_1(u_\mu)) > 0$)**.** In view of (120), we have

$$\overline{E}_\mu(v_1) \le \overline{I}_\mu. \tag{123}$$

Let i_0 be an index such that $F_\mu^{i_0} = \underline{F_\mu}$, and let us consider the function v_b defined by $v_b^i = v_1^i > 0$ for $i \neq i_0$ and $v_b^{i_0}$ such that $h\sum_{i=0}^{N-1} v_b^i = a$. By construction, $v_1^{i_0} = 1$ and $hv_b^{i_0} = a - \theta_\mu + h$, so

$$v_b^{i_0} \sim_{h\to 0} \frac{a-\theta_M}{h} > 0. \tag{124}$$

Hence, v_b is a test function for (118) and we have $\overline{I}_\mu \leq \overline{E}_\mu(v_b)$. Collecting this inequality with (123), we have

$$\overline{E}_\mu(v_1) \;\leq\; \overline{I}_\mu \;\leq\; \overline{E}_\mu(v_b). \tag{125}$$

Since $F_\mu^{i_0} = \underline{F_\mu}$, we have $\overline{E}_\mu(v_b) - \overline{E}_\mu(v_1) = h\left(W_{\rm LJ}(v_b^{i_0}) - W_{\rm LJ}(v_1^{i_0})\right)$. We know that $v_1^{i_0} = 1$. With (124), we obtain

$$0 \leq \overline{E}_\mu(v_b) - \overline{E}_\mu(v_1) \leq -hW_{\rm LJ}(1). \tag{126}$$

With (125) and (126), we have

$$\lim_{h\to 0} \overline{I}_\mu = \lim_{h\to 0} \overline{E}_\mu(v_1) = \int_\Omega W_{\rm LJ}(v_1(x)) + (F_M(x) - \inf F_M)v_1(x)\,{\rm d}x, \tag{127}$$

where $v_1(x)$ is defined by (43). We now prove a lower bound for $\overline{I}_\mu$. Since $\overline{I}_\mu = h\sum_{i=0}^{N-1}\left(W_{\rm LJ}(v_\mu^i) + (F_\mu^i - \underline{F_\mu})v_\mu^i\right)$, we have $\overline{I}_\mu \geq h\sum_{i=0}^{N-1}\left(W_{\rm LJ}(1) + (F_\mu^i - \underline{F_\mu})\right) + h\sum_{i\in G_1(u_\mu)}(F_\mu^i - \underline{F_\mu})(v_\mu^i - 1)$. The previous inequality implies $\overline{I}_\mu - h\sum_{i=0}^{N-1}\left(W_{\rm LJ}(1) + (F_\mu^i - \underline{F_\mu})\right) \geq -h\,{\rm Card}(G_1(u_\mu))\left(\sup_{0\leq i\leq N-1} F_\mu^i - \underline{F_\mu}\right)$. Letting h go to zero in the above inequality, we obtain, in view of (127),

$$\int_\Omega W_{\rm LJ}(v_1) + (F_M - \inf F_M)v_1 - \int_\Omega W_{\rm LJ}(1) + (F_M - \inf F_M) \geq -\liminf_{h\to 0}\left(h\,{\rm Card}(G_1(u_\mu))\left(\sup_{0\leq i\leq N-1} F_\mu^i - \underline{F_\mu}\right)\right).$$

Since $f \neq 0$, we see that $v_1(x) \neq 1$ somewhere in Ω. As $v_1(x)$ minimizes the function $W_{\rm LJ}(t) + (F_M(x) - \inf F_M)t$ on $[0, +\infty)$, we obtain $\liminf h\,{\rm Card}(G_1(u_\mu)) > 0$, and there exists $L_1 > 0$ such that, for h small enough, $h\,{\rm Card}(G_1(u_\mu)) \geq L_1$.

Step 2 (a first estimate of the Lagrange multiplier λ_μ^* and of v_μ)**.** In view of (125) and (126), we have $0 \leq \overline{I}_\mu - \overline{E}_\mu(v_1) \leq -hW_{\rm LJ}(1)$. Since $\overline{E}_\mu(v) = h\sum_{i=0}^{N-1} P_i(v^i)$ for any $v \in Y_\mu(a)$ (see (120)), we have

$$h\sum_{i\in G_1(u_\mu)}\left(P_i(v_\mu^i) - P_i(v_1^i)\right) + h\sum_{i\notin G_1(u_\mu)}\left(P_i(v_\mu^i) - P_i(v_1^i)\right) \leq -hW_{\rm LJ}(1). \tag{128}$$

Since $t \mapsto P_i(t)$ attains its minimum at v_1^i, we see that the left hand side of the above inequality is a sum of two nonnegative terms. We know that $v_1^i \leq 1$. Using the convexity of P_i on $(0, 1]$, one obtains

$$\forall i \in G_1(u_\mu),\quad P_i(v_\mu^i) - P_i(v_1^i) \geq C(v_\mu^i - v_1^i)^2, \tag{129}$$

where C stands (here and below) for a generic constant which does not depend on h. With (119) and (122), we obtain $v_\mu^i - v_1^i \geq C\lambda_\mu^*$ for some constant C. Inserting this information in (128) and (129), one obtains $(\lambda_\mu^*)^2\, h\, \mathrm{Card}(G_1(u_\mu)) \leq O(h)$. As $h\,\mathrm{Card}(G_1(u_\mu)) \geq L_1 > 0$, we have

$$0 < \lambda_\mu^* \leq C\sqrt{h}. \tag{130}$$

Collecting (119), (122) and (130), we infer that there exists a constant C independent of h such that, for all i in $G_1(u_\mu) \cup G_2(u_\mu)$, we have $|v_\mu^i - v_1^i| \leq C\lambda_\mu^*$, so

$$\begin{aligned} &\forall i \in G_1(u_\mu) \cup G_2(u_\mu),\ |v_\mu^i - v_1^i| \leq C\sqrt{h},\\ &\forall i \in G_3(u_\mu), \qquad v_\mu^i \geq \frac{C}{h^{1/14}}. \end{aligned} \tag{131}$$

Step 3 ($\mathrm{Card}\, G_3(u_\mu) = 1$)**.** For any $i \in G_1(u_\mu) \cup G_2(u_\mu)$, we see that v_1^i and v_μ^i belong to the interval $(0, 1 + C\sqrt{h}]$, on which W_{LJ} and P_i are convex. So inequality (129) is valid for all $i \in G_1(u_\mu) \cup G_2(u_\mu)$, *i.e.* for all $i \notin G_3(u_\mu)$. Thus, (128) implies on the one hand

$$C\,h \sum_{i \notin G_3(u_\mu)} (v_\mu^i - v_1^i)^2 \leq h \sum_{i \notin G_3(u_\mu)} \big(P_i(v_\mu^i) - P_i(v_1^i)\big) \leq -hW_{\mathrm{LJ}}(1). \tag{132}$$

On the other hand, for any $i \in G_3(u_\mu)$, $P_i(v_1^i) \leq P_i(1) = W_{\mathrm{LJ}}(1) + F_\mu^i - \underline{F_\mu}$ and, with (131),

$$P_i(v_\mu^i) \geq W_{\mathrm{LJ}}(v_\mu^i) + F_\mu^i - \underline{F_\mu} \geq W_{\mathrm{LJ}}\left(\frac{C}{h^{1/14}}\right) + F_\mu^i - \underline{F_\mu}.$$

This and (128) gives $\mathrm{Card}\, G_3(u_\mu)\big(W_{\mathrm{LJ}}\left(\frac{C}{h^{1/14}}\right) - W_{\mathrm{LJ}}(1)\big) \leq \sum_{i \in G_3(u_\mu)} \big(P_i(v_\mu^i) - P_i(v_1^i)\big) \leq -W_{\mathrm{LJ}}(1)$. So, for h small enough, $\mathrm{Card}\, G_3(u_\mu) \leq 1$. If $G_3(u_\mu) = \emptyset$, then, with (132), we obtain

$$0 \;<\; a - \theta_\mu \;=\; h\sum_{i=0}^{N-1} v_\mu^i - v_1^i \;\leq\; \sqrt{L}\,\sqrt{h\sum_{i=0}^{N-1}(v_\mu^i - v_1^i)^2} \;\leq\; O(\sqrt{h}),$$

and we come to a contradiction with $a > \theta_M = \lim_{h\to 0} \theta_\mu$. So $\mathrm{Card}\, G_3(u_\mu) = 1$, and we denote by i_μ its unique index: $G_3(u_\mu) = \{i_\mu\}$.

If $F_\mu^{i_\mu} > \underline{F_\mu}$, let i_0 be an index such that $F_\mu^{i_0} = \underline{F_\mu}$. By exchanging $v_\mu^{i_\mu}$ and $v_\mu^{i_0}$, one can lower the energy of v_μ. This is in contradiction with the fact that v_μ is minimizer. So $F_\mu^{i_\mu} = \underline{F_\mu}$.

Step 4 (identification of the Lagrange multiplier)**.** We have:
$a - \theta_M = a - \theta_\mu + o(1) = o(1) + h\sum_{i \notin G_3(u_\mu)}(v_\mu^i - v_1^i) + h(v_\mu^{i_\mu} - v_1^{i_\mu})$.
With (131), we see that $h\sum_{i \notin G_3(u_\mu)}(v_\mu^i - v_1^i) = o(1)$. With (119), we have $v_1^{i_\mu} = 1$, so $a - \theta_M = o(1) + hv_\mu^{i_\mu}$. Hence, $v_\mu^{i_\mu} \sim_{h\to 0} \frac{a-\theta_M}{h}$, which implies (52). As a consequence, $W_{\mathrm{LJ}}'(v_\mu^{i_\mu}) \sim Ch^7$. From (121), we obtain $\lambda_\mu^* = W_{\mathrm{LJ}}'(v_\mu^{i_\mu})$. So, for h small enough, we have $\lambda_\mu^* \in (0, h]$ and, since $h\sum v_\mu^i = a$, the Lagrange multiplier λ_μ^* satisfies (50). Since λ_μ, defined by Lemma 2.2, is the unique solution of (50), we have $\lambda_\mu^* = \lambda_\mu$. Collecting this equality with (121), we obtain (51). □

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