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ATOMISTIC-TO-CONTINUUM COUPLING APPROXIMATION OF A ONE-DIMENSIONAL TOY MODEL FOR DENSITY FUNCTIONAL THEORY*

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Abstract. We consider an atomistic model defined through an interaction field satisfying a variational principle and which can therefore be considered a toy model of (orbital-free) density functional theory. We investigate atomistic-to-continuum coupling mechanisms for this atomistic model, paying special attention to the dependence of the atomistic subproblem on the atomistic region boundary and the boundary conditions. We rigorously prove first-order error estimates for two related coupling mechanisms.

Key words. atomistic models, quasicontinuum method, coarse graining

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1. Introduction.

The quasicontinuum (QC) method and, more generally, atomistic/continuum (a/c) coupling methods are numerical coarse-graining techniques for the efficient simulation of phenomena and processes in materials at the nanoscale, such as defects, fracture, grain boundaries, or nanoindentation [18, 19, 16, 11]. Incompatibilities between the treatment of forces in atomistic and continuum models lead to difficulties in defining coupling mechanisms that do not introduce additional errors. Substantial effort has been made to understand this problem and to construct efficient and accurate a/c methods; see [17, 4, 15, 9, 20] for examples of formulations of computational methods and [1, 2, 3, 12, 13, 14] and the references therein for examples of analytical treatments. Formulations of a/c methods for atomistic models based on quantum mechanics were proposed in [8, 6], but, to the best of our knowledge, no rigorous analysis of these methods exists.

In the present article we formulate and analyze one-dimensional a/c methods for an atomistic model that is defined through an interaction field satisfying a linear variational principle. Our results are related to two classes of a/c methods: First, our work can be viewed as an analysis of (a simplified version of) the a/c method proposed by Iyer and Gavini [9], who use field-based versions of classical potentials to formulate their method. Second, the atomistic model we formulate can be considered a toy model of (orbital-free) density functional theory, and hence our work represents a preliminary step towards a rigorous analysis of the a/c methods described in [8, 6].

Our main results, stated in Theorems 5.5 and 6.6, are a priori error estimates for two closely related a/c couplings. While in a comparatively simple setting, the technical steps leading up these theorems address several important issues relevant for a/c coupling in the presence of fields, most prominently the dependence on the

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choice of boundary and boundary data for the interaction fields.

The article is structured as follows. In section 1 we formally motivate the atomistic model and introduce the necessary notation. In section 2 we give a precise formulation of the model with periodic boundary conditions and derive a "weak formulation" for the resulting forces on the particles. Section 3 is devoted to the analysis of the model in a bounded domain when the fields are subjected to Dirichlet boundary conditions. The Cauchy–Born continuum model is derived and analyzed in section 4. Finally, in sections 5 and 6 we propose two possible constructions of a/c methods based on different exchanges of boundary conditions between an atomistic and a continuum region, and we establish error estimates.

We will occasionally cite the extended preprint [10] to refer to details of certain arguments that we have omitted from the present work.

1.1. Field-based formulation of pair interactions. The following outline follows ideas presented in [9]. Let $\boldsymbol{y} = (y_1, \dots, y_N) \in \mathbb{R}^N$ represent the coordinates of N particles in one dimension. We consider an atomistic energy based on a pair-potential V,

$$\mathcal{E}(\boldsymbol{y}) = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} V(|y_i - y_j|).$$

The force on particle i is given by

$$-D_{y_i}\mathcal{E}(\boldsymbol{y}) = -\sum_{\substack{j=1 \\ j \neq i}}^{N} \operatorname{sign}(y_i - y_j) V'(|y_i - y_j|).$$

We note that the forces are nonlocal expressions in the sense that their computation involves summation over the other $N - 1$ particles.

Next, we make a few modifications to this model. First, we replace the pointwise particles with smooth, nonnegative, and compactly supported particle densities $\delta_\varepsilon(\cdot - y_i)$ (such that $\int_{\mathbb{R}} \delta_\varepsilon(x)\,\mathrm{d}x = 1$). This leads to

$$\mathcal{E}(\boldsymbol{y}) \approx \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \int_{\mathbb{R}} \int_{\mathbb{R}} \delta_\varepsilon(z - y_i) V(|z - x|) \delta_\varepsilon(x - y_j)\,\mathrm{d}z\,\mathrm{d}x.$$

To simplify the presentation further, we include the self-energies of the individual particle densities and define

$$\mathcal{E}_\varepsilon(\boldsymbol{y}) = \frac{1}{2} \sum_{i,j=1}^{N} \int_{\mathbb{R}} \int_{\mathbb{R}} \delta_\varepsilon(z - y_i) V(|z - x|) \delta_\varepsilon(x - y_j)\,\mathrm{d}z\,\mathrm{d}x.$$

This additional self-energy contribution does not affect the forces. It can be computed explicitly and subtracted from the energy later on. Upon introducing the field $\phi : \mathbb{R} \to \mathbb{R}$,

$$\phi(x) = \int_{\mathbb{R}} \rho_{\boldsymbol{y}}(z) V(|x - z|)\,\mathrm{d}z, \quad \text{where} \quad \rho_{\boldsymbol{y}}(z) = \sum_{i=1}^{N} \delta_\varepsilon(z - y_i), \tag{1.1}$$

we can rewrite the energy $\mathcal{E}_\varepsilon(\boldsymbol{y})$ in the form

$$\mathcal{E}_\varepsilon(\boldsymbol{y}) = \frac{1}{2}\int_{\mathbb{R}} \rho_{\boldsymbol{y}}(x)\phi(x)\,\mathrm{d}x.$$

It is now easy to see that the forces are given by the *local* expression

$$-D_{\boldsymbol{y}}\mathcal{E}_\varepsilon(\boldsymbol{y}) = -\int_{\mathbb{R}} D_{\boldsymbol{y}}\rho_{\boldsymbol{y}}(z)\phi(z)\,\mathrm{d}z.$$

Hence, if the field ϕ is known, then it becomes unnecessary to compute nonlocal sums over particles. The nonlocality of the interaction has been encoded in the field ϕ. However, it is now necessary to compute the field ϕ, which is defined via the convolution (1.1).

Suppose that the pair-potential V is the Green's function for a linear differential operator $L_V(\nabla)$; then, ϕ can alternatively be computed by solving the differential equation

$$L_V(\nabla)\phi = \rho_{\boldsymbol{y}}.$$

As an example we consider the Yukawa potential in one space dimension

$$V(x) = \frac{1}{2m}\mathrm{e}^{-m|x|} = \frac{1}{2\pi}\int_{\mathbb{R}} \frac{1}{k^2+m^2}\,\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k.$$

In this case ϕ can be obtained as the solution to

$$-\Delta\phi + m^2\phi = \rho_{\boldsymbol{y}}$$

or, equivalently, as a solution to the minimization problem

$$\phi = \arg\min_{\varphi}\left\{\frac{1}{2}\int_{\mathbb{R}} |\nabla\varphi|^2 + m^2\varphi^2\,\mathrm{d}x - \int_{\mathbb{R}} \rho_{\boldsymbol{y}}\varphi\,\mathrm{d}x\right\}.$$

The resulting interaction potential $\mathcal{E}_\varepsilon$ can also be written in the form

$$\mathcal{E}_\varepsilon(\boldsymbol{y}) = -\min_{\varphi}\left\{\frac{1}{2}\int_{\mathbb{R}} |\nabla\varphi|^2 + m^2\varphi^2\,\mathrm{d}x - \int_{\mathbb{R}} \rho_{\boldsymbol{y}}\varphi\,\mathrm{d}x\right\}. \tag{1.2}$$

The present work is devoted to the analysis of a/c approximations of (1.2) in a periodic one-dimensional setting. What distinguishes this analysis from previous analyses of a/c methods is that the coupling is achieved through an exchange of boundary conditions for the interaction field ϕ, rather than ghost-force removal ideas such as in [4, 15].

Remark 1. The interaction defined by (1.2) is purely repulsive. A purely attractive interaction can be obtained by changing the outer minus sign in the definition of $\mathcal{E}_\varepsilon$ to a plus sign. We could take linear combinations of the two energies of the form (1.2) with different parameters m to obtain a Morse potential interaction: $V(x) = \mathrm{e}^{-2m(|x|-1)} - 2\mathrm{e}^{-m(|x|-1)} = C^2\mathrm{e}^{-2m|x|} - 2C\mathrm{e}^{-m|x|}$, where $C = \mathrm{e}^m$. Indeed, following [9, sect. 4.1] we can show that, with this choice,

$$\begin{aligned}\mathcal{E}_\varepsilon(\boldsymbol{y}) &= \frac{1}{2}\sum_{i,j=1}^{N}\int_{\mathbb{R}}\int_{\mathbb{R}} \delta_\varepsilon(z-y_i)V(|z-x|)\delta_\varepsilon(x-y_j)\,\mathrm{d}z\,\mathrm{d}x\\ &= \inf_{\varphi}\int_{\mathbb{R}}\left\{\frac{1}{2}|\nabla^2\varphi|^2 + m^2|\nabla\varphi|^2 + \frac{1}{2}\alpha^4|\varphi|^2 - \rho_{\boldsymbol{y}}\varphi\right\}\mathrm{d}x.\end{aligned}$$

In particular, the field ϕ can now be obtained by solving a fourth-order differential equation. We anticipate no difficulties in generalizing our analysis to this case.

Even after introducing an attractive potential, our methods seem rather limited in their scope. We remark, however, that more general pair interactions can be approximated by linear combinations of exponential potentials [9].

Many-body interactions lead into the field of orbital-free density function theory. Generalizing our analysis to that extent would require more substantial modifications.

1.2. Notation. We consider an infinite chain of atoms on the one-dimensional lattice $\widehat{\boldsymbol{X}} = \varepsilon\mathbb{Z}$, where $\varepsilon = 2/(2N+1)$ is the reference lattice spacing. Moreover, to keep the analysis simple, we admit only $(2N+1)$-periodic displacements from the reference lattice (cf. [14]). Hence, we define the spaces of admissible displacements and deformations, respectively, by

$$\mathcal{U} = \big\{\boldsymbol{u} \in \mathbb{R}^{\mathbb{Z}} : u_{j+(2N+1)} = u_j \ \ \forall j \in \mathbb{Z}, \ \ \textstyle\sum_{j=-N}^{N} u_j = 0\big\},$$
$$\mathcal{Y} = F\widehat{\boldsymbol{X}} + \mathcal{U},$$

where $F > 0$ is a prescribed *macroscopic strain*. A deformation $\boldsymbol{y} \in \mathcal{Y}$ defines the computational domain

$$\Omega = (y_{-N-1}, y_N)$$

for the field variable ϕ. We note that the length of the interval is independent of $\boldsymbol{y}$.

We define the finite differences $\boldsymbol{y}', \boldsymbol{y}'' \in \mathcal{U}$ for $\boldsymbol{y} \in \mathcal{Y}$ or $\mathcal{U}$ by their respective components

$$y_j' = \frac{y_j - y_{j-1}}{\varepsilon}, \qquad y_j'' = \frac{y_{j+1} - 2y_j + y_{j-1}}{\varepsilon^2}.$$

Let us also define the weighted ℓ^2 scalar product and norm by

$$(\boldsymbol{u}, \boldsymbol{v})_\varepsilon = \varepsilon \sum_{\nu=-N}^{N} u_\nu v_\nu \quad \forall \boldsymbol{u}, \boldsymbol{v} \in \mathcal{U}, \qquad \|\boldsymbol{u}\|_{\ell^2_\varepsilon} := (\boldsymbol{u}, \boldsymbol{u})_\varepsilon^{1/2} \quad \forall \boldsymbol{u} \in \mathcal{U}. \tag{1.3}$$

The ℓ^∞-norm is defined in the obvious way:

$$\|\boldsymbol{u}\|_{\ell^\infty} = \max_{\nu=-N,\dots,N} |u_\nu| \quad \forall \boldsymbol{u} \in \mathcal{U}.$$

The space $\mathcal{U}$ equipped with the discrete Sobolev seminorm $\|\boldsymbol{u}\|_{\mathcal{U}^{1,2}} = \|\boldsymbol{u}'\|_{\ell^2_\varepsilon}$ will be denoted by $\mathcal{U}^{1,2}$ and its topological dual space by $\mathcal{U}^{-1,2}$. The norm on $\mathcal{U}^{-1,2}$ is given by

$$\|T\|_{\mathcal{U}^{-1,2}} = \sup_{\boldsymbol{u} \in \mathcal{U}^{1,2}} \frac{T \cdot \boldsymbol{u}}{\|\boldsymbol{u}\|_{\mathcal{U}^{1,2}}},$$

where, due to the finite-dimensional setting, we denote the duality pairing by $T \cdot u$.

For monotonically increasing $\boldsymbol{y} \in \mathcal{Y}$ (which we will write as $\boldsymbol{y}' > 0$) we denote by $\mathrm{S}(\boldsymbol{y}) \subset H^1(\Omega)$ the space of continuous functions that are linear on every interval $Q_i = (y_{i-1}, y_i)$, $i \in \{-N, \dots, N\}$. Furthermore, we define $\mathrm{S}_\#(\boldsymbol{y}) = \mathrm{S}(\boldsymbol{y}) \cap H^1_\#(\Omega)$ to be the subset of all periodic functions in $\mathrm{S}(\boldsymbol{y})$.

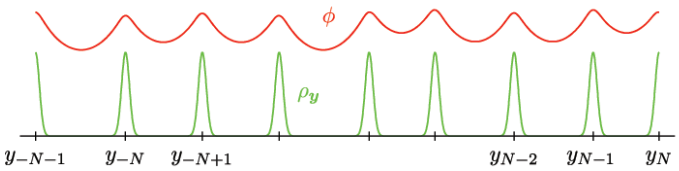

FIG. 2.1. *Sketch of the basic atomistic problem: the field ϕ is periodic in $\Omega = (y_{-N-1}, y_N)$, and $\rho_{\boldsymbol{y}}$ is a smooth particle density representing the atoms with positions given by $\boldsymbol{y} \in \mathcal{Y}$.*

2. Periodic boundary conditions. We now put the field-based interaction potential that was outlined above in a precise mathematical framework. Let the functional $I : H^1_\#(\Omega) \times \mathcal{Y} \to \mathbb{R}$ be defined by

$$I(\varphi, \boldsymbol{y}) = \int_\Omega \left(\tfrac{1}{2}\varepsilon^2 |\nabla\varphi|^2 + \tfrac{1}{2}m^2\varphi^2\right) \mathrm{d}x - \int_\Omega \rho_{\boldsymbol{y}}\varphi \,\mathrm{d}x, \quad \text{where}$$
$$\rho_{\boldsymbol{y}}(x) = \varepsilon \sum_{j\in\mathbb{Z}} \delta_\varepsilon(x - y_j) \quad \text{and} \quad \delta_\varepsilon(x) = \varepsilon^{-1}\delta_1(x/\varepsilon).$$

Here, δ_1 is a symmetric, nonnegative, regularized delta distribution with compact support $\left[-\frac{\varsigma_0}{2}, \frac{\varsigma_0}{2}\right]$, where $\varsigma_0 > 0$ and $\int_{\mathbb{R}} \delta_1 \,\mathrm{d}x = 1$; see Figure 2.1. We will frequently refer to the parameter ς_0, which is fixed throughout the paper.

We then define the interaction potential $\mathcal{E} : \mathcal{Y} \to \mathbb{R}$ by

$$\mathcal{E}(\boldsymbol{y}) = -\min_{\varphi\in H^1_\#(\Omega)} I(\varphi, \boldsymbol{y}). \tag{2.1}$$

The respective minimizer (see Figure 2.1)

$$\phi = \arg\min_{\varphi\in H^1_\#(\Omega)} I(\varphi, \boldsymbol{y})$$

is the periodic solution to the Euler–Lagrange equation

$$-\varepsilon^2\Delta\phi + m^2\phi = \rho_{\boldsymbol{y}} \quad \text{in } \Omega. \tag{2.2}$$

Although ϕ depends on $\boldsymbol{y}$, we will usually suppress this in our notation. It will always be clear from the context which configuration ϕ belongs to. It follows from (2.2) and integration by parts that

$$\mathcal{E}(\boldsymbol{y}) = \frac{1}{2}\int_\Omega \phi\rho_{\boldsymbol{y}} \,\mathrm{d}x.$$

To determine equilibrium configurations subject to a given external force $\boldsymbol{f} \in \mathcal{U}^{-1,2}$ (represented by the inner product $(\boldsymbol{f}, \cdot)_\varepsilon$) we need to minimize the total potential energy $E_{\boldsymbol{f}} : \mathcal{Y} \to \mathbb{R}$ defined by

$$E_{\boldsymbol{f}}(\boldsymbol{y}) = \mathcal{E}(\boldsymbol{y}) + (\boldsymbol{f}, \boldsymbol{y})_\varepsilon. \tag{2.3}$$

A minimizer $\bar{\boldsymbol{y}} \in \mathcal{Y}$ of (2.3) satisfies the following Euler–Lagrange equation in $\mathcal{U}^{-1,2}$:

$$DE_{\boldsymbol{f}}(\bar{\boldsymbol{y}}) = D\mathcal{E}(\bar{\boldsymbol{y}}) + \boldsymbol{f} = \boldsymbol{0}.$$

In the remainder of the section we analyze the derivatives of $\mathcal{E}$. Our main result is the "weak formulation" (2.6) of $D\mathcal{E}$, mimicking the weak form of an elliptic PDE. This result acts as a natural connection to the weak form of the Cauchy–Born equation, which we will derive in section 4.

We begin by computing a more classical representation of the forces.

PROPOSITION 2.1. *The potential $\mathcal{E} : \mathcal{Y} \to \mathbb{R}$ defined by* (2.1) *is twice continuously Fréchet differentiable. The components of the first derivative are given by*

$$D_{y_j}\mathcal{E}(\boldsymbol{y}) = -\varepsilon \int_\Omega \nabla\delta_\varepsilon(x - y_j)\phi(x)\,\mathrm{d}x \tag{2.4}$$

for $j \in \{-N, \dots, N-1\}$ and by

$$D_{y_N}\mathcal{E}(\boldsymbol{y}) = -\varepsilon \int_\Omega \big(\nabla\delta_\varepsilon(x - y_{-N-1}) + \nabla\delta_\varepsilon(x - y_N)\big)\phi(x)\,\mathrm{d}x. \tag{2.5}$$

Proof. The proof of this result is standard and can be found in [9], for example. The occurrence of both y_N and y_{-N-1} in (2.5) is due to the periodic boundary condition. Note that y_N is the "periodic image" of y_{-N-1}. ∎

We stress the fact that the forces $-D_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y})$ are local expressions. To calculate the force on atom j it is necessary to know ϕ in $\operatorname{supp}\delta_\varepsilon(\cdot - y_j)$, but there is no need to sum over all remaining atoms. This nonlocality is encoded in the field ϕ.

Next we establish the *weak formulation* for the forces on particles. A version of this calculation was already shown in [7], which used an interpolant for the displacement that is constant on the support of every $\delta_\varepsilon(\cdot - y_j)$. To avoid this restriction, we modify and extend the argument in [7]. For simplicity we assume that the supports of the densities of different particles do not intersect:

$$\operatorname{supp}\delta_\varepsilon(\cdot - y_i) \cap \operatorname{supp}\delta_\varepsilon(\cdot - y_j) = \emptyset \quad \forall i, j \in \mathbb{Z}, \quad i \neq j.$$

Removing this restriction would create substantial additional technical difficulties throughout the analysis.

Since $|\operatorname{supp}\delta_\varepsilon(\cdot - y_i)| = \varepsilon\varsigma_0$, this is equivalent to $|y_j - y_i| > \varepsilon\varsigma_0$ for $i \neq j$ or, if $\boldsymbol{y}$ is an increasing sequence, $y_j' > \varsigma_0$ for all $j \in \mathbb{Z}$.

LEMMA 2.2. *Let $\boldsymbol{y} \in \mathcal{Y}$ satisfy $\boldsymbol{y}' > \varsigma_0$, and let $\phi \in H^1_\#(\Omega)$ be the associated field, defined by* (2.2). *Let $\boldsymbol{u} = (u_j)_{j\in\mathbb{Z}} \in \mathcal{U}$ be a test vector and $u \in \mathrm{S}_\#(\boldsymbol{y})$ be the periodic piecewise linear interpolant of $\boldsymbol{u}$; that is, $u(y_j) = u_j$ for $j \in \mathbb{Z}$. Then,*

$$D\mathcal{E}(\boldsymbol{y})\cdot\boldsymbol{u} = \sum_{j=-N}^{N} D_{y_j}\mathcal{E}(\boldsymbol{y})\cdot u_j = \int_\Omega \sigma_{\boldsymbol{y}}(x)\nabla u(x)\,\mathrm{d}x, \tag{2.6}$$

where $\sigma_{\boldsymbol{y}} = \sigma_{\boldsymbol{y},1} + \sigma_{\boldsymbol{y},2}$ and

$$\begin{aligned} \sigma_{\boldsymbol{y},1}(x) &= \tfrac{1}{2}\varepsilon^2|\nabla\phi|^2 - \tfrac{1}{2}m^2\phi^2 + \rho_{\boldsymbol{y}}\phi, \\ \sigma_{\boldsymbol{y},2}(x) &= \varepsilon \sum_{j=-N-1}^{N} \phi(x)\nabla\delta_\varepsilon(x - y_j)(x - y_j). \end{aligned} \tag{2.7}$$

Proof. We begin by multiplying the derivative (2.4) for $j \in \{-N, \dots, N-1\}$ by

the component u_j:

$$\begin{aligned} D_{y_j}\mathcal{E}(\boldsymbol{y})u_j =& -\varepsilon u_j \int_\Omega \nabla\delta_\varepsilon(x-y_j)\phi(x)\,\mathrm{d}x \\ =& -\varepsilon\int_\Omega u(x)\nabla\delta_\varepsilon(x-y_j)\phi(x)\,\mathrm{d}x + \varepsilon\int_\Omega (u(x)-u_j)\nabla\delta_\varepsilon(x-y_j)\phi(x)\,\mathrm{d}x \\ =& \varepsilon\int_\Omega \delta_\varepsilon(x-y_j)u(x)\nabla\phi(x)\,\mathrm{d}x + \varepsilon\int_\Omega \delta_\varepsilon(x-y_j)\phi(x)\nabla u(x)\,\mathrm{d}x \\ &+\varepsilon\int_\Omega (u(x)-u_j)\nabla\delta_\varepsilon(x-y_j)\phi(x)\,\mathrm{d}x =: T_1^{(j)}+T_2^{(j)}+T_3^{(j)}. \end{aligned}$$

Here we have used integration by parts, but there are no boundary terms since u, ϕ, and $\rho_{\boldsymbol{y}}$ are periodic on Ω. Using (2.5) we obtain a similar expression for $D_{y_N}\mathcal{E}(\boldsymbol{y})u_N$. Summing over $j=-N,\dots,N$ we obtain

$$D\mathcal{E}(\boldsymbol{y})\cdot\boldsymbol{u} = \sum_{j=-N}^{N} D_{y_j}\mathcal{E}(\boldsymbol{y})\cdot u_j = T_1+T_2+T_3, \tag{2.8}$$

where $T_i=\sum_{j=-N}^{N} T_i^{(j)}$, $i\in\{1,2,3\}$. From $\rho_{\boldsymbol{y}}=\varepsilon\sum_{j\in\mathbb{Z}}\delta_\varepsilon(\cdot-y_j)$ it immediately follows that

$$T_2=\int_\Omega \rho_{\boldsymbol{y}}(x)\phi(x)\nabla u(x)\,\mathrm{d}x.$$

For T_1 we can carry out the following rearrangements:

$$\begin{aligned} T_1 &= \int_\Omega \rho_{\boldsymbol{y}} u\nabla\phi\,\mathrm{d}x = \int_\Omega \big(-\varepsilon^2\Delta\phi+m^2\phi\big)u\nabla\phi\,\mathrm{d}x \\ &= \int_\Omega \big(-\varepsilon^2\nabla\phi\Delta\phi+m^2\phi\nabla\phi\big)u\,\mathrm{d}x = \frac{1}{2}\int_\Omega \nabla\big(-\varepsilon^2|\nabla\phi|^2+m^2\phi^2\big)u\,\mathrm{d}x \\ &= \frac{1}{2}\int_\Omega \big(\varepsilon^2|\nabla\phi|^2-m^2\phi^2\big)\nabla u\,\mathrm{d}x. \end{aligned}$$

Here, we have again used integration by parts and the periodicity of all functions involved. We deduce that

$$T_1+T_2=\int_\Omega \sigma_{\boldsymbol{y},1}(x)\nabla u(x)\,\mathrm{d}x,$$

with $\sigma_{\boldsymbol{y},1}$ as defined in (2.7).

Before turning to T_3 we first note that, since u is piecewise linear,

$$u(x)=u_j+\frac{x-y_j}{y_j-y_{j-1}}(u_j-u_{j-1})=u_j+(x-y_j)\nabla u(x) \quad \text{for } x\in Q_j=(y_{j-1},y_j),$$
$$u(x)=u_j+\frac{x-y_j}{y_{j+1}-y_j}(u_{j+1}-u_j)=u_j+(x-y_j)\nabla u(x) \quad \text{for } x\in Q_{j+1}=(y_j,y_{j+1}).$$

Hence, T_3 in (2.8) can be written as

$$\begin{aligned} T_3 &= \varepsilon\sum_{j=-N-1}^{N}\int_\Omega \phi(x)\nabla\delta_\varepsilon(x-y_j)(u(x)-u_j)\,\mathrm{d}x \\ &= \varepsilon\sum_{j=-N-1}^{N}\int_\Omega \phi(x)\nabla\delta_\varepsilon(x-y_j)(x-y_j)\nabla u(x)\,\mathrm{d}x = \varepsilon\int_\Omega \sigma_{\boldsymbol{y},2}(x)\nabla u\,\mathrm{d}x, \end{aligned}$$

with $\sigma_{\boldsymbol{y},2}$ as defined in (2.7), which concludes the proof. ∎

Remark 2. 1. In more than one space dimension the above calculations can be generalized if a triangular, respectively, tetrahedral, mesh with the atomic positions as nodes is constructed. For example, this leads to

$$\sigma_{\boldsymbol{y},1}(x) = \left(-\tfrac{1}{2}\varepsilon^2|\nabla\phi|^2 - \tfrac{1}{2}m^2\phi^2 + \rho_{\boldsymbol{y}}\phi\right)\mathrm{id} \; + \varepsilon^2\nabla\phi\otimes\nabla\phi.$$

2. A closer look at the calculations in the proof of Lemma 2.2 shows that the weak form can be obtained for semilinear models $-\varepsilon^2\Delta\phi + F'(\phi) = \rho_{\boldsymbol{y}}$ with any convex function F. Even a fourth-order model of the form $\varepsilon^4\Delta^2\phi - \varepsilon^2\Delta\phi + F'(\phi) = \rho_{\boldsymbol{y}}$ admits a similar weak formulation.

As already suggested in the introduction the Green's function for the differential operator $-\varepsilon^2\Delta + m^2\mathrm{id}$ acting on functions defined on $\mathbb{R}$ is given by

$$G_\varepsilon(x) = \frac{1}{2\varepsilon m}\,\mathrm{e}^{-\frac{m}{\varepsilon}|x|}. \tag{2.9}$$

We therefore get the following explicit formulas for the function values $\phi(x)$ and $\nabla\phi(x)$ for $x \in \Omega$.

PROPOSITION 2.3. *Let $\boldsymbol{y} \in \mathcal{Y}$, and let $\phi = \arg\min_{\varphi\in H^1_\#(\Omega)} I(\varphi, \boldsymbol{y})$ be the corresponding interaction field. Then, for every $x \in \Omega$,*

$$\phi(x) = \int_{\mathbb{R}} G_\varepsilon(x-z)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z = \frac{1}{2m}\sum_{k\in\mathbb{Z}}\int_{\mathbb{R}} \delta_\varepsilon(z-y_k)\,\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z, \tag{2.10}$$

$$\nabla\phi(x) = \int_{\mathbb{R}} G_\varepsilon(x-z)\nabla\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z = \frac{1}{2m}\sum_{k\in\mathbb{Z}}\int_{\mathbb{R}} \nabla\delta_\varepsilon(z-y_k)\,\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z. \tag{2.11}$$

Proof. The proof of this proposition is similar to that of [5, Thm. 2.1]; see also the extended preprint [10, Prop. 2.4]. ∎

The following is a consequence of the simple exponential form of the Yukawa potential and some elementary properties of the exponential function in one dimension. Let $y_i, y_j \in \mathbb{R}$ satisfy $y_j > y_i + \varepsilon\varsigma_0$, so that the supports of particle densities representing the atoms i and j do not intersect. Then,

$$\begin{aligned}
&\int_{\mathbb{R}}\int_{\mathbb{R}} \delta_\varepsilon(z-y_j)\mathrm{e}^{-\frac{m}{\varepsilon}|z-x|}\delta_\varepsilon(x-y_i)\,\mathrm{d}x\,\mathrm{d}z \\
&= \int_{\mathbb{R}}\int_{\mathbb{R}} \delta_\varepsilon(z-y_j)\mathrm{e}^{-\frac{m}{\varepsilon}(z-x)}\delta_\varepsilon(x-y_i)\,\mathrm{d}x\,\mathrm{d}z \\
&= \mathrm{e}^{-\frac{m}{\varepsilon}(y_j-y_i)}\int_{\mathbb{R}} \mathrm{e}^{-\frac{m}{\varepsilon}(z-y_j)}\delta_\varepsilon(z-y_j)\,\mathrm{d}z \cdot \int_{\mathbb{R}} \mathrm{e}^{-\frac{m}{\varepsilon}(y_i-x)}\delta_\varepsilon(y_i-x)\,\mathrm{d}x \\
&= \mu^2\,\mathrm{e}^{-\frac{m}{\varepsilon}(y_j-y_i)}, \qquad (2.12)
\end{aligned}$$

where we have defined

$$\mu = \int_{\mathbb{R}} \delta_\varepsilon(x)\mathrm{e}^{-\frac{m}{\varepsilon}x}\,\mathrm{d}x = \int_{\mathbb{R}} \delta_\varepsilon(x)\mathrm{e}^{\frac{m}{\varepsilon}x}\,\mathrm{d}x = \int_{\mathbb{R}} \delta_1(x)\mathrm{e}^{mx}\,\mathrm{d}x.$$

Although we will frequently use this property (e.g., in Lemma 4.2), it is not essential for our reasoning. It merely makes some calculations more convenient.

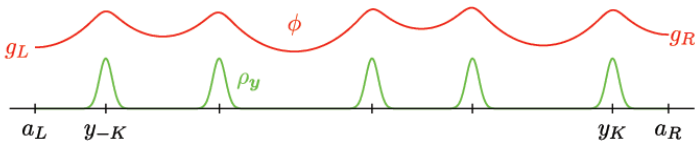

FIG. 3.1. *The atomistic model in the domain Ω_a with Dirichlet boundary conditions $g = [g_L\ g_R]^{\mathrm{T}}$.*

3. Dirichlet boundary conditions. In this section we consider a version of the model (2.1) in the domain $\Omega_a = (a_L, a_R) \subset \mathbb{R}$ subject to Dirichlet instead of periodic boundary conditions; cf. Figure 3.1. This concept will be used in sections 5 and 6, for the formulation of a/c methods, as the atomistic subproblem. We will study the dependence of this subproblem on the choice of boundary points a_L, a_R and on the choice of boundary data that we prescribe for the field variable ϕ at those points. The results we develop in this section will guide us in our treatment of the a/c interface in sections 5 and 6.

We set $a = [a_L\ a_R]^{\mathrm{T}} \in \mathbb{R}^2$ and $\Delta a = a_R - a_L$. Throughout section 3 we think of $\boldsymbol{y} = (y_{-K}, \dots, y_K)$ as an ordered element of Ω_a^{2K+1} such that $a_L < y_{-K} < \cdots < y_K < a_R$, where $K < N$. The particle density $\rho_{\boldsymbol{y}}$ is defined by

$$\rho_{\boldsymbol{y}} = \varepsilon \sum_{j=-K}^{K} \delta_\varepsilon(\cdot - y_j).$$

We shall assume throughout that the y_j are separated and lie well inside Ω_a in the sense that $\operatorname{supp} \rho_{\boldsymbol{y}} \cap \partial\Omega_a = \emptyset$ or, equivalently,

$$\begin{aligned} &y_i' \geq \varsigma_0 \qquad \text{for } i = -K+1, \dots, K, \\ &a_R - y_K > \varepsilon\varsigma_0/2 \quad \text{and} \quad y_{-K} - a_L > \varepsilon\varsigma_0/2. \end{aligned} \tag{3.1}$$

We impose the following boundary conditions on the resulting field $\phi : \Omega_a \to \mathbb{R}$:

$$\phi(a_L) = g_L, \qquad \phi(a_R) = g_R;$$

i.e., $\phi|_{\partial\Omega_a} = g$, with $g = [g_L\ g_R]^{\mathrm{T}} \in \mathbb{R}^2$. The interaction potential $\mathcal{E}_{a,g} : \Omega_a^{2K+1} \to \mathbb{R}$ is defined by

$$\mathcal{E}_{a,g}(\boldsymbol{y}) = - \min_{\substack{\varphi \in H^1(\Omega_a) \\ \varphi|_{\partial\Omega_a} = g}} I_a(\varphi, \boldsymbol{y}), \tag{3.2}$$

where $I_a : H^1(\Omega_a) \times \Omega_a^{2K+1} \to \mathbb{R}$ is given by

$$I_a(\varphi, \boldsymbol{y}) = \int_{a_L}^{a_R} \left(\tfrac{1}{2}\varepsilon^2 |\nabla\varphi|^2 + \tfrac{1}{2} m^2 \varphi^2\right) \mathrm{d}x - \int_{a_L}^{a_R} \rho_{\boldsymbol{y}} \varphi \, \mathrm{d}x. \tag{3.3}$$

For given $\boldsymbol{y}$ the minimizer ϕ is the weak solution to

$$\begin{aligned} -\varepsilon^2 \Delta\phi + m^2\phi &= \rho_{\boldsymbol{y}} \quad \text{in } \Omega_a, \\ \phi|_{\partial\Omega_a} &= g. \end{aligned} \tag{3.4}$$

We will frequently use the decomposition

$$\phi = \phi_0 + \xi_{a,g}, \tag{3.5}$$

where $\phi_0 \in H^1_0(\Omega_a)$ and $\xi_{a,g} \in H^1(\Omega_a)$, respectively, solve the boundary-value problems

$$\begin{aligned} -\varepsilon^2 \Delta \phi_0 + m^2 \phi_0 &= \rho_{\boldsymbol{y}} \quad \text{in } \Omega_a, \\ \phi_0|_{\partial\Omega_a} &= 0 \end{aligned}$$

and

$$\begin{aligned} -\varepsilon^2 \Delta \xi_{a,g} + m^2 \xi_{a,g} &= 0 \quad \text{in } \Omega_a, \\ \xi_{a,g}|_{\partial\Omega_a} &= g. \end{aligned} \tag{3.6}$$

This last boundary-value problem can be solved explicitly, which yields the following lemma.

LEMMA 3.1. *The solution $\xi_{a,g}$ of* (3.6) *is given by*

$$\xi_{a,g}(x) = c_L(a,g)\mathrm{e}^{-\frac{m}{\varepsilon}(x-a_L)} + c_R(a,g)\mathrm{e}^{-\frac{m}{\varepsilon}(a_R-x)}, \tag{3.7}$$

where the coefficients $c_L(a,g)$ and $c_R(a,g)$ are given by

$$c(a,g) = \begin{bmatrix} c_L(a,g) \\ c_R(a,g) \end{bmatrix} = \begin{bmatrix} 1 & \tau \\ \tau & 1 \end{bmatrix}^{-1} \begin{bmatrix} g_L \\ g_R \end{bmatrix} =: T_a^{-1} \cdot g \tag{3.8}$$

and we have defined $\tau = \exp(-\frac{m}{\varepsilon}\Delta a)$.

Note that, for $\Delta a \gg \varepsilon$, τ is exponentially small; hence we will often neglect terms of that order of magnitude. We will write $\mathcal{O}(\tau)$ for a quantity or function that is (uniformly) bounded above by $C\tau$ in modulus, where C is independent of ε and Δa. For example, we have $c(a,g) = g + \mathcal{O}(\tau)$.

Next, we compute the derivative of $\mathcal{E}_{a,g}$ with respect to the atomic coordinates. For these derivatives, we obtain a "weak" formulation of the same shape as in the periodic case (see Proposition 2.1).

If $\boldsymbol{y}' > 0$, then we denote by $\mathcal{S}(\boldsymbol{y} \cup a)$ the set of continuous, piecewise affine functions over the mesh given by the nodes $a_L, y_{-K}, \ldots, y_K, a_R$. Moreover, $\mathcal{S}_0(\boldsymbol{y} \cup a) = \mathcal{S}(\boldsymbol{y} \cup a) \cap H^1_0(\Omega_a)$.

PROPOSITION 3.2. *Let $a, g \in \mathbb{R}^2$, $a_L < a_R$; then $\mathcal{E}_{a,g} : \mathcal{Y} \to \mathbb{R}$ defined by* (3.2) *is continuously Fréchet differentiable at $\boldsymbol{y}$:*

(i) *The components of the first derivative are given by*

$$D_{y_j}\mathcal{E}_{a,g}(\boldsymbol{y}) = -\varepsilon \int_{\Omega_a} \nabla \delta_\varepsilon(x - y_j)\phi(x)\,\mathrm{d}x \qquad \text{for } i = -K, \ldots, K. \tag{3.9}$$

(ii) *Let $\boldsymbol{u} \in \mathcal{U}$ be a test vector, $u \in \mathrm{S}_0(\boldsymbol{y} \cup a)$ its interpolant, and let $\min \boldsymbol{y}' \geq \varsigma_0$; then,*

$$D_{\boldsymbol{y}}\mathcal{E}_{a,g}(\boldsymbol{y}) \cdot \boldsymbol{u} = \int_{\Omega_a} \sigma_{\boldsymbol{y}}(x) \nabla u(x)\,\mathrm{d}x, \tag{3.10}$$

where $\sigma_{\boldsymbol{y}}$ is given by (2.7).

Proof. The derivatives with respect to the coordinates $\boldsymbol{y}$ are easy to calculate along the same lines as in the proof of Proposition 2.1. The weak formulation can be obtained as in the periodic case (Lemma 2.2) using the fact that the interpolant u vanishes on $\partial\Omega_a$. ∎

Remark 3. We point out that, in general,

$$\mathcal{E}_{a,g}(\boldsymbol{y}) \neq \frac{1}{2}\int_{\Omega_a} \rho_{\boldsymbol{y}}\phi \,\mathrm{d}x.$$

However, we will see below, for example in (3.16), that $\mathcal{E}_{a,g}(\boldsymbol{y})$ can be written as the sum of a boundary data contribution and a term that is independent of g.

With a view to the subsequent derivation of a/c methods we will from now on interpret a and g as arguments to $\mathcal{E}_{a,g}$ rather than fixed parameters entering its definition. We consider the map $\Omega_a^{2K+1} \times \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}$, $(\boldsymbol{y}, a, g) \mapsto \mathcal{E}_{a,g}(\boldsymbol{y})$, and we obtain an expression of the derivatives of this map with respect to the boundary a and the boundary data g.

3.1. Dependence on the boundary positions. When formulating a/c methods in section 5 we will let the boundary a of the atomistic subdomain depend on the configuration $\boldsymbol{y}$. It is therefore necessary to understand the dependence of the energy $\mathcal{E}_{a,g}(\boldsymbol{y})$ on a. Our main result is that the derivative $D_a\mathcal{E}_{a,g}(\boldsymbol{y})$ can be combined with $D_{\boldsymbol{y}}\mathcal{E}_{a,g}(\boldsymbol{y})$ into a weak formulation reminiscent of (2.6). This will be a central building block for a/c methods.

PROPOSITION 3.3. *Suppose that* $\boldsymbol{y} \in \mathcal{Y}$, $\min \boldsymbol{y}' \geq \varsigma_0$. *Let* $h = [h_L\ h_R]^{\mathrm{T}} \in \mathbb{R}^2$ *and* $\boldsymbol{u} = (u_{-K}, \dots, u_K) \in \mathbb{R}^{2K+1}$ *be test vectors, and let* $u \in \mathrm{S}(\boldsymbol{y} \cup a)$ *denote the interpolant of* $\boldsymbol{u}$ *and* h *in the sense that*

$$u(a_L) = h_L, \quad u(a_R) = h_R, \quad \textit{and} \quad u(y_j) = u_j \quad \forall j \in \{-K, \dots, K\}.$$

Then,

$$D_a\mathcal{E}_{a,g}(\boldsymbol{y})\cdot h + D_{\boldsymbol{y}}\mathcal{E}_{a,g}(\boldsymbol{y})\cdot \boldsymbol{u} = \int_{\Omega_a} \sigma_{\boldsymbol{y}}(x)\nabla u(x)\,\mathrm{d}x,$$

where $\sigma_{\boldsymbol{y}}$ *is defined in* (2.7).

Proof. This is a direct consequence of the following two lemmas and (3.10). ∎

In the first auxiliary lemma we compute the derivative of $\mathcal{E}_{a,g}(\boldsymbol{y})$ with respect to $a = [a_L\ a_R]^{\mathrm{T}}$ while keeping the relative distances between the atoms constant. In other words we consider the change in $\mathcal{E}_{a,g}(\boldsymbol{y})$ when the whole domain Ω_a is stretched with the atom positions following this stretching. For $\boldsymbol{y} \in \Omega_a^{2K+1}$ let $\boldsymbol{X} = (X_{-K}, \dots, X_K) \in (0,1)^{2K+1}$ be given implicitly by $y_j = a_L + \Delta a X_j$ for all $j \in \{-K, \dots, K\}$. For fixed $g, \boldsymbol{X}$ we define

$$\begin{aligned} \widetilde{\mathcal{E}}(a) &:= \mathcal{E}_{a,g}(a_L + (a_R - a_L)\boldsymbol{X}), \\ \widetilde{D}_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y}) &:= D_{a_R}\widetilde{\mathcal{E}}(a). \end{aligned}$$

(We understand $a_L + (a_R - a_L)\boldsymbol{X}$ in a componentwise manner: $(a_L + \Delta a\boldsymbol{X})_j = a_L + \Delta a X_j$ for all $j \in \{-K, \dots, K\}$.) The derivative $\widetilde{D}_{a_L}\mathcal{E}_{a,g}(\boldsymbol{y})$ is defined analogously.

LEMMA 3.4. *Let* $\boldsymbol{y} \in \Omega_a^{2K+1}$ *satisfy* (3.1)*; then*

$$-\widetilde{D}_{a_L}\mathcal{E}_{a,g}(\boldsymbol{y}) = \widetilde{D}_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y}) = \frac{1}{\Delta a}\int_{\Omega_a} \sigma_{\boldsymbol{y}}(x)\,\mathrm{d}x. \tag{3.11}$$

Proof. We fix $\boldsymbol{X}$ and let $\boldsymbol{\eta}(a) := a_L + \Delta a\boldsymbol{X}$. We begin by transforming the prob-

lem to the unit interval $(0,1)$ using the transformation $x \mapsto X(x) = (x-a_L)/(a_R-a_L)$:

$$\begin{aligned}\widetilde{\mathcal{E}}(a) = \mathcal{E}_{a,g}(\boldsymbol{\eta}(a)) &= \int_{\Omega_a} \left(-\frac{1}{2}\varepsilon^2|\nabla\phi|^2 - \frac{1}{2}m^2\phi^2 + \rho_{\boldsymbol{\eta}(a)}\phi\right) \mathrm{d}x \\ &= \Delta a \int_0^1 \left(-\frac{\varepsilon^2}{2\Delta a^2}|\nabla\widehat{\phi}|^2 - \frac{m^2}{2}\widehat{\phi}^2 + \widehat{\rho}_{\boldsymbol{\eta}(a)}\widehat{\phi}\right) \mathrm{d}X.\end{aligned} \tag{3.12}$$

Here, $\widehat{\phi}(X) = \phi(x(X))$ and $\widehat{\rho}_{\boldsymbol{\eta}(a)}(X) = \rho_{\boldsymbol{\eta}(a)}(x(X))$. It follows as in Proposition 2.1 that, to compute $D_a\widetilde{\mathcal{E}}(a)$, it is sufficient to calculate the partial derivatives of the right-hand side with respect to a_R (the derivative of ϕ or $\widehat{\phi}$ with respect to a_R does not appear since ϕ is a minimizer of $I_a(\cdot,\boldsymbol{y})$). This leads to

$$\begin{aligned}D_{a_R}\widetilde{\mathcal{E}}(a) = &\int_0^1 \left(-\frac{\varepsilon^2}{2\Delta a^2}|\nabla\widehat{\phi}|^2 - \frac{m^2}{2}\widehat{\phi}^2 + \widehat{\rho}_{\boldsymbol{\eta}(a)}\widehat{\phi}\right) \mathrm{d}X + \Delta a \int_0^1 \frac{\varepsilon^2}{\Delta a^3}|\nabla\widehat{\phi}|^2 \,\mathrm{d}X \\ &+ \Delta a \int_0^1 \widehat{\phi} D_{a_R}\widehat{\rho}_{\boldsymbol{\eta}(a)} \,\mathrm{d}X.\end{aligned}$$

Transforming the first two integrals on the right-hand side back to the interval Ω_a we arrive at

$$\frac{1}{\Delta a}\mathcal{E}_{a,g}(\boldsymbol{y}) + \frac{\varepsilon^2}{\Delta a}\int_{\Omega_a}|\nabla\phi|^2 \,\mathrm{d}x = \frac{1}{\Delta a}\int_{\Omega_a}\sigma_{\boldsymbol{y},1}(x)\,\mathrm{d}x,$$

where $\sigma_{\boldsymbol{y},1}$ was given in (2.7).

It remains to differentiate $\widehat{\rho}_{\boldsymbol{\eta}(a)}$ with respect to a_R. By the definition of the transformation $x \mapsto X(x)$ we have

$$\begin{aligned}D_{a_R}\widehat{\rho}_{\boldsymbol{\eta}(a)}(X) &= \varepsilon D_{a_R}\sum_{j=-K}^{K}\delta_\varepsilon\big((a_R-a_L)(X-X_j)\big) \\ &= \varepsilon\sum_{j=-K}^{K}(X-X_j)\nabla\delta_\varepsilon\big((a_R-a_L)(X-X_j)\big).\end{aligned}$$

Using $\Delta a(X-X_j) = (x-y_j)$ we therefore get

$$\begin{aligned}\Delta a\int_0^1 \widehat{\phi}D_{a_R}\widehat{\rho}_{\boldsymbol{\eta}(a)}\,\mathrm{d}X &= \frac{\varepsilon}{\Delta a}\sum_{j=-K}^{K}\int_{\Omega_a}(x-y_j)\nabla\delta_\varepsilon(x-y_j)\phi(x)\,\mathrm{d}x \\ &= \frac{1}{\Delta a}\int_{\Omega_a}\sigma_{\boldsymbol{y},2}(x)\,\mathrm{d}x,\end{aligned}$$

with $\sigma_{\boldsymbol{y},2}(x)$ as given in (2.7).

To see that $D_{a_L}\widetilde{\mathcal{E}} = -D_{a_R}\widetilde{\mathcal{E}}$ we simply note that $\mathcal{E}(a)$ depends only on Δa, which can be seen from (3.12) and the definition of $\widehat{\rho}_{\boldsymbol{\eta}(a)}(X)$. ∎

We define $\theta_R \in \mathrm{S}(\boldsymbol{y}\cup a)$ to be the piecewise linear function with

$$\theta_R(a_R) = 1, \quad \theta_R(a_L) = 0, \quad \theta_R(y_j) = 0 \quad \forall j \in \{-K,\dots,K\}.$$

The function $\theta_L \in \mathrm{S}(\boldsymbol{y}\cup a)$ is defined analogously.

LEMMA 3.5. *Let $\boldsymbol{y} \in \Omega_a^{2K+1}$ satisfy (3.1); then, the derivatives of $\mathcal{E}_{a,g}(\boldsymbol{y})$ with respect to a_L, a_R (for fixed $\boldsymbol{y}$ and g) satisfy*

$$D_{a_L}\mathcal{E}_{a,g}(\boldsymbol{y}) = \int_{\Omega_a} \sigma_{\boldsymbol{y}}(x)\nabla\theta_L(x)\,\mathrm{d}x,$$
$$D_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y}) = \int_{\Omega_a} \sigma_{\boldsymbol{y}}(x)\nabla\theta_R(x)\,\mathrm{d}x.$$

Proof. Let Θ_R be the affine function defined on Ω_a with $\Theta_R(a_L) = 0$, $\Theta_R(a_R) = 1$. Since $\nabla\Theta_R(x) = \frac{1}{\Delta a}$, Lemma 3.4 yields

$$\widetilde{D}_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y}) = \int_{\Omega_a} \sigma_{\boldsymbol{y}}\nabla\Theta_R\,\mathrm{d}x = \int_{\Omega_a} \sigma_{\boldsymbol{y}}\nabla(\Theta_R - \theta_R)\,\mathrm{d}x + \int_{\Omega_a} \sigma_{\boldsymbol{y}}\nabla\theta_R\,\mathrm{d}x. \tag{3.13}$$

Now, we have $\Theta_R - \theta_R \in \mathrm{S}_0(\boldsymbol{y} \cup a)$ and hence, by Proposition 3.2,

$$\int_{\Omega_a} \sigma_{\boldsymbol{y}}(x)\nabla(\Theta_R - \theta_R)\,\mathrm{d}x = \sum_{j=-K}^{K} D_{y_j}\mathcal{E}_{a,g}(\boldsymbol{y})\Theta_R(y_j). \tag{3.14}$$

However, $\widetilde{D}_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y})$ was defined as the derivative with respect to a_R, while the relative distances of the atoms are kept constant. Thus, we see that

$$\widetilde{D}_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y}) = D_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y}) + \sum_{j=-K}^{K} D_{y_j}\mathcal{E}_{a,g}(\boldsymbol{y})\Theta_R(y_j).$$

Inserting this into (3.13) and using (3.14) then gives

$$\int_{\Omega_a} \sigma_{\boldsymbol{y}}(x)\nabla\theta_R\,\mathrm{d}x = D_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y}).$$

Similarly, we can show the expression stated for $D_{a_L}\mathcal{E}_{a,g}(\boldsymbol{y})$. ∎

3.2. Dependence on the boundary values. Next, we compute the derivative of $\mathcal{E}_{a,g}(\boldsymbol{y})$ with respect to the boundary conditions g when the configuration $\boldsymbol{y}$ and the boundary a are kept fixed. We define

$$\gamma_L(\boldsymbol{y}, a) = 2\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)G_\varepsilon(x - a_L)\,\mathrm{d}x \quad \text{and} \quad \gamma_R(\boldsymbol{y}, a) = 2\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)G_\varepsilon(a_R - x)\,\mathrm{d}x. \tag{3.15}$$

LEMMA 3.6. *The partial derivative of $\mathcal{E}_{a,g}(\boldsymbol{y})$ with respect to g is given by*

$$D_g\mathcal{E}_{a,g}(\boldsymbol{y}) = -m\varepsilon\left((1-\tau^2)\begin{bmatrix} c_L(a,g) \\ c_R(a,g)\end{bmatrix} - \begin{bmatrix}\gamma_L(\boldsymbol{y},a) \\ \gamma_R(\boldsymbol{y},a)\end{bmatrix}\right)^T \cdot T_a^{-1},$$

where T_a, $c(a,g) = [c_L(a,g)\ c_R(a,g)]^T$, and $\tau = \mathrm{e}^{-\frac{m}{\varepsilon}\Delta a}$ are defined in Lemma 3.1.

Proof. Throughout the proof we suppress the arguments of γ_L, γ_R, and c for ease of readability. We recall the additive decomposition $\phi = \phi_0 + \xi_{a,g}$ from (3.5). From $\phi_0 \in H_0^1(\Omega)$ and from the equation $-\varepsilon^2\Delta\xi_{a,g} + m^2\xi_{a,g} = 0$ it follows that $\varepsilon^2(\nabla\xi_{a,g}, \nabla\phi_0) + m^2(\xi_{a,g}, \phi_0) = 0$. Hence, a short calculation shows that the energy $\mathcal{E}_{a,g}(\boldsymbol{y})$ can be rewritten as

$$\mathcal{E}_{a,g}(\boldsymbol{y}) = -I_a(\phi, \boldsymbol{y}) = -I_a(\phi_0, \boldsymbol{y}) - I_a(\xi_{a,g}, \boldsymbol{y}). \tag{3.16}$$

The first term on the right-hand side does not depend on the boundary conditions g, and the second term is known explicitly: using $-\varepsilon^2\Delta\xi_{a,g} + m^2\xi_{a,g} = 0$, integration by parts, and the explicit formula (3.7) for $\xi_{a,g}$, we obtain

$$\begin{aligned}
I_a(\xi_{a,g}, \boldsymbol{y}) &= \int_{\Omega_a} \frac{1}{2}\big(\varepsilon^2|\nabla\xi_{a,g}|^2 + m^2\xi_{a,g}^2\big)\,\mathrm{d}x - \int_{\Omega_a} \rho_{\boldsymbol{y}}\xi_{a,g}\,\mathrm{d}x \\
&= \frac{\varepsilon^2}{2}\big(-\xi_{a,g}(a_L)\nabla\xi_{a,g}(a_L) + \xi_{a,g}(a_R)\nabla\xi_{a,g}(a_R)\big) - \int_{\Omega_a} \rho_{\boldsymbol{y}}\xi_{a,g}\,\mathrm{d}x \\
&= \frac{\varepsilon m}{2}\big(c_L^2 + c_R^2\big)\big(1 - \mathrm{e}^{-2\frac{m}{\varepsilon}\Delta a}\big) - \int_{\Omega_a} \rho_{\boldsymbol{y}}\big(c_L\mathrm{e}^{-\frac{m}{\varepsilon}(x-a_L)} + c_R\mathrm{e}^{-\frac{m}{\varepsilon}(a_R-x)}\big)\,\mathrm{d}x \\
&= m\varepsilon\bigg(\frac{c_L^2 + c_R^2}{2}\big(1-\tau^2\big) - \frac{2}{2m\varepsilon}\int_{\Omega_a} \rho_{\boldsymbol{y}}\big(c_L\mathrm{e}^{-\frac{m}{\varepsilon}(x-a_L)} + c_R\mathrm{e}^{-\frac{m}{\varepsilon}(a_R-x)}\big)\,\mathrm{d}x\bigg) \\
&= m\varepsilon\bigg(\frac{c_L^2 + c_R^2}{2}\big(1-\tau^2\big) - \big(c_L\gamma_L + c_R\gamma_R\big)\bigg).
\end{aligned}$$

Here we have used the Green's function G_ε from (2.9). Differentiating this expression with respect to c_L and c_R and applying the chain rule with $D_g c = T_a^{-1}$ yield the result. ∎

A useful auxiliary result for the analysis of a/c methods is the global Lipschitz continuity of the field ϕ with respect to variations in the boundary conditions g.

LEMMA 3.7. *Let $\phi_1, \phi_2 \in H^1(\Omega_a)$ be minimizers of $I_a(\cdot, \boldsymbol{y})$ subject to the boundary conditions $g_1 \in \mathbb{R}^2$, respectively, $g_2 \in \mathbb{R}^2$. Then,*

$$\begin{aligned}
|\phi_1(x) - \phi_2(x)| &\le \sqrt{2}\,|T_a^{-1}(g_1 - g_2)|\,\mathrm{e}^{-\frac{m}{\varepsilon}d_a(x)}, \\
\varepsilon|\nabla\phi_1(x) - \nabla\phi_2(x)| &\le \sqrt{2}\,m\,|T_a^{-1}(g_1 - g_2)|\,\mathrm{e}^{-\frac{m}{\varepsilon}d_a(x)},
\end{aligned}$$

where $d_a(x) := \min(x - a_L, a_R - x)$ denotes the distance to the boundary of Ω_a, for $x \in \Omega_a$.

Proof. We write both functions in the form $\phi_i = \phi_0 + \xi_{a,g_i}$, $i \in \{1, 2\}$. For $i = 1, 2$, let $c_i = T_a^{-1}g_i$ be the respective coefficients entering ξ_{a,g_i}; then,

$$\begin{aligned}
|\phi_1(x) - \phi_2(x)| &= |\xi_{a,g_1}(x) - \xi_{a,g_2}(x)| \\
&\le |c_{1,L} - c_{2,L}|\,\mathrm{e}^{-\frac{m}{\varepsilon}(x-a_L)} + |c_{1,R} - c_{2,R}|\,\mathrm{e}^{-\frac{m}{\varepsilon}(a_R-x)}.
\end{aligned}$$

This immediately yields the first bound. The bound for the derivatives is obtained similarly. ∎

3.3. "Optimal" boundary conditions. In this subsection we study a specific choice of boundary data g that will play an important role throughout the remainder of the paper.

We begin by noting that $D_g\mathcal{E}_{a,g}(\boldsymbol{y}) = 0$ if and only if

$$c_L(a, g) = \gamma_L(\boldsymbol{y}, a)/(1-\tau^2) \quad \text{and} \quad c_R(a, g) = \gamma_R(\boldsymbol{y}, a)/(1-\tau^2).$$

According to (3.8) this corresponds to the boundary conditions

$$g_L^* = \frac{1}{1-\tau}\frac{\gamma_L + \tau\gamma_R}{1+\tau} \quad \text{and} \quad g_R^* = \frac{1}{1-\tau}\frac{\tau\gamma_L + \gamma_R}{1+\tau}. \tag{3.17}$$

It can be seen from Lemma 3.6 that the boundary data contribution $I_a(\xi_{a,g}, \boldsymbol{y})$ to the energy $\mathcal{E}_{a,g}(\boldsymbol{y})$ is quadratic in g. For fixed configuration $\boldsymbol{y}$ and domain Ω_a the

boundary conditions $g = g^*(\boldsymbol{y}, a)$ minimize the boundary data contribution $I_a(\xi_{a,g}, \boldsymbol{y})$ to the energy $\mathcal{E}_{a,g}(\boldsymbol{y})$. This is equivalent to minimizing $I_a(\cdot, \boldsymbol{y})$ over $H^1(\Omega_a)$ and therefore leads to homogeneous Neumann boundary conditions for ϕ on $\partial\Omega_a$.

If $\Delta a \gg \varepsilon$, i.e., $\tau \ll 1$, then we have $\gamma_{L/R} = g^*_{L/R} + \mathcal{O}(\tau)$, and hence we can simplify

$$\begin{aligned} I_a(\xi_{a,g}, \boldsymbol{y}) &= m\varepsilon\big(\tfrac{1}{2}\big(g_L^2 + g_R^2\big) - \big(g_L g_L^* + g_R g_R^*\big)\big) + \mathcal{O}(\varepsilon\tau), \\ D_g\mathcal{E}_{a,g}(\boldsymbol{y}) &= m\varepsilon(g^* - g) + \mathcal{O}(\varepsilon\tau). \end{aligned} \tag{3.18}$$

In the remainder of this subsection, we take a closer look at the interaction potential $\mathcal{E}_{a,g}$ from (3.2) with the $\boldsymbol{y}$-dependent boundary conditions $g = g^*(\boldsymbol{y}, a)$ defined in (3.17).

PROPOSITION 3.8. *Let $\boldsymbol{y} \in \Omega_a^{2K+1}$. Then,*

$$\begin{aligned} \mathcal{E}_{a,g^*(\boldsymbol{y},a)}(\boldsymbol{y}) &= \frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x + \tau M_\tau(\gamma_L, \gamma_R) \\ &\quad + \frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)\big(\mathrm{e}^{-\frac{m}{\varepsilon}(2a_R - x - z)} + \mathrm{e}^{-\frac{m}{\varepsilon}(x+z-2a_L)}\big)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x, \end{aligned} \tag{3.19}$$

where $M_\tau(\gamma_L, \gamma_R)$ depends quadratically on γ_L and γ_R.

Expression (3.19) can be interpreted as the energy of the atoms represented by $\boldsymbol{y}$ interacting with each other plus the interaction with mirror atoms outside Ω_a. This mirror interaction was introduced by means of the boundary conditions $g = g^*$.

For the proof of the proposition it is convenient to use an explicit formula for the function values of $\phi_0 \in H^1_0(\Omega_a)$ from the decomposition (3.5). By Proposition 2.3, the Green's function for the equation $-\varepsilon^2\Delta\phi + m^2\phi = \rho_{\boldsymbol{y}}$ in $\mathbb{R}$ is given by $G_\varepsilon(x, y) = \frac{1}{2m\varepsilon}\mathrm{e}^{-\frac{m}{\varepsilon}|x-y|}$. We will now construct the Green's function $G_{\varepsilon,a}$ for the operator $-\varepsilon^2\Delta + m^2\mathrm{id}$ subject to homogeneous Dirichlet conditions on $\partial\Omega_a$.

LEMMA 3.9. *Let $\phi_0 \in H^1_0(\Omega_a)$ satisfy $-\varepsilon^2\Delta\phi_0 + m^2\phi_0 = \rho_{\boldsymbol{y}}$ in Ω_a. Then,*

$$\phi_0(x) = \int_{\Omega_a} G_{\varepsilon,a}(x, z)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z \quad \forall x \in \Omega_a, \tag{3.20}$$

where $G_{\varepsilon,a} = G^{(1)}_{\varepsilon,a} + \tau G^{(2)}_{\varepsilon,a}$, with $G^{(i)}_{\varepsilon,a}$, $i = 1, 2$, given by

$$\begin{aligned} G^{(1)}_{\varepsilon,a}(x, z) &= \frac{1}{2m\varepsilon}\Big(\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|} - \mathrm{e}^{-\frac{m}{\varepsilon}(x+z-2a_L)} - \mathrm{e}^{-\frac{m}{\varepsilon}(2a_R-x-z)}\Big), \\ G^{(2)}_{\varepsilon,a}(x, z) &= -\frac{1}{2m\varepsilon}\frac{1}{1-\tau^2}\Big(\tau\mathrm{e}^{-\frac{m}{\varepsilon}(x+z-2a_L)} + \tau\mathrm{e}^{-\frac{m}{\varepsilon}(2a_R-x-z)} \\ &\qquad - \mathrm{e}^{-\frac{m}{\varepsilon}(x-z+a_R-a_L)} - \mathrm{e}^{-\frac{m}{\varepsilon}(z-x+a_R-a_L)}\Big). \end{aligned}$$

Proof. The proof of this result is standard [5, Chap. 2.2.4]; see also [10, Lem. 3.10]. ∎

We remark that $G_{\varepsilon,a} = G^{(1)}_{\varepsilon,a} + \mathcal{O}(\tau)$.

Proof of Proposition 3.8. We have already seen in (3.16) that for any choice of boundary data $g \in \mathbb{R}^2$ the energy $\mathcal{E}_{a,g}(\boldsymbol{y})$ can be written as the sum of two terms

$$\mathcal{E}_{a,g}(\boldsymbol{y}) = -I_a(\phi, \boldsymbol{y}) = -I_a(\phi_0, \boldsymbol{y}) - I_a(\xi_{a,g}, \boldsymbol{y}),$$

where $I_a(\phi_0, \boldsymbol{y})$ is independent of the boundary conditions.

Calculation of $I_a(\phi_0, \boldsymbol{y})$. Since the function ϕ_0 is a minimizer of $I_a(\cdot, \boldsymbol{y})$ over $H^1_0(\Omega)$, we have with the expression (3.20) for $\phi_0(x)$ that

$$I_a(\phi_0, \boldsymbol{y}) = -\frac{1}{2}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}\phi_0 \,\mathrm{d}x = -\frac{1}{2}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x) G_{\varepsilon,a}(x,z)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x. \tag{3.21}$$

By the definition (3.15) of γ_L and γ_R we have

$$\begin{aligned}
\frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}(2a_R - x - z)}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}x\,\mathrm{d}z &= \frac{m\varepsilon}{4}\gamma_R^2,\\
\frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}(x + z - 2a_L)}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}x\,\mathrm{d}z &= \frac{m\varepsilon}{4}\gamma_L^2,\\
\frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}(z - x + a_R - a_L)}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}x\,\mathrm{d}z &= \frac{m\varepsilon}{4}\gamma_L\gamma_R.
\end{aligned} \tag{3.22}$$

Inserting the expression $G_{\varepsilon,a} = G^{(1)}_{\varepsilon,a} + \tau G^{(2)}_{\varepsilon,a}$ into (3.21) and using these equalities yields

$$\begin{aligned}
I_a(\phi_0, \boldsymbol{y}) = &-\frac{1}{2}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)G_\varepsilon(x,z)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x + \frac{m\varepsilon}{4}\big(\gamma_L^2 + \gamma_R^2\big)\\
&+ \frac{m\varepsilon}{4}\frac{\tau}{1-\tau^2}\big(\tau\gamma_L^2 + \tau\gamma_R^2 - 2\gamma_L\gamma_R\big).
\end{aligned}$$

Calculation of $I_a(\xi_{a,g^*(\boldsymbol{y},a)}, \boldsymbol{y})$. From Lemma 3.6 we know that for general $g \in \mathbb{R}^2$

$$I_a(\xi_{a,g}, \boldsymbol{y}) = m\varepsilon\bigg(\frac{c_L^2 + c_R^2}{2}\big(1-\tau^2\big) - \big(c_L\gamma_L + c_R\gamma_R\big)\bigg).$$

If $g = g^*(\boldsymbol{y}, a)$, then $c_L = \gamma_L/(1-\tau^2)$ and $c_R = \gamma_R/(1-\tau^2)$, as seen in (3.17). Hence,

$$I_a(\xi_{a,g^*(\boldsymbol{y},a)}, \boldsymbol{y}) = -\frac{m\varepsilon}{2}\frac{1}{1-\tau^2}\big(\gamma_L^2 + \gamma_R^2\big).$$

Isolating the dependence on τ gives

$$I_a(\xi_{a,g^*(\boldsymbol{y},a)}, \boldsymbol{y}) = -\frac{m\varepsilon}{2}\big(\gamma_L^2 + \gamma_R^2\big) - \frac{m\varepsilon}{2}\frac{\tau^2}{1-\tau^2}\big(\gamma_L^2 + \gamma_R^2\big). \tag{3.23}$$

Conclusion. Adding $-I_a(\xi_{a,g^*(\boldsymbol{y},a)}, \boldsymbol{y})$ as just obtained and $-I_a(\phi_0, \boldsymbol{y})$ from above we arrive at

$$\begin{aligned}
\mathcal{E}_{a,g^*(\boldsymbol{y},a)}(\boldsymbol{y}) = &\frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x + \frac{m\varepsilon}{4}\big(\gamma_L^2 + \gamma_R^2\big)\\
&- \frac{m\varepsilon}{4}\frac{\tau}{1-\tau^2}\big(\tau\gamma_L^2 + 2\gamma_L\gamma_R + \tau\gamma_R^2\big).
\end{aligned} \tag{3.24}$$

Defining $\tau M_\tau(\gamma_L, \gamma_R)$ to be the third term on the right-hand side and applying (3.22) yields (3.19). ∎

4. The Cauchy–Born approximation. The next building block for the design of a/c methods based on the model (2.1) is the respective continuum model. The goal of the present section is to derive this model and study its consistency error relative

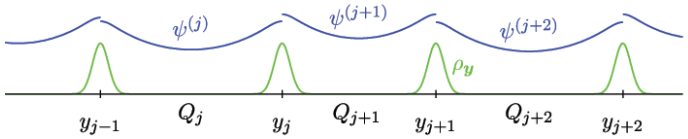

FIG. 4.1. *The Cauchy–Born approximation: independent periodic problems are solved on the cells* $Q_j = (y_{j-1}, y_j)$ *leading to locally defined fields* $\psi^{(j)}$.

to the full atomistic model and its stability. These results will enter the consistency and stability results on a/c couplings in sections 5 and 6.

Let $\boldsymbol{y} \in \mathcal{Y}$ satisfy $\min \boldsymbol{y}' > \varsigma_0$. The Cauchy–Born approximation is obtained by computing the energy of the cells $Q_j = (y_{j-1}, y_j)$ independently from one another, by treating each of them as part of a homogeneous chain (see Figure 4.1). We define the Cauchy–Born energy of the cell Q_j by

$$\mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y}) = -\min_{\psi \in H^1_{\#}(Q_j)} \left(\int_{Q_j} \left(\tfrac{1}{2}\varepsilon^2 |\nabla \psi|^2 + \tfrac{1}{2} m^2 \psi^2 \right) \mathrm{d}x - \int_{Q_j} \rho_{\boldsymbol{y}} \psi \, \mathrm{d}x \right). \tag{4.1}$$

Note that this energy depends only on the distance $(y_j - y_{j-1})$. The minimizer $\psi^{(j)}$ of (4.1) satisfies the equation $-\varepsilon^2 \Delta \psi^{(j)} + m^2 \psi^{(j)} = \rho_{\boldsymbol{y}}$ in Q_j and its $|Q_j|$-periodic extension to $\mathbb{R}$:

$$-\varepsilon^2 \Delta \psi^{(j)} + m^2 \psi^{(j)} = \rho_{\boldsymbol{y}^{(j)}} \quad \text{in } \mathbb{R}, \tag{4.2}$$

where we have defined the positions $\boldsymbol{y}^{(j)} = (y_k^{(j)})_{k \in \mathbb{Z}}$ of an infinite chain of equidistant atoms by

$$y_k^{(j)} = y_j + (k - j)(y_j - y_{j-1}) \quad \forall k \in \mathbb{Z}. \tag{4.3}$$

The Cauchy–Born approximation $\mathcal{E}^{\mathrm{cb}}(\boldsymbol{y})$ of the atomistic energy $\mathcal{E}(\boldsymbol{y})$ is then given by the sum over all cells

$$\mathcal{E}^{\mathrm{cb}}(\boldsymbol{y}) = \sum_{j=-N}^{N} \mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y}) = \frac{1}{2} \sum_{j=-N}^{N} \int_{Q_j} \rho_{\boldsymbol{y}} \psi^{(j)} \, \mathrm{d}x. \tag{4.4}$$

In the Cauchy–Born model we seek to minimize the total potential energy $E_{\boldsymbol{f}}^{\mathrm{cb}} : \mathcal{Y} \to \mathbb{R}$ defined by

$$E_{\boldsymbol{f}}^{\mathrm{cb}}(\boldsymbol{y}) = \mathcal{E}^{\mathrm{cb}}(\boldsymbol{y}) + (\boldsymbol{f}, \boldsymbol{y})_{\varepsilon}. \tag{4.5}$$

Whether the Cauchy–Born model is a good approximation to the exact atomistic model strongly depends on the regularity properties of minimizers of (4.5).

Let $\boldsymbol{u} \in \mathcal{U}$ be a test vector and $u \in \mathcal{S}_{\#}(\boldsymbol{y})$ be an interpolant of $\boldsymbol{u}$; i.e., $u(y_j) = u_j$ for $j \in \mathbb{Z}$. It follows as in Lemma 3.4 that the derivative of $\mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y})$ can be written in the form

$$D_{\boldsymbol{y}} \mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y}) \cdot \boldsymbol{u} = \frac{u_j - u_{j-1}}{y_j - y_{j-1}} \int_{Q_j} \sigma_{j,\boldsymbol{y}}^{\mathrm{cb}}(x) \, \mathrm{d}x = \int_{Q_j} \sigma_{j,\boldsymbol{y}}^{\mathrm{cb}}(x) \nabla u(x) \, \mathrm{d}x, \tag{4.6}$$

where the local continuum stress function $\sigma^{\rm cb}_{j,\boldsymbol{y}}$, in direct correspondence with (2.7), is

$$\begin{aligned}\sigma^{\rm cb}_{j,\boldsymbol{y}}(x) = {}& \tfrac{1}{2}\varepsilon^2|\nabla\psi^{(j)}(x)|^2 - \tfrac{1}{2}m^2\psi^{(j)}(x)^2 + \rho_{\boldsymbol{y}}(x)\psi^{(j)}(x)\\ &+ \varepsilon\sum_{j=-N-1}^{N}\psi^{(j)}(x)\nabla\delta_\varepsilon(x-y_j)(x-y_j).\end{aligned}\tag{4.7}$$

Furthermore, we define the Cauchy–Born stress function $\sigma^{\rm cb}_{\boldsymbol{y}}:\Omega\to\mathbb{R}$ by

$$\sigma^{\rm cb}_{\boldsymbol{y}}(x) = \sigma^{\rm cb}_{j,\boldsymbol{y}}(x) \quad \text{if} \quad x\in\Omega_j$$

for all $x\in\Omega$.

4.1. Consistency. Next, we turn to the consistency analysis of the Cauchy–Born approximation, for which we shall estimate the error of the Cauchy–Born forces in a norm suitable for the subsequent error analysis.

From (2.6) and (4.6) we deduce that

$$\begin{aligned}\big|\big(D\mathcal{E}(\boldsymbol{y}) - D\mathcal{E}^{\rm cb}(\boldsymbol{y})\big)\cdot\boldsymbol{u}\big| &\le \int_\Omega \big|\sigma_{\boldsymbol{y}}(x) - \sigma^{\rm cb}_{\boldsymbol{y}}(x)\big|\,|\nabla u(x)|\,{\rm d}x\\ &= \sum_{j=-N}^{N}\int_{Q_j}\big|\sigma_{\boldsymbol{y}}(x) - \sigma^{\rm cb}_{j,\boldsymbol{y}}(x)\big|\,|\nabla u(x)|\,{\rm d}x,\end{aligned}$$

where the stress functions $\sigma_{\boldsymbol{y}}$ and $\sigma^{\rm cb}_{j,\boldsymbol{y}}$ are given by (2.7) and (4.7), respectively. To investigate the modeling error $\big|\sigma_{\boldsymbol{y}}(x)-\sigma^{\rm cb}_{j,\boldsymbol{y}}(x)\big|$ incurred by going from the atomistic description to the Cauchy–Born approximation it is therefore sufficient to analyze $|\phi-\psi^{(j)}|$ and $|\nabla\phi-\nabla\psi^{(j)}|$ in Q_j for every $j\in\{-N,\dots,N\}$.

LEMMA 4.1. *Let $\boldsymbol{y}\in\ell^\infty(\mathbb{Z})$, and define $\boldsymbol{y}^{(j)} = (y^{(j)}_k)_{k\in\mathbb{Z}}$ by $y^{(j)}_k = y_j + \varepsilon y'_j(k-j)$ for all $k\in\mathbb{Z}$; then,*

$$\begin{aligned}&\big|y_n - y^{(j)}_n\big| \le (n-j)\varepsilon^2\|\boldsymbol{y}''\|_{\ell^1([j,n-1])} \qquad \text{for } n>j,\\ &\big|y_n - y^{(j)}_n\big| \le (j-1-n)\varepsilon^2\|\boldsymbol{y}''\|_{\ell^1([n+1,j-1])} \qquad \text{for } n<j-1.\end{aligned}$$

Proof. Assume, without loss of generality, that $n>j$. Since $y_{j-1} = y^{(j)}_{j-1}$ and $y_j = y^{(j)}_j$,

$$y_n - y^{(j)}_n = \varepsilon\sum_{k=j+1}^{n}\big(y'_k - (y^{(j)}_k)'\big) = \varepsilon^2\sum_{k=j+1}^{n}\sum_{l=j}^{k-1}\big(y''_l - (y^{(j)}_l)''\big) = \varepsilon^2\sum_{k=j+1}^{n}\sum_{l=j}^{k-1}y''_l,$$

where we have used that $(\boldsymbol{y}^{(j)})'$ is constant. Changing the order of summation we get

$$|y_n - y^{(j)}_n| \le \varepsilon^2\sum_{l=j}^{n-1}\sum_{k=l+1}^{n}|y''_l| = \varepsilon^2\sum_{l=j}^{n-1}(n-l)y''_l \le (n-j)\varepsilon^2\|\boldsymbol{y}''\|_{\ell^1([j,n-1])}. \qquad \square$$

In the next result we estimate the errors $|\phi(x)-\psi^{(j)}(x)|$, $|\nabla\phi(x)-\nabla\psi^{(j)}(x)|$ for x in the cell Q_j. As anticipated by Lemma 4.1 they depend on the second difference $\boldsymbol{y}''$.

LEMMA 4.2. *Let $\boldsymbol{y} \in \mathcal{Y}$ satisfy $\min \boldsymbol{y}' > \varsigma_0$. Let $\phi \in H^1_{\#}(\Omega)$ satisfy (2.2) and $\psi^{(j)} \in H^1_{\#}(Q_j)$ satisfy (4.2), respectively. Then,*

$$\begin{aligned}\big\|\phi - \psi^{(j)}\big\|_{L^\infty(Q_j)} &\le \mu\varepsilon \sum_{n=1}^{\infty} \|\boldsymbol{y}''\|_{\ell^1([j-n,j+n-1])} n \mathrm{e}^{-mn\min \boldsymbol{y}'},\\ \big\|\varepsilon\nabla\phi - \varepsilon\nabla\psi^{(j)}\big\|_{L^\infty(Q_j)} &\le m\mu\varepsilon \sum_{n=1}^{\infty} \|\boldsymbol{y}''\|_{\ell^1([j-n,j+n-1])} n \mathrm{e}^{-mn\min \boldsymbol{y}'}.\end{aligned}$$

Proof. From Proposition 2.3 we immediately deduce that, for all $x \in Q_j$,

$$\begin{aligned}\phi(x) &= \frac{1}{2m}\int_{\mathbb{R}} \sum_{k\in\mathbb{Z}} \delta_\varepsilon(z-y_k)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z,\\ \psi^{(j)}(x) &= \frac{1}{2m}\int_{\mathbb{R}} \sum_{k\in\mathbb{Z}} \delta_\varepsilon(z-y^{(j)}_k)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z.\end{aligned} \tag{4.8}$$

Since $y^{(j)}_j = y_j$ and $y^{(j)}_{j-1} = y_{j-1}$, the respective terms in the sums cancel. Hence, we get for $x \in Q_j$

$$\phi(x) - \psi^{(j)}(x) = \frac{1}{2m} \sum_{\substack{k\in\mathbb{Z}\\ k\neq j-1,j}} \int_{\mathbb{R}} \big(\delta_\varepsilon(z-y_k) - \delta_\varepsilon(z-y^{(j)}_k)\big)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z.$$

We now derive bounds on the individual terms in the sum. Note that (2.12) simplifies the following calculations, but due to the smoothness of the Green's function similar bounds can be obtained without it.

Let $k > j$. Then we have $|x-z| = z-x$ for all $z \in \operatorname{supp}\delta_\varepsilon(\cdot - y_k)$ and all $z \in \operatorname{supp}\delta_\varepsilon(\cdot - y^{(j)}_k)$. Thus, with (2.12),

$$\frac{1}{2m}\int_{\mathbb{R}} \big(\delta_\varepsilon(z-y_k) - \delta_\varepsilon(z-y^{(j)}_k)\big)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z = \frac{\mu}{2m}\big(\mathrm{e}^{-\frac{m}{\varepsilon}(y_k-x)} - \mathrm{e}^{-\frac{m}{\varepsilon}(y^{(j)}_k-x)}\big). \tag{4.9}$$

If $y^{(j)}_k \ge y_k$, then

$$\begin{aligned}\left|\frac{1}{2m}\int_{\mathbb{R}} \big(\delta_\varepsilon(z-y_k) - \delta_\varepsilon(z-y^{(j)}_k)\big)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z\right| &\le \frac{\mu}{2m}\mathrm{e}^{-\frac{m}{\varepsilon}(y_k-x)}\big(1-\mathrm{e}^{-\frac{m}{\varepsilon}(y^{(j)}_k-y_k)}\big)\\ &\le \frac{\mu}{2m}\mathrm{e}^{-\frac{m}{\varepsilon}(y_k-x)}\frac{m}{\varepsilon}(y^{(j)}_k - y_k).\end{aligned}$$

Using $(y_k - x) \ge (k-j)\varepsilon\min\boldsymbol{y}'$ for all $x \in Q_j$ and applying Lemma 4.1 leads to

$$\frac{\mu}{2\varepsilon}\mathrm{e}^{-\frac{m}{\varepsilon}(y_k-x)}\big|y_k - y^{(j)}_k\big| \le \frac{\mu\varepsilon}{2}\|\boldsymbol{y}''\|_{\ell^1([j,k-1])}(k-j)\mathrm{e}^{-(k-j)m\min\boldsymbol{y}'}.$$

The same bound on (4.9) can be obtained if $y^{(j)}_k \le y_k$.

For any $k < j-1$ we can use the same techniques to obtain that

$$\begin{aligned}&\left|\frac{1}{2m}\int_{\mathbb{R}} \big(\delta_\varepsilon(z-y_k) - \delta_\varepsilon(z-y^{(j)}_k)\big)\ \mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z\right|\\ &\qquad\le \frac{\mu\varepsilon}{2}\|\boldsymbol{y}''\|_{\ell^1([k+1,j-1])}(j-k-1)\mathrm{e}^{-(j-k-1)m\min\boldsymbol{y}'}.\end{aligned}$$

Summing over all $k \in \mathbb{Z}\backslash\{j-1, j\}$ we deduce that

$$\left|\phi(x) - \psi^{(j)}(x)\right| \leq \mu\varepsilon \sum_{n=1}^{\infty} \|\boldsymbol{y}''\|_{\ell^1([j-n,j+n-1])} n \mathrm{e}^{-mn \min \boldsymbol{y}'}.$$

The proof for the derivatives $\nabla\phi$, $\nabla\psi^{(j)}$ is analogous. ∎

We wish to prove modeling error estimates on $\left\|\sigma_{\boldsymbol{y}} - \sigma^{\mathrm{cb}}_{j,\boldsymbol{y}}\right\|_{L^\infty(Q_j)}$ in terms of $\left\|\phi - \psi^{(j)}\right\|_{L^\infty(Q_j)}$ and $\left\|\nabla\phi - \nabla\psi^{(j)}\right\|_{L^\infty(Q_j)}$. Since the stress functions $\sigma_{\boldsymbol{y}}$ and $\sigma^{\mathrm{cb}}_{j,\boldsymbol{y}}$ are quadratic in the fields ϕ and $\psi^{(j)}$, we need L^∞-bounds, which we establish in the next lemma.

LEMMA 4.3. *Let $\boldsymbol{y} \in \mathcal{Y}$, $\boldsymbol{y}' > \varsigma_0$, and let $\phi = \arg\min_{\varphi \in H^1_{\#}(\Omega)} I(\varphi, \boldsymbol{y})$ be the corresponding field. Then, there are continuous functions K_0, K_1 that depend implicitly on m (but are independent of ε and $\boldsymbol{y}$) such that*

$$\|\phi\|_{L^\infty(\Omega)} \leq K_0(m \min \boldsymbol{y}') \quad \textit{and} \quad \varepsilon\|\nabla\phi\|_{L^\infty(\Omega)} \leq K_1(m \min \boldsymbol{y}').$$

Proof. The stated estimates follow in a straightforward manner from the integral representation of the solution ϕ; see [10, Lem. 4.4] for the details. ∎

We can now prove the following modeling error estimates.

LEMMA 4.4. *Let $\sigma_{\boldsymbol{y}}$ and $\sigma^{\mathrm{cb}}_{j,\boldsymbol{y}}$ be given by (2.7), respectively, (4.7); then,*

$$\left\|\sigma_{\boldsymbol{y}} - \sigma^{\mathrm{cb}}_{j,\boldsymbol{y}}\right\|_{L^\infty(Q_j)} \leq C\big(\varepsilon \left\|\nabla\phi - \nabla\psi^{(j)}\right\|_{L^\infty(Q_j)} + \left\|\phi - \psi^{(j)}\right\|_{L^\infty(Q_j)}\big), \quad j = 1, \ldots, N,$$

where the constant C depends only on δ_1, $K_i = K_i(m\boldsymbol{y}')$, and on m.

Proof. From the definitions of the atomistic and continuum stress function we deduce that

$$\begin{aligned}
\sigma_{\boldsymbol{y}}(x) - \sigma^{\mathrm{cb}}_{j,\boldsymbol{y}}(x) = \; & -\tfrac{1}{2}\big(\varepsilon\nabla\phi(x) - \varepsilon\nabla\psi^{(j)}(x)\big)\big(\varepsilon\nabla\phi(x) + \varepsilon\nabla\psi^{(j)}(x)\big) \\
& + \tfrac{1}{2}m^2\big(\phi(x) - \psi^{(j)}(x)\big)\big(\phi(x) + \psi^{(j)}(x)\big) \\
& - \rho_{\boldsymbol{y}}(x)\big(\phi(x) - \psi^{(j)}(x)\big) \\
& - \big(\phi(x) - \psi^{(j)}(x)\big) \sum_{i=j-1}^{j} \varepsilon\nabla\delta_\varepsilon(x - y_i)(x - y_i)
\end{aligned}$$

for all $x \in Q_j$. With $\delta_\varepsilon(x) = \varepsilon^{-1}\delta_1(x/\varepsilon)$, the L^∞-bound on ϕ from Lemma 4.3, and the analogous bound for $\psi^{(j)}$ we get

$$\begin{aligned}
\tfrac{1}{2}\left|\varepsilon\nabla\phi(x) + \varepsilon\nabla\psi^{(j)}(x)\right| &\leq K_1(m \min \boldsymbol{y}'), \\
\tfrac{m^2}{2}\left|\phi(x) + \psi^{(j)}(x)\right| &\leq m^2 K_0(m \min \boldsymbol{y}'), \\
\|\rho_{\boldsymbol{y}}\|_{L^\infty} &\leq \|\delta_1\|_{L^\infty}, \\
\left|\varepsilon\nabla\delta_\varepsilon(x - y_i)(x - y_i)\right| &\leq \|\nabla\delta_1 \mathrm{id}\|_{L^\infty},
\end{aligned}$$

which implies the stated result. ∎

4.2. Stability. Besides consistency, the second crucial property of an approximation to a given model is its stability. The following auxiliary result establishes stability of the Cauchy–Born model (by proving that its Hessian is coercive in a suitable norm) and will also play a role in the stability analysis of a/c methods.

LEMMA 4.5. *Let $\boldsymbol{y} \in \mathcal{Y}$ satisfy $\min \boldsymbol{y}' > \varsigma_0$. Then, for all $j \in \{-N, \dots, N\}$,*

$$D^2\mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \geq \frac{m^2\mu^2}{2}\mathrm{e}^{-m\max \boldsymbol{y}'}\varepsilon|u_j'|^2 \quad \forall \boldsymbol{u} \in \mathcal{U}.$$

Proof. We first recall that $\mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y}) = \frac{1}{2}\int_{Q_j}\rho_{\boldsymbol{y}}\psi^{(j)}\,\mathrm{d}x$ because $\psi^{(j)}$ is a minimizer of (4.1). Extending $\psi^{(j)}$ $|Q_j|$-periodically to $\mathbb{R}$ and using the symmetry of the cell problem, we can rewrite this as

$$\mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y}) = \frac{\varepsilon}{2}\int_{\mathbb{R}}\delta_\varepsilon(x-y_j)\psi^{(j)}(x)\,\mathrm{d}x.$$

We now insert the explicit formula (4.8) for $\psi^{(j)}(x)$ and apply (2.12) to get

$$\begin{aligned}\mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y}) &= \frac{\varepsilon}{4m}\sum_{k\in\mathbb{Z}}\int_{\mathbb{R}}\int_{\mathbb{R}}\delta_\varepsilon(x-y_j)\delta_\varepsilon(z-y_k^{(j)})\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z\,\mathrm{d}x\\ &= \frac{\mu^2\varepsilon}{4m}\sum_{\substack{k\in\mathbb{Z}\\k\neq j}}\mathrm{e}^{-\frac{m}{\varepsilon}|y_j-y_k^{(j)}|} + \mathcal{E}_{\mathrm{self}} = \frac{\mu^2\varepsilon}{2m}\sum_{\nu=1}^{\infty}\mathrm{e}^{-m\,\nu\,y_j'} + \mathcal{E}_{\mathrm{self}},\end{aligned}$$

where the constant $\mathcal{E}_{\mathrm{self}}$ coming from $k=j$ in the sum represents the self-energies of the atoms in the cell Q_j. Here we have also used that $\left|y_k^{(j)} - y_j\right| = |k-j|y_j'$ for all $k \in \mathbb{Z}$. Differentiating twice leads to

$$\begin{aligned}D^2\mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] &= \frac{m\mu^2}{2}\varepsilon\sum_{\nu=1}^{\infty}\nu^2\mathrm{e}^{-\nu m y_j'}|u_j'|^2\\ &\geq \frac{m\mu^2}{2}\varepsilon|u_j'|^2\sum_{\nu=1}^{\infty}\nu^2\mathrm{e}^{-\nu m\max\boldsymbol{y}'} \geq \frac{m\mu^2}{2}\mathrm{e}^{-m\max\boldsymbol{y}'}\ \varepsilon|u_j'|^2.\end{aligned}$$

In the last step we have kept the term only for $\nu = 1$, which represents the nearest neighbor interactions. ∎

5. Atomistic-to-continuum coupling. The computation of the original atomistic energy $\mathcal{E}(\boldsymbol{y})$ involves the solution of the optimization problem (2.1) posed in the whole of $\Omega = (y_{-N-1}, y_N)$. Our goal is the construction of computationally cheaper, approximate energies $\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})$ such that minimizers $\bar{\boldsymbol{y}}^{\mathrm{ac}} \in \mathcal{Y}$ of

$$E_{\boldsymbol{f}}^{\mathrm{ac}}(\boldsymbol{y}) = \mathcal{E}^{\mathrm{ac}}(\boldsymbol{y}) + (\boldsymbol{f},\boldsymbol{y})_\varepsilon$$

are good approximations of minimizers $\bar{\boldsymbol{y}}$ of the energy $E_{\boldsymbol{f}}$ from (2.3).

Following the philosophy of a/c methods we approximate $\mathcal{E}(\boldsymbol{y})$ by the continuum model where $\boldsymbol{y}$ is smooth and a version of the atomistic model where $\boldsymbol{y}$ is nonsmooth. In the following we will implicitly assume that the configurations $\boldsymbol{y} \in \mathcal{Y}$ under consideration are smooth except in the segment $y_{-K}, \dots, y_K$ for some $K < N$. We divide Ω into an atomistic subdomain Ω^{at} such that $y_j \in \Omega^{\mathrm{at}}$ for all $j \in \{-K, \dots, K\}$ and the continuum domain $\Omega^{\mathrm{cb}} = \Omega\backslash\Omega^{\mathrm{at}}$. In Ω^{cb} we will use the Cauchy–Born approximation on a cell-by-cell basis. In Ω^{at} we will use the atomistic model with Dirichlet boundary conditions, as discussed in section 3.

This basic setting gives rise to a variety of possibilities, including the precise choice of $\partial\Omega^{\mathrm{at}}$ and the boundary conditions imposed on the atomistic subproblem.

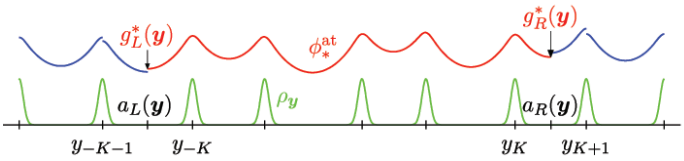

FIG. 5.1. *An illustration of the first a/c method. In* $\Omega^{\rm at} = (a_L(\boldsymbol{y}), a_R(\boldsymbol{y}))$ *the atomistic problem is solved with the Dirichlet boundary conditions* $g^*(\boldsymbol{y})$*. Outside* $\Omega^{\rm at}$ *the Cauchy–Born approximation is used in all cells* Q_j*.*

Both will in general depend on the configuration $\boldsymbol{y}$. Our main objective for $\mathcal{E}^{\rm ac}$ is the existence of a weak formulation in the sense that

$$D\mathcal{E}^{\rm ac}(\boldsymbol{y})\cdot\boldsymbol{u} = \int_\Omega \sigma_{\boldsymbol{y}}^{\rm ac}(x)\nabla u(x)\,{\rm d}x,$$

where $u \in \mathcal{S}_\#(\boldsymbol{y})$ is a piecewise linear interpolant of $\boldsymbol{u} \in \mathcal{U}$ and $\sigma_{\boldsymbol{y}}^{\rm ac}$ is a stress function to be determined. If this weak formulation can be obtained, the consistency analysis reduces to error estimates on fields, as already seen in Lemma 4.4.

Throughout this section, $\phi \in H^1_\#(\Omega)$ denotes the solution of the original minimization problem (2.1) for a given configuration $\boldsymbol{y} \in \mathcal{Y}$.

The remainder of the section is organized as follows: In section 5.1 we formulate an a/c coupling in which the field in the atomistic region is obtained from the "optimal" boundary data given by $g = g_*$. (Since this choice is impractical in higher dimensions, we consider deviations from this choice in section 6.) In section 5.2 we establish a consistency error estimate for the a/c force and in section 5.3 a stability estimate, and in Theorem 5.5 we combine these results to form an a priori error estimate for the solution of the a/c method.

5.1. An a/c method with optimal boundary conditions. We place the boundary a of the atomistic subproblem halfway between the interface atoms, that is, $a = a(\boldsymbol{y}) = [a_L(\boldsymbol{y})\ a_R(\boldsymbol{y})]^{\rm T}$, where

$$a_L(\boldsymbol{y}) = \frac{y_{-K-1} + y_{-K}}{2}, \qquad a_R(\boldsymbol{y}) = \frac{y_K + y_{K+1}}{2}.$$

Let $\Omega^{\rm at} = (a_L(\boldsymbol{y}), a_R(\boldsymbol{y}))$ and $\Omega^{\rm cb} = \Omega\backslash\Omega^{\rm at}$. We write the a/c energy $\mathcal{E}^{\rm ac}(\boldsymbol{y})$ as the sum of a continuum and an atomistic part,

$$\mathcal{E}^{\rm ac}(\boldsymbol{y}) = \mathcal{E}_*^{\rm cb}(\boldsymbol{y}) + \mathcal{E}_*^{\rm at}(\boldsymbol{y}), \tag{5.1}$$

which are introduced below.

Due to the choice of $a(\boldsymbol{y})$ we have two half cells, $(y_{-K-1}, a_L(\boldsymbol{y}))$ and $(a_R(\boldsymbol{y}), y_{K+1})$, in the continuum region $\Omega^{\rm cb}$ (see Figure 5.1). Since the cell problems are symmetric, the Cauchy–Born energies of these half cells are given by $\frac{1}{2}\mathcal{E}^{\rm cb}_{-K}(\boldsymbol{y})$ and $\frac{1}{2}\mathcal{E}^{\rm cb}_{K+1}(\boldsymbol{y})$, respectively. Hence, the continuum contribution to the energy $\mathcal{E}^{\rm ac}$ is defined by

$$\mathcal{E}_*^{\rm cb}(\boldsymbol{y}) = \sum_{j=-N+1}^{-K-1} \mathcal{E}_j^{\rm cb}(\boldsymbol{y}) + \tfrac{1}{2}\mathcal{E}^{\rm cb}_{-K}(\boldsymbol{y}) + \tfrac{1}{2}\mathcal{E}^{\rm cb}_{K+1}(\boldsymbol{y}) + \sum_{j=K+2}^{N} \mathcal{E}_j^{\rm cb}(\boldsymbol{y}). \tag{5.2}$$

The coordinates of the atoms in the atomistic region $\Omega^{\rm at}$ are represented by

$$\boldsymbol{y}_{\rm at} = (y_{-K}, \ldots, y_K)^{\rm T}.$$

For the definition of $\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y})$ we consider the minimization problem (3.2) on the atomistic domain Ω^{at} subject to the "optimal" Dirichlet boundary conditions $g^*(\boldsymbol{y}) = [g_L^*(\boldsymbol{y})\ g_R^*(\boldsymbol{y})]^{\mathrm{T}}$ (cf. (3.17)). In correspondence with (3.17) they are given by

$$g_L^*(\boldsymbol{y}) = \frac{1}{1-\tau}\frac{\gamma_L(\boldsymbol{y}) + \tau\gamma_R(\boldsymbol{y})}{1+\tau}, \qquad g_R^*(\boldsymbol{y}) = \frac{1}{1-\tau}\frac{\tau\gamma_L(\boldsymbol{y}) + \gamma_R(\boldsymbol{y})}{1+\tau},$$

where $\tau = \mathrm{e}^{-\frac{m}{\varepsilon}\Delta a(\boldsymbol{y})}$, and γ_L, γ_R are defined in (3.15). The energy contribution from the atomistic subproblem is thus given by

$$\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y}) = \mathcal{E}_{a(\boldsymbol{y}),g^*(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}}) = -\inf\Big\{I_{a(\boldsymbol{y})}(\varphi, \boldsymbol{y}_{\mathrm{at}}) : \quad \varphi \in H^1(\Omega^{\mathrm{at}}), \quad \varphi|_{\partial\Omega^{\mathrm{at}}} = g^*(\boldsymbol{y})\Big\},$$

where $I_{a(\boldsymbol{y})}$ is defined as in (3.3). We denote the solution of this optimization problem by $\phi_{\mathrm{at}}^* \in H^1(\Omega^{\mathrm{at}})$. It satisfies the boundary-value problem

$$\begin{aligned} -\varepsilon^2\Delta\phi_{\mathrm{at}}^* + m^2\phi_{\mathrm{at}}^* &= \rho_{\boldsymbol{y}} \ \text{ in } \Omega^{\mathrm{at}}, \\ \phi_{\mathrm{at}}^*|_{\partial\Omega^{\mathrm{at}}} &= g^*(\boldsymbol{y}). \end{aligned}$$

From a computational point of view $g^*(\boldsymbol{y})$ is also a convenient choice since this is equivalent to homogeneous Neumann boundary conditions. In section 3.3 we deduced a clear interpretation of the effect of this choice of boundary data: besides the interaction among themselves, the atoms in Ω^{at} interact with mirror atoms outside Ω^{at}. This is closely related to the geometric reconstruction idea for classical potentials [17, 4].

In analogy to (2.3) we search for minimizers of the total potential energy

$$E_{\boldsymbol{f}}^{\mathrm{ac}}(\boldsymbol{y}) = \mathcal{E}^{\mathrm{ac}}(\boldsymbol{y}) + (\boldsymbol{f}, \boldsymbol{y})_\varepsilon \tag{5.3}$$

in $\mathcal{Y}$, where $\boldsymbol{f} \in \mathcal{U}^{-1,2}$ represents an external force. Formally, a minimizer $\bar{\boldsymbol{y}}^{\mathrm{ac}}$ satisfies the following Euler–Lagrange equation in $\mathcal{U}^{-1,2}$:

$$DE_{\boldsymbol{f}}^{\mathrm{ac}}(\boldsymbol{y}) = D\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y}) + \boldsymbol{f} = \boldsymbol{0}.$$

Throughout the remainder of this article we assume that the atomistic domain Ω^{at} is large compared with ε, that is, $\Delta a \gg \varepsilon$, and hence terms of order $\mathcal{O}(\tau)$ are exponentially small. To keep the notation more compact we will not give precise estimates of τ-dependent terms arising from the atomistic domain explicitly but include an $\mathcal{O}(\tau)$ where necessary.

5.2. Consistency. In order to study the consistency properties of the a/c energy $\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})$ from (5.1) we first need to calculate its derivative. Having established weak formulations for the derivatives of $\mathcal{E}$ and $\mathcal{E}^{\mathrm{cb}}$, as well as $\mathcal{E}_{a,g}$, we will prove that the a/c energy $\mathcal{E}^{\mathrm{ac}}$ admits a similar reformulation of $D\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})\cdot\boldsymbol{u}$. For this we have to take into account that both the boundary of the atomistic domain Ω^{at} and the boundary conditions depend on $\boldsymbol{y}$. The necessary preparations were carried out in section 3.

LEMMA 5.1. *Let $\boldsymbol{y} \in \mathcal{Y}$ satisfy $\min \boldsymbol{y}' > \varsigma_0$. Furthermore, let $\boldsymbol{u} \in \mathcal{U}$ be a test vector and $u \in \mathrm{S}_{\#}(\boldsymbol{y})$ be an interpolant of $\boldsymbol{u}$; then,*

$$D\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})\cdot\boldsymbol{u} = \int_\Omega \sigma_{\boldsymbol{y}}^{\mathrm{ac}}(x)\nabla u(x)\,\mathrm{d}x, \qquad \text{where } \sigma_{\boldsymbol{y}}^{\mathrm{ac}}(x) = \begin{cases} \sigma_{\boldsymbol{y}}^{\mathrm{cb}}(x) & \text{if } x \in \Omega^{\mathrm{cb}}, \\ \sigma_{\boldsymbol{y},*}^{\mathrm{at}}(x) & \text{if } x \in \Omega^{\mathrm{at}}, \end{cases} \tag{5.4}$$

and $\sigma_{\boldsymbol{y},*}^{\mathrm{at}}(x)$ is given by (2.7) with $\phi = \phi_{\mathrm{at}}^*$.

Proof. 1. *Continuum contribution.* From section 4 we already have the equality

$$D\mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y})\cdot\boldsymbol{u} = \int_{Q_j} \sigma_{\boldsymbol{y},j}^{\mathrm{cb}}(x)\nabla u(x)\,\mathrm{d}x,$$

$j \in \{-N,\dots,-K-1\}\cup\{K+2,\dots,N\}$. For the contribution $\frac{1}{2}\mathcal{E}_{-K}^{\mathrm{cb}}(\boldsymbol{y})$ from the half cell $(y_{-K-1}, a_L(\boldsymbol{y}))$ we make use of the symmetry of the cell problems. Since $\nabla u|_{Q_{-K}}$ is constant, $a_L(\boldsymbol{y})$ is the midpoint of $Q_{-K} = (y_{-K-1}, y_{-K})$, and $\sigma_{\boldsymbol{y},-K}^{\mathrm{cb}}$ is symmetric in Q_{-K}, we deduce that

$$\frac{1}{2}D\mathcal{E}_{-K}^{\mathrm{cb}}(\boldsymbol{y})\cdot\boldsymbol{u} = \frac{1}{2}\int_{Q_{-K}} \sigma_{\boldsymbol{y},-K}^{\mathrm{cb}}(x)\nabla u(x)\,\mathrm{d}x = \int_{y_{-K-1}}^{a_L(\boldsymbol{y})} \sigma_{\boldsymbol{y},-K}^{\mathrm{cb}}(x)\nabla u(x)\,\mathrm{d}x.$$

We treat $\frac{1}{2}\mathcal{E}_{K+1}^{\mathrm{cb}}(\boldsymbol{y})$ analogously. Hence,

$$D\mathcal{E}_*^{\mathrm{cb}}(\boldsymbol{y})\cdot\boldsymbol{u} = \int_{\Omega^{\mathrm{cb}}} \sigma_{\boldsymbol{y}}^{\mathrm{cb}}(x)\nabla u(x)\,\mathrm{d}x,$$

where $\sigma_{\boldsymbol{y}}^{\mathrm{cb}}(x) = \sigma_{\boldsymbol{y},j}^{\mathrm{cb}}(x)$ if $x \in Q_j$.

2. *Atomistic contribution.* To calculate the derivative $D\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y})$ we use the chain rule and the derivatives that were provided in section 3. Applying Proposition 3.3 (with $h_L = (u_{-K-1}+u_{-K})/2$, $h_R = (u_K+u_{K+1})/2$ because of $D_{\boldsymbol{y}}a(\boldsymbol{y})\cdot\boldsymbol{u} = a(\boldsymbol{u})$), we get

$$\begin{aligned} D\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y})\cdot\boldsymbol{u} &= D_{\boldsymbol{y}}\mathcal{E}_{a(\boldsymbol{y}),g^*(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})\cdot\boldsymbol{u}_{\mathrm{at}} + D_a\mathcal{E}_{a(\boldsymbol{y}),g^*(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})\cdot D_{\boldsymbol{y}}a(\boldsymbol{y})\cdot\boldsymbol{u} \\ &= \int_{\Omega^{\mathrm{at}}} \sigma_{\boldsymbol{y},*}^{\mathrm{at}}(x)\nabla u(x)\,\mathrm{d}x, \end{aligned} \tag{5.5}$$

where the stress $\sigma_{\boldsymbol{y},*}^{\mathrm{at}}$ is given by (2.7) with $\phi = \phi_{\mathrm{at}}^*$ and $\boldsymbol{u}_{\mathrm{at}} = (u_{-K},\dots,u_K) \in \mathbb{R}^{2K+1}$ is the section of $\boldsymbol{u}$ corresponding to the atoms in the atomistic region. Note that the choice of boundary conditions implies $D_g\mathcal{E}_{a(\boldsymbol{y}),g^*(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}}) = 0$; cf. (3.17). ∎

Remark 4. The weak form (5.4) of the derivative $D\mathcal{E}^{\mathrm{ac}}$ already implies that there are no ghost forces for homogeneous deformations; i.e., $D\mathcal{E}^{\mathrm{ac}}(F\widehat{\boldsymbol{X}}) = 0$ for all $F > 0$. If the atoms are equidistant, then $g_L^*(\boldsymbol{y}) = \phi(a_L)$ and $g_R^*(\boldsymbol{y}) = \phi(a_R)$ and thus also $\phi_{\mathrm{at}}^* = \phi$ in Ω^{at}. Moreover, it is clear that $\psi^{(j)} = \phi$ for all j. Hence, we obtain that $\sigma_{\boldsymbol{y}}^{\mathrm{ac}}(x) = \sigma_{\boldsymbol{y}}(x)$ for all $x \in \Omega$, which implies that $D\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y}) = D\mathcal{E}(\boldsymbol{y}) = 0$ for all $\boldsymbol{y} = F\widehat{\boldsymbol{X}} \in \mathcal{Y}$ representing homogeneous deformations (i.e., that the method exhibits no ghost forces).

Absence of ghost forces does not immediately imply *consistency* of the a/c method; rather, it has to be shown separately. This we do next. Because of the structure of the weak formulation (5.4), the analysis boils down to estimating the errors between the field ϕ coming from the original atomistic model and the fields $\psi^{(j)}$, respectively, ϕ_{at}^*.

THEOREM 5.2. *Let $\boldsymbol{y} \in \mathcal{Y}$ be such that $\min \boldsymbol{y}' \geq s_0 > \varsigma_0$; then, for all $\boldsymbol{u} \in \mathcal{U}$ with interpolants $u \in \mathcal{S}_{\#}(\boldsymbol{y})$,*

$$\left|\left(D\mathcal{E}(\boldsymbol{y}) - D\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})\right)\cdot\boldsymbol{u}\right| \leq C\left(\varepsilon\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}} + \tau\right)\|\nabla u\|_{L^2},$$

where $C = C(s_0)$ and the weighted ℓ^2_{w,s_0}-norm is defined by

$$\|\boldsymbol{y}''\|^2_{\ell^2_{w,s_0}} := \varepsilon\sum_{j=-N}^{N} w_j\left|y_j''\right|^2, \tag{5.6}$$

with weights $w_j := \mathrm{e}^{-ms_0\mathrm{dist}(j,\{-K,K\})}$ *for* $j = -K,\dots,K$ *and* $w_j = 1$ *otherwise.*

Proof. Using the weak formulation (5.4) of $D\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})$ we obtain

$$\begin{aligned}\big|\big(D_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y}) - D_{\boldsymbol{y}}\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})\big)\cdot\boldsymbol{u}\big| &= \left|\int_\Omega \big(\sigma_{\boldsymbol{y}}(x) - \sigma_{\boldsymbol{y}}^{\mathrm{qc}}(x)\big)\nabla u(x)\,\mathrm{d}x\right| \\ &\le \|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y}}^{\mathrm{qc}}\|_{L^2(\Omega)}\,\|\nabla u\|_{L^2} \\ &\le \left(\sum_{j=-N}^{N} \varepsilon\|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y}}^{\mathrm{qc}}\|^2_{L^\infty(Q_j)}\right)^{1/2}\cdot\|\nabla u\|_{L^2}\,. \end{aligned} \tag{5.7}$$

For Q_j belonging to the continuum region Lemmas 4.4 and 4.2 imply

$$\begin{aligned}\|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y}}^{\mathrm{ac}}\|_{L^\infty(Q_j)} &\le C\varepsilon\sum_{n=1}^{\infty}\|\boldsymbol{y}''\|_{\ell^1([j-n,j+n-1])}n\mathrm{e}^{-mns_0} \\ &\le C\varepsilon\sum_{n=1}^{\infty}\|\boldsymbol{y}''\|_{\ell^2([j-n,j+n-1])}n^{3/2}\mathrm{e}^{-mns_0} \\ &\le C\varepsilon\left(\sum_{n=1}^{\infty}\|\boldsymbol{y}''\|^2_{\ell^2([j-n,j+n-1])}\mathrm{e}^{-mns_0}\right)^{1/2}, \end{aligned} \tag{5.8}$$

where the constant changes on each line, we have employed the Cauchy–Schwarz inequality twice, and we used the fact that the series $\sum_{n=1}^{\infty} n^3\mathrm{e}^{-mns_0}$ is convergent.

Summing over all cells belonging to the continuum region and interchanging the order of summation we obtain

$$\begin{aligned}\sum_{\substack{j\in\{-N,\dots,N\}\\ \setminus\{-K+1,\dots,K\}}} \varepsilon\|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y}}^{\mathrm{qc}}\|^2_{L^\infty(Q_j)} &\le C\varepsilon^3\sum_{\substack{j\in\{-N,\dots,N\}\\ \setminus\{-K+1,\dots,K\}}}\sum_{n=1}^{\infty}\|\boldsymbol{y}''\|^2_{\ell^2([j-n,j+n-1])}\mathrm{e}^{-mns_0} \\ &\le C\varepsilon^3\sum_{k=-N}^{N}\widetilde{w}_k|y_k''|^2, \end{aligned}$$

where

$$\widetilde{w}_k = \sum_{\substack{j\in\{-N,\dots,N\}\\ \setminus\{-K+1,\dots,K\}}}\ \sum_{\substack{n=1,\dots,\infty\\ k\in[j-n,j+n-1]}} \mathrm{e}^{-mns_0}.$$

This is a geometric series from which we can factor out $\mathrm{e}^{-ms_0\mathrm{dist}(k,\{-K,K\})}$, and hence we obtain $\widetilde{w}_k \le Cw_k$, which gives

$$\sum_{j\notin\{-K+1,\dots,K\}} \varepsilon\|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y}}^{\mathrm{qc}}\|^2_{L^\infty(Q_j)} \le C\varepsilon^3\sum_{k=-N}^{N} w_k|y_k''|^2. \tag{5.9}$$

To compute the consistency error of the weak form in the atomistic region we need to bound the difference $\big\|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y}}^{\mathrm{qc}}\big\|_{L^\infty(Q_j)} = \big\|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y},*}^{\mathrm{at}}\big\|_{L^\infty(Q_j)}$ for $Q_j \subset \Omega^{\mathrm{at}}$. Using the same arguments as in the proof of Lemma 4.4 we obtain

$$\big\|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y},*}^{\mathrm{at}}\big\|_{L^\infty(Q_j)} \le C\big(\|\phi - \phi^*_{\mathrm{at}}\|_{L^\infty(Q_j)} + \varepsilon\|\nabla\phi - \nabla\phi^*_{\mathrm{at}}\|_{L^\infty(Q_j)}\big).$$

Lemma 3.7 implies

$$\left\|\sigma_{\boldsymbol{y}} - \sigma^{\rm at}_{\boldsymbol{y},*}\right\|_{L^\infty(Q_j)} \leq C\big(|\phi(a_L) - g^*_L(\boldsymbol{y})| + |\phi(a_R) - g^*_R(\boldsymbol{y})|\big)\mathrm{e}^{-\frac{m}{\varepsilon}\min_{x\in Q_j} d_a(x)}.$$

Next, we recall from (3.17) and (3.15) that $g^*_R = \gamma^*_R + \mathcal{O}(\tau)$, which is given by

$$\gamma_R(\boldsymbol{y}) = \int_{\mathbb{R}} \rho^{\rm refl}_{\boldsymbol{y}}(x) G_\varepsilon(a_R - x)\,\mathrm{d}x + \mathcal{O}(\tau), \tag{5.10}$$

where $\rho^{\rm refl}_{\boldsymbol{y}}(z) = \sum_{j\in\mathbb{Z}} \delta_\varepsilon(z - y^{\rm refl}_j)$ and $\boldsymbol{y}^{\rm refl}$ is a reflected and periodized extension of $(y_j)_{j=-K}^K$, defined by

$$\begin{aligned} y^{\rm refl}_j &:= y_j \qquad \text{for } j = -K,\dots,K,\\ y^{\rm refl}_{K+j} &:= 2a_R - y_{K-j+1} \qquad \text{for } j = 1,\dots,2K+1, \end{aligned}$$

and this reflected configuration of $4K+2$ atoms is then repeated periodically. (Note, however, that only the reflection is required to obtain (5.10).)

Hence, we obtain

$$\begin{aligned} \big|\phi(a_R) - g^*_R(\boldsymbol{y})\big| &= \big|\phi(a_R) - \gamma_L(\boldsymbol{y})\big| + \mathcal{O}(\tau)\\ &\leq \frac{1}{2m\varepsilon}\left|\int_{\mathbb{R}} \big(\rho_{\boldsymbol{y}}(z) - \rho^{\rm refl}_{\boldsymbol{y}}(z)\big)\,\mathrm{e}^{-\frac{m}{\varepsilon}|a_R - z|}\,\mathrm{d}z\right| + \mathcal{O}(\tau). \end{aligned}$$

Minor modifications of the proofs of Lemmas 4.2 and 4.1 yield

$$\begin{aligned} \big|\phi(a_R) - g^*_R(\boldsymbol{y})\big| &\leq \frac{C}{\varepsilon}\sum_{j=K+1}^{\infty} \big|y^{\rm refl}_j - y_j\big|\mathrm{e}^{-\frac{m}{\varepsilon}(\min(y^{\rm refl}_j, y_j) - a_R)} + \mathcal{O}(\tau)\\ &\leq C\varepsilon\sum_{n=1}^{\infty} \|\boldsymbol{y}''\|_{\ell^1([K-n+1,K+n])} n\mathrm{e}^{-mns_0} + \mathcal{O}(\tau). \end{aligned} \tag{5.11}$$

An analogous result holds for $|\phi(a_L) - g^*_L(\boldsymbol{y})|$. It is now straightforward to see that the consistency error committed in the atomistic region can be bounded above in the same way as the consistency error committed in the continuum region (in fact it is dominated by (5.9)). This completes the proof. ∎

5.3. Stability. The special choice $g^*(\boldsymbol{y})$ of boundary conditions for the atomistic subproblem allows for an elementary stability analysis of $\mathcal{E}^{\rm ac}(\boldsymbol{y})$ that draws from the ideas we used in section 3.3. We recall from Proposition 3.8 that

$$\begin{aligned} \mathcal{E}^{\rm at}_*(\boldsymbol{y}) = \frac{1}{4m\varepsilon}\int_{\Omega^{\rm at}}\int_{\Omega^{\rm at}} \rho_{\boldsymbol{y}}(x)\big(&\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|} + \mathrm{e}^{-\frac{m}{\varepsilon}(2a_R(\boldsymbol{y}) - x - z)}\\ &+ \mathrm{e}^{-\frac{m}{\varepsilon}(x+z-2a_L(\boldsymbol{y}))}\big)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x + \mathcal{O}(\tau). \end{aligned}$$

The next result addresses the differentiability of γ_L and γ_R. We show that the derivatives satisfy certain bounds.

LEMMA 5.3. *Let $\boldsymbol{y} \in \Omega_a^{2K+1}$ satisfy $y_{i+1} - y_i > \varepsilon\varsigma_0$ for all $i \in \{-K+1,\dots,K\}$, $a_R - y_K > \varepsilon\varsigma_0/2$, and $y_{-K} - a_L > \varepsilon\varsigma_0/2$. Then, $\gamma_L(\boldsymbol{y}, a)$ is twice continuously differentiable with respect to $\boldsymbol{y}$ and a and there exists $C(m\min\boldsymbol{y}')$ (independent of ε)*

such that

$$\big|D\gamma_L(\boldsymbol{y},a)\cdot(\boldsymbol{u},h)\big| \le C(m\min \boldsymbol{y}')\left(\left(\frac{u_{-K}-h_L}{\varepsilon}\right)^2 + \sum_{k=-K+1}^{K}(u_k')^2\right)^{1/2},$$

$$\big|D^2\gamma_L(\boldsymbol{y},a)\cdot\big[(\boldsymbol{u},h),(\boldsymbol{u},h)\big]\big| \le C(m\min \boldsymbol{y}')\left(\left(\frac{u_{-K}-h_L}{\varepsilon}\right)^2 + \sum_{k=-K+1}^{K}(u_k')^2\right)$$

for all $\boldsymbol{u}\in\mathcal{U}$ *and* $h\in\mathbb{R}^2$. *Analogous bounds hold for* $\gamma_R(\boldsymbol{y},a)$.

Proof. The proof is based on the observation that

$$\begin{aligned}\gamma_L(\boldsymbol{y},a) &= \frac{1}{m}\sum_{j=-K}^{K}\int_{\Omega_a} \mathrm{e}^{-\frac{m}{\varepsilon}(x-a_L)}\delta_\varepsilon(x-y_j)\,\mathrm{d}x\\ &= \frac{\mu}{m}\mathrm{e}^{-\frac{m}{\varepsilon}(y_{-K}-a_L)}\sum_{j=-K}^{K}\mathrm{e}^{-\frac{m}{\varepsilon}(y_j-y_{-K})}.\end{aligned}$$

The rest of the proof is a straightforward computation; see [10, Lem. 5.3] for the details. ∎

The τ-dependent terms in $\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y}) = \mathcal{E}_{a(\boldsymbol{y}),g^*(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})$ from (3.24) contain only $\gamma_L(\boldsymbol{y})$ and $\gamma_R(\boldsymbol{y})$, whose derivatives are bounded by Lemma 5.3. The derivatives of these τ-dependent terms are therefore still of order $\mathcal{O}(\tau)$ and will be neglected in the proof of the following result.

LEMMA 5.4. *Let* $\boldsymbol{y}\in\mathcal{Y}$ *satisfy* $\min \boldsymbol{y}' > \varsigma_0$. *Then,*

$$D^2\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \ge \Big(\frac{m\mu^2}{2}\mathrm{e}^{-m\max \boldsymbol{y}'} - \mathcal{O}(\tau)\Big)\|\boldsymbol{u}'\|_{\ell^2_\varepsilon}^2 \quad \forall \boldsymbol{u}\in\mathcal{U}.$$

Proof. We treat continuum and atomistic contributions independently and start with the former. Lemma 4.5 states that

$$D^2\mathcal{E}_j^{\mathrm{cb}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \ge \frac{m^2\mu^2}{2}\mathrm{e}^{-m\max \boldsymbol{y}'}\varepsilon|u_j'|^2$$

for all $j=-N,\dots,N$. Hence, the definition (5.2) of $\mathcal{E}_*^{\mathrm{cb}}$ directly implies that

$$D^2\mathcal{E}_*^{\mathrm{cb}}(\boldsymbol{y})[\boldsymbol{u},\boldsymbol{u}] \ge \mathrm{e}^{-m\max \boldsymbol{y}'}\frac{m^2\mu^2}{2}\varepsilon\left(\sum_{j=-N}^{-K-1}|u_j'|^2 + \frac{1}{2}\big(|u_{-K}'|^2+|u_{K+1}'|^2\big) + \sum_{j=K+2}^{N}|u_j'|^2\right).$$

Let us now turn to the atomistic part $\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y})$. From section 3.3 we know that for the given choice of boundary conditions and $a(\boldsymbol{y})$ we can write the energy of the atomistic part as

$$\begin{aligned}\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y}) &= \frac{\varepsilon}{4m}\sum_{i,j=-K}^{K}\int_{\Omega^{\mathrm{at}}}\int_{\Omega^{\mathrm{at}}}\delta_\varepsilon(x-y_i)\big(\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}+\mathrm{e}^{-\frac{m}{\varepsilon}(x+z-y_{-K-1}-y_{-K})}\\ &\qquad + \mathrm{e}^{-\frac{m}{\varepsilon}(y_{K+1}+y_K-x-z)}\big)\delta_\varepsilon(z-y_j)\,\mathrm{d}z\,\mathrm{d}x\\ &= \frac{\varepsilon\mu^2}{4m}\sum_{i,j=-K}^{K}\big(\mathrm{e}^{-\frac{m}{\varepsilon}|y_i-y_j|}+\mathrm{e}^{-\frac{m}{\varepsilon}(y_i+y_j-y_{-K}-y_{-K-1})}\\ &\qquad + \mathrm{e}^{-\frac{m}{\varepsilon}(y_K+y_{K+1}-y_i-y_j)}\big) + \mathcal{E}_{\mathrm{self}} + \mathcal{O}(\tau),\end{aligned} \tag{5.12}$$

where the constant $\mathcal{E}_{\text{self}}$ accounts for the self-energies of the atoms $\{-K,\dots,K\}$. Differentiating twice and keeping only contributions from nearest neighbor interactions leads directly to

$$D^2\mathcal{E}^{\text{at}}_*(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \geq \mathrm{e}^{-m\max \boldsymbol{y}'}\frac{m\mu^2}{2}\,\varepsilon\left(\frac{1}{2}|u'_{-K}|^2+\sum_{i=-K+1}^{K}|u'_i|^2+\frac{1}{2}|u'_{K+1}|^2\right)-\mathcal{O}(\tau).$$

Adding the lower bounds for $D^2\mathcal{E}^{\text{cb}}_*(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}]$ and $D^2\mathcal{E}^{\text{at}}_*(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}]$ we arrive at

$$\begin{aligned} D^2\mathcal{E}^{\text{ac}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] &= \big(D^2\mathcal{E}^{\text{cb}}_*(\boldsymbol{y})+D^2\mathcal{E}^{\text{at}}_*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}]\\ &\geq \left(\mathrm{e}^{-m\max \boldsymbol{y}'}\frac{m\mu^2}{2}-\mathcal{O}(\tau)\right)\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon}\end{aligned}$$

for all $\boldsymbol{u}\in\mathcal{U}$, as desired. ∎

5.4. Error estimates. Combining the consistency and stability results we obtain the following error estimate. We note that the upper bound on the error depends on the smoothness of $\bar{\boldsymbol{y}}$ in the continuum region, but that the dependence on $\bar{\boldsymbol{y}}$ in the atomistic region decays exponentially with distance to the a/c interface. In realistic higher-dimensional models such an estimate would make it possible to allow defects in the atomistic region without affecting the error estimate.

THEOREM 5.5. *Suppose that* $\bar{\boldsymbol{y}}\in\arg\min E_{\boldsymbol{f}}$ *and* $\bar{\boldsymbol{y}}_{\text{ac}}\in\arg\min E^{\text{ac}}_{\boldsymbol{f}}$ *satisfy*

$$\min \bar{\boldsymbol{y}}', \min \bar{\boldsymbol{y}}'_{\text{ac}} \geq s_0 \geq \varsigma_0 \quad \textit{and} \quad \max \bar{\boldsymbol{y}}', \max \bar{\boldsymbol{y}}'_{\text{ac}} \leq S_0 < +\infty. \tag{5.13}$$

There exist constants c *and* $C=C(s_0,S_0)$ *such that if* $\Delta a \geq c\log(S_0)$, *then*

$$\big\|\bar{\boldsymbol{y}}'-\bar{\boldsymbol{y}}'_{\text{ac}}\big\|_{\ell^2_\varepsilon} \leq C\Big(\varepsilon\big\|\bar{\boldsymbol{y}}''\|_{\ell^2_{w,s_0}}+\tau\Big), \tag{5.14}$$

where $\tau=\mathrm{e}^{-\frac{m}{\varepsilon}\Delta a(\boldsymbol{y})}$ *is defined in* (3.15).

Proof. From Lemma 5.4 it is clear that there exists a constant c such that, for $\Delta a\geq c$, we have

$$D^2\mathcal{E}^{\text{ac}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \geq \frac{m\mu^2}{4}\mathrm{e}^{-mS_0}\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon} \quad \forall \boldsymbol{u}\in\mathcal{U}, \quad \forall \boldsymbol{y}\in\mathcal{Y}, \boldsymbol{y}'\leq S_0.$$

In particular, this holds for all $\boldsymbol{y}\in\operatorname{conv}\{\bar{\boldsymbol{y}},\bar{\boldsymbol{y}}_{\text{ac}}\}$. Let $c_0=\frac{m\mu^2}{4}\mathrm{e}^{-mS_0}$.

Let $\boldsymbol{u}=\bar{\boldsymbol{y}}-\bar{\boldsymbol{y}}_{\text{ac}}$; then we can choose $\boldsymbol{y}\in\operatorname{conv}\{\bar{\boldsymbol{y}},\bar{\boldsymbol{y}}_{\text{ac}}\}$ such that

$$c_0\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon} \leq D^2\mathcal{E}^{\text{ac}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] = \big(D\mathcal{E}^{\text{ac}}(\bar{\boldsymbol{y}})-D\mathcal{E}^{\text{ac}}(\bar{\boldsymbol{y}}_{\text{ac}})\big)[\boldsymbol{u}].$$

Employing the consistency estimate of Theorem 5.2 we obtain the stated result. ∎

Remark 5. With some additional work it is possible to avoid assuming the existence of $\bar{\boldsymbol{y}}_{\text{ac}}$ but to deduce it from an inverse function theorem–type argument [14, 10].

6. Boundary conditions from cell problems. The boundary conditions $g^*(\boldsymbol{y})$ we imposed on the atomistic subproblem in section 5.1 gave rise to a method without ghost forces and whose analysis was relatively straightforward. The reasons for this is the clean weak formulation (5.4) of $D\mathcal{E}^{\text{ac}}$ and the convenient stability properties established in Lemma 5.4. We now investigate how this situation changes if computationally cheaper boundary conditions are chosen. The following construction may also provide a starting point for generalizations to higher dimensions.

For example, a canonical choice, which requires no additional computational effort, is

$$g_L(\boldsymbol{y}) = \psi^{(-K)}(a_L) \quad \text{and} \quad g_R(\boldsymbol{y}) = \psi^{(K+1)}(a_R), \tag{6.1}$$

where we still assume $a_L(\boldsymbol{y}) = \frac{1}{2}(y_{-K-1} + y_{-K})$ and $a_R(\boldsymbol{y}) = \frac{1}{2}(y_K + y_{K+1})$. In this case, we have the following result, which suggests that the additional error committed can be controlled.

LEMMA 6.1. *Let* $\min \boldsymbol{y} \geq s_0 \geq \varsigma_0$*, and let* $g_{L/R}$ *be given by* (6.1)*; then,*

$$\big|g(\boldsymbol{y}) - g^*(\boldsymbol{y})\big| \leq C\big(\varepsilon^{1/2}\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}} + \tau\big). \tag{6.2}$$

Proof. Without loss of generality we focus on g_R only. Upon first estimating

$$\big|g_R(\boldsymbol{y}) - g_R^*(\boldsymbol{y})\big| \leq \big|\psi^{(K+1)}(a_R) - \phi(a_R)\big| + \big|\phi(a_R) - g_R^*(\boldsymbol{y})\big|,$$

and then employing (5.11) and Lemma 4.2, we obtain

$$\big|g_R(\boldsymbol{y}) - g_R^*(\boldsymbol{y})\big| \leq C\varepsilon \sum_{n=1}^{\infty} \|\boldsymbol{y}''\|_{\ell^1([K-n+1,K+n])} n\mathrm{e}^{-mns_0} + \mathcal{O}(\tau).$$

Applying the same argument as in (5.8) to (5.9), we obtain the upper bound (6.2). ∎

Motivated by Lemma 6.1 we define a second a/c energy $\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})$ by

$$\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y}) = \mathcal{E}_*^{\mathrm{cb}}(\boldsymbol{y}) + \mathcal{E}^{\mathrm{at}}(\boldsymbol{y}), \tag{6.3}$$

where $\mathcal{E}_*^{\mathrm{cb}}(\boldsymbol{y})$ is the same as in the method discussed in section 5.1 (see (5.2)) and

$$\begin{aligned}\mathcal{E}^{\mathrm{at}}(\boldsymbol{y}) &= \mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}}) \\ &= -\inf\Big\{I_{a(\boldsymbol{y})}(\varphi, \boldsymbol{y}_{\mathrm{at}}) : \quad \varphi \in H^1(\Omega^{\mathrm{at}}), \quad \varphi|_{\partial\Omega^{\mathrm{at}}} = g(\boldsymbol{y})\Big\}.\end{aligned}$$

We denote the minimizer for given $\boldsymbol{y}$ by $\phi_{\mathrm{at}} \in H^1(\Omega^{\mathrm{at}})$.

In the remainder of this section we will analyze the error between an atomistic minimizer $\bar{\boldsymbol{y}} \in \arg\min E_{\boldsymbol{f}}$ and an a/c minimizer $\bar{\boldsymbol{y}}_{\mathrm{ac}} \in \arg\min E_{\boldsymbol{f}}^{\mathrm{ac}}$, using a strategy similar to that in section 5. Our main result is Theorem 6.6. The difference in the choice of boundary data g will be controlled using Lemma 6.1 and the following additional auxiliary result.

LEMMA 6.2. *Let* $\min \boldsymbol{y}' \geq s_0 \geq \varsigma_0$*. Let* $g_R(\boldsymbol{y})$ *be defined by* (6.1)*; then, it can be equivalently written as*

$$g_R(\boldsymbol{y}) = \frac{1}{2m} \sum_{k\in\mathbb{Z}} \int_{\mathbb{R}} \delta_\varepsilon\bigg(z - \bigg(k + \frac{1}{2}\bigg)\varepsilon y'_{K+1}\bigg)\mathrm{e}^{-\frac{m}{\varepsilon}|z|}\,\mathrm{d}z. \tag{6.4}$$

In particular, g_R *is twice Fréchet differentiable with respect to* $\boldsymbol{y}$*, and there exists a constant* $C = C(s_0)$ *such that, for all* $\boldsymbol{y} \in \mathcal{Y}$ *with* $\min \boldsymbol{y}' \geq s_0 \geq \varsigma_0$*,*

$$\big|D_{\boldsymbol{y}} g_R(\boldsymbol{y}) \cdot \boldsymbol{u}\big| \leq C|u'_{K+1}| \quad \text{and} \quad \big|D^2_{\boldsymbol{y}} g_R(\boldsymbol{y}) \cdot [\boldsymbol{u}, \boldsymbol{u}]\big| \leq C|u'_{K+1}|^2 \quad \forall \boldsymbol{u} \in \mathcal{U}.$$

Analogous results hold for $g_L(\boldsymbol{y})$*.*

Proof. Recall from (4.8) that

$$g_R(\boldsymbol{y}) = \psi^{(K+1)}(a_R) = \frac{1}{2m} \sum_{k\in\mathbb{Z}} \int_{\mathbb{R}} \delta_\varepsilon(z - y_{K+k}^{(K+1)})\mathrm{e}^{-\frac{m}{\varepsilon}|a_R - z|}\,\mathrm{d}z,$$

where $y_j^{(K+1)}$ denotes the periodic extension defined in (4.3). We use the identities

$$y_{K+k}^{(K+1)} = y_K + k\varepsilon y'_{K+1} \quad \text{and} \quad a_R = y_K + \tfrac{1}{2}\varepsilon y'_{K+1}$$

to obtain

$$g_R(\boldsymbol{y}) = \frac{1}{2m}\sum_{k\in\mathbb{Z}}\int_{\mathbb{R}} \delta_\varepsilon(z - y_K - k\varepsilon y'_{K+1})\mathrm{e}^{-\frac{m}{\varepsilon}|y_K+\frac{1}{2}\varepsilon y'_{K+1}-z|}\,\mathrm{d}z.$$

Shifting the integration by $(y_K + \frac{1}{2}\varepsilon y'_{K+1})$ we obtain (6.4).

The bound on the first and second derivatives follows as in Lemma 5.3; the key observation is that $\delta_\varepsilon = \mathcal{O}(\varepsilon^{-1})$ is balanced against the ε preceding y'_{K+1} in its argument. ∎

6.1. Consistency. A crucial difference between the a/c energy (6.3) and the energy from section 5.1 is that now the derivative of the atomistic energy with respect to the boundary conditions does not vanish.

Since the continuum contribution to $D\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})\cdot\boldsymbol{u}$ is the same as in section 5.1, we need only analyze $D\mathcal{E}^{\mathrm{at}}(\boldsymbol{y})$. Using the chain rule we obtain

$$\begin{aligned} D\mathcal{E}^{\mathrm{at}}(\boldsymbol{y})\cdot\boldsymbol{u} = {} & D_{\boldsymbol{y}_{\mathrm{at}}}\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})\cdot\boldsymbol{u}_{\mathrm{at}} + D_a\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})\cdot a(\boldsymbol{u}) \\ & + D_g\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})\cdot(D_{\boldsymbol{y}}g(\boldsymbol{y})\cdot\boldsymbol{u}). \end{aligned}$$

The same reasoning as in section 5.1 gives for the first two terms on the right-hand side

$$D_{\boldsymbol{y}_{\mathrm{at}}}\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})\cdot\boldsymbol{u}_{\mathrm{at}} + D_a\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})\cdot a(\boldsymbol{u}) = \int_{\Omega^{\mathrm{at}}} \sigma^{\mathrm{at}}_{\boldsymbol{y}}(x)\nabla u(x)\,\mathrm{d}x, \tag{6.5}$$

where $\sigma^{\mathrm{at}}_{\boldsymbol{y}}(x)$ is given by (2.7) with $\phi = \phi_{\mathrm{at}}$.

Next, we turn our attention to the term $D_g\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})\cdot(D_{\boldsymbol{y}}g(\boldsymbol{y})\cdot\boldsymbol{u})$. We recall from Lemma 3.6 that (for $\Delta a \gg \varepsilon$)

$$D_g\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}}) = -m\varepsilon\big[g_L(\boldsymbol{y}) - g_L^*(\boldsymbol{y}),\ \ g_R(\boldsymbol{y}) - g_R^*(\boldsymbol{y})\big] + \mathcal{O}(\varepsilon\tau).$$

Combining this result with Lemmas 6.2 and 6.1 we obtain

$$\begin{aligned} \big|D_g\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})\cdot(D_{\boldsymbol{y}}g(\boldsymbol{y})\cdot\boldsymbol{u})\big| &\le C\varepsilon\Big(|g_L - g_L^*| + |g_R - g_R^*| + \tau\Big) \\ &\qquad \cdot\big(|u'_{-K}|^2 + |u'_{K+1}|^2\big)^{1/2} \\ &\le C\Big(\varepsilon\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}} + \tau\Big)\cdot\|\boldsymbol{u}'\|_{\ell^2_\varepsilon}, \end{aligned} \tag{6.6}$$

where $C = C(\min\boldsymbol{y}')$, and we have estimated $\varepsilon^{1/2}\tau \le \tau$. Equipped with these estimates we obtain the following consistency result.

LEMMA 6.3. *Let $\boldsymbol{y} \in \mathcal{Y}$ with $\min\boldsymbol{y}' \ge s_0 \ge \varsigma_0$; then, there exists a constant $C = C(s_0)$ such that*

$$\Big|D\mathcal{E}(\boldsymbol{y})\cdot\boldsymbol{u} - D\mathcal{E}^{\mathrm{at}}(\boldsymbol{y})\cdot\boldsymbol{u}\Big| \le C\Big(\varepsilon\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}} + \tau\Big)\,\|\nabla u\|_{L^2} \quad \forall\boldsymbol{u}\in\mathcal{U},$$

where we have used the same notation as in Theorem 5.2.

Proof. From (6.5) and (6.6) we obtain that

$$\begin{aligned}
&\Big|D\mathcal{E}(\boldsymbol{y})\cdot\boldsymbol{u} - D\mathcal{E}^{\mathrm{at}}(\boldsymbol{y})\cdot\boldsymbol{u}\Big| \\
&\le \Bigg[\Big(\varepsilon \sum_{\substack{j=-N,\dots,N\\ j\notin\{-K+1,\dots,K\}}} \big\|\sigma_{\boldsymbol{y}} - \sigma^{\mathrm{cb}}_{j,\boldsymbol{y}}\big\|^2_{L^\infty(Q_j)} + \big\|\sigma_{\boldsymbol{y}} - \sigma^{\mathrm{at}}_{\boldsymbol{y}}\big\|^2_{L^2(a_L,a_R)}\Big)^{1/2} \\
&\qquad\qquad + C\big(\varepsilon\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}} + \tau\big)\Bigg]\cdot\|\nabla u\|_{L^2}.
\end{aligned}$$

The first group in the upper bound was already estimated in the proof of Theorem 5.2, and the second group, $\|\sigma_{\boldsymbol{y}} - \sigma^{\mathrm{at}}_{\boldsymbol{y}}\|_{L^2(a_L,a_R)}$, can be treated analogously to the term $\|\sigma_{\boldsymbol{y}} - \sigma^{\mathrm{at}}_{\boldsymbol{y},*}\|_{L^2(a_L,a_R)}$ in the proof of Theorem 5.2. ∎

6.2. Stability. We wish to compute a lower bound on $D^2\mathcal{E}^{\mathrm{ac}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}]$ for some given $\boldsymbol{y}\in\mathcal{Y}$ with $\varsigma_0 \le s_0 \le \boldsymbol{y}' \le S_0$. Since the continuum part of the energy is the same as in the first method, we address only the stability of the atomistic subproblem with the given choice of boundary data. We write the second derivative of the energy $\mathcal{E}^{\mathrm{at}}$ in the form

$$D^2\mathcal{E}^{\mathrm{at}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] = D^2\mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] + \big(D^2\mathcal{E}^{\mathrm{at}}(\boldsymbol{y}) - D^2\mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}]$$

and use the coercivity of $D^2\mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y})$: we know from Lemma 5.4 that

$$D^2\mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \ge \mathrm{e}^{-m\max\boldsymbol{y}'}\frac{m\mu^2}{2}\,\varepsilon\left(\frac{1}{2}|u'_{-K}|^2 + \sum_{i=-K+1}^{K}|u'_i|^2 + \frac{1}{2}|u'_{K+1}|^2\right) - \mathcal{O}(\tau)$$

for all $\boldsymbol{u}\in\mathcal{U}$; hence we are left to analyze the difference $D^2\mathcal{E}^{\mathrm{at}}(\boldsymbol{y}) - D^2\mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y})$. We will *not* show that this difference is small; rather, we will only be able to bound it below by a controllable quantity. This is reminiscent of similar observations made in [14].

LEMMA 6.4. *Let $\boldsymbol{y}\in\mathcal{Y}$ such that $\min\boldsymbol{y}' \ge s_0 \ge \varsigma_0$; then, there exists a constant $C = C(s_0)$ such that*

$$\big(D^2\mathcal{E}^{\mathrm{at}}(\boldsymbol{y}) - D^2\mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}] \ge -C\big(\varepsilon^{1/2}\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}} + \tau\big).$$

Proof. The difference between the energies $\mathcal{E}^{\mathrm{at}}(\boldsymbol{y})$ and $\mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y})$ consists only of effects from the boundary conditions. We have, by (3.18),

$$\begin{aligned}
\mathcal{E}^{\mathrm{at}}(\boldsymbol{y}) - \mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y}) &= -I_{a(\boldsymbol{y})}(\xi_{a(\boldsymbol{y}),g(\boldsymbol{y})},\boldsymbol{y}) + I_{a(\boldsymbol{y})}(\xi_{a(\boldsymbol{y}),g^*(\boldsymbol{y})},\boldsymbol{y}) \\
&= \frac{m\varepsilon}{2}\big|g(\boldsymbol{y}) - g^*(\boldsymbol{y})\big|^2 + \mathcal{O}(\varepsilon\tau).
\end{aligned}$$

As in section 5.3, one can verify that the $\mathcal{O}(\tau)$ term remains of that same order in the first and second derivatives. This implies that

$$\begin{aligned}
\big(D^2\mathcal{E}^{\mathrm{at}}(\boldsymbol{y}) - D^2\mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}] &= m\varepsilon\big(g(\boldsymbol{y}) - g^*(\boldsymbol{y})\big)^{\mathrm{T}}\big[\big(D^2g(\boldsymbol{y}) - D^2g^*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}]\big] \\
&\quad + 2m\varepsilon\big|\big(Dg(\boldsymbol{y}) - Dg^*(\boldsymbol{y})\big)\cdot\boldsymbol{u}\big|^2 + \mathcal{O}(\tau\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon}) \\
&\ge m\varepsilon\big(g(\boldsymbol{y}) - g^*(\boldsymbol{y})\big)^{\mathrm{T}}\big[\big(D^2g(\boldsymbol{y}) - D^2g^*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}]\big] + \mathcal{O}(\tau\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon}). \qquad (6.7)
\end{aligned}$$

We now employ Lemma 6.2 to bound $D^2 g(\boldsymbol{y})$, Lemma 5.3 to bound $D^2 g^*$ (up to another $\mathcal{O}(\tau)$ error), and Lemma 6.1 to bound $g - g^*$, which yields

$$\big(D^2\mathcal{E}^{\rm at}(\boldsymbol{y}) - D^2\mathcal{E}^{\rm at}_*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}] \geq -C\big(\varepsilon^{1/2}\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}} + \tau\big)\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon},$$

where $C = C(\min \boldsymbol{y}')$. ∎

From Lemmas 6.4 and 5.4 we immediately obtain the following corollary, which states that if S_0 is moderate, $\boldsymbol{y}$ "smooth" in a neighborhood of the interfaces $a_{L/R}$ and in the continuum region, and if the atomistic region is sufficiently large, then $D^2\mathcal{E}^{\rm ac}(\boldsymbol{y})$ is stable.

COROLLARY 6.5. *Let $\boldsymbol{y} \in \mathcal{Y}$ satisfy $\min \boldsymbol{y}' \geq s_0 \geq \varsigma_0$ and $\max \boldsymbol{y}' \leq S_0$; then, there exists a constant $C = C(s_0)$ such that*

$$D^2\mathcal{E}^{\rm ac}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \geq \Big(\frac{m\mu^2}{2}\,{\rm e}^{-mS_0} - C\big(\varepsilon^{1/2}\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}} + \tau\big)\Big)\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon} \quad \forall \boldsymbol{u} \in \mathcal{U}.$$

Remark 6. The scaling $\varepsilon^{1/2}$ is due to the fact that the additional error committed is concentrated in a region of length ε.

6.3. Error estimates. Repeating the proof of Theorem 5.5 verbatim, but replacing the consistency and stability estimates from section 5 with those derived in Lemma 6.3 and Corollary 6.5, we obtain the following error estimates for the modified a/c method.

We note that the result is qualitatively identical to Theorem 5.5, except for the additional requirement that $\tau + \varepsilon^{1/2}\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}}$ be sufficiently small. This condition allows us to control the perturbation to the stability constant derived in Corollary 6.5 by appropriately choosing the location of the interface.

THEOREM 6.6. *Recall the notation introduced in Theorem 5.2. Suppose that $\bar{\boldsymbol{y}} \in \arg\min E_{\boldsymbol{f}}$ and $\bar{\boldsymbol{y}}_{\rm ac} \in \arg\min E^{\rm ac}_{\boldsymbol{f}}$, where $\mathcal{E}^{\rm ac}$ is defined in* (6.3)*, satisfy*

$$\min \bar{\boldsymbol{y}}', \min \bar{\boldsymbol{y}}'_{\rm ac} \geq s_0 \geq \varsigma_0 \quad \text{and} \quad \max \bar{\boldsymbol{y}}', \max \bar{\boldsymbol{y}}'_{\rm ac} \leq S_0 < +\infty. \tag{6.8}$$

There exist constants c and $C = C(s_0, S_0)$ such that if $\tau + \varepsilon^{1/2}\|\boldsymbol{y}''\|_{\ell^2_{w,s_0}} \leq c{\rm e}^{-mS_0}$ (in particular, K must be sufficiently large), then

$$\big\|\bar{\boldsymbol{y}}' - \bar{\boldsymbol{y}}'_{\rm ac}\big\|_{\ell^2_\varepsilon} \leq C\Big(\varepsilon\big\|\bar{\boldsymbol{y}}''\|_{\ell^2_{w,s_0}} + \tau\Big). \tag{6.9}$$

7. Conclusions and outlook. We have presented a rigorous error analysis of two atomistic-to-continuum coupling methods for a field-based interaction potential in one space dimension.

For both of the two a/c methods we discussed we chose $\boldsymbol{y}$-dependent boundaries $a(\boldsymbol{y})$ of the atomistic subdomain $\Omega^{\rm at}$. In other words we fixed the position of the boundary in the Lagrangian domain. This leads to convenient weak formulations of $D\mathcal{E}^{\rm ac}(\boldsymbol{y})$. An obvious alternative, which is particularly relevant for higher dimensions, is the choice of $\boldsymbol{y}$-independent a. We have not investigated this further; however, see [10] for some preliminary remarks.

We also remark that we heavily utilized the one-dimensional setting in several places in the analysis. A generalization of both the numerical methods and their analysis is therefore nontrivial. In particular, we can see no straightforward generalization of the reflection boundary conditions $g^*(\boldsymbol{y})$. A possible way forward would be to give an alternative analysis of the second method described in section 6 that does not utilize these reflection techniques.

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