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Key words and phrases: density functional theory, atomistic-to-continuum coupling, coarse graining, a priori error analysis

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Abstract

We consider an atomistic interaction potential in one dimension given through a minimization problem, which gives rise to a field. The forces on atoms are in this case given by local expressions involving this field. A convenient feature of this model is the existence of a weak formulation for the forces, which provides a natural connection point for the coupling with a continuum model. We suggest Quasicontinuum-like coupling mechanisms that are based on a decomposition of the domain into an atomistic and a continuum region. In the continuum region we use an approximation based on the Cauchy–Born rule. In the atomistic subdomain a version of the atomistic model with Dirichlet boundary conditions is applied. Special attention has to be paid to the dependence of the atomistic subproblem on the boundary and the boundary conditions. Applying concepts from nonlinear analysis we show existence and convergence of solutions to the Quasicontinuum approximation.

1 Introduction

{sec:SM_Intro}

In the present article we formulate and analyze one-dimensional QC methods for an atomistic interaction that is mediated by a field.

The article is structured as follows. In Section 1 we give a literature review, motivate the atomistic model, and introduce the necessary notation. In Section 2 we formulate the model in a more precise mathematical way 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 respective continuum model is derived and analyzed in Section 4 using the Cauchy–Born approximation. Finally, in Section 5 we propose different possibilities for constructing QC methods that are based on exchange of boundary conditions and prove convergence. The article closes with an outlook on possible extensions and open problems in Section 6.

1.1 Literature Review

Some applications of the QC method can be found in [35, 36, 33, 25]. Phenomena investigated include defects, fracture, grain boundaries, and nano-indentation.

As mentioned in the Introduction, the most direct energy-based way of QC coupling leads to inconsistencies in the form of ghost forces. Naturally, a lot of work has therefore gone into the design of methods that do not exhibit these unphysical forces. Most of these approaches are based on a more careful treatment of interactions between atoms in the atomistic and the continuum part. For example, in [34] the quasi-nonlocal QC method was suggested. There, a layer of so-called quasi-nonlocal atoms is introduced between the atomistic and the continuum region. These quasi-nonlocal atoms interact normally with neighbours in the atomistic region, whereas interactions with atoms in the continuum region are replaced with virtual atoms whose positions are obtained by extrapolating nearest neighbour positions. A conceptually similar but more general philosophy based on reconstruction schemes for atomic environments is followed in [15].

In [19] the quasi-nonlocal QC method was extended to arbitrary finite-range interactions in one space dimension. A similar, bond-based approach was suggested in 1D and 2D in [32]. A method directly based on the coarse-graining idea is presented in [22].

Although the QC method was originally developed in the 1990s, attempts at its analysis have started only recently. Early results addressed the coarse-graining step in 1D [20, 29] and 2D [21]. In [29] *a priori* and *a posteriori* error bounds for the resulting Galerkin approximation are proved. An analysis of the decay of ghost force induced errors away from the interface is provided in [8].

To obtain actual convergence results for QC-like methods, it is in general not sufficient to show the absence of ghost forces. Following a classical paradigm of numerical analysis, many rigorous approaches have focused on the issues of consistency and stability of a QC method. The issue of stability was investigated for the one-dimensional standard energy-based QC method and the quasi-nonlocal QC methods in [10]. The authors show that besides its inconsistency the standard energy-based QC method also has unsatisfactory stability properties compared with the original atomistic model and the quasi-nonlocal QC method. Rigorous error analysis for the quasi-nonlocal QC method was performed in one space dimension [26, 27, 9, 19]. The quasi-nonlocal QC method has excellent consistency and stability properties and convergence can be obtained, see [27, 19].

Methods based on summation rules instead of the Cauchy–Born approximation to reduce the complexity were analyzed in [24]. Theoretical results in connection with force-based QC methods can be found in [7, 12, 13, 11]. The standard force-based QC method has excellent consistency properties. However, the analysis of stability is more involved. Linearizations of the involved operators are nonnormal and generally not positive definite. The choice of topology turns out to be crucial for obtaining stability [11]. Convergence of the force-based QC method in 1D is proved in [12].

A way of coupling a density functional based atomistic model with a semi-empirical simulation was suggested in [6]. The authors independently use a DFT model in a subdomain and an embedded atom potential (EAM) in the remainder of the domain. The actual coupling is achieved by introducing an interaction energy, which involves a phenomenological electron density in the EAM region as input. These ideas have also been combined with a standard QC method resulting in a model with a quantum mechanical, a classical atomistic and a continuum region [23]. A very similar approach is given in [38, 30]. There, phenomenological electron densities in a patch region are used as boundary conditions for the density functional simulation. The Cauchy–Born approximation of OFDFT provides the continuum model.

Some rigorous mathematical results concerning the continuum and thermodynamic limits of different atomistic models are provided in [4, 3, 5]. In [3] the authors rigorously derive continuum models from pair-potentials and Thomas–Fermi type models. In [4] also a limiting process based on Γ-convergence is analyzed. In [1, 2] the authors analyze models that couple an atomistic nearest neighbour and a continuum energy in one space dimension. The domain is divided into two regions and there is no underlying QC mesh. The message of the articles is that the natural way of coupling the two models leads to failure in the sense that if fracture arises, it does so in the continuum part rather than the atomistic part. The authors then propose a modified coupling that leads to the correct behaviour.

In [14] the authors derive the continuum limits for the Thomas–Fermi–von Weizsäcker and the Kohn–Sham functionals by separating the two scales involved: the scale of the macroscopic displacement field and the scale of the electron density. In the second part of the article two different versions of coupling between the TFW functional and its continuum limit are suggested.

Both are based on decomposing the computational domain into a nonsmooth part (where atomistic detail is needed) and a smooth part (where the approximation by the continuum limit is thought to be accurate). In the first coupling method, the TFW model is used in the whole domain, however, the electron density in the smooth domain is obtained from local cell problems. This approach is shown not to give ghost forces. The second coupling method is obtained by replacing the energy of the smooth region by its Cauchy–Born approximation. This time there are ghost forces due to the unsymmetric treatment of the Coulomb interaction.

1.2 Outline of the Field-Based Model

{sec:SM_Atomistic}

We now motivate a basic atomistic interaction that is mediated by a field. The following ideas were first outlined in [18]. There, a coarse-grained version of the model was suggested as a potential alternative to classical QC coupling.

We start our considerations with a simple atomistic energy based on a pair-potential V in one dimension. Let $\boldsymbol{y} = (y_1, \ldots, y_N) \in \mathbb{R}^N$ represent the coordinates of N particles. We consider the energy

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

Obviously, 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 the 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. We introduce the field $\phi : \mathbb{R} \to \mathbb{R}$ through

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

{eq:phiconvolution}

Then, the energy $\mathcal{E}_\varepsilon(\boldsymbol{y})$ can be written in the following form

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

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

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

By knowing the field ϕ it is unnecessary to compute the force on one particle by adding up the forces that are exerted by all other particles. The nonlocality of the interaction has been encoded in the field ϕ. However, we have replaced the problem of nonlocality with the necessity to calculate the field ϕ, which is defined on the whole of $\mathbb{R}$, via the convolution (1.1).

If the pair-potential V is the Green's function belonging to a linear partial differential operator $L_V(\nabla)$, then ϕ can be computed by solving an equation with right-hand side $\rho_{\boldsymbol{y}}$:

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

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

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

In this case ϕ can be obtained as the solution to

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

or, equivalently, 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 interaction potential $\mathcal{E}_\varepsilon$ takes the form

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

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 combine two energies of the form (1.2) with different parameters m to model an interaction similar to Morse's potential $V(|x|) = \mathrm{e}^{-2|x|} - 2\mathrm{e}^{-|x|}$.

The present article is devoted to the analysis of QC approximations of (1.2) in a periodic one-dimensional setting. The basic idea of QC coupling in this case is as follows. The computational domain is divided into an atomistic and a continuum region. In the continuum region, we use the standard Cauchy–Born approximation of $\mathcal{E}_\varepsilon$. For the atomistic part we use a version of (1.2) on a bounded domain Ω^{at} subject to certain boundary conditions. Both the boundary and the boundary data will be allowed to depend on the configuration $\boldsymbol{y}$.

1.3 Notation

{sec:SM_Notation}

When working with atomistic models, boundaries have to be treated carefully. Strictly speaking they represent defects that lead to boundary layers in the displacement. To avoid these difficulties we look at an infinite chain of atoms on the one-dimensional lattice $\widehat{\boldsymbol{X}} = \varepsilon\mathbb{Z}$, where $\varepsilon > 0$ is the reference lattice spacing. Moreover, to keep the functional analysis simple, we consider only $(2N+1)$-periodic displacements from the reference lattice (see also [27]). Let

$$\mathcal{U} = \left\{\boldsymbol{u}\in\mathbb{R}^{\mathbb{Z}} : u_{j+(2N+1)} = u_j \quad \forall j\in\mathbb{Z},\quad \sum_{j=-N}^{N} u_j = 0\right\}$$

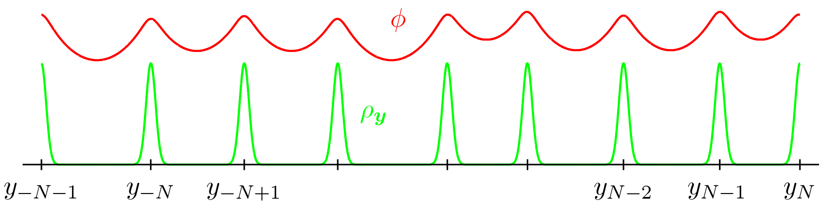

Figure 2.1: Sketch of the basic atomistic problem: the field ϕ is periodic in $\Omega = (y_{-N-1}, y_N)$ and $\rho_{\boldsymbol{y}}$ is a smooth particle density representing the atoms with positions given by $\boldsymbol{y} \in \mathcal{Y}$. {fig:QC1}

and define

$$\mathcal{Y} = F\widehat{\boldsymbol{X}} + \mathcal{U}$$

with a macroscopic deformation gradient $F > 0$. As a computational domain we use the interval

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

To keep the reference length of the interval constant we set $\varepsilon = 2/(2N+1)$.

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 Sobolev-like norm $\|\boldsymbol{u}\|_{\mathcal{U}^{1,2}} = \|\boldsymbol{u}'\|_{\ell^2_\varepsilon}$ 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

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

For monotonously 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 $\mathrm{S}(\boldsymbol{y})$.

2 Periodic Boundary Conditions

{SM:ModelPeriodic}

We now put the field-based interaction potential that was outlined above in a precise mathematical framework. For this, we define the functional $I : H^1_\#(\Omega) \times \mathcal{Y} \to \mathbb{R}$ by

$$I(\varphi, \boldsymbol{y}) = \int_\Omega \Big(\tfrac{1}{2}\varepsilon^2 |\nabla\varphi|^2 + \tfrac{1}{2} m^2 \varphi^2 \Big) \,\mathrm{d}x - \int_\Omega \rho_{\boldsymbol{y}} \varphi \,\mathrm{d}x,$$

where

$$\rho_{\boldsymbol{y}}(x) = \varepsilon \sum_{j\in\mathbb{Z}} Z_j \delta_\varepsilon(x - y_j), \quad \text{and} \quad \delta_\varepsilon(x) = \varepsilon^{-1}\delta_1(x/\varepsilon).$$

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. To avoid cluttering we set $Z_j = 1$ for all $j \in \mathbb{Z}$.

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

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

The respective minimizer (see Figure 2.1)

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

is obviously the periodic solution to the Euler–Lagrange equation

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

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 immediately 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 $\boldsymbol{f} \in \mathcal{U}^{-1,2}$ we need to minimize the total potential energy $E_{\boldsymbol{f}} : \mathcal{Y} \to \mathbb{R}$ defined by

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

A minimizer $\bar{\boldsymbol{y}} \in \mathcal{Y}$ of (2.3) will satisfy the Euler–Lagrange equation

$$DE_{\boldsymbol{f}}(\bar{\boldsymbol{y}}) = D\mathcal{E}(\bar{\boldsymbol{y}}) + \boldsymbol{f} = 0 \quad \in \mathcal{U}^{-1,2}.$$

In the following we address the derivatives of $\mathcal{E}$. Our main observation is a "weak" formulation for the first derivative $D\mathcal{E}$ that acts as a natural connection point for the coupling with a continuum model.

{prop:periodicderiv

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*

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

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

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

We again 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 $\operatorname{supp}\delta(\cdot - y_j)$ 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. This very much resembles the structure of the continuum equations and will be the basis for the QC coupling in Section 5. A version of this calculation was already shown in [17]. There, the author worked with an interpolant that was assumed constant on the support of every $\delta_\varepsilon(\cdot - y_j)$.

For simplicity we assume that the supports of the densities of different particles do not intersect:

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

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 monotonously increasing $y_j' > \varsigma_0$ for all $j \in \mathbb{Z}$.

{lemma:weakformulat

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

$$u(y_j) = u_j \quad \forall j \in \{-N-1, \dots, N\}. \tag{2.6}$$ {eq:uuinterpolant}

Then,

$$D\mathcal{E}(\boldsymbol{y})\cdot\boldsymbol{u} = \sum_{j=-N}^{N} D_{y_j}\mathcal{E}(\boldsymbol{y})\cdot u_j = \int_\Omega \sigma_{\boldsymbol{y}}(x)\nabla u(x)\,\mathrm{d}x\,, \tag{2.7}$$ {eq:per_weakform}

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

$$\begin{aligned} \sigma_{\boldsymbol{y},1}(x) &= \tfrac{1}{2}\varepsilon^2|\nabla\phi|^2 - \tfrac{1}{2}m^2\phi^2 + \rho_{\boldsymbol{y}}\phi, \\ \sigma_{\boldsymbol{y},2}(x) &= \varepsilon \sum_{j=-N-1}^{N} \phi(x)\nabla\delta_\varepsilon(x - y_j)(x - y_j). \end{aligned} \tag{2.8}$$ {eq:sigmaat12}

Proof. Let $u \in \mathrm{S}_\#(\boldsymbol{y})$ be the interpolant of $\boldsymbol{u}$ satisfying (2.6). We start 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

$$D\mathcal{E}(\boldsymbol{y})\cdot\boldsymbol{u} = \sum_{j=-N}^{N} D_{y_j}\mathcal{E}(\boldsymbol{y})\cdot u_j = T_1 + T_2 + T_3, \tag{2.9}$$ {eq:T123}

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 (2.8).

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

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

Hence, T_3 in the above equation (2.9) 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 (2.8), which concludes the proof. □

Remark 2.3. 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

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

A closer look at the calculations in the above proof also 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 weak formulation in a similar vein. □

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

$$G_\varepsilon(x) = \frac{1}{2\varepsilon m}\,\mathrm{e}^{-\frac{m}{\varepsilon}|x|}. \tag{2.10}$$ {eq:greensfunction}

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

{prop:phiexpression

Proposition 2.4. *Let* $\boldsymbol{y} \in \mathcal{Y}$ *be given and* $\phi = \arg\min_{\varphi \in H^1_\#(\Omega)} I(\varphi, \boldsymbol{y})$ *be the corresponding interaction field. Then, for every* $x \in \Omega$,

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

$$\nabla\phi(x) = \int_{\mathbb{R}} G_\varepsilon(x-z)\nabla\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z = \frac{1}{2m}\sum_{k\in\mathbb{Z}}\int_{\mathbb{R}} \nabla\delta_\varepsilon(z-y_k)\,\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z. \tag{2.12}$$ {eq:dphiGreensf}

Proof. The proof of this proposition is straightforward and can be found in the appendix. □

Using the fact that $\rho_{\boldsymbol{y}}$ is $|\Omega|$-periodic we can write the integral (2.11) over $\mathbb{R}$ as an integral over Ω by introducing a periodic Green's function $G^\#_{\varepsilon,\Omega}$:

$$\phi(x) = \int_{\mathbb{R}} \rho_{\boldsymbol{y}}(z) G_\varepsilon(x-z)\,\mathrm{d}z = \int_\Omega \rho_{\boldsymbol{y}}(z) G^\#_{\varepsilon,\Omega}(x-z)\,\mathrm{d}z,$$

where $G^\#_{\varepsilon,\Omega}$ is given by

$$G^\#_{\varepsilon,\Omega}(x) = \frac{1}{2m\varepsilon}\sum_{\nu\in\mathbb{Z}} \mathrm{e}^{-\frac{m}{\varepsilon}|x-\nu|\Omega||}.$$

The energy $\mathcal{E}(\boldsymbol{y})$ then takes the form

$$\mathcal{E}(\boldsymbol{y}) = \frac{1}{2}\int_\Omega \rho_{\boldsymbol{y}}(x)\phi(x)\,\mathrm{d}x = \frac{1}{2}\int_\Omega\int_\Omega \rho_{\boldsymbol{y}}(x) G^\#_{\varepsilon,\Omega}(x-z)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}x\;\mathrm{d}z. \tag{2.13}$$ {eq:EwithperiodicG}

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

$$\begin{aligned}\int_{\mathbb{R}}\int_{\mathbb{R}} \delta_\varepsilon(z-y_j)\mathrm{e}^{-\frac{m}{\varepsilon}|z-x|}\delta_\varepsilon(x-y_i)\,\mathrm{d}x\;\mathrm{d}z &= \int_{\mathbb{R}}\int_{\mathbb{R}} \delta_\varepsilon(z-y_j)\mathrm{e}^{-\frac{m}{\varepsilon}(z-x)}\delta_\varepsilon(x-y_i)\,\mathrm{d}x\;\mathrm{d}z\\ &= \mathrm{e}^{-\frac{m}{\varepsilon}(y_j-y_i)}\int_{\mathbb{R}} \mathrm{e}^{-\frac{m}{\varepsilon}(z-y_j)}\delta_\varepsilon(z-y_j)\,\mathrm{d}z\\ &\qquad\cdot\int_{\mathbb{R}} \mathrm{e}^{-\frac{m}{\varepsilon}(y_i-x)}\delta_\varepsilon(y_i-x)\,\mathrm{d}x\\ &= \mu^2\,\mathrm{e}^{-\frac{m}{\varepsilon}(y_j-y_i)},\end{aligned} \tag{2.14}$$ {eq:mueffcalculatio

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, it is not essential for our reasoning. It merely makes some calculations more convenient. We point out that $\mu = \mathcal{O}(\mathrm{e}^m)$.

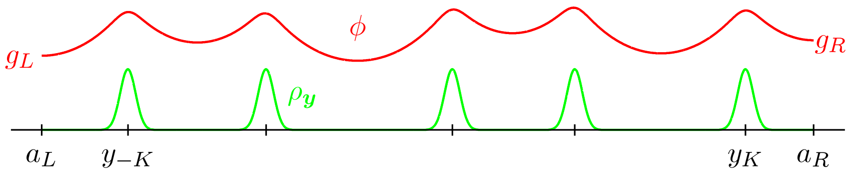

Figure 3.1: The atomistic model in the domain Ω_a with Dirichlet boundary conditions $g = [g_L\ g_R]^T$. {fig:QCDirichlet}

3 Dirichlet Boundary Conditions

{sec:SMDirBCs}

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. This concept will later be used as the atomistic subproblem of QC methods. We set $a = [a_L\ a_R]^T \in \mathbb{R}^2$ and $\Delta a = a_R - a_L$. Throughout the present Section 3 we think of $\boldsymbol{y} = (y_{-K}, \dots, y_K)$ as an ordered element of Ω_a^{2K+1} such that $a_L < y_{-K} < \cdots < y_K < a_R$. The particle density $\rho_{\boldsymbol{y}}$ is canonically defined by

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

For simplicity we assume that the y_j lie well inside Ω_a in the sense that $\operatorname{supp} \rho_{\boldsymbol{y}} \cap \partial\Omega_a = \emptyset$ or, equivalently, $y_{-K} - a_L > \varsigma_0/2$ and $a_R - y_K > \varsigma_0/2$.

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

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

or $\phi|_{\partial\Omega_a} = g$, for $g = [g_L\ g_R]^T \in \mathbb{R}^2$. Then we define the interaction potential $\mathcal{E}_{a,g} : \Omega_a^{2K+1} \to \mathbb{R}$ via

$$\mathcal{E}_{a,g}(\boldsymbol{y}) = - \min_{\substack{\varphi \in H^1(\Omega_a) \\ \varphi|_{\partial\Omega_a} = g}} I_a(\varphi, \boldsymbol{y}), \tag{3.1}$$ {eq:Ebdd}

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

$$I_a(\varphi, \boldsymbol{y}) = \int_{a_L}^{a_R} \left(\tfrac{1}{2}\varepsilon^2 |\nabla\varphi|^2 + \tfrac{1}{2} m^2 \varphi^2\right) \mathrm{d}x - \int_{a_L}^{a_R} \rho_{\boldsymbol{y}} \varphi \,\mathrm{d}x\,. \tag{3.2}$$ {eq:I_a}

For given $\boldsymbol{y}$ the minimizer $\phi = \arg\min_{\varphi \in \xi_{a,g} + H_0^1(\Omega_a)} I_a(\varphi, \boldsymbol{y})$ is the weak solution to

$$\begin{aligned} -\varepsilon^2 \Delta\phi + m^2 \phi &= \rho_{\boldsymbol{y}} \quad \text{in } \Omega_a, \\ \phi|_{\partial\Omega_a} &= g. \end{aligned} \tag{3.3}$$ {eq:phiboundedequat

We will frequently use the decomposition

$$\phi = \phi_0 + \xi_{a,g}, \tag{3.4}$$ {eq:phi_Dir_additiv

where $\phi_0 \in H_0^1(\Omega_a)$ 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

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

It is easy to show that $\xi_{a,g}$ has the form

$$\xi_{a,g}(x) = c_L(a,g) \mathrm{e}^{-\frac{m}{\varepsilon}(x-a_L)} + c_R(a,g) \mathrm{e}^{-\frac{m}{\varepsilon}(a_R-x)}, \tag{3.5}$$ {eq:xi_g}

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

$$c(a,g) = \begin{bmatrix} c_L(a,g) \\ c_R(a,g) \end{bmatrix} = \begin{bmatrix} \frac{1}{1-\tau^2} & -\frac{\tau}{1-\tau^2} \\ -\frac{\tau}{1-\tau^2} & \frac{1}{1-\tau^2} \end{bmatrix} \begin{bmatrix} g_L \\ g_R \end{bmatrix} = T_a \cdot g \tag{3.6}$$ {eq:cofg}

and we have defined

$$\tau = \mathrm{e}^{-\frac{m}{\varepsilon}\Delta a}.$$

We note that if $|\Omega_a| = \Delta a = a_R - a_L$ is large compared with ε, we get $\tau \approx 0$ and therefore $c(a,g) \approx g$ because of the exponential decay of the Green's function.

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 $\boldsymbol{y}$ is monotonously increasing in the sense that $y_{-K} < \cdots < y_K$, we denote by $S(\boldsymbol{y} \cup a)$ the set of continuous, piecewise affine functions over the mesh given by the nodes $a_L, y_{-K}, \ldots, y_K, a_R$. Moreover, $S_0(\boldsymbol{y} \cup a) = S(\boldsymbol{y} \cup a) \cap \mathrm{H}^1_0(\Omega)$.

{lem:weakformbounde

Proposition 3.1. *Let $a, g \in \mathbb{R}^2$ and $\boldsymbol{y} \in \mathcal{Y}$ be given. The potential $\mathcal{E}_{a,g} : \mathcal{Y} \to \mathbb{R}$ defined by (3.1) is continuously Fréchet differentiable.*
(i) The components of the first derivative are given by

$$D_{y_j} \mathcal{E}_{a,g}(\boldsymbol{y}) = -\varepsilon \int_{\Omega_a} \nabla \delta_\varepsilon(x - y_j) \phi(x) \,\mathrm{d}x \tag{3.7}$$ {eq:nablaVbdd}

for $j = -K, \ldots, K$.
(ii) Let $\boldsymbol{u} \in \mathcal{U}$ be a test vector and $u \in \mathrm{S}_0(\boldsymbol{y} \cup a)$ an interpolant of $\boldsymbol{u}$ in the sense that

$$u(a_L) = u(a_R) = 0 \quad \text{and} \quad u(y_j) = u_j \quad \forall j \in \{-K, \ldots, K\}.$$

Then, if $y_{i+1} - y_i > \varsigma_0$ for all $i \in \{-K+1, \ldots, K\}$, $a_R - y_K > \varsigma_0/2$, and $y_{-K} - a_L > \varsigma_0/2$, we have

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

where $\sigma_{\boldsymbol{y}}$ is given by (2.8).

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 $\partial\Omega_a$. □

It is worth pointing out that for $g \neq 0$ 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 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 QC methods we will from now on interpret a and g as arguments to $\mathcal{E}_{a,g}$ rather than fixed parameters entering its definition. In other words we consider the mapping $\Omega_a^{2K+1} \times \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}$, $(\boldsymbol{y}, a, g) \mapsto \mathcal{E}_{a,g}(\boldsymbol{y})$. For future reference we derive the derivatives of this mapping with respect to the boundary a and the boundary data g.

3.1 Dependence on the Boundary

When formulating QC methods in Section 5 we will let the boundary a of the atomistic subdomain depend on the configuration $\boldsymbol{y}$. Therefore, we need 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 (2.7). This will be a central building block for QC methods.

{cor:Ebdd_weakform}

Proposition 3.2. *Let $\boldsymbol{y} \in \mathcal{Y}$ 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 $y_{-K} - a_L > \varepsilon\varsigma_0/2$. Let $\boldsymbol{u} = (u_{-K}, \dots, u_K) \in \mathbb{R}^{2K+1}$ and $h = [h_L\ h_R]^T \in \mathbb{R}^2$ be test vectors. Moreover, let $u \in \mathrm{S}(\boldsymbol{y} \cup a)$ be the interpolant of $\boldsymbol{u}$ and h in the sense that*

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

Then,

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

Proof. This is a direct consequence of the following two lemmas. □

For the first auxiliary lemma it is convenient to define a derivative of $\mathcal{E}_{a,g}(\boldsymbol{y})$ with respect to $a = [a_L\ a_R]^T$ when the relative distances between the atoms are kept 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 given $\boldsymbol{y} \in \Omega_a^{2K+1}$ let $\boldsymbol{X} = (X_{-K}, \dots, X_K) \in (0,1)^{2K+1}$ be determined by $y_j = a_L + (a_R - a_L)X_j$ for all $j \in \{-K, \dots, K\}$. Then, for fixed g and $\boldsymbol{X}$ we define

$$\widetilde{\mathcal{E}}(a) := \mathcal{E}_{a,g}(a_L + (a_R - a_L)\boldsymbol{X}) \tag{3.8}$$

and

$$\widetilde{D}_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y}) := D_{a_R}\widetilde{\mathcal{E}}(a).$$

Here, we interpret the sum $a_L + (a_R - a_L)\boldsymbol{X}$ 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, from which it is immediately clear that $\widetilde{D}_{a_L}\mathcal{E}_{a,g}(\boldsymbol{y}) = -\widetilde{D}_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y})$.

{lemma:DEyN}

Lemma 3.3. *Let $\boldsymbol{y} \in \Omega_a^{2K+1}$. Then*

$$\widetilde{D}_{a_R}\mathcal{E}_{a,g}(\boldsymbol{y}) = \frac{1}{\Delta a}\int_{\Omega_a} \sigma_{\boldsymbol{y}}(x)\,\mathrm{d}x\,. \tag{3.9}$$ {eq:DtildeEyN}

Proof. First, we set $\boldsymbol{\eta}(a) = a_L + \Delta a\boldsymbol{X}$. We begin by transforming the problem to the unit interval $(0,1)$ using the transformation $x \mapsto X(x) = (x - a_L)/(a_R - a_L)$:

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

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 calculate $D_a\widetilde{\mathcal{E}}(a)$ 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

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

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 (2.8).

What remains to be done is differentiating $\widehat{\rho}_{\boldsymbol{\eta}(a)}$ 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 (2.8). □

We can now derive a weak form for the derivative $D_a\mathcal{E}_{a,g}(\boldsymbol{y})$. Therefore, we define $\theta_R \in \mathrm{S}(\boldsymbol{y} \cup a)$ to be the piecewise linear function with

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

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

Lemma 3.4. *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 $y_{-K} - a_L > \varepsilon\varsigma_0/2$. The derivatives of $\mathcal{E}_{a,g}(\boldsymbol{y})$ with respect to a_L, a_R (for fixed $\boldsymbol{y}$ and g) satisfy*

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

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 3.3 yields

$$\widetilde{D}_{a_R}\mathcal{E}_{a,\boldsymbol{y}}(\boldsymbol{y}) = \int_{\Omega_a} \sigma_{\boldsymbol{y}} \nabla \Theta_R \, \mathrm{d}x \; = \int_{\Omega_a} \sigma_{\boldsymbol{y}} \nabla (\Theta_R - \theta_R) \, \mathrm{d}x \; + \int_{\Omega_a} \sigma_{\boldsymbol{y}} \nabla \theta_R \, \mathrm{d}x \, . \tag{3.10}$$

{eq:Thetatheta}

Now, we have $\Theta_R - \theta_R \in \mathrm{S}_0(\boldsymbol{y} \cup a)$ and hence, by Proposition 3.1,

$$\int_{\Omega_a} \sigma_{\boldsymbol{y}}(x) \nabla(\Theta_R - \theta_R) \,\mathrm{d}x \;=\; \sum_{j=-K}^{K} D_{y_j} \mathcal{E}_{a,g}(\boldsymbol{y}) \Theta_R(y_j). \tag{3.11}$$ {eq:Thetatheta2}

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

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

Inserting this into (3.10) and using (3.11) 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 Conditions

Next, we deal with 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. Knowing this derivative is important for subsequent QC coupling because the boundary data will in general depend on $\boldsymbol{y}$. We define

$$\begin{aligned} \gamma_L(\boldsymbol{y}, a) &= 2 \int_{\Omega_a} \rho_{\boldsymbol{y}}(x) G_\varepsilon(x - a_L) \,\mathrm{d}x \,, \\ \gamma_R(\boldsymbol{y}, a) &= 2 \int_{\Omega_a} \rho_{\boldsymbol{y}}(x) G_\varepsilon(a_R - x) \,\mathrm{d}x \,. \end{aligned} \tag{3.12}$$ {eq:gammaLgammaR}

{lemma:depbdrycond}

Lemma 3.5. *The partial derivative of $\mathcal{E}_{a,g}(\boldsymbol{y})$ with respect to g is given by:*

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

where T_a and $c(a,g) = [c_L(a,g)\ c_R(a,g)]^T$ were given in (3.6) *and* $\tau = \mathrm{e}^{-\frac{m}{\varepsilon} \Delta a}$.

Proof. Throughout the proof we suppress the arguments of γ_L, γ_R, and c for readability. We recall the additive decomposition $\phi = \phi_0 + \xi_{a,g}$ from (3.4). It follows from $-\varepsilon^2 \Delta \xi_{a,g} + m^2 \xi_{a,g} = 0$ and $\phi_0 \in \mathrm{H}^1_0(\Omega)$ that $\varepsilon^2 (\nabla \xi_{a,g}, \nabla \phi_0) + m^2 (\xi_{a,g}, \phi_0) = 0$. Hence, a quick calculation shows that the energy $\mathcal{E}_{a,g}(\boldsymbol{y})$ can be written in the following additive way:

$$\mathcal{E}_{a,g}(\boldsymbol{y}) = -I_a(\phi, \boldsymbol{y}) = -I_a(\phi_0, \boldsymbol{y}) - I_a(\xi_{a,g}, \boldsymbol{y}). \tag{3.13}$$ {eq:Eintbdry}

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 (3.5) for $\xi_{a,g}$, we get

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

Here we have used the Green's function G_ε from (2.10). Differentiating this expression with respect to c_L and c_R and applying the chain rule with $D_g c = T_a$ yield the result. □

{remark:refl}

Remark 3.6. We remark that $D_g \mathcal{E}_{a,g}(\boldsymbol{y}) = 0$ if and only if $c_L(a,g) = \gamma_L(\boldsymbol{y}, a)/(1-\tau^2)$ and $c_R(a,g) = \gamma_R(\boldsymbol{y}, a)/(1-\tau^2)$. According to (3.6) this corresponds to the boundary conditions

$$
g_L^*(\boldsymbol{y}, a) = \frac{1}{1-\tau}\,\frac{\gamma_L(\boldsymbol{y}, a) + \tau\gamma_R(\boldsymbol{y}, a)}{1+\tau}, \qquad g_R^*(\boldsymbol{y}, a) = \frac{1}{1-\tau}\,\frac{\tau\gamma_L(\boldsymbol{y}, a) + \gamma_R(\boldsymbol{y}, a)}{1+\tau}. \tag{3.14}
$$

{eq:g*}

In other words the boundary conditions are weighted averages of the values $\frac{1}{1-\tau}\gamma_L(\boldsymbol{y}, a)$ and $\frac{1}{1-\tau}\gamma_R(\boldsymbol{y}, a)$. □

Remark 3.7. As seen in Lemma 3.5 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 $\nabla\phi = 0$ on $\partial\Omega_a$. □

If the domain Ω_a is large and hence $\tau \approx 0$, then $\gamma_L(\boldsymbol{y}, a) \approx g_L^*(\boldsymbol{y}, a)$ and $\gamma_R(\boldsymbol{y}, a) \approx g_R^*(\boldsymbol{y}, a)$. We can then simplify the expression for $I_a(\xi_{a,g}, \boldsymbol{y})$ given in the proof of Lemma 3.5:

$$
\begin{aligned}
I_a(\xi_{a,g}, \boldsymbol{y}) &= m\varepsilon\bigg(\frac{c_L(a,g)^2 + c_R(a,g)^2}{2}\big(1-\tau^2\big) - \big(c_L(a,g)\gamma_L(\boldsymbol{y}, a) + c_R(a,g)\gamma_R(\boldsymbol{y}, a)\big)\bigg) \\
&= m\varepsilon\bigg(\frac{g_L^2 + g_R^2}{2} - \big(g_L g_L^*(\boldsymbol{y}, a) + g_R g_R^*(\boldsymbol{y}, a)\big)\bigg) + \mathcal{O}(\tau).
\end{aligned} \tag{3.15}
$$

{eq:Isimpleexpressi

A useful fact for the analysis of QC methods is the global Lipschitz continuity of the solution ϕ in the L^∞-norm with respect to the boundary conditions g for fixed $\boldsymbol{y}$ and a. This is direct result of the exponential decay of the Green's function.

{lemma:maxprinc}

Lemma 3.8. *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,*

$$
\begin{aligned}
\|\phi_1 - \phi_2\|_{L^\infty} &\le \sqrt{2}|T_a|\,|g_1 - g_2|, \\
\varepsilon\|\nabla\phi_1 - \nabla\phi_2\|_{L^\infty} &\le \sqrt{2}m|T_a|\,|g_1 - g_2|.
\end{aligned}
$$

Proof. We write both functions in the form $\phi_i = \phi_0 + \xi_{a,g_i}$, $i \in \{1,2\}$. Let $c_1 = [c_{1,L}\ c_{1,R}]^T, c_2 = [c_{2,L}\ c_{2,R}]^T$ be the respective coefficients entering ξ_{a,g_i}, $i \in \{1,2\}$. Hence, we get

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

uniformly in x. Taking the supremum over $x \in \Omega_a$ yields the bound for $\|\phi_1 - \phi_2\|_{L^\infty}$. The bound for the derivatives is obtained similarly. □

The bound given in the previous result is rather crude. The effects from the boundary data decay exponentially away from $\partial\Omega_a$, and hence $|\phi_1(x) - \phi_2(x)|$ is much smaller well inside Ω_a.

3.3 A Special Case

{sec:specialcase}

In this short section we take a look at the interaction potential $\mathcal{E}_{a,g}$ from (3.1) with the $\boldsymbol{y}$-dependent boundary conditions $g = g^*(\boldsymbol{y}, a)$ from Remark 3.6. This will be a useful starting point for the design of QC methods in Section 5.

Proposition 3.9. *Let $\boldsymbol{y} \in \Omega_a^{2K+1}$. Then,*

$$\begin{aligned}\mathcal{E}_{a,g^*(\boldsymbol{y},a)}(\boldsymbol{y}) = &\frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x \ + \tau M_\tau(\gamma_L, \gamma_R) \\ &+ \frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a} \rho_{\boldsymbol{y}}(x)\big(\mathrm{e}^{-\frac{m}{\varepsilon}(2a_R-x-z)} + \mathrm{e}^{-\frac{m}{\varepsilon}(x+z-2a_L)}\big)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x\end{aligned} \tag{3.16}$$

{eq:Eg*}

where $M_\tau(\gamma_L, \gamma_R)$ depends quadratically on γ_L and γ_R. {prop:Eg*}

Expression (3.16) 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.

For the proof of the proposition, it is convenient to use an explicit formula for the function values of $\phi_0 \in H_0^1(\Omega_a)$ from the decomposition (3.4). As we saw in Proposition 2.4, the Green's function for the equation $-\varepsilon^2\Delta\phi + m^2\phi = \rho_{\boldsymbol{y}}$ in $\mathbb{R}$ is given by $G_\varepsilon(x,y) = \frac{1}{2m\varepsilon}\mathrm{e}^{-\frac{m}{\varepsilon}|x-y|}$. This could be used to obtain an explicit formula for $\phi(x)$ in the periodic case. We will now construct the Green's function $G_{\varepsilon,a}$ for the operator $-\varepsilon^2\Delta + m^2 id$ subject to homogeneous Dirichlet conditions on $\partial\Omega_a$. Following a simple construction (see appendix or [16, Chapter 2.2.4]) we obtain

$$G_{\varepsilon,a}(x,z) = G^{(1)}_{\varepsilon,a}(x,z) + \tau G^{(2)}_{\varepsilon,a}(x,z), \tag{3.17}$$

{eq:GaG1G2}

where

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

If the domain Ω_a is large compared with ε, that is $\Delta a \gg \varepsilon$, we have $G_{\varepsilon,a} \approx G^{(1)}_{\varepsilon,a}$. To make the following formulas more readable we suppress the arguments of γ_L and γ_R from (3.12). We get the following result.

{lemma:Greensfuncti

Lemma 3.10. *Let $\phi_0 \in H_0^1(\Omega_a)$ satisfy $-\varepsilon^2\Delta\phi_0 + m^2\phi_0 = \rho_{\boldsymbol{y}}$ in Ω_a. Then,*

$$\phi_0(x) = \int_{\Omega_a} G_{\varepsilon,a}(x,z)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z \quad \forall x \in \Omega_a. \tag{3.18}$$ {eq:phiphi0xiGreens

Proof. The proof is provided in the appendix. □

Proof of Proposition 3.9. We have already seen in (3.13) 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 $\mathrm{H}_0^1(\Omega)$, we have with the expression (3.18) for $\phi_0(x)$ that

$$I_a(\phi_0,\boldsymbol{y}) = -\frac{1}{2}\int_{\Omega_a}\int_{\Omega_a}\rho_{\boldsymbol{y}}\phi_0\,\mathrm{d}x = -\frac{1}{2}\int_{\Omega_a}\int_{\Omega_a}\rho_{\boldsymbol{y}}(x)G_{\varepsilon,a}(x,z)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x\,. \tag{3.19}$$ {eq:IaLRphi0temp}

By the definition (3.12) of γ_L and γ_R we have

$$\begin{aligned}\frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a}\rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}(2a_R-x-z)}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}x\;\mathrm{d}z &= \frac{m\varepsilon}{4}\gamma_R^2,\\ \frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a}\rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}(x+z-2a_L)}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}x\;\mathrm{d}z &= \frac{m\varepsilon}{4}\gamma_L^2,\\ \frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a}\rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}(z-x+a_R-a_L)}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}x\;\mathrm{d}z &= \frac{m\varepsilon}{4}\gamma_L\gamma_R.\end{aligned} \tag{3.20}$$ {eq:gammaLsquared}

Inserting the expression (3.17) for $G_{\varepsilon,a}$ into (3.19) 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 3.5 we know that for general g

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

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 Remark 3.6. 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

$$I_a(\xi_{a,g^*(\boldsymbol{y},a)},\boldsymbol{y}) = -\frac{m\varepsilon}{2}\big(\gamma_L^2+\gamma_R^2\big) - \frac{m\varepsilon}{2}\frac{\tau^2}{1-\tau^2}\big(\gamma_L^2+\gamma_R^2\big). \tag{3.21}$$ {eq:Ixia}

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

$$\begin{aligned}\mathcal{E}_{a,g^*(\boldsymbol{y},a)}(\boldsymbol{y}) = &\frac{1}{4m\varepsilon}\int_{\Omega_a}\int_{\Omega_a}\rho_{\boldsymbol{y}}(x)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z\,\mathrm{d}x + \frac{m\varepsilon}{4}\,\big(\gamma_L^2+\gamma_R^2\big)\\ &-\frac{m\varepsilon}{4}\frac{\tau}{1-\tau^2}\big(\tau\gamma_L^2+2\gamma_L\gamma_R+\tau\gamma_R^2\big).\end{aligned} \tag{3.22}$$ {eq:Eagwithtau}

Defining $\tau M_\tau(\gamma_L,\gamma_R)$ to be the third term on the right-hand side and applying (3.20) yields (3.16). □

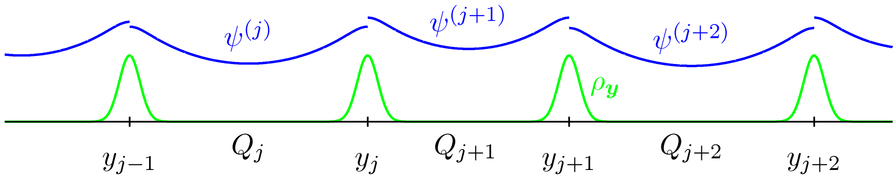

Figure 4.1: The Cauchy–Born approximation: independent periodic problems are solved on the cells $Q_j = (y_{j-1}, y_j)$ leading to locally defined fields $\psi^{(j)}$. {fig:QCCB}

4 The Cauchy–Born Approximation

{sec:SM_CB}

The next building block we need for the design of QC methods based on the model (2.1) is the respective continuum model, which will be derived using the Cauchy–Born approximation. Let $\boldsymbol{y} \in \mathcal{Y}$ satisfy $\min \boldsymbol{y}' > \varsigma_0$. As outlined in the Introduction the Cauchy–Born approximation consists in considering the cells $Q_j = (y_{j-1}, y_j)$ one by one and computing their energy as if they were part of an infinite chain with homogeneous deformation. This is equivalent to solving the periodic minimization problem restricted to Q_j (see Figure 4.1). We therefore define the Cauchy–Born energy of the cell Q_j by

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

Note that this energy only depends on the distance $(y_j - y_{j-1})$. The minimizer $\psi^{(j)}$ of the above problem (4.1) obviously 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 $\mathbb{R}$:

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

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

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

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

$$\mathcal{E}^{cb}(\boldsymbol{y}) = \sum_{j=-N}^{N} \mathcal{E}_j^{cb}(\boldsymbol{y}) = \frac{1}{2} \sum_{j=-N}^{N} \int_{Q_j} \rho_{\boldsymbol{y}} \psi^{(j)} \,\mathrm{d}x \,. \tag{4.3}$$ {eq:CBenergy}

Whether $\mathcal{E}^{cb}(\boldsymbol{y})$ is a good approximation of $\mathcal{E}(\boldsymbol{y})$ strongly depends on the regularity properties of $\boldsymbol{y}$. As we will see below, if $\boldsymbol{y}$ is smooth, i.e., the second difference $\boldsymbol{y}''$ is small, then $|\mathcal{E}^{cb}(\boldsymbol{y}) - \mathcal{E}(\boldsymbol{y})|$ is small.

Let $\boldsymbol{u} \in \mathcal{U}$ be a test vector and $u \in S_\#(\boldsymbol{y})$ an interpolant of $\boldsymbol{u}$ in the sense of (2.6). It follows as in Lemma 3.3 that the derivative of $\mathcal{E}_j^{cb}(\boldsymbol{y})$ can be written in the form

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

where the local continuum stress function $\sigma_{j,\boldsymbol{y}}^{cb}$, in direct correspondence with (2.8), is

$$\begin{aligned} \sigma_{j,\boldsymbol{y}}^{\mathrm{cb}}(x) &= \tfrac{1}{2}\varepsilon^2 |\nabla\psi^{(j)}(x)|^2 - \tfrac{1}{2} m^2 \psi^{(j)}(x)^2 + \rho_{\boldsymbol{y}}(x) \psi^{(j)}(x) \\ &\quad + \varepsilon \sum_{j=-N-1}^{N} \psi^{(j)}(x) \nabla \delta_\varepsilon(x - y_j)(x - y_j). \end{aligned} \tag{4.4}$$ {eq:contstress}

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

$$\sigma_{\boldsymbol{y}}^{cb}(x) = \sigma_{j,\boldsymbol{y}}^{\mathrm{cb}}(x) \quad \text{if} \ \ x \in \Omega_j$$

for all $x \in \Omega$.

4.1 Consistency

Next, we turn to the consistency analysis of the Cauchy–Born approximation, for which we thoroughly analyze the modelling error incurred. From the previous sections we deduce that

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

where the stress functions $\sigma_{\boldsymbol{y}}$ and $\sigma_{j,\boldsymbol{y}}^{\mathrm{cb}}$ are given by (2.8) and (4.4), respectively. The difference between $\sigma_{\boldsymbol{y}}$ and $\sigma_{j,\boldsymbol{y}}^{\mathrm{cb}}$ is that the fields $\psi^{(j)}$ entering $\sigma_{j,\boldsymbol{y}}^{cb}$ are calculated independently on every cell Q_j. To investigate the modelling error $\big|\sigma_{\boldsymbol{y}}(x) - \sigma_{j,\boldsymbol{y}}^{cb}(x)\big|$ incurred by going from the atomistic description to the Cauchy–Born approximation it is hence sufficient to analyze $|\phi - \psi^{(j)}|$ and $|\nabla\phi - \nabla\psi^{(j)}|$ in Q_j for every $j \in \{-N, \ldots, N\}$.

First, we provide a technical lemma.

{lemma:ypp}

Lemma 4.1. *Let* $\boldsymbol{y} \in \ell^\infty(\mathbb{Z})$ *and define* $\boldsymbol{y}^{(j)} = (y_k^{(j)})_{k\in\mathbb{Z}}$ *by* $y_k^{(j)} = y_j + \varepsilon y_j'(k-j)$ *for all* $k \in \mathbb{Z}$. *Then, for* $n > j$:

$$\big|y_n - y_n^{(j)}\big| \leq (n-j)^2\varepsilon^2\|\boldsymbol{y}''\|_{\ell^\infty([j,n-1])}.$$

If $n < j-1$, *then*

$$\big|y_n - y_n^{(j)}\big| \leq (j-1-n)^2\varepsilon^2\|\boldsymbol{y}''\|_{\ell^\infty([n+1,j-1])}.$$

Proof. Since $y_{j-1} = y_{j-1}^{(j)}$ and $y_j = y_j^{(j)}$ we get for $n > j$:

$$y_n - y_n^{(j)} = \varepsilon \sum_{k=j+1}^{n} \big(y_k' - (y_k^{(j)})'\big) = \varepsilon^2 \sum_{k=j+1}^{n}\sum_{l=j}^{k-1}\big(y_l'' - (y_l^{(j)})''\big) = \varepsilon^2 \sum_{k=j+1}^{n}\sum_{l=j}^{k-1} y_l'',$$

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

$$y_n - y_n^{(j)} = \varepsilon^2 \sum_{l=j}^{n-1}\sum_{k=l+1}^{n} y_l'' = \varepsilon^2 \sum_{l=j}^{n-1}(n-l)y_l''.$$

So, we deduce that

$$\big|y_n - y_n^{(j)}\big| \leq (n-j)^2\varepsilon^2\|\boldsymbol{y}''\|_{\ell^\infty([j,n-1])}.$$

If $n < j-1$, we obtain with similar steps

$$y_n - y_n^{(j)} = -\varepsilon \sum_{k=n+1}^{j-1} (y_k' - (y_k^{(j)})') = \varepsilon^2 \sum_{k=n+1}^{j-1}\sum_{l=k}^{j-1} y_l'',$$

which implies that

$$\big|y_n - y_n^{(j)}\big| \leq (j-n-1)^2\varepsilon^2\|\boldsymbol{y}''\|_{\ell^\infty([n+1,j-1])},$$

as desired. □

The next result addresses 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 it depends on the second difference $\boldsymbol{y}''$.

{lemma:psijconverge

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,*

$$\left\|\phi-\psi^{(j)}\right\|_{L^\infty(Q_j)}\le\mu\varepsilon\sum_{n=1}^{\infty}\|\boldsymbol{y}''\|_{\ell^\infty([j-n,j+n-1])}n^2\mathrm{e}^{-mn\min\boldsymbol{y}'},\quad\textit{and}$$

$$\left\|\varepsilon\nabla\phi-\varepsilon\nabla\psi^{(j)}\right\|_{L^\infty(Q_j)}\le m\mu\varepsilon\sum_{n=1}^{\infty}\|\boldsymbol{y}''\|_{\ell^\infty([j-n,j+n-1])}n^2\mathrm{e}^{-mn\min\boldsymbol{y}'}.$$

Proof. From Proposition 2.4 we immediately deduce that, for all $x\in Q_j$,

$$\begin{aligned}\phi(x)&=\frac{1}{2m}\int_{\mathbb{R}}\sum_{k\in\mathbb{Z}}\delta_\varepsilon(z-y_k)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z,\\ \psi^{(j)}(x)&=\frac{1}{2m}\int_{\mathbb{R}}\sum_{k\in\mathbb{Z}}\delta_\varepsilon(z-y_k^{(j)})\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z.\end{aligned}\tag{4.5}$$ {eq:phiandpsij}

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

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

We now derive bounds on the individual terms in the sum. Note that (2.14) simplifies the following calculations but due to the smoothness of the Green's function similar bounds can be obtained without it.

Step 1. Let $k>j$. Then we have $|x-z|=z-x$ for all $z\in\operatorname{supp}\delta_\varepsilon(\cdot-y_k)$ and all $z\in\operatorname{supp}\delta_\varepsilon(\cdot-y_k^{(j)})$. Thus, with (2.14),

$$\frac{1}{2m}\int_{\mathbb{R}}\big(\delta_\varepsilon(z-y_k)-\delta_\varepsilon(z-y_k^{(j)})\big)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z=\frac{\mu}{2m}\big(\mathrm{e}^{-\frac{m}{\varepsilon}(y_k-x)}-\mathrm{e}^{-\frac{m}{\varepsilon}(y_k^{(j)}-x)}\big).\tag{4.6}$$ {eq:phiminuspsi}

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

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

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

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

The same bound on (4.6) can be obtained if $y_k^{(j)}\le y_k$.

Step 2. For any $k<j-1$ we can use the same techniques to obtain that

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

Step 3. Summing over all $k \in \mathbb{Z}\backslash\{j-1, j\}$ we deduce that

$$\left|\phi(x) - \psi^{(j)}(x)\right| \leq \mu\varepsilon \sum_{n=1}^{\infty} \|\boldsymbol{y}''\|_{\ell^\infty([j-n,j+n-1])} n^2 \mathrm{e}^{-mn\min\boldsymbol{y}'}.$$

Step 4. The derivatives of ϕ, $\psi^{(j)}$ in $Q_j = [y_{j-1}, y_j]$ are given by

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

For $k > j$, respectively, $k < j-1$ the exponential factor can in both cases be replaced with $\mathrm{e}^{-\frac{m}{\varepsilon}(z-x)}$, respectively, $\mathrm{e}^{-\frac{m}{\varepsilon}(x-z)}$. Integration by parts leads to the same situation as above with one power of ε less and a factor of m more. □

The next result is only a slight modification of the previous one. The idea is to only treat the modelling error from a finite number of neighbouring atoms explicitly and to find an upper bound on the contribution from atoms that are further away from Q_j.

{lemma:psijerroreM}

Lemma 4.3. *Let $\phi \in H^1_\#(\Omega)$ satisfy* (2.2) *and $\psi^{(j)} \in H^1_\#(Q_j)$ satisfy* (4.2)*, respectively. Then, for any $M \in \mathbb{N}$:*

$$\left\|\phi - \psi^{(j)}\right\|_{L^\infty(Q_j)} \leq \varepsilon\mu \sum_{n=1}^{M-1} \|\boldsymbol{y}''\|_{\ell^\infty(j-n,j+n-1)} n^2 \mathrm{e}^{-mn\min\boldsymbol{y}'} + \frac{2\mu}{m}\frac{\mathrm{e}^{-mM\min\boldsymbol{y}'}}{1-\mathrm{e}^{-m\min\boldsymbol{y}'}}$$

and

$$\varepsilon\left\|\nabla\phi - \nabla\psi^{(j)}\right\|_{L^\infty(Q_j)} \leq \varepsilon m\mu \sum_{n=1}^{M-1} \|\boldsymbol{y}''\|_{\ell^\infty(j-n,j+n-1)} n^2 \mathrm{e}^{-mn\min\boldsymbol{y}'} + 2\mu\frac{\mathrm{e}^{-mM\min\boldsymbol{y}'}}{1-\mathrm{e}^{-m\min\boldsymbol{y}'}}.$$

Proof. The first error part is derived as in the previous lemma. We then look at the contribution to $\phi(x)$ from the atoms in y_k for $k \geq j+M$:

$$\begin{aligned}\frac{1}{2m}\int_{\mathbb{R}} \delta_\varepsilon(z-y_k)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z &= \frac{1}{2m}\int_{\mathbb{R}} \delta_\varepsilon(z-y_k)\mathrm{e}^{-\frac{m}{\varepsilon}(z-y_k)}\mathrm{e}^{-\frac{m}{\varepsilon}(y_k-x)}\,\mathrm{d}z \\ &= \frac{\mu}{2m}\mathrm{e}^{-\frac{m}{\varepsilon}(y_k-x)} \\ &\leq \frac{\mu}{2m}\mathrm{e}^{-m(k-j)\min\boldsymbol{y}'} \\ &\leq \frac{\mu}{2m}\mathrm{e}^{-mM\min\boldsymbol{y}'}\mathrm{e}^{-m(k-M-j)\min\boldsymbol{y}'}.\end{aligned}$$

Summing over $k \geq M+j$ we hence get

$$\frac{1}{2m}\sum_{k=j+M}^{\infty}\int_{\mathbb{R}} \delta_\varepsilon(z-y_k)\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z \leq \frac{\mu}{2m}\frac{\mathrm{e}^{-mM\min\boldsymbol{y}'}}{1-\mathrm{e}^{-m\min\boldsymbol{y}'}}.$$

The same bound can be obtained for the sum over all $k \leq j-M-1$. Similarly we deal with the contributions of these k to $\psi^{(j)}$. The triangle inequality then shows the bound on $\left\|\phi-\psi^{(j)}\right\|_{L^\infty(Q_j)}$. The proof for the bound on $\varepsilon\left\|\nabla\phi - \nabla\psi^{(j)}\right\|_{L^\infty(Q_j)}$ works analogously. □

The following result establishes L^∞-bounds on ϕ and $\nabla\phi$ that only depend on $m \min \boldsymbol{y}'$.

Lemma 4.4. *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, independent of ε, such that*

$$\|\phi\|_{L^\infty(\Omega)} \le K_0(m \min \boldsymbol{y}'),$$
$$\varepsilon\|\nabla\phi\|_{L^\infty(\Omega)} \le K_1(m \min \boldsymbol{y}').$$

{lemma:phiLinftynor

Proof. Let $x \in [y_{j-1}, y_j]$. Then, (2.11) and (2.14) imply that

$$\begin{aligned}|\phi(x)| &= \frac{1}{2m}\sum_{k\in\mathbb{Z}}\int_{\mathbb{R}} \delta_\varepsilon(z-y_k)\,\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z,\\ &= \frac{1}{2m}\int_{\mathbb{R}}\big(\delta_\varepsilon(z-y_{j-1})+\delta_\varepsilon(z-y_j)\big)\,\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}\,\mathrm{d}z + \frac{\mu}{2m}\sum_{\substack{k\in\mathbb{Z}\\ k\neq j-1,j}} \mathrm{e}^{-\frac{m}{\varepsilon}|x-y_k|}.\end{aligned}$$

Since $|x-y_k| \ge (k-j)\varepsilon\min\boldsymbol{y}'$ for all $k > j$, and $|x-y_k| \ge (j-1-k)\varepsilon\min\boldsymbol{y}'$ for all $k < j-1$,

$$\begin{aligned}\phi(x) &\le \frac{1}{m}\int_{\mathbb{R}}\delta_\varepsilon(z)\mathrm{e}^{-\frac{m}{\varepsilon}|z|}\,\mathrm{d}z + \frac{\mu}{m}\sum_{\nu=1}^{\infty}\mathrm{e}^{-\nu m\min\boldsymbol{y}'}\\ &= \frac{1}{m}\int_{\mathbb{R}}\delta_\varepsilon(z)\mathrm{e}^{-\frac{m}{\varepsilon}|z|}\,\mathrm{d}z + \frac{\mu}{m}\frac{\mathrm{e}^{-m\min\boldsymbol{y}'}}{1-\mathrm{e}^{-m\min\boldsymbol{y}'}} \le K_0(m\min\boldsymbol{y}').\end{aligned}$$

The integral term here is bounded since $\mathrm{e}^{-\frac{m}{\varepsilon}|z|}$ is bounded and $\int_{\mathbb{R}}\delta_\varepsilon(z)\,\mathrm{d}z = 1$. Similarly we obtain, with (2.12), that

$$\varepsilon|\nabla\phi(x)| \le \frac{1}{m}\int_{\mathbb{R}}\varepsilon|\nabla\delta_\varepsilon(z)|\mathrm{e}^{-\frac{m}{\varepsilon}|z|}\,\mathrm{d}z + \mu\frac{\mathrm{e}^{-m\min\boldsymbol{y}'}}{1-\mathrm{e}^{-m\min\boldsymbol{y}'}} \le K_1(m\min\boldsymbol{y}'),$$

where we have used that $\int_{\mathbb{R}}\varepsilon|\nabla\delta_\varepsilon(z)|\,\mathrm{d}z$ is uniformly bounded in ε. □

Note that both K_0 and K_1 also implicitly depend on m. However, we think of m as fixed and therefore suppress this dependence. The parameter m determines the range of the interaction and therefore also $\boldsymbol{y}'$. Instances of $m\boldsymbol{y}'$ will appear frequently in the analysis of the QC method.

The quadratic nature of the model (2.1) results in stress functions $\sigma_{\boldsymbol{y}}$ and $\sigma^{cb}_{j,\boldsymbol{y}}$ that are quadratic in the fields ϕ and $\psi^{(j)}$, respectively. Together with L^∞-bounds on ϕ and $\psi^{(j)}$ this allows us to easily bound the modelling error $\big\|\sigma_{\boldsymbol{y}} - \sigma^{cb}_{j,\boldsymbol{y}}\big\|_{L^\infty(Q_j)}$ in terms of $\big\|\phi - \psi^{(j)}\big\|_{L^\infty(Q_j)}$ and $\big\|\nabla\phi - \nabla\psi^{(j)}\big\|_{L^\infty(Q_j)}$.

Lemma 4.5. *Let $\sigma_{\boldsymbol{y}}$ and $\sigma^{cb}_{j,\boldsymbol{y}}$ be given by (2.8), respectively, (4.4). Then, for all $j \in \{-N, \dots, N\}$*

$$\begin{aligned}\big\|\sigma_{\boldsymbol{y}} - \sigma^{cb}_{j,\boldsymbol{y}}\big\|_{L^\infty(Q_j)} &\le K_1(m\min\boldsymbol{y}')\,\varepsilon\,\big\|\nabla\phi - \nabla\psi^{(j)}\big\|_{L^\infty(Q_j)}\\ &\quad + \big(m^2K_0(m\min\boldsymbol{y}') + C\big)\big\|\phi - \psi^{(j)}\big\|_{L^\infty(Q_j)},\end{aligned}$$

where the constant C only depends on δ_1.

{lemma:contstressco

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 4.4, and a similar bound for $\psi^{(j)}$ we get

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

which implies the stated result. □

4.2 Stability

Besides consistency, the second crucial property of an approximation to a given model is stability. In the present case, we need to determine under which conditions $D^2\mathcal{E}^{\mathrm{cb}}(\boldsymbol{y})$ is positive definite.

Lemma 4.6. *Let $\boldsymbol{y} \in \mathcal{Y}$ satisfy $\boldsymbol{y}' > \varsigma_0$. Then, for all $j \in \{-N, \dots, N\}$,*

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

{lemma:cbstability}

Proof. We first recall that $\mathcal{E}^{cb}_j(\boldsymbol{y}) = \frac{1}{2}\int_{Q_j} \rho_{\boldsymbol{y}}\psi^{(j)}\,\mathrm{d}x$ 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

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

We now insert the explicit formula (4.5) for $\psi^{(j)}(x)$ and apply (2.14) to get

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

where the constant $\mathcal{E}_{self}$ 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 $\big|y^{(j)}_k - y_j\big| = |k - j|y_j'$ for all $k \in \mathbb{Z}$. Differentiating twice leads to

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

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

Finally, we prove a Lipschitz bound for the second derivatives $D^2\mathcal{E}_j^{cb}$.

{lemma:DDEcbLipschi

Lemma 4.7. *Let $\boldsymbol{y}_1, \boldsymbol{y}_2 \in \mathcal{Y}$. If $\min \boldsymbol{y}_1' \geq s_0 > \varsigma_0$ and $\min \boldsymbol{y}_2' \geq s_0$, then for all $j \in \{-N,\dots,N\}$*

$$\big|\big(D^2\mathcal{E}_j^{cb}(\boldsymbol{y}_1) - D^2\mathcal{E}_j^{cb}(\boldsymbol{y}_2)\big)\cdot[\boldsymbol{u},\boldsymbol{u}]\big| \leq \frac{m^2\mu^2}{2}\big(\varepsilon|u_j'|^2\big)\big\|\boldsymbol{y}_1' - \boldsymbol{y}_2'\big\|_{\ell^\infty}\sum_{\nu=1}^{\infty}\nu^3\mathrm{e}^{-\nu m s_0} \quad \forall \boldsymbol{u}\in\mathcal{U}.$$

Proof. The derivative $D^2\mathcal{E}_j^{cb}$ was calculated in the previous proof. Hence,

$$\big(D^2\mathcal{E}_j^{cb}(\boldsymbol{y}_1) - D^2\mathcal{E}_j^{cb}(\boldsymbol{y}_2)\big)\cdot[\boldsymbol{u},\boldsymbol{u}] = \frac{m\mu^2}{2}\,\varepsilon\sum_{\nu=1}^{\infty}\nu^2\big(\mathrm{e}^{-\nu m y_{1,j}'} - \mathrm{e}^{-\nu m y_{2,j}'}\big)|u_j'|^2.$$

Since by assumption $y_{1,j}' \geq s_0$ and $y_{2,j}' \geq s_0$, we get with the Mean Value Theorem

$$\big|\mathrm{e}^{-\nu m y_{1,j}'} - \mathrm{e}^{-\nu m y_{2,j}'}\big| \leq \nu m \mathrm{e}^{-\nu m s_0}|y_{1,j}' - y_{2,j}'|.$$

Inserting this in the previous equation concludes the proof. □

5 Quasicontinuum Coupling

{Sec:QCCoupling}

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 $\mathcal{E}^{qc}(\boldsymbol{y})$ such that $\mathcal{E}(\boldsymbol{y}) \approx \mathcal{E}^{qc}(\boldsymbol{y})$ for all relevant $\boldsymbol{y}$ and minimizers $\bar{\boldsymbol{y}}^{qc} \in \mathcal{Y}$ of

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

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

Following the basic philosophy of the QC method we need to approximate $\mathcal{E}(\boldsymbol{y})$ using 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 $\Omega^{cb} = \Omega\backslash\Omega^{\mathrm{at}}$. In Ω^{cb} we will use the Cauchy–Born approximation on a cell-by-cell basis. On the other hand, in Ω^{at} we will use the atomistic model with Dirichlet boundary conditions as discussed in Section 3.

This basic outset 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. Both will in general depend

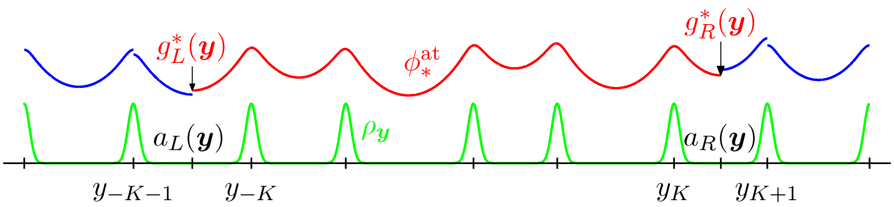

Figure 5.1: An illustration of the first QC method. In $\Omega^{\rm at} = (a_L(\boldsymbol{y}), a_R(\boldsymbol{y}))$ the atomistic problem is solved with the Dirichlet boundary conditions $g^*(\boldsymbol{y})$. Outside $\Omega^{\rm at}$ the Cauchy–Born approximation is used in all cells Q_j. {fig:QC_Method1}

on the configuration $\boldsymbol{y}$. Our main objective for $\mathcal{E}^{qc}$ is the existence of a weak formulation in the sense that

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

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

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

5.1 A Method With Optimal Boundary Conditions

{sec:firstmethod}

For the first QC method we place the boundary a of the atomistic subproblem halfway between the interface atoms, that is $a = a(\boldsymbol{y}) = [a_L(\boldsymbol{y})\ a_R(\boldsymbol{y})]^T$ with[1]

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

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

$$\mathcal{E}^{\rm qc}(\boldsymbol{y}) = \mathcal{E}_*^{\rm cb}(\boldsymbol{y}) + \mathcal{E}_*^{\rm at}(\boldsymbol{y}), \tag{5.1}$$ {eq:EQC_Method1}

which are introduced below.

We note that because of the definition of $a(\boldsymbol{y})$ there are 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 on all Q_j are symmetric, the Cauchy–Born energies of these half cells are given by $\frac{1}{2}\mathcal{E}^{\rm cb}_{-K}(\boldsymbol{y})$ and $\frac{1}{2}\mathcal{E}^{\rm cb}_{K+1}(\boldsymbol{y})$. The continuum part of the energy $\mathcal{E}^{\rm qc}$ is then defined by

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

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

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

[1]The analysis presented in this section immediately carries over to the choice $a_L(\boldsymbol{y}) = y_{-K}$ and $a_R(\boldsymbol{y}) = y_K$.

For the definition of $\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y})$ we consider the minimization problem (3.1) on the atomistic domain Ω^{at} subject to the Dirichlet boundary conditions $g^*(\boldsymbol{y}) = [g_L^*(\boldsymbol{y})\ g_R^*(\boldsymbol{y})]^T$. In correspondence with Remark 3.6 and Section 3.3 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 (see also (3.12))

$$\gamma_L(\boldsymbol{y}) = 2\int_{a_L(\boldsymbol{y})}^{a_R(\boldsymbol{y})} \rho_{\boldsymbol{y}}(x) G_\varepsilon(x - a_L)\,\mathrm{d}x\,, \qquad \gamma_R(\boldsymbol{y}) = 2\int_{a_L(\boldsymbol{y})}^{a_R(\boldsymbol{y})} \rho_{\boldsymbol{y}}(x) G_\varepsilon(a_R - x)\,\mathrm{d}x\,.$$

The energy contribution from the atomistic subproblem is thus given by

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

where $I_{a(\boldsymbol{y})}$ is defined as in (3.2). We denote the solution of this optimization problem by $\phi_{\mathrm{at}}^* \in H^1(\Omega^{\mathrm{at}})$. It satisfies the boundary value problem

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

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}.

We stress that $g^*(\boldsymbol{y})$ and hence $\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y})$ only depend on the components $y_{-K-1}, \ldots, y_{K+1}$. Only the four components y_{-K-1}, y_{-K}, y_K, and y_{K+1} enter both $\mathcal{E}_*^{\mathrm{at}}$ and $\mathcal{E}_*^{cb}$.

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

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

{eq:totalenergyminQ

in $\mathcal{Y}$, where $\boldsymbol{f} \in \mathcal{U}^{-1,2}$ represents an external force. A minimizer $\bar{\boldsymbol{y}}^{qc}$ will satisfy the Euler–Lagrange equation

$$DE_{\boldsymbol{f}}^{qc}(\boldsymbol{y}) = D\mathcal{E}^{qc}(\boldsymbol{y}) + \boldsymbol{f} = 0 \quad \in \mathcal{U}^{-1,2}.$$

Throughout the remainder of this article we assume that the atomistic domain Ω^{at} is large compared with ε:

$$a_R(\boldsymbol{y}) - a_L(\boldsymbol{y}) \gg \varepsilon \quad \text{such that} \quad \tau = \mathrm{e}^{-\frac{m}{\varepsilon}\Delta a(\boldsymbol{y})} \approx 0.$$

To keep the formulas slightly more compact we therefore do not keep track of the τ-dependent terms arising from the atomistic domain explicitly but include an $\mathcal{O}(\tau)$ where necessary.

5.1.1 Consistency

In order to study the consistency properties of the QC energy $\mathcal{E}^{\mathrm{qc}}(\boldsymbol{y})$ from (5.1) we first need to calculate its derivative. Having established weak formulations for the derivatives of $\mathcal{E}$, $\mathcal{E}^{\mathrm{cb}}$, as well as $\mathcal{E}_{a,g}$, we will prove that the Quasicontinuum energy $\mathcal{E}^{qc}$ admits a similar reformulation of $D\mathcal{E}^{qc}(\boldsymbol{y}) \cdot \boldsymbol{u}$. 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 $u \in \mathrm{S}_\#(\boldsymbol{y})$ an interpolant of $\boldsymbol{u}$ in the sense of* (2.6)*. Then,*

$$D\mathcal{E}^{qc}(\boldsymbol{y})\cdot\boldsymbol{u} = \int_\Omega \sigma^{qc}_{\boldsymbol{y}}(x)\nabla u(x)\,\mathrm{d}x\,, \tag{5.4}$$ {eq:QCweakform1}

where

$$\sigma^{qc}_{\boldsymbol{y}}(x) = \begin{cases} \sigma^{cb}_{\boldsymbol{y}}(x) & \text{if } x \in \Omega^{\mathrm{cb}}, \\ \sigma^{\mathrm{at}}_{\boldsymbol{y},*}(x) & \text{if } x \in \Omega^{\mathrm{at}}, \end{cases}$$

and $\sigma^{\mathrm{at}}_{\boldsymbol{y},*}(x)$ is given by (2.8) *with $\phi = \phi^*_{\mathrm{at}}$.* {lemma:Method0WeakF

Proof. Continuum Contribution. From Section 4 we already have the equality

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

$j \in \{-N,\dots,-K-1\} \cup \{K+2,\dots,N\}$. For the contribution $\frac{1}{2}\mathcal{E}^{\mathrm{cb}}_{-K}(\boldsymbol{y})$ 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 $\sigma^{\mathrm{cb}}_{\boldsymbol{y},-K}$ is symmetric in Q_{-K}, we deduce that

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

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

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

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

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 3.2 (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

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

where the stress $\sigma^{\mathrm{at}}_{\boldsymbol{y},*}$ is given by (2.8) 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 $D_g\mathcal{E}_{a(\boldsymbol{y}),g^*(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}}) = 0$ as seen in Remark 3.6. □

We point out that the weak form (5.4) of the derivative $D\mathcal{E}^{qc}$ already implies that there are no ghost forces for homogeneous deformations $\boldsymbol{y}$. 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}. It is obvious that $\psi^{(j)} = \phi$ in Q_j for all $j \in \{-N,\dots,-K-1\} \cup \{K+2,\dots,N\}$. Summarizing, we get $\sigma^{qc}_{\boldsymbol{y}}(x) = \sigma_{\boldsymbol{y}}(x)$ for all $x \in \Omega$, which implies that there are no ghost forces, that is, $D\mathcal{E}^{qc}(\boldsymbol{y}) = 0$ for all $\boldsymbol{y} = F\widehat{\boldsymbol{X}} \in \mathcal{Y}$ representing homogeneous deformations.

Next, we prove consistency of the QC method. Because of the structure of the weak formulation (5.4), the analysis comes down to estimating the errors between the field ϕ coming from the original atomistic model and the fields $\psi^{(j)}$, respectively, ϕ^*_{at}.

For $M \in \mathbb{N}$ we define the index set

$$\mathcal{C}_M = \{-N, \dots, -K + M - 1\} \cup \{K - M + 1, \dots, N\}. \tag{5.6}$$ {eq:CM}

This set represents all atoms in the continuum region plus $2M$ atoms at the two ends of the atomistic region.

Lemma 5.2. *Let $\boldsymbol{y} \in \mathcal{Y}$ be given and assume $\min \boldsymbol{y}' \geq s_0 > \varsigma_0$. Then, there exists $C > 0$ such that*

$$\big|\big(D\mathcal{E}(\boldsymbol{y}) - D\mathcal{E}^{qc}(\boldsymbol{y})\big)\cdot \boldsymbol{u}\big| \leq C\big(\varepsilon \|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mMs_0}\big)\|\nabla u\|_{L^2},$$

for all $\boldsymbol{u} \in \mathcal{U}$, where $u \in S_\#(\boldsymbol{y})$ denotes an interpolant of $\boldsymbol{u}$ in the sense of (2.6). The constant C depends only on s_0 and δ_1. {Lemma:Method0Consi

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

$$\begin{aligned}
\big|\big(D_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y}) - D_{\boldsymbol{y}}\mathcal{E}^{\rm qc}(\boldsymbol{y})\big)\cdot \boldsymbol{u}\big| &= \left|\int_\Omega \big(\sigma_{\boldsymbol{y}}(x) - \sigma^{\rm qc}_{\boldsymbol{y}}(x)\big)\nabla u(x)\,\mathrm{d}x\right| \\
&\leq \|\sigma_{\boldsymbol{y}} - \sigma^{\rm qc}_{\boldsymbol{y}}\|_{\mathrm{L}^2(\Omega)}\,\|\nabla u\|_{\mathrm{L}^2} \\
&\leq |\Omega|^{1/2}\|\sigma_{\boldsymbol{y}} - \sigma^{\rm qc}_{\boldsymbol{y}}\|_{\mathrm{L}^\infty(\Omega)}\,\|\nabla u\|_{\mathrm{L}^2}\,.
\end{aligned} \tag{5.7}$$ {eq:DEqcminusDE}

We therefore need to find error bounds for $\|\sigma_{\boldsymbol{y}} - \sigma^{\rm qc}_{\boldsymbol{y}}\|_{\mathrm{L}^\infty(\Omega)}$ both in the atomistic and the continuum region.

Continuum Contribution. Since $\min \boldsymbol{y}' \geq s_0 > \varsigma_0$, Lemma 4.3 implies that

$$\varepsilon\big\|\nabla\phi - \nabla\psi^{(j)}\big\|_{L^\infty(Q_j)} + \big\|\phi - \psi^{(j)}\big\|_{L^\infty(Q_j)} \leq C\Big(\varepsilon\|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mM\min \boldsymbol{y}'}\Big)$$

uniformly in j, where C only depends on ms_0. Note that compared with Lemma 4.3 we have taken the ℓ^∞-norm of $\boldsymbol{y}''$ over the index set $\mathcal{C}_M$, which contains the continuum atoms as well as $2M$ atoms at the two ends of the atomistic domain. Referring to Lemma 4.5 we deduce that

$$\big\|\sigma_{\boldsymbol{y}} - \sigma^{\rm qc}_{\boldsymbol{y}}\big\|_{\mathrm{L}^\infty(\Omega^{\rm cb})} = \big\|\sigma_{\boldsymbol{y}} - \sigma^{\rm cb}_{\boldsymbol{y}}\big\|_{\mathrm{L}^\infty(\Omega^{\rm cb})} \leq C\Big(\varepsilon\|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mM\min \boldsymbol{y}'}\Big),$$

where C depends on δ_1 and $m\min \boldsymbol{y}'$, respectively, ms_0.

Atomistic Contribution. This time we need a bound on the difference $\big\|\sigma_{\boldsymbol{y}} - \sigma^{\rm qc}_{\boldsymbol{y}}\big\|_{\mathrm{L}^\infty(\Omega^{\rm at})} = \big\|\sigma_{\boldsymbol{y}} - \sigma^{\rm at}_{\boldsymbol{y},*}\big\|_{\mathrm{L}^\infty(\Omega^{\rm at})}$. For this we first address the error $|\phi(x) - \phi^*_{\rm at}(x)|$, $x \in \Omega^{\rm at}$. The functions ϕ and $\phi^*_{\rm at}$ satisfy the equations $-\varepsilon^2\Delta\phi + m^2\phi = \rho_{\boldsymbol{y}}$, respectively, $-\varepsilon^2\Delta\phi^*_{\rm at} + m^2\phi^*_{\rm at} = \rho_{\boldsymbol{y}}$ in $\Omega^{\rm at}$. However, the boundary conditions are different: $\phi(a_L)$ and $\phi(a_R)$ for ϕ, respectively, $g^*_L(\boldsymbol{y})$ and $g^*_R(\boldsymbol{y})$ for $\phi^*_{\rm at}$. According to Lemma 3.8 we thus get

$$\|\phi - \phi^*_{\rm at}\|_{L^\infty(\Omega^{\rm at})} + \varepsilon\|\nabla\phi - \nabla\phi^*_{\rm at}\|_{L^\infty(\Omega^{\rm at})} \leq C\big(\big|\phi(a_L) - g^*_L(\boldsymbol{y})\big| + \big|\phi(a_R) - g^*_R(\boldsymbol{y})\big|\big).$$

The definitions of $g^*(\boldsymbol{y})$, $\gamma_L(\boldsymbol{y})$, and $\gamma_R(\boldsymbol{y})$ imply

$$\big|\gamma_L(\boldsymbol{y}) - g^*_L(\boldsymbol{y})\big| = \mathcal{O}(\tau), \quad \big|\gamma_R(\boldsymbol{y}) - g^*_R(\boldsymbol{y})\big| = \mathcal{O}(\tau).$$

For the value $\gamma_R(\boldsymbol{y})$, for example, we obtained in Remark 3.6 the equality

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

where $\rho^{\mathrm{refl}}_{\boldsymbol{y},R}$ is a reflected and periodized extension of $\rho_{\boldsymbol{y}}|_{\Omega^{\mathrm{at}}}$. This then leads to

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

Using the same ideas as in Lemmas 4.2 and 4.3 we can then show that

$$|\phi(a_R) - g^*_R(\boldsymbol{y})| \le C\varepsilon\|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)} + C\mathrm{e}^{-mM\min \boldsymbol{y}'} + \mathcal{O}(\tau),$$

where the constants only depend on $m \min \boldsymbol{y}'$. The same bound can be obtained for $|\phi(a_L) - g^*_L(\boldsymbol{y})|$. This then implies that

$$\|\phi - \phi^*_{\mathrm{at}}\|_{L^\infty(\Omega^{\mathrm{at}})} + \varepsilon\|\nabla\phi - \nabla\phi^*_{\mathrm{at}}\|_{L^\infty(\Omega^{\mathrm{at}})} \le C\big(\varepsilon\|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mM\min\boldsymbol{y}'} + \tau\big)$$

and hence

$$\big\|\sigma_{\boldsymbol{y}} - \sigma^{\mathrm{qc}}_{\boldsymbol{y}}\big\|_{\mathrm{L}^\infty(\Omega^{\mathrm{at}})} = \big\|\sigma_{\boldsymbol{y}} - \sigma^{\mathrm{at}}_{\boldsymbol{y},*}\big\|_{\mathrm{L}^\infty(\Omega^{\mathrm{at}})} \le C\big(\varepsilon\|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mMs_0} + \tau\big),$$

where C only depends on $m\min\boldsymbol{y}'$. Together with (5.7) and $\tau \le \mathrm{e}^{-mMs_0}$ this completes the proof. □

5.1.2 Stability

The special choice $g^*(\boldsymbol{y})$ of boundary conditions for the atomistic subproblem allows for an elementary stability analysis of $\mathcal{E}^{\mathrm{qc}}(\boldsymbol{y})$ that draws from the ideas we used in Section 3.3. We recall that

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

The next result addresses the differentiability of γ_L and γ_R. We show that the derivatives satisfy certain bounds. Calculations like these are typical for this type of atomistic model.

{lemma:gammaLR}

Lemma 5.3. *Let $\boldsymbol{y} \in \Omega^{2K+1}_a$ 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,*

$$\gamma_L(\boldsymbol{y}, a) \le \frac{\mu}{m}\frac{1}{1-\mathrm{e}^{-m\min\boldsymbol{y}'}}, \qquad \gamma_R(\boldsymbol{y}, a) \le \frac{\mu}{m}\frac{1}{1-\mathrm{e}^{-m\min\boldsymbol{y}'}}.$$

Moreover, $\gamma_L(\boldsymbol{y})$ is twice continuously differentiable with respect to $\boldsymbol{y}$ and a and there exists $C(m\min\boldsymbol{y}')$ (independent of ε) such that

$$\begin{aligned}\big|D\gamma_L(\boldsymbol{y}, a)\cdot(\boldsymbol{u}, h)\big| &\le C(m\min\boldsymbol{y}')\bigg(\Big(\frac{u_{-K} - h_L}{\varepsilon}\Big)^2 + \sum_{k=-K+1}^{K}(u'_k)^2\bigg)^{1/2},\\ \big|D^2\gamma_L(\boldsymbol{y}, a)\cdot\big[(\boldsymbol{u}, h), (\boldsymbol{u}, h)\big]\big| &\le C(m\min\boldsymbol{y}')\bigg(\Big(\frac{u_{-K} - h_L}{\varepsilon}\Big)^2 + \sum_{k=-K+1}^{K}(u'_k)^2\bigg)\end{aligned}$$

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

Proof. We start with the following observation

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

Using $y_j - y_{-K} \le (j+K) \min \boldsymbol{y}'$ for $j = -K, \dots, K$ we directly infer that

$$\gamma_L(\boldsymbol{y}, a) \le \frac{\mu}{m} \sum_{j=-K}^{K} \mathrm{e}^{-\frac{m}{\varepsilon}(y_j - y_{-K})} \le \frac{\mu}{m} \frac{1 - \mathrm{e}^{-(2K+1)m \min \boldsymbol{y}'}}{1 - \mathrm{e}^{-m \min \boldsymbol{y}'}} \le \frac{\mu}{m} \frac{1}{1 - \mathrm{e}^{-m \min \boldsymbol{y}'}}.$$

Differentiating gives

$$\begin{aligned} D_{a_L} \gamma_L(\boldsymbol{y}, a) h_L + D_{\boldsymbol{y}} \gamma_L(\boldsymbol{y}, a) \cdot \boldsymbol{u} &= \, -\mu \sum_{j=-K}^{K} \mathrm{e}^{-\frac{m}{\varepsilon}(y_j - a_L)} \frac{u_j - h_L}{\varepsilon}, \\ D^2 \gamma_L(\boldsymbol{y}, a) \cdot \big[(\boldsymbol{u}, h), (\boldsymbol{u}, h)\big] &= m\mu \sum_{j=-K}^{K} \mathrm{e}^{-\frac{m}{\varepsilon}(y_j - a_L)} \frac{(u_j - h_L)^2}{\varepsilon^2}. \end{aligned}$$

We show the stated bound for the second derivative. The one for the first derivative is obtained similarly. We have

$$\begin{aligned} \Big(\frac{u_j - h_L}{\varepsilon}\Big)^2 &= \Big(\frac{u_{-K} - h_L}{\varepsilon} + \sum_{k=-K+1}^{j} u_k'\Big)^2 \\ &\le 2\Big(\frac{u_{-K} - h_L}{\varepsilon}\Big)^2 + 2(j+K) \sum_{k=-K+1}^{j} (u_k')^2. \end{aligned}$$

Therefore,

$$\begin{aligned} D^2 \gamma_L(\boldsymbol{y}, a) \cdot \big[(\boldsymbol{u}, h), (\boldsymbol{u}, h)\big] \le 2m\mu \sum_{j=-K}^{K} (j+K) \mathrm{e}^{-(j+K)m \min \boldsymbol{y}'} \\ \cdot \bigg(\Big(\frac{u_{-K} - h_L}{\varepsilon}\Big)^2 + \sum_{k=-K+1}^{K} (u_k')^2\bigg), \end{aligned}$$

which is the desired bound. □

The τ-dependent terms in $\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y}) = \mathcal{E}_{a(\boldsymbol{y}), g^*(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}})$ from (3.22) only contain $\gamma_L(\boldsymbol{y})$ 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*

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

{lemma:QCStabMethod

Proof. We treat continuum and atomistic contributions independently and start with the former. Lemma 4.6 states that

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

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

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

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

$$\begin{aligned}\mathcal{E}_*^{\mathrm{at}}(\boldsymbol{y}) &= \frac{\varepsilon}{4m}\sum_{i,j=-K}^{K}\int_{\Omega^{\mathrm{at}}}\int_{\Omega^{\mathrm{at}}}\delta_\varepsilon(x-y_i)\big(\mathrm{e}^{-\frac{m}{\varepsilon}|x-z|}+\mathrm{e}^{-\frac{m}{\varepsilon}(x+z-y_{-K-1}-y_{-K})}\\ &\qquad\qquad +\mathrm{e}^{-\frac{m}{\varepsilon}(y_{K+1}+y_K-x-z)}\big)\delta_\varepsilon(z-y_j)\,\mathrm{d}z\,\mathrm{d}x\\ &= \frac{\varepsilon\mu^2}{4m}\sum_{i,j=-K}^{K}\big(\mathrm{e}^{-\frac{m}{\varepsilon}|y_i-y_j|}+\mathrm{e}^{-\frac{m}{\varepsilon}(y_i+y_j-y_{-K}-y_{-K-1})}\\ &\qquad\qquad +\mathrm{e}^{-\frac{m}{\varepsilon}(y_K+y_{K+1}-y_i-y_j)}\big)+\mathcal{E}_{self}+\mathcal{O}(\tau),\end{aligned} \tag{5.8}$$

{eq:E*atlong}

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

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

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

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

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

Next, we provide a Lipschitz continuity result for the second derivative $D^2\mathcal{E}^{qc}$.

{eq:Eqc_Lipschitz}

Lemma 5.5. *Let $\boldsymbol{y}_1,\boldsymbol{y}_2\in\mathcal{Y}$. If $\min\boldsymbol{y}_1'\geq s_0>\varsigma_0$ and $\min\boldsymbol{y}_2'\geq s_0$, then*

$$\big\|D^2\mathcal{E}^{qc}(\boldsymbol{y}_1)-D^2\mathcal{E}^{qc}(\boldsymbol{y}_2)\big\|\leq L(s_0)\|\boldsymbol{y}_1'-\boldsymbol{y}_2'\|_{\ell^\infty}.$$

Proof. The Lipschitz continuity of $D^2\mathcal{E}_*^{cb}$ follows from Lemma 4.7. Thus, we only have to consider the atomistic part $\mathcal{E}_*^{\mathrm{at}}$ given in a convenient form in (5.8). We present the proof for the part

$$\mathcal{E}_0^{\mathrm{at}}(\boldsymbol{y})=\frac{\varepsilon\mu^2}{4m}\sum_{i,j=-K}^{K}\mathrm{e}^{-\frac{m}{\varepsilon}|y_i-y_j|}+\mathcal{E}_{self}.$$

The parts involving $\mathrm{e}^{-\frac{m}{\varepsilon}(y_i+y_j-y_{-K}-y_{-K-1})}$ and $\mathrm{e}^{-\frac{m}{\varepsilon}(y_K+y_{K+1}-y_i-y_j)}$ can be treated analogously. Differentiating $\mathcal{E}_0^{\mathrm{at}}(\boldsymbol{y})$ twice leads to

$$\big(D^2\mathcal{E}_0^{\mathrm{at}}(\boldsymbol{y}_1)-D^2\mathcal{E}_0^{\mathrm{at}}(\boldsymbol{y}_2)\big)\cdot[\boldsymbol{u},\boldsymbol{u}]=\frac{m\varepsilon\mu^2}{4}\sum_{\substack{i,j=-K\\ i\neq j}}^{K}\big(\mathrm{e}^{-\frac{m}{\varepsilon}|y_{1,i}-y_{1,j}|}-\mathrm{e}^{-\frac{m}{\varepsilon}|y_{2,i}-y_{2,j}|}\big)\frac{(u_i-u_j)^2}{\varepsilon^2}.$$

Next, we analyze the first factor inside the sum. Since $y'_{1,i} \geq s_0$ and $y'_{2,i} \geq s_0$ for all $i \in \{-N, \dots, N\}$ we have $|y_{1,i} - y_{1,j}| \geq |i-j|\varepsilon s_0$, $|y_{2,i} - y_{2,j}| \geq |i-j|\varepsilon s_0$ for all $i, j \in \{-K, \dots, K\}$ and therefore by the Mean Value Theorem

$$\begin{aligned}\left|\mathrm{e}^{-\frac{m}{\varepsilon}|y_{1,i}-y_{1,j}|} - \mathrm{e}^{-\frac{m}{\varepsilon}|y_{2,i}-y_{2,j}|}\right| &\leq m\mathrm{e}^{-m|i-j|s_0}\varepsilon^{-1}\big|y_{1,i} - y_{1,j} - (y_{2,i} - y_{2,j})\big| \\ &= m\mathrm{e}^{-m|i-j|s_0}\left|\sum_{\nu=i+1}^{j}\big(y'_{1,\nu} - y'_{2,\nu}\big)\right| \\ &\leq m\mathrm{e}^{-m|i-j|s_0}|j-i|\,\big\|\boldsymbol{y}'_1 - \boldsymbol{y}'_2\big\|_{\ell^\infty}.\end{aligned}$$

Hence,

$$\big|\big(D^2\mathcal{E}_0^{\mathrm{at}}(\boldsymbol{y}_1) - D^2\mathcal{E}_0^{\mathrm{at}}(\boldsymbol{y}_2)\big)\cdot[\boldsymbol{u}, \boldsymbol{u}]\big| \leq \frac{m^2\varepsilon\mu^2}{4}\big\|\boldsymbol{y}'_1 - \boldsymbol{y}'_2\big\|_{\ell^\infty}\sum_{\substack{i,j=-K\\ i\neq j}}^{K}\mathrm{e}^{-m|i-j|s_0}|j-i|\frac{(u_i - u_j)^2}{\varepsilon^2}.$$

The idea now is to show that the sum on the right-hand side is bounded by a function of s_0 times $\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon}$. Elementary rearrangments lead to

$$\begin{aligned}\sum_{\substack{i,j=-K\\ i\neq j}}^{K}\mathrm{e}^{-m|i-j|s_0}|j-i|\frac{(u_i - u_j)^2}{\varepsilon^2} &= 2\sum_{i=-K}^{K}\sum_{j=i+1}^{K}\mathrm{e}^{-m|i-j|s_0}|j-i|\frac{(u_i - u_j)^2}{\varepsilon^2} \\ &= 2\sum_{i=-K}^{K}\sum_{\nu=1}^{K-i}\mathrm{e}^{-m\nu s_0}\nu\frac{(u_{i+\nu} - u_i)^2}{\varepsilon^2} \\ &= 2\sum_{\nu=1}^{2K}\mathrm{e}^{-m\nu s_0}\nu\sum_{i=-K}^{K-\nu}\frac{(u_{i+\nu} - u_i)^2}{\varepsilon^2}.\end{aligned}$$

We note that, for all $\nu \in \mathbb{N}$,

$$\frac{(u_{i+\nu} - u_i)^2}{\varepsilon^2} = \left(\sum_{\kappa=i+1}^{i+\nu}u'_\kappa\right)^2 \leq \nu\sum_{\kappa=i+1}^{i+\nu}|u'_\kappa|^2.$$

Using this we obtain

$$\begin{aligned}2\sum_{\nu=1}^{2K}\mathrm{e}^{-m\nu s_0}\nu\sum_{i=-K}^{K-\nu}\frac{(u_{i+\nu} - u_i)^2}{\varepsilon^2} &\leq 2\sum_{\nu=1}^{2K}\mathrm{e}^{-m\nu s_0}\nu^2\sum_{i=-K}^{K-\nu}\sum_{\kappa=i+1}^{i+\nu}|u'_\kappa|^2 \\ &\leq 2\varepsilon^{-1}\sum_{\nu=1}^{\infty}\mathrm{e}^{-m\nu s_0}\nu^3\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon},\end{aligned}$$

where in the last step we have changed the summation order over j and κ and summed over $j = -K, \dots, K$. Summarizing, we have shown that

$$\big|\big(D^2\mathcal{E}_0^{\mathrm{at}}(\boldsymbol{y}_1) - D^2\mathcal{E}_0^{\mathrm{at}}(\boldsymbol{y}_2)\big)\cdot[\boldsymbol{u}, \boldsymbol{u}]\big| \leq \frac{2m^2\mu^2}{4}\big\|\boldsymbol{y}'_1 - \boldsymbol{y}'_2\big\|_{\ell^\infty}\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon}\sum_{\nu=1}^{\infty}\nu^3\mathrm{e}^{-m\nu s_0}.$$

Taking the supremum over $\boldsymbol{u} \in \mathcal{U}$ concludes the proof. □

5.1.3 Existence and Convergence

Before stating and proving the main result, we provide a lemma that relates the difference of $\boldsymbol{u} \in \mathcal{U}$ to the derivative of its interpolant $u \in S_\#(\boldsymbol{y})$.

{lemma:gradientu}

Lemma 5.6. *Let $\boldsymbol{u} \in \mathcal{U}$ be a test vector and $u \in \mathrm{S}_\#(\boldsymbol{y})$ an interpolant of $\boldsymbol{u}$ in the sense of (2.6). Then,*

$$\|\nabla u\|_{L^2} \leq \frac{1}{(\min \boldsymbol{y}')^{1/2}} \|\boldsymbol{u}'\|_{\ell^2_\varepsilon}.$$

Proof. By the definition of the interpolant u we have

$$\begin{aligned}\int_\Omega |\nabla u|^2 \,\mathrm{d}x &= \sum_{i=-N}^{N} \int_{y_{i-1}}^{y_i} \left(\frac{u_i - u_{i-1}}{y_i - y_{i-1}}\right)^2 \mathrm{d}x \\ &= \varepsilon \sum_{i=-N}^{N} \frac{(u_i - u_{i-1})^2}{\varepsilon^2} \frac{\varepsilon}{y_i - y_{i-1}} = \varepsilon \sum_{i=-N}^{N} \frac{|u_i'|^2}{y_i'}.\end{aligned}$$

Taking the square root concludes the proof. □

We are finally ready to prove an existence and convergence result. The proof consists in showing that all conditions in Lemma A.1 are satisfied, see for example [27, Theorem 8]. The parameter $M \in \mathbb{N}_0$ provides some flexibility. It can be adjusted so that the conditions are satisfied. The theorem can informally be paraphrased as follows: if the minimizer $\bar{\boldsymbol{y}} \in \arg\min E_{\boldsymbol{f}}$ of the original atomistic problem is sufficiently smooth in the neighbourhood $\mathcal{C}_M$ of the atoms in the continuum region and M is sufficiently large, then there exists a solution $\bar{\boldsymbol{y}}_{qc} \in \mathcal{Y}$ to the QC approximated problem that is a good approximation to $\bar{\boldsymbol{y}}$.

Theorem 5.7. *Let $\bar{\boldsymbol{y}} \in \arg\min E_{\boldsymbol{f}}$ satisfy $\min \bar{\boldsymbol{y}}' \geq s_0 > \varsigma_0$ and $\max \bar{\boldsymbol{y}}' \leq S_0$. Then, there exists $\lambda(s_0, S_0) > 0$ such that, if, for some $M \in \mathbb{N}$,*

$$\varepsilon^{1/2} \|\bar{\boldsymbol{y}}''\|_{\ell^\infty(\mathcal{C}_M)} + \varepsilon^{-1/2} \mathrm{e}^{-mMs_0} \leq \lambda(s_0, S_0), \tag{5.9}$$ {smallcondition}

then there exists a solution $\bar{\boldsymbol{y}}_{qc} \in \mathcal{Y}$ to

$$DE^{qc}_{\boldsymbol{f}}(\bar{\boldsymbol{y}}^{qc}) = 0 \quad in \;\; \mathcal{U}^{-1,2},$$

that satisfies

$$\left\|\bar{\boldsymbol{y}}' - \bar{\boldsymbol{y}}'_{qc}\right\|_{\ell^2_\varepsilon} \leq C(s_0, S_0)\big(\varepsilon \|\bar{\boldsymbol{y}}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mMs_0} + \tau\big).$$

{Theorem:QC1Converg

Proof. First, we define $\mathcal{F} : \mathcal{U}^{1,2} \to \mathcal{U}^{-1,2}$ by $\mathcal{F}(\boldsymbol{w}) = DE^{qc}_{\boldsymbol{f}}(\bar{\boldsymbol{y}} + \boldsymbol{w})$ for $\boldsymbol{w} \in \mathcal{U}$, where the spaces $\mathcal{U}^{1,2}$ and $\mathcal{U}^{-1,2}$ were introduced in Section 1.3. We need to show that $\mathcal{F}(\boldsymbol{w}) = 0$ has a solution $\boldsymbol{w} \in A = \{\boldsymbol{w} \in \mathcal{U} : \min(\bar{\boldsymbol{y}}' + \boldsymbol{w}') \geq \varsigma_0\}$.

Step 1. Consistency. The analysis from Lemma 5.2 together with Lemma 5.6 shows that

$$\|\mathcal{F}(0)\|_{\mathcal{U}^{-1,2}} = \left\|DE^{qc}_{\boldsymbol{f}}(\bar{\boldsymbol{y}})\right\|_{\mathcal{U}^{-1,2}} = \left\|D\mathcal{E}^{qc}(\bar{\boldsymbol{y}}) - D\mathcal{E}(\bar{\boldsymbol{y}})\right\|_{\mathcal{U}^{-1,2}} \leq \eta,$$

where

$$\eta = \frac{C(ms_0)}{s_0}\big(\varepsilon \|\bar{\boldsymbol{y}}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mMs_0} + \tau\big).$$

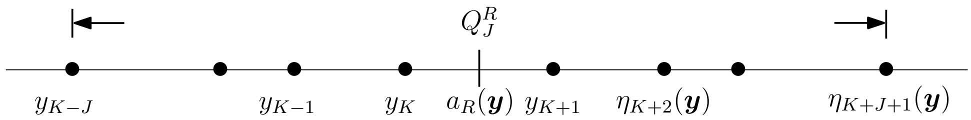

Figure 5.2: Illustration of the problem in the interval $Q_J^R = (y_{K-J}, 2a_R(\boldsymbol{y}) - y_{K-J})$ used to compute $g_R(\boldsymbol{y})$. {fig:QC2}

Step 2. Stability. Lemma 5.4 states that

$$D^2\mathcal{E}^{qc}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \geq \Big(\frac{m\mu^2}{2}\mathrm{e}^{-mS_0} - \mathcal{O}(\tau)\Big)\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon} =: \vartheta\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon} \quad \forall \boldsymbol{u} \in \mathcal{U},$$

which immediately translates to

$$\big\|D\mathcal{F}(0)^{-1}\big\|_{Lin(\mathcal{U}^{-1,2},\mathcal{U}^{1,2})} \leq \vartheta^{-1}.$$

Step 3. Lipschitz bound. The next step is to show the existence of a Lipschitz constant for $D\mathcal{F}$ in the neighbourhood $B_{2\eta\vartheta}(0)$. For all $\boldsymbol{w} \in \mathcal{U}$ with $\|\boldsymbol{w}'\|_{\ell^2_\varepsilon} \leq 2\eta\vartheta$ we get with an inverse inequality

$$\|\boldsymbol{w}'\|_{\ell^\infty} \leq \varepsilon^{-1/2}\|\boldsymbol{w}'\|_{\ell^2_\varepsilon} \leq 2\varepsilon^{-1/2}\eta\vartheta.$$

Let $0 < \delta < 1$. If $2\varepsilon^{-1/2}\eta\vartheta \leq (1-\delta)s_0$, we hence have $\min(\bar{\boldsymbol{y}}' + \boldsymbol{w}') \geq \delta s_0$ for all $\boldsymbol{w}$ with $\|\boldsymbol{w}'\|_{\ell^2_\varepsilon} \leq 2\eta\vartheta$. Knowing that $\bar{\boldsymbol{y}}' + \boldsymbol{w}'$ is bounded below, we can apply the Lipschitz bound from Lemma 5.5:

$$\begin{aligned}\big\|D^2\mathcal{E}^{qc}(\boldsymbol{y}+\boldsymbol{w}_1) - D^2\mathcal{E}^{qc}(\boldsymbol{y}+\boldsymbol{w}_2)\big\| &\leq L(\delta s_0)\|\boldsymbol{w}_1' - \boldsymbol{w}_2'\|_{\ell^\infty} \\ &\leq L_\varepsilon\|\boldsymbol{w}_1' - \boldsymbol{w}_2'\|_{\ell^2_\varepsilon},\end{aligned}$$

where $L_\varepsilon = \varepsilon^{-1/2}L(\delta s_0)$.

Step 4. Conclusion. What remains to be done is to ensure that $2L_\varepsilon\eta\vartheta < 1$. Looking at the product of these values, we see that for sufficiently small $\varepsilon^{-1/2}(\varepsilon\|\bar{\boldsymbol{y}}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mMs_0} + \tau)$, this can be satisfied. Lemma A.1 then guarantees the existence of $\bar{\boldsymbol{y}}_{qc} \in \mathcal{Y}$ such that $DE^{qc}_{\boldsymbol{f}}(\bar{\boldsymbol{y}}_{qc}) = 0$. The configuration $\bar{\boldsymbol{y}}_{qc}$ is a minimizer of $E^{qc}_{\boldsymbol{f}}$ since $D^2E^{qc}_{\boldsymbol{f}}(\bar{\boldsymbol{y}}_{qc})$ is positive definite. $\square$

Referring to (5.9) we note that the magnitude of M depends on ε. The condition (5.9) can be satisfied if, for example, $M \sim -\log\varepsilon$.

5.2 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 whose analysis turned out to be straightforward. The reasons for this lie in the clean weak formulation (5.4) of $D\mathcal{E}^{qc}$ and the convenient stability properties established in Lemma 5.4. We now investigate how this situation changes if the boundary conditions chosen are approximations of $g^*(\boldsymbol{y})$ that can be computed easily. The following construction may also be easier to generalize to higher dimensions. We still set $a_L(\boldsymbol{y}) = \frac{1}{2}(y_{-K-1} + y_{-K})$ and $a_R(\boldsymbol{y}) = \frac{1}{2}(y_K + y_{K+1})$.

We recall from Remark 3.6 that $g^*_R(\boldsymbol{y})$ could (up to $\mathcal{O}(\tau)$) be interpreted as the field value in a_R produced by the symmetric particle density $\rho^{refl}_{\boldsymbol{y},R}$. Loosely speaking, we now cut off this distribution and extend it periodically so that the new boundary conditions $g(\boldsymbol{y}) = [g_L(\boldsymbol{y})\ g_R(\boldsymbol{y})]^T$

can be obtained by solving periodic problems on certain domains. The presentation will be kept more informal than before.

A computationally cheap option to obtain $g(\boldsymbol{y})$ is given by

$$g_L(\boldsymbol{y}) = \psi^{(-K)}(a_L), \qquad g_R(\boldsymbol{y}) = \psi^{(K+1)}(a_R), \tag{5.10}$$

where $\psi^{(-K)}$ and $\psi^{(K+1)}$ are the fields from the Cauchy–Born approximations in the cells Q_{-K}, respectively, Q_{K+1}. These two cell problems have to be solved in any case to compute the energy of the continuum part. This particular choice of $g(\boldsymbol{y})$ would therefore not cause additional computational costs.

More generally, for $J \in \mathbb{N}_0$ we define the computational cell

$$Q_J^R = \big(y_{K-J}, 2a_R - y_{K-J}\big).$$

For $J = 0$ this is just the cell Q_{K+1}. We will see that the magnitude of J is unimportant for the consistency of the method, but J does enter the stability analysis.

Let us introduce the linear operator $\boldsymbol{\eta} : \mathbb{R}^{\mathbb{Z}} \to \mathbb{R}^{\mathbb{Z}}$ mapping $\boldsymbol{y}$ to $\boldsymbol{\eta}(\boldsymbol{y}) = (\eta_j(\boldsymbol{y}))_{j\in\mathbb{Z}}$. We define the components

$$\eta_{K-J}(\boldsymbol{y}) = y_{K-J}, \quad \ldots, \quad \eta_{K+1}(\boldsymbol{y}) = y_{K+1},$$

and (see Figure 5.2)

$$\eta_{K+2}(\boldsymbol{y}) = 2a_R(\boldsymbol{y}) - y_{K-1}, \quad \ldots, \quad \eta_{K+J+1}(\boldsymbol{y}) = 2a_R(\boldsymbol{y}) - y_{K-J}.$$

Note that the components $\eta_{K+2}(\boldsymbol{y})$, ... , $\eta_{K+J+1}(\boldsymbol{y})$ are mirror images of the coordinates $\eta_{K-1}(\boldsymbol{y})$, ... , $\eta_{K-J}(\boldsymbol{y})$ across $a_R(\boldsymbol{y})$.

Next, we define the missing components of $\boldsymbol{\eta}(\boldsymbol{y})$ by periodic extension:

$$\eta_{K+(2J+2)\nu+j}(\boldsymbol{y}) = \eta_{K+j}(\boldsymbol{y}) + \nu|Q_J^R| \quad \forall j \in \{-J, \ldots, J+1\}, \ \ \forall \nu \in \mathbb{Z}.$$

The boundary condition $g_R(\boldsymbol{y})$ is now obtained by solving the periodic problem

$$-\varepsilon^2\Delta\widetilde{\psi}_R + m^2\widetilde{\psi}_R = \rho_{\boldsymbol{\eta}(\boldsymbol{y})} \quad \text{in } Q_J^R$$

or, equivalently,

$$-\varepsilon^2\Delta\widetilde{\psi}_R + m^2\widetilde{\psi}_R = \rho_{\boldsymbol{\eta}(\boldsymbol{y})} \quad \text{in } \mathbb{R} \tag{5.11}$$ {eq:tildepsi}

and setting

$$g_R(\boldsymbol{y}) = \widetilde{\psi}_R(a_R). \tag{5.12}$$ {psitilde}

The left-hand boundary condition $g_L(\boldsymbol{y})$ is defined analogously. We set $g(\boldsymbol{y}) = [g_L(\boldsymbol{y})\ g_R(\boldsymbol{y})]^T$.

We then define a second Quasicontinuum energy $\mathcal{E}^{\rm qc}(\boldsymbol{y})$ as follows

$$\mathcal{E}^{\rm qc}(\boldsymbol{y}) = \mathcal{E}^{\rm cb}_*(\boldsymbol{y}) + \mathcal{E}^{\rm at}(\boldsymbol{y}), \tag{5.13}$$ {eq:EnergyMethod2}

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

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

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

5.2.1 Consistency Analysis

A crucial difference between the QC energy (5.13) and the energy from Section 5.1 is that now the derivative of the atomistic energy with respect to the boundary conditions in general does not vanish. We therefore have to ensure that the term $D_g\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\rm at})D_{\boldsymbol{y}}g(\boldsymbol{y})\cdot\boldsymbol{u}$ emerging in $D\mathcal{E}^{qc}(\boldsymbol{y})$ can still be included in the weak formulation.

Weak Formulation. Let $\boldsymbol{u}\in\mathcal{U}$ be a test vector and $u\in \mathrm{S}_{\#}(\boldsymbol{y})$ an interpolant of $\boldsymbol{u}$. The goal now is to show that

$$D\mathcal{E}^{qc}(\boldsymbol{y})\cdot\boldsymbol{u} = \int_\Omega \sigma^{qc}_{\boldsymbol{y}}(x)\nabla u(x)\,\mathrm{d}x + \int_\Omega \sigma^{qc}_{g(\boldsymbol{y})}\nabla u\,\mathrm{d}x\,, \tag{5.14}$$

{eq:weakformQCM2}

where

$$\sigma^{qc}_{\boldsymbol{y}}(x) = \begin{cases} \sigma^{cb}_{\boldsymbol{y}}(x) & \text{if } x\in\Omega^{\rm cb},\\ \sigma^{\rm at}_{\boldsymbol{y}}(x) & \text{if } x\in\Omega^{\rm at},\end{cases}$$

and $\sigma^{\rm at}_{\boldsymbol{y}}(x)$ is given by (2.8) with $\phi=\phi_{\rm at}$. The additional term $\sigma^{qc}_{g(\boldsymbol{y})}$ in (5.14) satisfies

$$\big\|\sigma^{qc}_{g(\boldsymbol{y})}\big\|_{L^\infty} \le C\big|g(\boldsymbol{y})-g^*(\boldsymbol{y})\big|, \tag{5.15}$$

{eq:boundonsigmaqcg

where C depends on $m\min\boldsymbol{y}'$ and $\max\boldsymbol{y}'$.

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

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

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

$$D_{\boldsymbol{y}_{\rm at}}\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\rm at})\cdot\boldsymbol{u}_{\rm at} + D_a\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\rm at})\cdot a(\boldsymbol{u}) = \int_{\Omega^{\rm at}} \sigma^{\rm at}_{\boldsymbol{y}}(x)\nabla u(x)\,\mathrm{d}x\,, \tag{5.16}$$

{eq:firstTermQC2}

where $\sigma^{\rm at}_{\boldsymbol{y}}(x)$ is given by (2.8) with $\phi=\phi_{\rm at}$.

Next, we turn our attention to the term $D_g\mathcal{E}_{a(\boldsymbol{y}),g(\boldsymbol{y})}(\boldsymbol{y}_{\rm at})\cdot D_{\boldsymbol{y}}g(\boldsymbol{y})\cdot\boldsymbol{u}_{\rm at}$ and start by considering $D_{\boldsymbol{y}}g_R(\boldsymbol{y})\cdot\boldsymbol{u}$. Going back to Remark 3.6 we recall that

$$\begin{aligned} g^*_R(\boldsymbol{y}) = \gamma_R(\boldsymbol{y}) + \mathcal{O}(\tau) &= \frac{1}{m}\int_\Omega \sum_{j=-K}^{K} \delta_\varepsilon(x-y_j)\mathrm{e}^{-\frac{m}{\varepsilon}(a_R(\boldsymbol{y})-x)}\,\mathrm{d}x + \mathcal{O}(\tau)\\ &= \frac{\mu}{m}\sum_{j=0}^{\infty}\mathrm{e}^{-\frac{m}{2\varepsilon}(y_K+y_{K+1}-2y_{K-j})} + \mathcal{O}(\tau). \end{aligned} \tag{5.17}$$

{eq:method2g*}

Here, we have extended the sum to infinity for convenience. This gives rise to an additional error of order $\mathcal{O}(\tau)$. Since we still assume that the atomistic domain $\Omega^{\rm at} = \big(a_L(\boldsymbol{y}), a_R(\boldsymbol{y})\big)$ is large, the error thus incurred is small. Similarly, it follows from (5.11) that the definition (5.12) of $g_R(\boldsymbol{y})$ is equivalent to

$$g_R(\boldsymbol{y}) = \frac{\mu}{m}\sum_{j=0}^{\infty}\mathrm{e}^{-\frac{m}{2\varepsilon}(y_K+y_{K+1}-2\eta_{K-j}(\boldsymbol{y}))}. \tag{5.18}$$

{eq:gofbymethod2}

Depending on the properties of $\boldsymbol{y}$ we have $g(\boldsymbol{y}) \approx g^*(\boldsymbol{y})$ but g only depends on $2J+4$ entries of $\boldsymbol{y}$ whereas g^* depends on $\{y_{-K-1}, \dots, y_{K+1}\}$. We note that $\eta_{K-j}(\boldsymbol{y})$ can, for $j \in \mathbb{N}_0$, be expressed in the form

$$\eta_{K-j}(\boldsymbol{y}) = y_K - \varepsilon \sum_{i=0}^{J} k_i^{(j)} y'_{K+1-i},$$

where

$$k_i^{(j)} \in \mathbb{N}_0 \quad \text{for all } i \in \{0, \dots, J\} \text{ and all } j \in \mathbb{N}_0, \quad \text{and } \sum_{i=0}^{J} k_i^{(j)} = j.$$

In words: the distance between $\eta_{K-j}(\boldsymbol{y})$ and y_K is the sum of multiples of the distances $y_{K+1-J} - y_{K-J}, \dots, y_{K+1} - y_K$. This is a direct consequence of the definition of $\boldsymbol{\eta}(\boldsymbol{y})$ in terms of reflection and periodization. Differentiating (5.18) then leads to

$$\begin{aligned} D_{\boldsymbol{y}} g_R(\boldsymbol{y}) \cdot \boldsymbol{u} &= \frac{-\mu}{2} \sum_{j=0}^{\infty} \mathrm{e}^{-\frac{m}{2\varepsilon}(y_K + y_{K+1} - 2\eta_{K-j}(\boldsymbol{y}))} \frac{u_K + u_{K+1} - 2\eta_{K-j}(\boldsymbol{u})}{\varepsilon} \\ &= \frac{-\mu}{2} \sum_{j=0}^{\infty} \mathrm{e}^{-\frac{m}{2\varepsilon}(y_K + y_{K+1} - 2\eta_{K-j}(\boldsymbol{y}))} \Big(u'_{K+1} + 2 \sum_{i=0}^{J} k_i^{(j)} u'_{K+1-i} \Big) \\ &= \frac{-\mu}{2} \sum_{i=0}^{J} \sum_{j=0}^{\infty} \mathrm{e}^{-\frac{m}{2\varepsilon}(y_K + y_{K+1} - 2\eta_{K-j}(\boldsymbol{y}))} \Big(\tfrac{1}{J+1} u'_{K+1} + 2 k_i^{(j)} u'_{K+1-i} \Big) \\ &= \sum_{i=0}^{J} \mu^R_{K+1-i}(\boldsymbol{y}) u'_{K+1-i}. \end{aligned} \tag{5.19}$$

{eq:Dbygcalculation

Here, we have defined

$$\mu^R_{K+1-i}(\boldsymbol{y}) = -\frac{\mu}{2} \sum_{j=0}^{\infty} \mathrm{e}^{-\frac{m}{2\varepsilon}(y_K + y_{K+1} - 2\eta_{K-j}(\boldsymbol{y}))} \Big(2k_i^{(j)} + \delta_{i,0} \tfrac{1}{J+1} \Big) \quad \forall j \in \{0, \dots, J\}.$$

It is clear from their definition that $k_i^{(j)} \le j$ for all $i \in \{0, \dots, J\}$ and all $j \in \mathbb{N}_0$. Thus, we get the following bound for $\mu^R_{K+1-i}(\boldsymbol{y})$:

$$\begin{aligned} |\mu^R_{K+1-i}(\boldsymbol{y})| &= \left| \frac{\mu}{2} \sum_{j=0}^{\infty} \mathrm{e}^{-\frac{m}{2\varepsilon}(y_K + y_{K+1} - 2\eta_{K-j}(\boldsymbol{y}))} \Big(2k_i^{(j)} + \delta_{i,0} \tfrac{1}{J+1} \Big) \right| \\ &\le \frac{\mu}{2} \sum_{j=0}^{\infty} (2j+1) \mathrm{e}^{-m(j+1/2) \min \boldsymbol{y}'}. \end{aligned} \tag{5.20}$$

{eq:mudefo}

Similar considerations can be carried out at the left-hand boundary for $g_L(\boldsymbol{y})$.

We recall from Lemma 3.5 that (for $\tau \approx 0$)

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

Multiplying this with (5.19) we deduce that the contribution to $D\mathcal{E}^{qc}(\boldsymbol{y})$ from the boundary data takes the form

$$D_g \mathcal{E}_{a(\boldsymbol{y}), g(\boldsymbol{y})}(\boldsymbol{y}_{\mathrm{at}}) \cdot D_{\boldsymbol{y}} g(\boldsymbol{y}) \cdot \boldsymbol{u} = \int_\Omega \sigma^{\mathrm{qc}}_{g(\boldsymbol{y})}(x) \nabla u(x) \, \mathrm{d}x + \mathcal{O}(\tau), \tag{5.21}$$

{eq:extraTermQC2}

where the additional stress function $\sigma^{\rm qc}_{g(\boldsymbol{y})}$ is piecewise constant and nonzero in neighbourhoods of the atomistic/continuum interface $\partial\Omega^{\rm at}$:

$$\sigma^{\rm qc}_{g(\boldsymbol{y})}(x) = \begin{cases} y_i' m\mu_i^L(\boldsymbol{y})\big(g_L^*(\boldsymbol{y}) - g_L(\boldsymbol{y})\big) & \text{if } x \in Q_i, \quad i \in \{-K,\dots,-K+J\}, \\ y_i' m\mu_i^R(\boldsymbol{y})\big(g_R^*(\boldsymbol{y}) - g_R(\boldsymbol{y})\big) & \text{if } x \in Q_i, \quad i \in \{K-J+1,\dots,K+1\}, \\ 0, & \text{otherwise.} \end{cases}$$

Here, we have used that $u_i' = y_i' \nabla u|_{Q_i}$. Adding (5.16) and (5.21) completes the proof of (5.14). The L^∞-bound (5.15) follows immediately from (5.20) and the definition of $\sigma^{\rm qc}_{g(\boldsymbol{y})}(x)$.

Consistency. As in Lemma 5.2 the consistency proof for given $\boldsymbol{y} \in \mathcal{Y}$ consists in finding an appropriate bound on $\|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y}}^{qc}\|_{L^\infty(\Omega)}$. In the atomistic region $\Omega^{\rm at}$ we therefore need to estimate the errors $\|\phi - \phi_{\rm at}\|_{L^\infty(\Omega^{\rm at})}$ and $\|\nabla\phi - \nabla\phi_{\rm at}\|_{L^\infty(\Omega^{\rm at})}$. Lemma 3.8 gives

$$\begin{aligned} \|\phi - \phi_{\rm at}\|_{L^\infty(\Omega^{\rm at})} + \varepsilon\|\nabla\phi - \nabla\phi_{\rm at}\|_{L^\infty(\Omega^{\rm at})} &\le C\big(|\phi(a_L) - \phi_{\rm at}(a_L)| + |\phi(a_R) - \phi_{\rm at}(a_R)|\big) \\ &= C\big(|\phi(a_L) - g_L(\boldsymbol{y})| + |\phi(a_R) - g_R(\boldsymbol{y})|\big). \end{aligned}$$

Using the definitions of $g_L(\boldsymbol{y})$ and $g_R(\boldsymbol{y})$, and techniques similar to the ones used in the proof of Lemma 4.2 it can be shown that

$$\|\phi - \phi_{\rm at}\|_{L^\infty(\Omega^{\rm at})} + \varepsilon\|\nabla\phi - \nabla\phi_{\rm at}\|_{L^\infty(\Omega^{\rm at})} \le C\big(\varepsilon\|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mM\min\boldsymbol{y}'} + \tau\big)$$

as well as

$$|g(\boldsymbol{y}) - g^*(\boldsymbol{y})| \le C\big(\varepsilon\|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mM\min\boldsymbol{y}'}\big)$$

for $M \in \mathbb{N}$ and $\mathcal{C}_M$ as defined in (5.6). From this we then deduce consistency in the sense that

$$\|\sigma_{\boldsymbol{y}} - \sigma_{\boldsymbol{y}}^{qc}\|_{L^\infty(\Omega)} + \|\sigma^{\rm qc}_{g(\boldsymbol{y})}\|_{L^\infty(\Omega^{\rm at})} \le C\big(\varepsilon\|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)} + \mathrm{e}^{-mM\min\boldsymbol{y}'} + \tau\big).$$

Note that we have used (5.15).

5.2.2 Stability Analysis

The stability analysis for the QC energy (5.13) is slightly more involved than for the method discussed in Section 5.1. Let $\boldsymbol{y} \in \mathcal{Y}$ be given. Our main observation is that for sufficiently large J there exists a constant $C(m\min\boldsymbol{y}', \max\boldsymbol{y}')$ such that

$$D^2\mathcal{E}^{\rm qc}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \ge C(m\min\boldsymbol{y}', \max\boldsymbol{y}')\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon} \qquad \forall \boldsymbol{u} \in \mathcal{U}^{1,2}.$$

Since the continuum part of the energy is the same as in the first method, we only have to look at stability of the atomistic subproblem with the given choice of boundary data. The idea is to write the second derivative of the energy $\mathcal{E}^{\rm at}$ in the form

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

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

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

for all $\boldsymbol{u} \in \mathcal{U}$. Hence, our aim is to show that the difference $\|D^2\mathcal{E}^{\rm at}(\boldsymbol{y}) - D^2\mathcal{E}^{\rm at}_*(\boldsymbol{y})\|$ is sufficiently small not to break stability.

The difference between the energies $\mathcal{E}^{\rm at}(\boldsymbol{y})$ and $\mathcal{E}^{\rm at}_*(\boldsymbol{y})$ only consists in effects from the boundary conditions and we have, by (3.15),

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

This implies that

$$\begin{aligned}\big(D^2\mathcal{E}^{\rm at}(\boldsymbol{y}) - D^2\mathcal{E}^{\rm at}_*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}] = m\varepsilon\big(g(\boldsymbol{y}) - g^*(\boldsymbol{y})\big)^T\big[\big(D^2g(\boldsymbol{y}) - D^2g^*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}]\big]\\ + 2m\varepsilon\big|\big(Dg(\boldsymbol{y}) - Dg^*(\boldsymbol{y})\big)\cdot\boldsymbol{u}\big|^2 + \mathcal{O}(\tau).\end{aligned} \tag{5.22}$$ {eq:D2EmD2E}

We will show that $\varepsilon\big|\big(D^2g(\boldsymbol{y}) - D^2g^*(\boldsymbol{y})\big)\cdot[\boldsymbol{u},\boldsymbol{u}]\big|$ is bounded so that the first term on the right-hand side is bounded by $C\big|g(\boldsymbol{y}) - g^*(\boldsymbol{y})\big|$. The second term, $2m\varepsilon\big|(Dg(\boldsymbol{y}) - Dg^*(\boldsymbol{y}))\cdot\boldsymbol{u}\big|$, is positive for all $\boldsymbol{u}\in\mathcal{U}$ and therefore does not affect the positive definiteness of $D^2\mathcal{E}^{\rm at}(\boldsymbol{y})$. If, however, two energies $\mathcal{E}_1$ and $\mathcal{E}_2$ generating a purely repulsive, respectively, a purely attractive interaction are combined to obtain a Morse-like interaction potential, then these terms $\big|(Dg(\boldsymbol{y}) - Dg^*(\boldsymbol{y}))\cdot\boldsymbol{u}\big|$ are relevant for the overall stability analysis. For this reason we provide a bound below. We show that $\big|(Dg(\boldsymbol{y}) - Dg^*(\boldsymbol{y}))\cdot\boldsymbol{u}\big|$ decreases as the sizes of the cells Q^L_J, Q^R_J, on which the boundary conditions $g(\boldsymbol{y})$ are computed, increases.

First, we address the first term on the right-hand side of (5.22). Differentiating gives

$$\begin{aligned}D^2g^*_R(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] &= \frac{m\mu}{4}\sum_{j=0}^{\infty}\mathrm{e}^{-\frac{m}{2\varepsilon}(y_K+y_{K+1}-2y_{K-j})}\left(\frac{u_K+u_{K+1}-2u_{K-j}}{\varepsilon}\right)^2\\ &= \frac{m\mu}{4}\sum_{j=0}^{\infty}\mathrm{e}^{-\frac{m}{2\varepsilon}(y_K+y_{K+1}-2y_{K-j})}\left(u'_{K+1} - 2\sum_{i=0}^{j}u'_{K-j}\right)^2\end{aligned}$$

and, similarly,

$$D^2g_R(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] = \frac{m\mu}{4}\sum_{j=0}^{\infty}\mathrm{e}^{-\frac{m}{2\varepsilon}(y_K+y_{K+1}-2\eta_{K-j}(\boldsymbol{y}))}\left(u'_{K+1} - 2\sum_{i=0}^{J}k_i^{(j)}u'_{K+1-j}\right)^2.$$

A calculation very similar to the one given in the proof of Lemma 5.3 leads to

$$\varepsilon\big(\big|D^2g_R(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}]\big| + \big|D^2g^*_R(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}]\big|\big) \le C(m\min\boldsymbol{y}')\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon},$$

which implies, for the first term on the right-hand side of (5.22)

$$m\varepsilon\big|\big(g(\boldsymbol{y}) - g^*(\boldsymbol{y})\big)^T\big(D^2(g(\boldsymbol{y}) - g^*(\boldsymbol{y}))\cdot[\boldsymbol{u},\boldsymbol{u}]\big)\big| \le C(m\min\boldsymbol{y}')\big|g(\boldsymbol{y}) - g^*(\boldsymbol{y})\big|\|\boldsymbol{u}'\|^2_{\ell^2_\varepsilon}$$

for all $\boldsymbol{u}\in\mathcal{U}$.

Now we analyze the second term $2m\varepsilon\big(D_{\boldsymbol{y}}(g(\boldsymbol{y}) - g^*(\boldsymbol{y}))\cdot\boldsymbol{u}\big)^2$ on the right-hand side of (5.22). We recall from (5.17), respectively, (5.18) that

$$\begin{aligned}Dg_R(\boldsymbol{y})\cdot\boldsymbol{u} &= \frac{-\mu}{2}\sum_{j=0}^{\infty}\mathrm{e}^{-\frac{m}{2\varepsilon}(y_K+y_{K+1}-2\eta_{K-j}(\boldsymbol{y}))}\frac{u_K+u_{K+1}-2\eta_{K-j}(\boldsymbol{u})}{\varepsilon},\\ Dg^*_R(\boldsymbol{y})\cdot\boldsymbol{u} &= \frac{-\mu}{2}\sum_{j=0}^{\infty}\mathrm{e}^{-\frac{m}{2\varepsilon}(y_K+y_{K+1}-2y_{K-j})}\frac{u_K+u_{K+1}-2u_{K-j}}{\varepsilon}.\end{aligned}$$

As a direct result of the construction of $\boldsymbol{\eta}$ the first $J+1$ terms in the above sums are equal. A quick calculation then shows that

$$\varepsilon\big|\big(Dg(\boldsymbol{y}) - Dg^*(\boldsymbol{y})\big)\cdot\boldsymbol{u}\big|^2 \le C(m\min\boldsymbol{y}')\mathrm{e}^{-m(2J+1)\min\boldsymbol{y}'}\|\boldsymbol{u}'\|_{\ell^2_\varepsilon}^2.$$

Summarizing, we have shown that

$$\big\|D^2\mathcal{E}^{\mathrm{at}}(\boldsymbol{y}) - D^2\mathcal{E}^{\mathrm{at}}_*(\boldsymbol{y})\big\| \le C(m\min\boldsymbol{y}')\big(|g(\boldsymbol{y}) - g^*(\boldsymbol{y})| + \mathrm{e}^{-m(2J+1)\min\boldsymbol{y}'}\big),$$

from which we deduce that

$$D^2\mathcal{E}^{\mathrm{qc}}(\boldsymbol{y})\cdot[\boldsymbol{u},\boldsymbol{u}] \ge C(m\min\boldsymbol{y}')\|\boldsymbol{u}'\|_{\ell^2_\varepsilon}^2 \quad \forall\boldsymbol{u}\in\mathcal{U}^{1,2}$$

for sufficiently small $\|\boldsymbol{y}''\|_{\ell^\infty(\mathcal{C}_M)}$ and sufficiently large M and J.

A convergence result analogous to Theorem 5.7 can be proven using the same techniques based on the Implicit Function Theorem.

6 Conclusions and Outlook

{sec:SM_Outlook}

In this article we have presented a rigorous analysis of a particular way of Quasicontinuum like coupling for a linear, field-based interaction potential in one space dimension. The starting point for the design of coupling methods was a weak formulation of the forces arising from the atomistic model. This provided a natural connection point to the corresponding continuum model. We believe that the present work in a comparably simple setting addresses several important questions relevant for QC coupling in the presence of fields: most prominently the dependence of minimization problems on the boundary and boundary data.

We close the article with some comments on open questions. This model being evidently basic from the outset, there is a lot of scope for further work.

For the two QC methods we discussed we chose $\boldsymbol{y}$-dependent boundaries $a(\boldsymbol{y})$ of the atomistic subdomain Ω^{at}. In other words we fixed the position of the boundary in the Lagrange picture. This lead to very convenient weak formulations of $D\mathcal{E}^{qc}(\boldsymbol{y})$. An obvious alternative (particularly relevant for higher dimensions) is the choice of $\boldsymbol{y}$-independent a. We note that this, however, comes with additional technical difficulties. Let $\boldsymbol{y}\in\mathcal{Y}$ and assume that $y_{-K-1} < a_L < y_{-K}$. Then, the Cauchy–Born energy of the interval (y_{-K-1}, a_L) in the continuum region Ω^{cb} is given by

$$-\int_{y_{-K-1}}^{a_L}\big(\tfrac12\varepsilon^2|\nabla\psi^{(-K)}|^2 + \tfrac12 m^2(\psi^{(-K)})^2 - \rho_{\boldsymbol{y}}\psi^{(-K)}\big)\,\mathrm{d}x$$
$$= \frac12\int_{y_{-K-1}}^{a_L}\rho_{\boldsymbol{y}}\psi^{(-K)}\,\mathrm{d}x - \frac{\varepsilon^2}{2}\psi^{(-K)}(a_L)\nabla\psi^{(-K)}(a_L),$$

where $\psi^{(-K)}$ is the Cauchy–Born field on the cell Q_{-K}. To calculate the derivative of this energy contribution, it is hence necessary to know $D_{a_L}\psi^{(-K)}(a_L)$ and $D_{a_L}\nabla\psi^{(-K)}(a_L)$ explicitly and include the resulting terms into the weak formulation of $D\mathcal{E}^{qc}(\boldsymbol{y})$.

It has to be stressed that our analysis heavily utilized explicitly known Green's functions. In particular, the one dimensional setting allowed us to fully understand the dependence of certain minimization problems with respect to the domain and the boundary conditions. Depending on the geometry of the domains Ω and Ω^{at} the construction of Green's functions in higher dimensions might be impossible. More work therefore needs to be done to understand this particular issue in higher dimensions.

Both QC methods we presented were based on boundary conditions on the atomistic subproblem that led to the complete decoupling of the continuum region and the atomistic region. The atomistic energy part $\mathcal{E}^{\text{at}}(\boldsymbol{y})$ only depended on the components $y_{-K-1}, \ldots, y_{K+1}$. In the case of the first method the effect of the boundary conditions $g^*(\boldsymbol{y})$ could elegantly be interpreted as the interaction with mirror atoms outside the atomistic subdomain Ω^{at}. A generalization of this framework to higher dimensions is likely to involve more complicated geometrical constructions, and may even turn out to be impossible.

As described previously, the weak formulation of $D\mathcal{E}(\boldsymbol{y}) \cdot \boldsymbol{u}$ can be derived for more general field-based models even in more than one space dimension. In the case of nonlinear models the analysis needs significant modification because the solution operator for the resulting partial differential equations is not given by a convolution with the Green's function.

A Proofs and Auxiliary Results

Proof of Proposition 2.1. First we note that the map $\boldsymbol{y} \mapsto \rho_{\boldsymbol{y}}(x)$ from $\mathcal{Y}$ to $\mathbb{R}$ is continuously differentiable for all x and $D_{\boldsymbol{y}}\rho_{\boldsymbol{y}}(x)$ is uniformly bounded in x. Since $\Omega = (y_{-N-1}, y_N)$ depends on $\boldsymbol{y}$ but $|\Omega| = 2F$ is fixed, we will only look at the internal atoms represented by $\widetilde{\boldsymbol{y}} = (y_{-N}, \ldots, y_{N-1})$. The derivative with respect to y_N follows from periodicity or by simply shifting Ω to the right by one atom.

For every fixed $\boldsymbol{y} \in \mathcal{Y}$ there is a unique minimizer $\phi(\boldsymbol{y})$ of $I(\cdot, \boldsymbol{y})$ (we are slightly abusing notation here and briefly interpret ϕ as a function from $\mathcal{Y}$ to $H^1_\#(\Omega)$). For every $\boldsymbol{y} \in \mathcal{Y}$ the function $\phi(\boldsymbol{y}) \in H^1_\#(\Omega)$ satisfies the Euler–Lagrange equation $D_\phi I(\phi(\boldsymbol{y}), \boldsymbol{y}) = 0$. Since $D_{\phi\phi} I(\phi, \boldsymbol{y}) = -\varepsilon^2\Delta + m^2\text{id}$ is positive definite for all ϕ and all $\boldsymbol{y}$, the function $\widetilde{\boldsymbol{y}} \mapsto \phi(\boldsymbol{y})$ is differentiable by Theorem 4.B in [37]. We interpret the derivative $D_{\widetilde{\boldsymbol{y}}}\phi(\boldsymbol{y}) = \big(D_{y_{-N}}\phi(\boldsymbol{y}), \ldots, D_{y_{N-1}}\phi(\boldsymbol{y})\big)$ as a vector of $2N$ functions from $H^1_\#(\Omega)$. Using the chain rule we then calculate the derivative $D_{\widetilde{\boldsymbol{y}}}\mathcal{E}(\boldsymbol{y})$ to be

$$D_{\widetilde{\boldsymbol{y}}}\mathcal{E}(\boldsymbol{y}) = D_\phi I(\phi(\boldsymbol{y}), \boldsymbol{y}) D_{\widetilde{\boldsymbol{y}}}\phi(\boldsymbol{y}) + D_{\widetilde{\boldsymbol{y}}} I(\phi(\boldsymbol{y}), \boldsymbol{y}) = D_{\widetilde{\boldsymbol{y}}} I(\phi(\boldsymbol{y}), \boldsymbol{y}).$$

Because ϕ is a minimizer of $I(\cdot, \boldsymbol{y})$ (and therefore $D_\phi I(\phi(\boldsymbol{y}), \boldsymbol{y}) = 0$) to calculate the derivative of $\mathcal{E}$ it is sufficient to calculate the partial derivative of I with respect to $\widetilde{\boldsymbol{y}}$. By uniform differentiability of $\rho_{\boldsymbol{y}}(x)$ with respect to $\boldsymbol{y}$ and continuity of ϕ we can differentiate under the integral sign [31, Theorem 9.42] and arrive at

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

The expression (2.4) for $j = -N, \ldots, N-1$ then follows directly from

$$D_{y_j}\rho_{\boldsymbol{y}}(x) = \varepsilon D_{y_j}\delta_\varepsilon(x - y_j) = -\varepsilon\nabla\delta_\varepsilon(x - y_j)$$

for all $x \in \Omega$. □

Proof of Proposition 2.4. The proof is similar to the one given for Theorem 2.1 in [16]. We start by constructing the solution $\phi_0 : \mathbb{R} \to \mathbb{R}$ to $-\varepsilon^2\Delta\phi_0 + m^2\phi_0 = \rho^c_{\boldsymbol{y}}$ in $\mathbb{R}$ for the compactly supported right-hand side $\rho^c_{\boldsymbol{y}} = \varepsilon\sum_{j=-N}^{N}\delta_\varepsilon(\cdot - y_j) \in C^\infty_0(\mathbb{R})$, i.e., the particle density of the atoms $\{-N, \ldots, N\}$. The periodic solution ϕ will be obtained by adding shifted versions of ϕ_0.

Let $\phi_0 : \mathbb{R} \to \mathbb{R}$ be defined by

$$\phi_0(x) = \int_{\mathbb{R}} G_\varepsilon(z)\rho^c_{\boldsymbol{y}}(x - z)\,\mathrm{d}z. \qquad \text{(A.1)}$$ {eq:phi0defo}

Moreover, let $\delta > 0$ be small. Since $\rho^c_{\boldsymbol{y}} \in C_0^\infty(\mathbb{R})$ and G_ε is continuous we can differentiate under the integral sign [31, Theorem 9.42]:

$$\begin{aligned}\Delta\phi_0(x) &= \int_{\mathbb{R}} G_\varepsilon(z)\Delta\rho^c_{\boldsymbol{y}}(x-z)\,\mathrm{d}z \\ &= \int_{B_\delta(0)} G_\varepsilon(z)\Delta\rho^c_{\boldsymbol{y}}(x-z)\,\mathrm{d}z + \int_{\mathbb{R}\setminus B_\delta(0)} G_\varepsilon(z)\Delta\rho^c_{\boldsymbol{y}}(x-z)\,\mathrm{d}z.\end{aligned}$$

The first term on the right-hand side is $\mathcal{O}(\delta)$ as G_ε is bounded. For the second term we have

$$\begin{aligned}\int_{\mathbb{R}\setminus B_\delta(0)} G_\varepsilon(z)\Delta\rho^c_{\boldsymbol{y}}(x-z)\,\mathrm{d}z = &-\int_{\mathbb{R}\setminus B_\delta(0)} \nabla G_\varepsilon(z)\nabla\rho^c_{\boldsymbol{y}}(x-z)\,\mathrm{d}z \\ &+ G_\varepsilon(\delta)\big(\nabla\rho^c_{\boldsymbol{y}}(x-\delta) - \nabla\rho^c_{\boldsymbol{y}}(x+\delta)\big).\end{aligned}$$

The second term on the right-hand side of this equation is $\mathcal{O}(\delta)$ since $\nabla\rho^c_{\boldsymbol{y}}$ is globally Lipschitz continuous. Continuing with integration by parts yields

$$\begin{aligned}-\int_{\mathbb{R}\setminus B_\delta(0)} \nabla G_\varepsilon(z)\nabla\rho^c_{\boldsymbol{y}}(x-z)\,\mathrm{d}z = &\int_{\mathbb{R}\setminus B_\delta(0)} \Delta G_\varepsilon(z)\rho^c_{\boldsymbol{y}}(x-z)\,\mathrm{d}z \\ &+ \nabla G_\varepsilon(-\delta)\rho^c_{\boldsymbol{y}}(x-\delta) - \nabla G_\varepsilon(\delta)\rho^c_{\boldsymbol{y}}(x+\delta) \\ = &-\frac{m^2}{\varepsilon^2}\phi_0(x) + \frac{1}{\varepsilon^2}\rho^c_{\boldsymbol{y}}(x) + \mathcal{O}(\delta).\end{aligned}$$

Here, we have used that $-\varepsilon^2\Delta G_\varepsilon(x) + m^2 G_\varepsilon(x) = 0$ for $x \neq 0$ and $\nabla G_\varepsilon(\pm\delta) = \mp\frac{1}{2\varepsilon^2}\mathrm{e}^{\mp\frac{m}{\varepsilon}\delta}$. Letting $\delta \to 0$ shows that $-\varepsilon^2\Delta\phi_0 + m^2\phi_0 = \rho^c_{\boldsymbol{y}}$ in $\mathbb{R}$.

Next, we need to construct the $|\Omega|$-periodic solution ϕ. Because of the exponential decay of G_ε it is straightforward to verify that the series

$$\phi(x) = \sum_{j\in\mathbb{Z}} \phi_0(x + j|\Omega|)$$

converges uniformly on every compact subset of $\mathbb{R}$. Moreover, ϕ is Ω-periodic and solves the equation $-\varepsilon^2\Delta\phi + m^2\phi = \rho_{\boldsymbol{y}}$ in Ω. A simple change of coordinates in the integral (A.1) defining ϕ_0 implies (2.11).

Due to the exponential decay of the Green's function we can differentiate under the integral sign to get

$$\nabla\phi(x) = \nabla\int_{\mathbb{R}} \rho_{\boldsymbol{y}}(x-z)G_\varepsilon(z)\,\mathrm{d}z = \int_{\mathbb{R}} \nabla\rho_{\boldsymbol{y}}(x-z)G_\varepsilon(z)\,\mathrm{d}z = \int_{\mathbb{R}} \nabla\rho_{\boldsymbol{y}}(z)G_\varepsilon(x-z)\,\mathrm{d}z$$

for all $x \in \Omega$, which is equivalent to (2.12). □

Proof of Lemma 3.10. In the present 1D setting it is straightforward to determine $G_{\varepsilon,a}$, see for example [16, Chapter 2.2.4]. We have

$$G_{\varepsilon,a}(x,z) = G_\varepsilon(x,z) - H_{\varepsilon,a}(x,z),$$

where, for every fixed x, $H_{\varepsilon,a}(x,\cdot)$ solves the boundary value problem

$$\begin{aligned}-\varepsilon^2\Delta_z H_{\varepsilon,a}(x,\cdot) + m^2 H_{\varepsilon,a}(x,\cdot) &= 0 \quad \text{in } \Omega, \\ H_{\varepsilon,a}(x,a_L) &= G_\varepsilon(a_L - x), \\ H_{\varepsilon,a}(x,a_R) &= G_\varepsilon(a_R - x).\end{aligned}$$

The same ideas that led to formula (3.5) for $\xi_{a,g}$ yield

$$\begin{aligned} H_{\varepsilon,a}(x,z) = & \begin{bmatrix} \mathrm{e}^{-\frac{m}{\varepsilon}(z-a_L)} & \mathrm{e}^{-\frac{m}{\varepsilon}(a_R-z)} \end{bmatrix} \cdot T_a \cdot \begin{bmatrix} \frac{1}{2m\varepsilon}\,\mathrm{e}^{-\frac{m}{\varepsilon}(x-a_L)} \\ \frac{1}{2m\varepsilon}\,\mathrm{e}^{-\frac{m}{\varepsilon}(a_R-x)} \end{bmatrix} \\ = & \frac{1}{2m\varepsilon}\frac{1}{1-\tau^2}\big(\mathrm{e}^{-\frac{m}{\varepsilon}(x+z-2a_L)} + \mathrm{e}^{-\frac{m}{\varepsilon}(2a_R-x-z)} \\ & \qquad - \tau\mathrm{e}^{-\frac{m}{\varepsilon}(x-z+a_R-a_L)} - \tau\mathrm{e}^{-\frac{m}{\varepsilon}(z-x+a_R-a_L)}\big). \end{aligned}$$

It follows immediately from its definition that $H_{\varepsilon,a}$ satisfies

$$-\varepsilon^2\Delta_x H_{\varepsilon,a}(\cdot,z) + m^2 H_{\varepsilon,a}(\cdot,z) = 0$$

in Ω_a for all fixed z. The proof of Proposition 2.4 can then easily be generalized to show that the function ζ defined by

$$\zeta(x) = \int_{\Omega_a} \big(G_\varepsilon(x,z) - H_{\varepsilon,a}(x,z)\big)\rho_{\boldsymbol{y}}(z)\,\mathrm{d}z$$

for $x \in \Omega_a$ satisfies $-\varepsilon^2\Delta\zeta + m^2\zeta = \rho_{\boldsymbol{y}}$ in Ω_a. It remains to show that ζ attains the appropriate values on the boundary $\partial\Omega_a$. We note that

$$\begin{aligned} H_{\varepsilon,a}(a_R,z) &= \frac{1}{2m\varepsilon}\frac{1}{1-\tau^2}\big(\tau\mathrm{e}^{-\frac{m}{\varepsilon}(z-a_L)} + \mathrm{e}^{-\frac{m}{\varepsilon}(a_R-z)} - \tau^2\mathrm{e}^{-\frac{m}{\varepsilon}(a_R-z)} - \tau\mathrm{e}^{-\frac{m}{\varepsilon}(z-a_L)}\big) \\ &= \frac{1}{2m\varepsilon}\,\mathrm{e}^{-\frac{m}{\varepsilon}(a_R-z)}. \end{aligned}$$

With $G_\varepsilon(a_R,z) = \frac{1}{2m\varepsilon}\,\mathrm{e}^{-\frac{m}{\varepsilon}(a_R-z)}$ this implies $G_{\varepsilon,a}(a_R,z) = 0$. Similarly we get $G_{\varepsilon,a}(a_L,z) = 0$. Therefore, $\zeta(a_R) = 0$ and $\zeta(a_L) = 0$ and we conclude that $\phi_0 = \zeta$. □

We state a useful, general existence result from [27, 28]. This represents a practical version of the Inverse Function Theorem.

Lemma A.1. *Let X, Y be Banach spaces, A an open subset of X, and let $\mathcal{F} : A \to Y$ be Fréchet differentiable. Suppose that $x_0 \in A$ satisfies the conditions*

$$\begin{aligned} \|\mathcal{F}(x_0)\|_Y &\le \eta, \\ \big\|D\mathcal{F}(x_0)^{-1}\big\|_{\mathrm{Lin}(X,Y)} &\le \vartheta, \\ \overline{B_{2\eta\vartheta}(x_0)} &\subset A, \\ \|D\mathcal{F}(x_1) - D\mathcal{F}(x_2)\|_{\mathrm{Lin}(X,Y)} &\le L\|x_1 - x_2\|_X \quad \text{for } \ \|x_i - x_0\|_X \le 2\eta\vartheta, \\ 2L\vartheta^2\eta &< 1. \end{aligned}$$

Then, there exists $x \in X$ such that $\mathcal{F}(x) = 0$ and $\|x - x_0\| \le 2\eta\vartheta$. □ {Lemma:Christoph}

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