ANALYSIS OF A ONE-DIMENSIONAL NONLOCAL QUASICONTINUUM METHOD

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Abstract. The accuracy of the quasicontinuum method is analyzed using a series of models with increasing complexity. It is demonstrated that the existence of the ghost force may lead to large errors. It is also shown that the ghost force removal strategy proposed by E, Lu and Yang leads to a version of the quasicontinuum method with uniform accuracy.

Key words. Quasicontinuum method, ghost force, geometrically consistent scheme

AMS subject classifications. 65N12, 65N06, 74G20, 74G15

1. Introduction. The quasicontinuum (QC) method [33] is among the most successful multiscale methods for modeling the mechanical deformation of crystalline solids. It is designed to deal with situations when the crystal is undergoing mostly elastic deformation except at isolated regions with defects. The QC method is usually formulated as an adaptive finite element method. But instead of relying on a continuum model, the QC method is based on an atomistic model. Its main ingredients are: adaptive selection of representative atoms (rep-atoms), with fewer atoms selected in regions with smooth deformation; division of the whole sample into local and nonlocal regions, with the defects covered by the nonlocal regions; and the application of the Cauchy-Born (CB) approximation in the local region as a device for reducing the complexity involved in computing the total energy of the system.

The quasicontinuum method has several distinct advantages. First of all, it has a reasonably simple formulation. In fact, it can be considered as a natural extension of adaptive finite element methods in which one simply uses the atomistic model where the mesh is refined to the atomic scale. Secondly, in the QC method, the treatment in different regions is based on the same model, the atomistic model, with the additional Cauchy-Born approximation used in the local region. For this reason, it is also considered to be more seamless than methods that are based on an explicit coupling between continuum and atomistic models. We refer to the review articles [6, 21] for a discussion of methods that are based on explicitly coupling atomistic and continuum models.

However, this does not mean that the QC method is free of the problems that one encounters when formulating coupled atomistic-continuum methodologies. In some sense, one may also regard the QC method as an example of such a strategy, with the local region playing the role of the continuum region, and the Cauchy-Born nonlinear elasticity model playing the role of the continuum model. In particular, the issue of consistency between the continuum and atomistic models across the coupling interface is very much manifested in the accuracy at the local-nonlocal interface for the QC method. This is the issue we will focus on in this paper. In fact, even though the atomistic models are used in both the local and the nonlocal regions, the Cauchy-Born approximation made in the local regions means that the effective model in this

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region is a nearest neighbor model for the rep-atoms, whereas the atomistic model itself generally involves non-nearest neighbor interactions (hence for the term *local* and *nonlocal* regions). This disparity creates problems at the local-nonlocal interface.

From the general perspective of multiscale, multi-physics modeling, particularly the issue of consistency between continuum and atomistic models across the continuum atomistic interface, the QC method provides the simplest example for understanding such issues. It is now well-known that the inconsistency between the local and nonlocal regions is manifested in the existence of the so-called ghost forces, which are the forces that the atoms experience at their equilibrium positions. We will demonstrate that the ghost force may lead to finite size error of the gradient of the solution. We will also show that the ghost force removal strategy proposed in [7] does result in a version of the QC method that is uniformly accurate across the interface.

Two ways of removing the ghost force have been proposed. The simplest way is to correct the forces by adding or subtracting some "deadload" [28]. This is called "force-based correction". This is easy to implement since one only needs to calculate the magnitude of the ghost forces and substrate them from the system as a correction. Dobson and Luskin [4] have shown the convergence of the iterations for this version of QC. Explicit error estimates can be found in [24].

In this study we will focus on another approach for removing the ghost forces, the geometrically consistent scheme [7]. This scheme depends only on the lattice structure of the system and works for all existing empirical potentials with arbitrary interaction range. It generalizes the quasi-nonlocal approach proposed earlier [29]. We will prove uniformly first order accuracy for the QC method that satisfies the geometrically consistent condition. We will focus primarily on one-dimensional models. This is because a lot of insight can already be gained by studying such models. It is possible to extend the results presented in this paper to high dimensional case with planar local-nonlocal interfaces, and we will outline the ideas for such an extension later. However, doing a good job of that requires a substantial amount of more work. Therefore we will postpone a detailed discussion of the high dimensional results to a later publication.

Since we are primarily interested in the error induced at the local-nonlocal interface, we will assume that every atom is a rep-atom. To understand the QC method fully, we also need to study the coarsening process, in particular the transition between the atom-based and element-based summation rules. There, the presence of corners seems to present some real difficulty, as was pointed out in [7].

The paper is organized as follows. In § 2, we give a brief review of the QC method. In § 3, we demonstrate the existence of the"ghost force" and its consequences. In § 4, we introduce the existing strategies for ghost forces removal and in § 5, we present detailed analysis of the geometrically consistent schemes. Conclusions are drawn in the last section. Some omitted proofs of § 3 are given in the Appendix.

2. Review of the Quasicontinuum Method. We start with a brief review of the QC method. The main objective of the QC method is to systematically coarsen an atomistic description by a judicious introduction of kinematic constraints. These kinematic constraints are selected and designed so as to preserve full atomistic resolution where required, e.g., in the vicinity of lattice defects, and to treat collectively large numbers of atoms in regions where the deformation field varies slowly on the scale of the lattice. The essential building blocks are: i) a reduced representation of the solid using rep-atoms; ii) the use of summation rules in order to efficiently compute the total energy of the system; iii) and the use of adaptive criteria in order to tailor the computational mesh to the structure of the deformation field.

The method starts with an underlying atomistic model of the material which is considered to be accurate. In principle, this atomistic model can be a quantum-mechanically based description such as a tight-binding model or models based on the density functional theory [14], but in the present paper we will focus on atomistic models using empirical potentials.

We will denote by $\boldsymbol{y}_i$ and $\boldsymbol{x}_i$ the positions of the i-th atom in the deformed and undeformed configurations, respectively. For simple crystalline solids, the undeformed state can be represented as the collection of points with the form

$$\boldsymbol{x} = n_1\boldsymbol{A}_1 + n_2\boldsymbol{A}_2 + n_3\boldsymbol{A}_3,$$

where $\boldsymbol{A}_1$, $\boldsymbol{A}_2$ and $\boldsymbol{A}_3$ are the basis vectors, and n_1, n_2 and n_3 are integers. The displacement vector for the i-th atom is defined as

$$\boldsymbol{u}_i = \boldsymbol{y}_i - \boldsymbol{x}_i.$$

The total energy of the system can be written as a sum over the energy of each atom

$$E^{\text{tot}}(\boldsymbol{y}) = \sum_{i=1}^{N} E_i(\boldsymbol{y}) = \sum_{i=1}^{N} E_i(\{\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_N\}),$$

where E_i is the energy associated with the i-th atom, which depends on the positions of the other atoms as well, and N is the number of atoms in the solid.

If some external load is applied to the system, the total energy of the system can be written as

$$\Phi(\boldsymbol{y}) = E^{\text{tot}}(\boldsymbol{y}) - \sum_{i=1}^{N} \boldsymbol{f}_i\boldsymbol{y}_i,$$

where $-\boldsymbol{f}_i\boldsymbol{y}_i$ is the work done by the external force $\boldsymbol{f}_i$ on the i-th atom.

The actual displacement of the atoms can in principle be found by minimizing the above total energy functional. In practice, this is often very expensive and uninformative: the computational cost is very large; the information of interest is often buried together with a huge amount of uninteresting data. In the QC method, one makes the observation that in regions where the atomic displacement is rather smooth, there is no need to include every atom as an independent degree of freedom, since the deformation in these regions can be represented with satisfactory accuracy by a much smaller set of rep-atoms. This idea is implemented in the QC method through a set of kinematic constraints–reducing the number of degrees of freedom by introducing rep-atoms and representing the displacement of all other atoms in terms of the displacement of the rep-atoms.

The rep-atoms are usually the vertices of the underlying finite element triangulation. They are selected using an adaptive mesh refinement strategy. Piecewise linear finite elements are used and the mesh size is denoted by h.

The kinematic constraint for the displacement of the atoms is given by

$$\boldsymbol{u}^h(\boldsymbol{x}_i) = \sum_{j=1}^{N_{\text{rep}}} S_j(\boldsymbol{x}_i)\boldsymbol{u}_j,$$

where $S_j(\boldsymbol{x})$ is the basis function associated with the j-th rep-atom, and N_{rep} is the number of rep-atoms. In general, we expect N_{rep} to be much smaller than N.

The total energy of such a system is now a function of the positions (displacement) of the rep-atoms only. However, to compute this energy by direct summation using the original atomistic model still requires visiting all the atoms. The QC method bypasses this by introducing approximate summation rules.

In the QC method, the computational domain is divided into local and nonlocal regions according to the smoothness of the displacement field $\boldsymbol{u}^h$. Inside the nonlocal region where deformation is large, all the atoms are rep-atoms, hence the energy associated with these atoms can be computed using direct summation. Inside the local region, the total energy is computed by using the Cauchy-Born rule on each element [3]. For simple crystals, the CB rule works as follows (there is a simple generalization to complex crystals, see [34, 30, 10]). Let $F = \nabla \boldsymbol{u}$ be the deformation gradient tensor of a uniform deformation, and $E_0(F)$ be the energy of the unit cell in a deformed lattice when its lattice vectors are deformed according to F, i.e.,

$$\boldsymbol{a}_i = F\boldsymbol{A}_i.$$

The strain energy density at F is given by

$$W_{\mathrm{CB}}(F) = \frac{E_0(F)}{\Omega_0},$$

where Ω_0 is the volume of the unit cell at the equilibrium state. The total energy associated with an element is simply the energy density evaluated at the deformation gradient F_e associated with the element and multiplied by the volume of the element Ω_e. The total potential energy in the local region is simply the sum of the energies on each element:

$$E^{\mathrm{local}} = \sum_{e=1}^{N_{\mathrm{element}}} \Omega_e W_{\mathrm{CB}}(F_e).$$

The total potential energy of the system for the QC method is the sum of the energy of the local and nonlocal regions:

$$E^{\mathrm{tot}}_{\mathrm{QC}} = E^{\mathrm{local}} + E^{\mathrm{nonlocal}}.$$

This formulation of the summation rule introduces an inconsistency across the local/nonlocal interface: the energy in the local region is computed for each element, whereas the energy in the nonlocal region is naturally computed for each rep-atom. Formally, the energy of the local region can be rewritten as a sum over all the rep-atoms:

$$E^{\mathrm{local}} = \sum_i \omega_i E^{\mathrm{el}}_i,$$

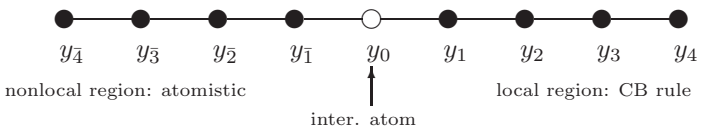
where the energy associated with each local atom is defined as

$$E^{\mathrm{el}}_i = \frac{1}{\omega_i} \sum_e \omega_{i,e} W_{\mathrm{CB}}(F_e),$$

where the weights $\omega_{i,e}$ satisfy $\omega_i = \sum_e \omega_{i,e}$. However, this may introduce inconsistency at the interface where the transition takes place.

An alternative way of approximating the energy is the cluster-based summation rule proposed by Knap and Ortiz [16].

FIG. 3.1. *1D chain*



The error in the QC method comes from two main sources. In the local region the error comes mainly from the kinematic constraint and the CB rule used. This source of error can be understood following the work of E and Ming [8, 9, 10]. More interesting is the error introduced at the interface between the local and nonlocal regions, where "ghost forces" may arise.

3. Ghost Forces.

3.1. Illustration of the ghost force. Consider a one-dimensional chain shown in Fig. 3.1, with a pairwise potential V_0. The first step in the QC method is coarse-graining, i.e., selecting rep-atoms. Since we are focusing on the interface between the continuum and atomistic regions, we will consider the case when every atom is a rep-atom. The first N atoms indexed by $-N, \ldots, -1$ will make up the nonlocal region in which the original atomistic model will be used. The atoms indexed by $1, \ldots, N$ will make up the local region in which the Cauchy-Born continuum model will be used. The atom indexed by 0 separates the two regions. For convenience, we will sometimes use $\bar{i}$ to replace $-i$ as the subscript, and use r_{ij} to denote the distance between the i-th and the j-th atoms.

If the interaction is limited to the nearest neighbor, the CB rule is the same as the atomistic model (direct summation). In this case, there is no ghost force. However, if the interaction range contains the next nearest neighbor, then the energies associated with the atoms near the interface are (in the absence of the external force):

$$
\begin{aligned}
E_{\bar{3}} &= \frac{1}{2}\big(V_0(r_{\bar{5}\bar{3}}) + V_0(r_{\bar{4}\bar{3}}) + V_0(r_{\bar{3}\bar{2}}) + V_0(r_{\bar{3}\bar{1}})\big),\\
E_{\bar{2}} &= \frac{1}{2}\big(V_0(r_{\bar{4}\bar{2}}) + V_0(r_{\bar{3}\bar{2}}) + V_0(r_{\bar{2}\bar{1}}) + V_0(r_{\bar{2}0})\big),\\
E_{\bar{1}} &= \frac{1}{2}\big(V_0(r_{\bar{3}\bar{1}}) + V_0(r_{\bar{2}\bar{1}}) + V_0(r_{\bar{1}0}) + V_0(r_{\bar{1}1})\big),\\
E_0 &= \frac{1}{2}\big(V_0(r_{\bar{2}0}) + V_0(r_{\bar{1}0}) + V_0(r_{01}) + V_0(2r_{01})\big),\\
E_1 &= \frac{1}{2}\big(V_0(2r_{01}) + V_0(r_{01}) + V_0(r_{12}) + V_0(2r_{12})\big),\\
E_2 &= \frac{1}{2}\big(V_0(2r_{12}) + V_0(r_{12}) + V_0(r_{23}) + V_0(2r_{23})\big).
\end{aligned}
$$

Therefore, the forces on the atoms with indices $\bar{1}, 0$ and 1 are given by

$$
\begin{aligned}
f_{\bar{1}} &= -V_0'(r_{\bar{3}\bar{1}}) - V_0'(r_{\bar{2}\bar{1}}) + V_0'(r_{\bar{1}0}) + \frac{1}{2}V_0'(r_{\bar{1}1}),\\
f_0 &= -V_0'(r_{\bar{2}0}) - V_0'(r_{\bar{1}0}) + V_0'(r_{01}) + 2V_0'(2r_{01}),\\
f_1 &= -\frac{1}{2}V_0'(r_{\bar{1}1}) - 2V_0'(2r_{01}) - V_0'(r_{01}) + V_0'(r_{12}) + 2V_0'(2r_{12}).
\end{aligned}
$$

FIG. 3.2. *Ghost force for the original QC solution with V_0 the Lennard-Jones potential*

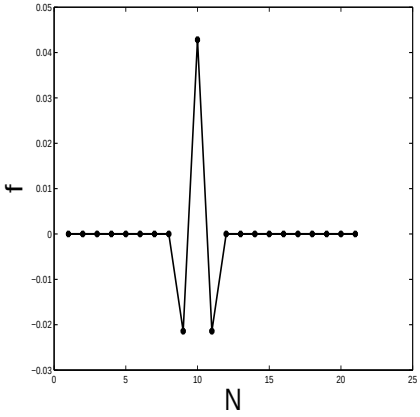
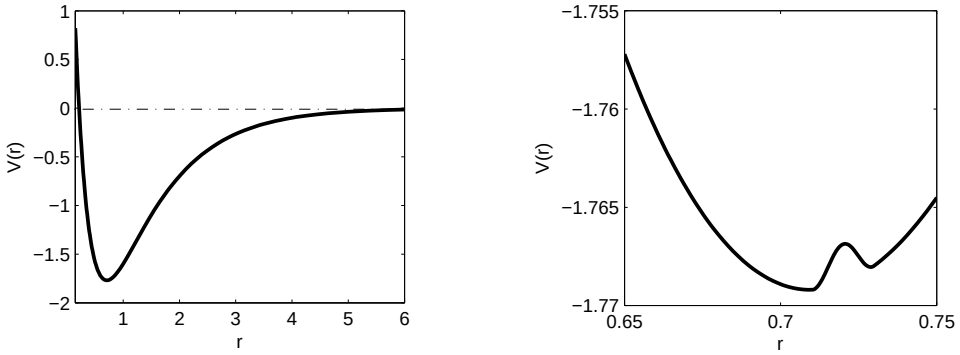


FIG. 3.3. *Conventional (left) and modified (right) Morse potential*



At the equilibrium state, we have

$$f_{\bar{1}} = -\frac{1}{2}V_0'(2\epsilon), \quad f_0 = V_0'(2\epsilon), \quad f_1 = -\frac{1}{2}V_0'(2\epsilon),$$

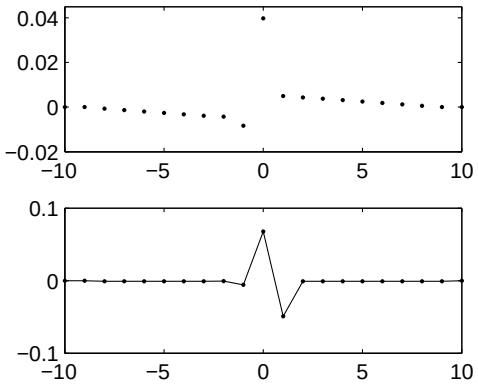
where $\epsilon = x_1 - x_0$ is the equilibrium bond length. We refer to Fig. 3.2 for the demonstration of the ghost force when V_0 is the Lennard-Jones potential [18].

From this example, we see that ghost force arises due to the asymmetry in calculating the energies in the local and nonlocal regions. The energy associated with the atom $\bar{1}$ depends on y_1, but the energy associated with the atom 1 does not depend on $y_{\bar{1}}$.

Next, let us examine the effect of the ghost force. First, let us discuss a simple example. We consider a one-dimensional chain with 21 atoms in total, interacting with the modified Morse-potential (see below) and next nearest neighbor interaction. The atoms are indexed by $-10, \ldots, 10$, where the 0-th atom is the interfacial atom. On the left side, we use the atomistic model. On the right-hand side, we use the Cauchy-Born continuum model. The QC solution $\boldsymbol{y} = (y_{-10}, \ldots, y_{10})$ is a local minimizer of $E^{\rm tot}(\boldsymbol{w})$ subject to the boundary condition

$$w_i = i\epsilon, \quad i = -11, -12, 11,$$

FIG. 3.4. *Displacement (upper) and deformation gradient (lower) of each atom for the original QC*



where $E^{\text{tot}}(\boldsymbol{w})$ is defined as:

$$E^{\text{tot}}(\boldsymbol{w}) = \sum_{i=-11}^{10} V_0(|w_i - w_{i+1}|) + \sum_{i=-12}^{-2} V_0(|w_i - w_{i+2}|) + \frac{1}{2} V_0(|w_{\bar{1}} - w_1|) + \sum_{i=0}^{10} V_0(2|w_i - w_{i+1}|).$$

Here V_0 is a modified *Morse potential* [25] (see Fig. 3.3) defined as:

$$V_0(r) = D_e\Big[e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}\Big] + \delta\Big[\cos\big(100\pi(r-0.72)\big) + 1\Big]$$

for $0.71 < r < 0.73$,

$$V_0(r) = D_e\Big[e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}\Big]$$

for $r \le 0.71$ or $r \ge 0.73$. Here a is a constant with dimension of the reciprocal of distance, and r_e is atomic length scale parameter, D_e is the well depth of the potential, and the parameter a controls the "width" of the potential. We rescale the potential and simply set $r_e = 1.0$, $D_e = 1.0$, and $a = 1.0$. The main feature of the modification is to create a second well for the potential. δ is the parameter that determines the height of the barrier between two wells in the modified Morse potential and is set to be $\delta = 10^{-3}$. The equilibrium distance between neighboring atoms is adjusted to be approximately 0.70965.

Figure 3.4 shows the displacement and the deformation gradient of each atom. One can see that the maximum strain in this particular example is as large as 6.8%, which occurs near the interface (the $\bar{1}$-th atom). Since there is no external force applied to the system, this strain is entirely due to the numerical error introduced by the QC formulation, or equivalently, by the ghost force. Such error may push the system to the basin of attraction of another nearby minimum. Physically, this suggests that it may cause unphysical dislocation nucleation around the tip of a propagating crack [39]. Moreover, we have confirmed that the system will not switch back to the

original state even if we switch the QC formulation back to a full atomistic description. Whether this actually occurs in more realistic simulations is still a subject of debate. But the possibilities are certainly there.

3.2. Explicit solution of the original QC method. In this subsection, we estimate the error caused by the ghost force in the case when there is an external force. For the case when there is no external force, we compute *explicitly* the error, which allows us to see exactly how the error caused by the ghost force looks like. To this end, we assume the interaction potential is harmonic

$$V_0(x_1, x_2) = \frac{1}{2}(x_1 - x_2)^2,$$

and consider the next nearest neighbor interaction. Let ϵ be the equilibrium bond length, we assume that $2N\epsilon = 1$ and $\overline{r} = r/\epsilon$, we rescale the potential as $V(\overline{r}) = V_0(r)$. The atomistic problem is: find the minimizer $\boldsymbol{y}^\epsilon = (y^\epsilon_{N-2}, \ldots, y^\epsilon_{N+2}) \in \mathcal{S}$ that satisfies

$$\boldsymbol{y}^\epsilon = \operatorname*{argmin}_{\boldsymbol{w}\in\mathcal{S}}\{E^{\rm tot}(\boldsymbol{w}) - \langle\, \boldsymbol{f}, \boldsymbol{w}\rangle\}, \tag{3.1}$$

where

$$E^{\rm tot}(\boldsymbol{w}) = \sum_{i=-N-1}^{N} V\left(\left|\frac{w_i - w_{i+1}}{\epsilon}\right|\right) + \sum_{i=-N-2}^{N} V\left(\left|\frac{w_i - w_{i+2}}{\epsilon}\right|\right),$$

$\boldsymbol{f}$ is the external force and $\langle\, \boldsymbol{f}, \boldsymbol{w}\rangle \equiv \sum_{i=-N}^{N} f_i w_i$. The admissible set $\mathcal{S}$ is defined by

$$\mathcal{S} = \{\, \boldsymbol{z} \in \mathbb{R}^{2N+5} \mid z_i = i\epsilon, \quad i = N+1, N+2, -N-1, -N-2\,\}. \tag{3.2}$$

The QC solution $\boldsymbol{y}_{\rm qc} = (y_{-N}, \ldots, y_N)$ is the minimizer that satisfies (3.1) with $E^{\rm tot}(\boldsymbol{w})$ replaced by

$$\begin{aligned} E^{\rm qc}(\boldsymbol{w}) = &\sum_{i=-N-1}^{N} V\left(\left|\frac{w_i - w_{i+1}}{\epsilon}\right|\right) + \sum_{i=-N-2}^{-2} V\left(\left|\frac{w_i - w_{i+2}}{\epsilon}\right|\right) \\ &+ \frac{1}{2}V\left(\left|\frac{w_{\bar{1}} - w_1}{\epsilon}\right|\right) + \sum_{i=0}^{N} V\left(2\left|\frac{w_i - w_{i+1}}{\epsilon}\right|\right). \end{aligned}$$

It is clear to see that $\boldsymbol{y}^\epsilon$ satisfies the Euler-Lagrangian equations:

$$-\frac{\partial E^{\rm tot}}{\partial w_i} = f_i.$$

Using the boundary condition (3.2), we write the above equations as

$$\epsilon^{-2}\left(4y^\epsilon_{-N} - y^\epsilon_{-N+1} - y^\epsilon_{-N+2}\right) = \epsilon^{-2}(x_{-N-1} + x_{-N-2}) + f_{-N} = -(2N+3)/\epsilon + f_{-N}.$$

Similarly,

$$\begin{aligned} \epsilon^{-2}\left(-y^\epsilon_{-N} + 4y^\epsilon_{-N+1} - y^\epsilon_{-N+2} - y^\epsilon_{-N+3}\right) &= \epsilon^{-2}x_{-N-1} + f_{-N+1} \\ &= -(N+1)/\epsilon + f_{-N+1}, \end{aligned}$$

and

$$\epsilon^{-2}\left(4y_N^\epsilon - y_{N-1}^\epsilon - y_{N-2}^\epsilon\right) = (2N+3)/\epsilon + f_N,$$
$$\epsilon^{-2}\left(-y_N^\epsilon + 4y_{N-1}^\epsilon - y_{N-2}^\epsilon - y_{N-3}^\epsilon\right) = (N+1)/\epsilon + f_{N-1}.$$

For $i = -N+3, \ldots, N-2$,

$$\epsilon^{-2}\left(-y_{i-2}^\epsilon - y_{i-1}^\epsilon + 4y_i^\epsilon - y_{i+1}^\epsilon - y_{i+2}^\epsilon\right) = f_i,$$

We can write these equations in a compact form as:

$$\mathcal{B}\boldsymbol{y}^\epsilon = \widehat{\boldsymbol{f}}, \tag{3.3}$$

where

$$\widehat{f}_{-N} = -(2N+3)/\epsilon + f_{-N}, \quad \widehat{f}_{-N+1} = -(N+1)/\epsilon + f_{-N+1},$$
$$\widehat{f}_{N-1} = (N+1)/\epsilon + f_{N-1}, \quad \widehat{f}_N = (2N+3)/\epsilon + f_N,$$
$$\widehat{f}_i = f_i, \quad i = -N+2, \ldots, N-2.$$

Similarly, $\boldsymbol{y}_{\rm qc}$ satisfies the Euler-Lagrangian equations:

$$-\frac{\partial E^{\rm qc}}{\partial w_i} = f_i.$$

Proceeding along the same line that leads to (3.3), we write the above equations as

$$\epsilon^{-2}\left(4y_{-N} - y_{-N+1} - y_{-N+2}\right) = -(2N+3)/\epsilon + f_{-N},$$
$$\epsilon^{-2}\left(-y_{-N} + 4y_{-N+1} - y_{-N+2} - y_{-N+3}\right) = -(N+1)/\epsilon + f_{-N+1},$$

and for $i = -N+3, \ldots, -2$,

$$\epsilon^{-2}\left(-y_{i-2} - y_{i-1} + 4y_i - y_{i+1} - y_{i+2}\right) = f_i.$$

Near the interface, we have

$$\begin{cases} \epsilon^{-2}\left(-y_{\bar{3}} - y_{\bar{2}} + \frac{7}{2}y_{\bar{1}} - y_0 - \frac{1}{2}y_1\right) = f_{\bar{1}}, \\ \epsilon^{-2}\left(-y_{\bar{2}} - y_{\bar{1}} + 7y_0 - 5y_1\right) = f_0, \\ \epsilon^{-2}\left(-\frac{1}{2}y_{\bar{1}} - 5y_0 + \frac{21}{2}y_1 - 5y_2\right) = f_1. \end{cases}$$

For $i = 2, \ldots, N-1$,

$$\epsilon^{-2}\left(-5y_{i-1} + 10y_i - 5y_{i+1}\right) = f_i,$$

and for the boundary atom N,

$$\epsilon^{-2}\left(-5y_{N-1} + 10y_N\right) = (5N+5)/\epsilon + f_N.$$

We may write these equations in a compact form as:

$$\mathcal{A}\boldsymbol{y}_{\rm qc} = \widetilde{\boldsymbol{f}}, \tag{3.4}$$

where $\widetilde{f}_i = \widehat{f}_i$ for $i = -N, \ldots, N-2$ and $\widetilde{f}_{N-1} = f_{N-1}, \widetilde{f}_N = (5N+5)/\epsilon + f_N$. To avoid the influence of the boundary atoms, we change the $(N-1)$-th and the N-th equations of (3.4) to the same with (3.3) and still denote the solution by $\boldsymbol{y}_{\rm qc}$, the equations (3.4) changes to

$$\widehat{\mathcal{A}}\boldsymbol{y}_{\rm qc} = \widehat{\boldsymbol{f}}, \tag{3.5}$$

where

$$\widehat{\mathcal{A}}_{i,j} = \begin{cases} \mathcal{A}_{i,j} & \text{if} \quad i = -N, \ldots, N-2, j = -N, \ldots, N, \\ \mathcal{B}_{i,j} & \text{if} \quad i = N-1, N, j = -N, \ldots, N. \end{cases}$$

THEOREM 3.1. *For $i = -N, \ldots, N-1$,*

$$|D^+(\boldsymbol{y}_{qc} - \boldsymbol{y}^\epsilon)_i| \le C \left(\left| \frac{3-\sqrt{5}}{2} \right|^{|i|} + \epsilon \right) \big(\| \boldsymbol{f} \|_\infty + 1 \big), \tag{3.6}$$

where $\boldsymbol{y}_{qc}$ is the QC solution (3.5) *and $\boldsymbol{y}^\epsilon$ is the solution of the atomistic model* (3.3)*. The forward difference quotient operator D^+ is defined as $D^+ y_i = (y_{i+1} - y_i)/\epsilon$ and $\|\boldsymbol{f}\|_\infty \equiv \max_{-N \le i \le N} |f_i|$.*

We start with the following identity:

$$\mathcal{B}(\boldsymbol{y}_{\rm qc} - \boldsymbol{y}^\epsilon) = \mathcal{B}\boldsymbol{y}_{\rm qc} - \widehat{\boldsymbol{f}} = (\mathcal{B} - \widehat{\mathcal{A}})\boldsymbol{y}_{\rm qc} \equiv \boldsymbol{F}, \tag{3.7}$$

where $\boldsymbol{F} \in \mathbb{R}^{2N+1}$ that is given by

$$\begin{cases} F_i = 0, \quad i = -N, \ldots, \bar{2}, N-1, N, \\ F_{\bar{1}} = -\dfrac{1}{2\epsilon} D^+(y_{\bar{1}} + y_0), \quad F_0 = -(D^+)^2 y_0 + \dfrac{2}{\epsilon} D^+ y_0, \\ F_1 = -\epsilon^2 (D^+)^4 y_{\bar{1}} - \dfrac{1}{2\epsilon} D^+(y_{\bar{1}} + y_0), \quad F_2 = -\epsilon^2 (D^+)^4 y_0, \\ F_i = \dfrac{\epsilon^2}{5} (D^+)^2 f_{i-1}, \quad i = 3, \ldots, N-2. \end{cases}$$

Using (3.7) we obtain the following explicit expression of the error in terms of the Green's difference function [35] that is defined by

$$\mathcal{G} = \epsilon^{-2} \mathcal{B}^{-1}.$$

LEMMA 3.2. *Let $\boldsymbol{y}_{qc}$ and $\boldsymbol{y}^\epsilon$ be the solutions of* (3.5) *and* (3.3)*, respectively, then*

$$\begin{aligned} D^+(\boldsymbol{y}_{qc} - \boldsymbol{y}^\epsilon)_i = & -\frac{\epsilon^4}{5} \sum_{j=1}^{N-3} D_1 D_2 \mathcal{G}_{i,j} D^+ f_j + \frac{\epsilon^3}{5} \big(D_1 \mathcal{G}_{i,N-2} D^+ f_{N-2} - D_1 D_2 \mathcal{G}_{i,0} f_1 \big) \\ & + \epsilon^2 D_1 D_2 \Big[\frac{1}{2} \mathcal{G}_{i,\bar{1}} + \frac{3}{5} \mathcal{G}_{i,0} - \frac{1}{10} \mathcal{G}_{i,1} \Big] D^+(y_0 + y_{\bar{1}}) \\ & - 2\epsilon^2 D_1 D_2 \mathcal{G}_{i,0} D^+ y_0, \end{aligned} \tag{3.8}$$

where $D_1 \mathcal{G}_{i,j} = \epsilon^{-1}(\mathcal{G}_{i+1,j} - \mathcal{G}_{i,j})$ and $D_2 \mathcal{G}_{i,j} = \epsilon^{-1}(\mathcal{G}_{i,j+1} - \mathcal{G}_{i,j})$.

Proof. It is clear to see $y_i - y_i^\epsilon = \epsilon^2 \sum_{j=-N}^{N} \mathcal{G}_{i,j} F_j = \epsilon^2 \sum_{j=\bar{1}}^{N-2} \mathcal{G}_{i,j} F_j$. Summation by parts, we obtain

$$\sum_{j=3}^{N-2} \mathcal{G}_{i,j} F_j = -\frac{\epsilon^2}{5} \sum_{j=3}^{N-3} D_2 \mathcal{G}_{i,j} D^+ f_j + \frac{\epsilon}{5} (\mathcal{G}_{i,N-2} D^+ f_{N-2} - \mathcal{G}_{i,3} D^+ f_2). \tag{3.9}$$

A direct calculation gives

$$\sum_{j=\bar{1}}^{2} F_j = -\epsilon (D^+)^3 y_1, \qquad \sum_{j=\bar{1}}^{1} F_j = -\epsilon (D^+)^3 y_0. \tag{3.10}$$

Using the first identity of (3.10), we get

$$\begin{aligned} \sum_{j=\bar{1}}^{2} \mathcal{G}_{i,j} F_j &= -\epsilon \mathcal{G}_{i,2} (D^+)^3 y_1 + \sum_{j=\bar{1}}^{1} (\mathcal{G}_{i,j} - \mathcal{G}_{i,2}) F_j \\ &= -\epsilon \mathcal{G}_{i,2} (D^+)^3 y_1 - \epsilon D_2 \mathcal{G}_{i,1} (F_{\bar{1}} + F_0 + F_1) \\ &\quad - \epsilon D_2 \mathcal{G}_{i,0} F_0 - \epsilon D_2 (\mathcal{G}_{i,\bar{1}} + \mathcal{G}_{i,0}) F_{\bar{1}}. \end{aligned}$$

Using the second identity of (3.10) and the expressions of $F_{\bar{1}}$ and F_0, we obtain

$$\begin{aligned} \sum_{j=\bar{1}}^{1} (\mathcal{G}_{i,j} - \mathcal{G}_{i,2}) F_j &= \epsilon D_2 \mathcal{G}_{i,1} ((D^+)^2 y_1 - (D^+)^2 y_0) + \epsilon D_2 \mathcal{G}_{i,0} (D^+)^2 y_0 \\ &\quad - 2 D_2 \mathcal{G}_{i,0} D^+ y_0 + (1/2) D_2 (\mathcal{G}_{i,\bar{1}} + \mathcal{G}_{i,0}) D^+ (y_{\bar{1}} + y_0) \\ &= \epsilon D_2 \mathcal{G}_{i,1} (D^+)^2 y_1 - \epsilon^2 D_2^2 \mathcal{G}_{i,0} (D^+)^2 y_0 \\ &\quad - 2 D_2 \mathcal{G}_{i,0} D^+ y_0 + \frac{1}{2} D_2 (\mathcal{G}_{i,\bar{1}} + \mathcal{G}_{i,0}) D^+ (y_{\bar{1}} + y_0). \end{aligned}$$

Using the $(N+3)$-th, $(N+4)$-th and $(N+5)$-th equations of (3.5), we get

$$(D^+)^2 y_1 = -\frac{f_2}{5}, \quad (D^+)^3 y_1 = -\frac{D^+ f_2}{5}, \quad (D^+)^2 y_0 = -\frac{f_1}{5} + \frac{1}{10\epsilon} D^+ (y_{\bar{1}} + y_0),$$

which together with the above equation leads to

$$\begin{aligned} \sum_{j=\bar{1}}^{2} \mathcal{G}_{i,j} F_j &= \frac{\epsilon}{5} \mathcal{G}_{i,2} D^+ f_2 - \frac{\epsilon}{5} D_2 \mathcal{G}_{i,1} f_2 + \frac{\epsilon^2}{5} D_2^2 \mathcal{G}_{i,0} f_1 \\ &\quad - 2 D_2 \mathcal{G}_{i,0} D^+ y_0 + \Big[\frac{1}{2} D_2 (\mathcal{G}_{i,\bar{1}} + \mathcal{G}_{i,0}) - \frac{\epsilon}{10} D_2^2 \mathcal{G}_{i,0} \Big] D^+ (y_{\bar{1}} + y_0). \end{aligned}$$

This equation and (3.9) gives

$$\begin{aligned} y_i - y_i^\epsilon &= -\frac{\epsilon^4}{5} \sum_{j=1}^{N-3} D_2 \mathcal{G}_{i,j} D^+ f_j + \frac{\epsilon^3}{5} \left(\mathcal{G}_{i,N-2} D^+ f_{N-2} - D_2 \mathcal{G}_{i,0} f_1 \right) \\ &\quad + \epsilon^2 D_2 \Big[\frac{1}{2} \mathcal{G}_{i,\bar{1}} + \frac{3}{5} \mathcal{G}_{i,0} - \frac{1}{10} \mathcal{G}_{i,1} \Big] D^+ (y_{\bar{1}} + y_0) + 2\epsilon^2 D_2 \mathcal{G}_{i,0} D^+ y_0. \end{aligned}$$

The identity (3.8) immediately follows from the above equation. □

It remains to bound $\mathcal{G}, D^+y_{\bar{1}}$ and D^+y_0. We estimate D^+y_0 and $D^+y_{\bar{1}}$ in the following lemma and postpone the proof to Appendix B.

LEMMA 3.3. *There exists a constant C such that*

$$|D^+y_0| + |D^+y_{\bar{1}}| \le C(\| \boldsymbol{f} \|_\infty + 1). \tag{3.11}$$

To estimate the Green's difference function $\mathcal{G}$, we resort to its explicit expression that will be given below. By definition, it is clear that for $i = -N+2, \dots, N-2$,

$$\begin{cases} 4\mathcal{G}_{i,-N} - \mathcal{G}_{i,-N+1} - \mathcal{G}_{i,-N+2} = 0, \\ -\mathcal{G}_{i,-N} + 4\mathcal{G}_{i,-N+1} - \mathcal{G}_{i,-N+2} - \mathcal{G}_{i,-N+3} = 0, \\ -\mathcal{G}_{i,j-2} - \mathcal{G}_{i,j-1} + 4\mathcal{G}_{i,j} - \mathcal{G}_{i,j+1} - \mathcal{G}_{i,j+2} = \delta_{j,i}, \quad j = -N+2, \dots, N-2, \\ -\mathcal{G}_{i,N-3} - \mathcal{G}_{i,N-2} + 4\mathcal{G}_{i,N-1} - \mathcal{G}_{i,N} = 0, \\ -\mathcal{G}_{i,N-2} - \mathcal{G}_{i,N-1} + 4\mathcal{G}_{i,N} = 0. \end{cases} \tag{3.12}$$

From the theory of recurrence equation, we get

$$\begin{cases} \mathcal{G}_{i,j} = \alpha_i F_{N+j}(\omega_1) + \beta_i F_{N+j}(\omega_2), \quad j = -N, \dots, i+1, \\ \mathcal{G}_{i,j} = \gamma_i F_{N-j}(\omega_1) + \delta_i F_{N-j}(\omega_2), \quad j = i-1, \dots, N, \end{cases} \tag{3.13}$$

where $F_m(z) = f(z) + g(z)m + z^m, m \in \mathbb{Z}$ with

$$f(z) = 14 + 5z, \quad g(z) = 11 + 4z, \qquad \omega_1 = (-3+\sqrt{5})/2, \quad \omega_2 = (-3-\sqrt{5})/2.$$

To determine the unknown parameters $\alpha_i, \beta_i, \gamma_i$ and δ_i in (3.13), we equate the expressions of $\mathcal{G}_{i,j}$ for $j = i-1, i, i+1$, and use the i-th equation of (3.12) To this end, we firstly prove an auxiliary identity.

LEMMA 3.4. *For $z = \omega_1, \omega_2$, and $i \in \mathbb{Z}$, we have*

$$\begin{aligned} F_{i-3}(z) + F_{i-2}(z) + F_i(z) + F_{i+1}(z) &= 4F_{i-1}(z), \\ F_i(z) + F_{i+2}(z) - 2F_{i+1}(z) &= -5z^{i+1}. \end{aligned} \tag{3.14}$$

Proof. It follows from $z^2 + 3z + 1 = 0,\ z = \omega_1, \omega_2$ that

$$z^{i+1} + z^i = -2z^i - z^{i-1} \quad \text{and} \quad z^{i-3} + z^{i-2} = -2z^{i-2} - z^{i-1}.$$

Adding up these two identities, we obtain

$$z^{i+1} + z^i + z^{i-3} + z^{i-2} = -2(z^i + z^{i-2}) - 2z^{i-1} = 6z^{i-1} - 2z^{i-1} = 4z^{i-1},$$

which together with the definition of $F_i(z)$ gives the identity $(3.14)_1$.

Proceeding in the same way, we obtain $(3.14)_2$. □

Using the i-th equation of (3.12), we obtain

$$\begin{aligned} &[4F_{N+i}(\omega_1) - F_{N+i-2}(\omega_1) - F_{N+i-1}(\omega_1) - F_{N+i+1}(\omega_1)]\alpha_i \\ &+ [4F_{N+i}(\omega_2) - F_{N+i-2}(\omega_2) - F_{N+i-1}(\omega_2) - F_{N+i+1}(\omega_2)]\beta_i \\ &- F_{N-i-2}(\omega_1)\gamma_i - F_{N-i-2}(\omega_2)\delta_i = 1. \end{aligned}$$

By $(3.14)_1$, we write the above equation as

$$F_{N+i+2}(\omega_1)\alpha_i + F_{N+i+2}(\omega_2)\beta_i - F_{N-i-2}(\omega_1)\gamma_i - F_{N-i-2}(\omega_2)\delta_i = 1.$$

The above equation together with the equations obtained by equating the expressions for $\mathcal{G}_{i,i-1}, \mathcal{G}_{i,i}$ and $\mathcal{G}_{i,i+1}$ gives

$$\begin{pmatrix} F_{N+i-1}(\omega_1) & F_{N+i-1}(\omega_2) & -F_{N-i+1}(\omega_1) & -F_{N-i+1}(\omega_2) \\ F_{N+i}(\omega_1) & F_{N+i}(\omega_2) & -F_{N-i}(\omega_1) & -F_{N-i}(\omega_2) \\ F_{N+i+1}(\omega_1) & F_{N+i+1}(\omega_2) & -F_{N-i-1}(\omega_1) & -F_{N-i-1}(\omega_2) \\ F_{N+i+2}(\omega_1) & F_{N+i+2}(\omega_2) & -F_{N-i-2}(\omega_1) & -F_{N-i-2}(\omega_2) \end{pmatrix} \begin{pmatrix} \alpha_i \\ \beta_i \\ \gamma_i \\ \delta_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

Denote the above (4×4)-matrix by A. Solving the above linear system and substituting $\alpha_i, \beta_i, \gamma_i$ and δ_i into (3.13), we obtain the explicit expression of $\mathcal{G}_{i,j}$.

LEMMA 3.5. *For $i = -N+2, \ldots, N-2$, let $i \wedge j = \min(i,j)$ and $i \vee j = \max(i,j)$,*

$$\mathcal{G}_{i,j} = \gamma_{i\wedge j}(\omega_1, \omega_2) F_{N-i\vee j}(\omega_1) + \gamma_{i\wedge j}(\omega_2, \omega_1) F_{N-i\vee j}(\omega_2), \tag{3.15}$$

where

$$\begin{aligned} \gamma_i(\omega_1, \omega_2) = \Big\{ & 5[g(\omega_2) + \omega_2^{2N} g(\omega_1)][\omega_1^{N+i} f(\omega_2) - \omega_2^{N+i} f(\omega_1) + (N+i)(\omega_1 - \omega_2)] \\ & + 5[\omega_1 - \omega_2 + \omega_2^{N+i} g(\omega_1) - \omega_1^{N+i} g(\omega_2)] \\ & \times [\omega_2^{2N} f(\omega_1) - f(\omega_2) - 2N g(\omega_2)] \Big\} (\det A)^{-1}, \end{aligned} \tag{3.16}$$

and

$$\det A = 50(\omega_1 - \omega_2)[\omega_1^N g(\omega_2) + \omega_2^N g(\omega_1)][\omega_2^N F_N(\omega_1) - \omega_1^N F_N(\omega_2)]. \tag{3.17}$$

For the cases when $i = -N, -N+1, N-1, N$, we have

LEMMA 3.6. *For $j = -N, \ldots, N$,*

$$\begin{aligned} \mathcal{G}_{-N,j} &= -j - N - 1 + \frac{1}{\triangle(\omega_1, \omega_2)} \left(\triangle_1(\omega_2) F_{N+j}(\omega_1) - \triangle_1(\omega_1) F_{N+j}(\omega_2) \right), \\ \mathcal{G}_{-N+1,j} &= 2(N+1+j) + 1 + \frac{1}{\triangle(\omega_1, \omega_2)} \left(\triangle_2(\omega_2) F_{N+j}(\omega_1) - \triangle_2(\omega_1) F_{N+j}(\omega_2) \right), \\ \mathcal{G}_{N,j} &= \mathcal{G}_{-N,-j}, \quad \mathcal{G}_{N-1,j} = \mathcal{G}_{-N+1,-j}, \end{aligned}$$

with $\triangle(\omega_1, \omega_2) = F_{2N+1}(\omega_1) F_{2N+2}(\omega_2) - F_{2N+1}(\omega_2) F_{2N+2}(\omega_1)$ and

$$\begin{cases} \triangle_1(z) = (2N+2) F_{2N+2}(z) - (2N+3) F_{2N+1}(z), \\ \triangle_2(z) = -(4N+5) F_{2N+2}(z) + (4N+7) F_{2N+1}(z), \end{cases} \quad z = \omega_1, \omega_2.$$

By Lemma 3.5 and Lemma 3.6, we get the following estimates for $\mathcal{G}$ and its forward difference quotient, the proof is postponed to Appendix A.

LEMMA 3.7. *There exists a constant C such that*

$$\begin{aligned} & 0 \le \mathcal{G}_{i,j} \le C\epsilon (N+1+i\wedge j)(N+1-i\vee j), \quad i,j = -N, \ldots, N, \\ & |D_1 D_2 \mathcal{G}_{i,j}| \le C\epsilon^{-2} \left(\epsilon + |\omega_1|^{|i-j|} \right) \quad i,j = -N, \ldots, N-1. \end{aligned} \tag{3.18}$$

Combining the estimates (3.11), (3.18) and the explicit expression of the error (3.8), we are ready to prove Theorem 3.1.

Proof of Theorem 3.1 Using $(3.18)_1$, we get

$$|D_1\mathcal{G}_{i,N-2}| \le (|\mathcal{G}_{i+1,N-2}| + |\mathcal{G}_{i,N-2}|)/\epsilon \le C\epsilon^{-1}.$$

A direct calculation gives

$$\sum_{j=1}^{N-3} |\omega_1|^{|i-j|} \le \frac{1+|\omega_1|}{1-|\omega_1|}, \quad i = -N, \dots, N.$$

Using the above two estimates, $(3.18)_2$ and the fact that $|D^+ f_i| \le \| \boldsymbol{f} \|_\infty/\epsilon$, we bound the first three terms in the right-hand side of (3.8) as

$$\begin{aligned}
&\left| -\frac{\epsilon^4}{5} \sum_{j=1}^{N-3} D_1 D_2 \mathcal{G}_{i,j} D^+ f_j + \frac{\epsilon^3}{5} \left(D_1 \mathcal{G}_{i,N-2} D^+ f_{N-3} - D_1 D_2 \mathcal{G}_{i,0} f_1 \right) \right| \\
&\le C\epsilon \left(\sum_{j=1}^{N-3} |\omega_1|^{|i-j|} \right) \| \boldsymbol{f} \|_\infty + C\epsilon \| \boldsymbol{f} \|_\infty + C(\epsilon^2 + \epsilon |\omega_1|^{|i|}) \| \boldsymbol{f} \|_\infty \\
&\le C\epsilon \| \boldsymbol{f} \|_\infty.
\end{aligned}$$

Using Lemma 3.7 and (3.11), we estimate the last two terms in (3.8) as

$$\begin{aligned}
&\left| \epsilon^2 D_1 D_2 \Big[\frac{1}{2} \mathcal{G}_{i,\bar{1}} + \frac{3}{5} \mathcal{G}_{i,0} - \frac{1}{10} \mathcal{G}_{i,1} \Big] D^+ (y_0 + y_{\bar{1}}) - 2\epsilon^2 D_1 D_2 \mathcal{G}_{i,0} D^+ y_0 \right| \\
&\le C(\epsilon + |\omega_1|^{|i|})(\| \boldsymbol{f} \|_\infty + 1).
\end{aligned}$$

A combination of the above two inequalities leads to (3.6). □

Next we turn to the case when there is no external force. In this special case, a simpler expression (see Lemma 3.8 below) can be found for the error of the QC method, as was firstly noted by Dobson and Luskin [5] in a slightly different set-up, although we derived this result independently. In the absence of the external force, the atomistic system is at the equilibrium state, i.e., $\boldsymbol{y}^\epsilon = \boldsymbol{x}$. It is easy to see that

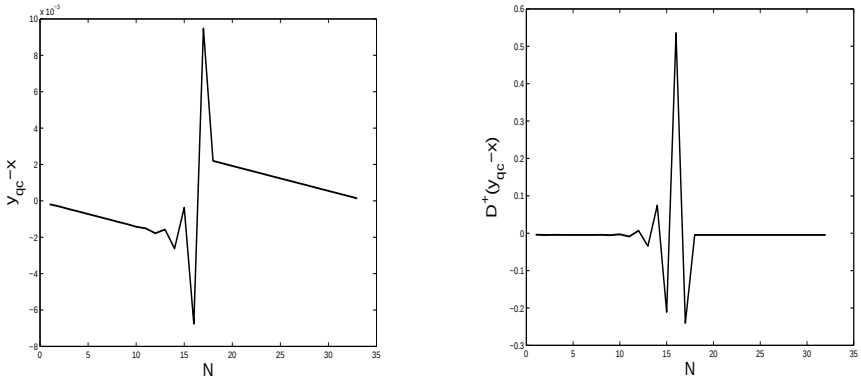
$$\mathcal{A}(\boldsymbol{y}_{\rm QC} - \boldsymbol{x}) = \boldsymbol{h}, \tag{3.19}$$

where $h_{\bar{1}} = -1/\epsilon, h_0 = 2/\epsilon, h_1 = -1/\epsilon$, and $h_i = 0$ otherwise. The difference between $\boldsymbol{y}_{\rm QC}$ and $\boldsymbol{x}$ is the error of the QC method. This error is given explicitly by the following lemma. The basic strategy for deriving the explicit expression of such error is the same as the above procedure to find the explicit formula of the Green's difference function. It consists of two steps. Firstly we get a general expression by the recurrence equation with certain unknown parameters; secondly, we match the equations near the "interface" to determine such parameters.

LEMMA 3.8. *Let $\boldsymbol{y}_{QC}$ be the solution of* (3.4)*, and $\widehat{\boldsymbol{y}}^{\,\epsilon} \equiv \boldsymbol{y}_{QC} - \boldsymbol{x}$. Define $\gamma = \alpha g(\omega_1) + \beta g(\omega_2)$, where α and β are two parameters that satisfy* (3.24) *below. Then*

$$\widehat{y}_i^{\,\epsilon} = \begin{cases} (i+N)\gamma + \alpha f(\omega_1) + \beta f(\omega_2) + \alpha\omega_1^{i+N} + \beta\omega_2^{i+N}, & \text{if} \quad i = -N, \dots, 0, \\ (i-N-1)\gamma, & \text{if} \quad i = 1, \dots, N, \end{cases} \tag{3.20}$$

FIG. 3.5. *Error profile for the original QC solution with* $N = 16$



(a) Profile for $\boldsymbol{y}_{\rm qc} - \boldsymbol{x}$ (b) Profile for $D^+(\boldsymbol{y}_{\rm qc} - \boldsymbol{x})$

and

(3.21)
$$D^+\widehat{y}_i^{\,\epsilon} = \begin{cases} \dfrac{\gamma}{\epsilon} + \dfrac{\alpha}{\epsilon}\omega_1^{i+N}(\omega_1 - 1) + \dfrac{\beta}{\epsilon}\omega_2^{i+N}(\omega_2 - 1), & \text{if} \quad i = -N, \ldots, \bar{1}, \\ -\dfrac{2\gamma}{\epsilon}N - \dfrac{\alpha f(\omega_1) + \beta f(\omega_2)}{\epsilon} - \dfrac{\alpha\omega_1^N + \beta\omega_2^N}{\epsilon}, & \text{if} \quad i = 0, \\ \gamma/\epsilon, & \text{if} \quad i = 1, \ldots, N-1. \end{cases}$$

Proof. From the theory of recurrence relations, we have

(3.22)
$$\widehat{y}_i^{\,\epsilon} = \begin{cases} \alpha F_{i+N}(\omega_1) + \beta F_{i+N}(\omega_2), & i = -N, \ldots, 0, \\ \gamma(i - N - 1), & i = 1, \ldots, N. \end{cases}$$

Summing up the $\bar{1}$-th, 0-th and $1-$th equations, we obtain

$$5(\widehat{y}_2^{\,\epsilon} - \widehat{y}_1^{\,\epsilon}) = 2\widehat{y}_{\bar{1}}^{\,\epsilon} + \widehat{y}_0^{\,\epsilon} - 2\widehat{y}_{\bar{2}}^{\,\epsilon} - \widehat{y}_{\bar{3}}^{\,\epsilon}.$$

Substituting (3.22) into the above equation we obtain

$$\alpha(2F_{N-1} - 2F_{N-2} + F_N - F_{N-3})(\omega_1) + \beta(2F_{N-1} - 2F_{N-2} + F_N - F_{N-3})(\omega_2) = 5\gamma.$$

A direct calculation gives: for $z = \omega_1, \omega_2$,

$$(2F_{N-1} - 2F_{N-2} + F_N - F_{N-3})(z) = 5g(z).$$

Combining the above two equations leads to

(3.23)
$$\gamma = \alpha g(\omega_1) + \beta g(\omega_2),$$

which together with (3.22) gives (3.20). A direct calculation gives (3.21). ∎

The equations (3.20) and (3.21) give the asymptotic error profile that is consistent with the "exact" profiles plotted in Fig. 3.5 even without knowing the exact values of α, β and γ.

Now we use the QC equations near the interface to determine the coefficients. Using the equation for $i = \bar{1}$, we get

$$\alpha\left(\frac{7}{2}F_{N-1} - F_{N-2} - F_{N-3} - F_N\right)(\omega_1) + \beta\left(\frac{7}{2}F_{N-1} - F_{N-2} - F_{N-3} - F_N\right)(\omega_2) + \frac{N}{2}\gamma = -\epsilon,$$

using (3.14), we write the above equation as

$$\alpha(F_{N+1} - F_{N-1}/2)(\omega_1) + \beta(F_{N+1} - F_{N-1}/2)(\omega_2) + \frac{N}{2}\gamma = -\epsilon.$$

Using the equation for $i = 1$, we get

$$\alpha\left(-5F_N - \frac{1}{2}F_{N-1}\right)(\omega_1) + \beta\left(-5F_N - \frac{1}{2}F_{N-1}\right)(\omega_2) - \left(\frac{11}{2}N + 5\right)\gamma = -\epsilon.$$

Combining the above two equations, we obtain that α and β satisfy the following (2×2)-linear system:

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} -\epsilon \\ \epsilon \end{pmatrix}, \tag{3.24}$$

where $M_{11} = R(\omega_1), M_{12} = R(\omega_2), M_{21} = S(\omega_1)$ and $M_{22} = S(\omega_2)$ with

$$\begin{aligned} R(z) &= F_{N+1}(z) - \frac{1}{2}F_{N-1}(z) + \frac{N}{2}g(z), \\ S(z) &= 5F_N(z) + \frac{1}{2}F_{N-1}(z) + \left(\frac{11}{2}N + 5\right)g(z). \end{aligned}$$

Solving the above equations, we obtain

$$\begin{aligned} \alpha &= -[6f(\omega_2) + (2-\omega_1)\omega_2^N + 6(2N+1)g(\omega_2)]\epsilon/\triangle(\omega_1,\omega_2), \\ \beta &= \quad [6f(\omega_1) + (2-\omega_2)\omega_1^N + 6(2N+1)g(\omega_1)]\epsilon/\triangle(\omega_1,\omega_2), \end{aligned}$$

where

$$\begin{aligned} \triangle(\omega_1,\omega_2) &= R(\omega_1)S(\omega_2) - R(\omega_2)S(\omega_1) \\ &= (N+1/2)g(\omega_1)(17\omega_1+38)\omega_2^N - (N+1/2)g(\omega_2)(17\omega_2+38)\omega_1^N \\ &\quad - \frac{1}{2}(74+191\omega_2)\omega_2^N + \frac{1}{2}(74+191\omega_1)\omega_1^N + 12(\omega_1-\omega_2). \end{aligned}$$

Using (3.23), we obtain

$$\gamma = \Big[6(\omega_2-\omega_1) - (2-\omega_1)g(\omega_1)\omega_2^N + (2-\omega_2)g(\omega_2)\omega_1^N\Big]\epsilon/\triangle(\omega_1,\omega_2).$$

It is easy to deduce that

$$\begin{aligned} &\alpha = \frac{(\omega_1-2)\omega_2^N}{\triangle(\omega_1,\omega_2)}\epsilon + \mathcal{O}(\epsilon|\omega_1|^N), \quad \beta = \frac{6(2N+1)g(\omega_1)}{\triangle(\omega_1,\omega_2)}\epsilon + \mathcal{O}(\epsilon^2|\omega_1|^N), \\ &\gamma = \frac{(\omega_1-2)g(\omega_1)\omega_2^N}{\triangle(\omega_1,\omega_2)}\,\epsilon + \mathcal{O}(\epsilon^2|\omega_1|^N). \end{aligned} \tag{3.25}$$

This leads to

THEOREM 3.9. *Let $\boldsymbol{y}_{qc}$ be the solution of* (3.4). *Then,*

$$\begin{aligned} &|D^+(y_i - x_i)| \le C\left(\epsilon + |\omega_1|^{|i|}\right), \qquad i = -N, \ldots, 0, \\ &|D^+(y_i - x_i)| \le C\epsilon, \qquad i = 1, \ldots, N. \end{aligned} \tag{3.26}$$

Moreover, we have

$$D^+(y_{\bar{1}} - x_{\bar{1}}) \ge \frac{9(\sqrt{5}-1)}{17+5\sqrt{5}}, \qquad N \ge 4. \tag{3.27}$$

A direct consequence of the above result is the characterization of the width of the polluted region around the interface, that is, the region beyond which $|D^+(\boldsymbol{y}_{\rm qc} - \boldsymbol{x})| = \mathcal{O}(\epsilon)$.

COROLLARY 3.10. *Let $\boldsymbol{y}_{qc}$ be the solution of* (3.4). *Then*

$$|D^+(y_i - x_i)| \le C\epsilon, \qquad i = -N, \ldots, -\left\lceil \left| \frac{\ln \epsilon}{\ln(3+\sqrt{5})/2} \right| \right\rceil \quad or \quad i = 1, \ldots, N.$$

REMARK 3.11. *Since the equilibrium bond length is ϵ, it follows from the above corollary that the width of the interface is $\mathcal{O}(\epsilon|\ln\epsilon|)$ (see [22]). Essentially the same result was presented firstly in print by Dobson and Luskin in their recent manuscript [5].*

Proof of Theorem 3.9 Our starting point is (3.21). For $i = -N, \ldots, \bar{1}$, we obtain

$$|D^+(y_i - x_i)| \le C(\epsilon + |\omega_1|^{-i}).$$

For $i = 0$, using (3.25), we obtain

$$|D^+\widehat{y}_0^{\epsilon}| \le \left| \frac{g(\omega_1)(2N(2-\omega_1) - 12N)\omega_2^N}{\triangle(\omega_1, \omega_2)} \right| + C(\epsilon + |\omega_1|^{2N}) \le C(\epsilon + 1).$$

For $i = 1, \ldots, N$, we have

$$|D^+\widehat{y}_i^{\epsilon}| \le C\epsilon.$$

The above three equations gives (3.26).

For $i = \bar{1}$, we have

$$D^+(y_{\bar{1}} - x_{\bar{1}}) = P(\omega_1, \omega_2)\omega_1^N / (\triangle(\omega_1, \omega_2)\omega_1^N),$$

where

$$\begin{aligned} P(\omega_1, \omega_2)\omega_1^N = {} & 6(2N+1)g(\omega_1)(1-\omega_1) - 6(2N+1)g(\omega_2)(1-\omega_2)\omega_1^{2N} \\ & - [6(1-\omega_2)f(\omega_2) + (\omega_2 - 2)g(\omega_2)]\omega_1^{2N} + 7(\omega_2 - \omega_1)\omega_1^N \\ & + 6(1-\omega_1)f(\omega_1) + (\omega_1 - 2)g(\omega_1). \end{aligned}$$

It is easy to have

$$P(\omega_1, \omega_2)\omega_1^N \ge 6(2N+1)g(\omega_1)(1-\omega_1).$$

Next,

$$\omega_1^N \triangle(\omega_1,\omega_2) = (N+1/2)g(\omega_1)(17\omega_1+38) - (N+1/2)g(\omega_2)(17\omega_2+38)\omega_1^{2N} - \frac{1}{2}(74+191\omega_2) + \frac{1}{2}(74+191\omega_1)\omega_1^{2N} + 12(\omega_1-\omega_2)\omega_1^N.$$

We have

$$0 < \omega_1^N \triangle(\omega_1,\omega_2) \le (N+3/2)g(\omega_1)(17\omega_1+38).$$

This implies

$$D^+(y_{\bar{1}} - x_{\bar{1}}) \ge \frac{12N+6}{N+3/2}\frac{1-\omega_1}{17\omega_1+38}.$$

This implies (3.27) since $N \ge 4$. □

Before going further, let us introduce some notations. For any vector $\boldsymbol{z} = (z_{-N},\ldots,z_N) \in \mathbb{R}^{2N+1}$, we define the backward difference quotient $D^- z_i \equiv (z_i - z_{i-1})/\epsilon$, the central difference quotient $\widehat{D} \equiv (D^+ + D^-)/2$, and the higher-order forward difference quotient operator $(D^+)^k \equiv [(E-I)/\epsilon]^k$ for any $k \in \mathbb{N}$, where E is the forward shift operator. We will use $\langle\cdot,\cdot\rangle$ to denote the standard Euclidean inner product unless otherwise stated. We define a discrete rescaled H^1 norm as

$$\| \boldsymbol{z} \|_d \equiv \left(\epsilon^{-2} z_{-N}^2 + \epsilon^{-2} z_N^2 + \sum_{i=-N}^{N} |D^+ z_i|^2 \right)^{1/2}. \tag{3.28}$$

By Cauchy-Schwartz inequality, we have

$$|z_{N-1}| \le \sqrt{2}\epsilon \| \boldsymbol{z} \|_d, \quad |z_{N-2}| \le \sqrt{3}\,\epsilon \| \boldsymbol{z} \|_d, \quad |z_{N-3}| \le 2\epsilon \| \boldsymbol{z} \|_d. \tag{3.29}$$

4. Removal of Ghost Forces.

4.1. Quasi-nonlocal QC method. To remove the ghost force, Shimokawa, Mortensen, Schiøz and Jacbosen [29] introduced the concept of quasi-nonlocal atoms. Roughly speaking, a quasi-nonlocal atom acts like a nonlocal atom on the nonlocal side of the interface, while it acts like a local atom on the local side of the interface. For the case of next nearest neighbor interaction, the introduction of the quasi-nonlocal atoms is sufficient to remove the ghost-force. For the one-dimensional chain as Fig. 3.1, if the interaction range contains the next nearest neighbor, then the energies associated with the atoms near the interface are (in the absence of the external force):

$$\begin{aligned}
E_{\bar{1}} &= \frac{1}{2}\big(V_0(r_{\bar{3}\bar{1}}) + V_0(r_{\bar{2}\bar{1}}) + V_0(r_{\bar{1}0}) + V_0(r_{\bar{1}1})\big),\\
E_0 &= \frac{1}{2}\big(V_0(r_{\bar{2}0}) + V_0(r_{\bar{1}0}) + V_0(r_{01}) + V_0(2r_{01})\big),\\
E_1 &= \frac{1}{2}\big(V_0(r_{\bar{1}1}) + V_0(r_{01}) + V_0(r_{12}) + V_0(2r_{12})\big),\\
E_2 &= \frac{1}{2}\big(V_0(2r_{12}) + V_0(r_{12}) + V_0(r_{23}) + V_0(2r_{23})\big).
\end{aligned}$$

The forces for the atoms indexed by $i = -N, \ldots, \bar{2}, 2, \ldots, N$ are the same as the original QC method, while the forces for the interfacial atoms $\bar{1}, 0$ and 1 are:

$$f_{\bar{1}} = -\frac{1}{\epsilon}\Big\{V'\left(D^- y_{\bar{1}}\right) + V'\left(2\widehat{D} y_{\bar{2}}\right) + V'\left(-D^+ y_{\bar{1}}\right) + V'\left(-2\widehat{D} y_0\right)\Big\},$$
$$f_0 = -\frac{1}{\epsilon}\Big\{V'\left(2\widehat{D} y_{\bar{1}}\right) + V'\left(D^- y_0\right) + V'\left(-D^+ y_0\right) + V'\left(-2D^+ y_0\right)\Big\},$$
$$f_1 = -\frac{1}{\epsilon}\Big\{V'\left(D^- y_1\right) + V'\left(2\widehat{D} y_1\right) + V'\left(2D^- y_1\right) + V'\left(-D^+ y_1\right) + 2V'\left(-2D^+ y_1\right)\Big\}.$$

At the equilibrium state, we have

$$f_{\bar{1}} = f_0 = f_1 = 0.$$

Therefore, there is no ghost force.

4.2. Geometrically consistent reconstruction scheme. In [7], the authors introduced the concept of geometrically consistent scheme as a general strategy for removing the ghost force. This is a concept that depends only on the geometry of the lattice, not the details of the potential. Moreover, this scheme has an underlying variational formulation.

As we have addressed in § 2, computing the energy of the whole system is equivalent to computing the site energy for each rep-atom. For this reason, it suffices to reconstruct the local environment of each rep-atom. We can then compute the associated energy using the atomic potential. Denote by $R_i(j)$ the reconstruction of the relative position of the j-th atom with respect to the i-th atom. Well inside the nonlocal region, we may simply use the position of nearby rep-atom, i.e.,

$$R_i(j) = R_i^{\mathrm{a}}(j) \equiv (y_j - y_i)/\epsilon.$$

Inside the local region, we may use the position of the nearest rep-atom, i.e.,

$$R_i(j) = R_i^{\mathrm{CB}}(j) \equiv |j - i|(y_{i+\mathrm{sgn}(j-i)} - y_i)/\epsilon.$$

At the local-nonlocal interface, one needs to reconstruct the relative atomic positions with respect to each rep-atom, inside its interaction range.

In [7], the authors introduced the geometrically consistent condition. As to the one-dimensional chain, this condition becomes:

Definition 4.1. *The reconstruction scheme is geometrically consistent if for all k and n,*

$$\sum_{|r_i(j)|=R_n} \frac{\partial R_i(j)}{\partial y_k} = 0, \qquad \textit{for all} \quad i, \tag{4.1}$$

where $r_i(j) = x_j - x_i$ denotes the relative position of atom j with respect to atom i at the equilibrium state, and R_n is the distance between atom i and atom j.

To find reconstruction schemes that are geometrically consistent, instead of using either $R_i^{\mathrm{a}}(j)$ or $R_i^{\mathrm{CB}}(j)$, we allow linear combination of $R_i^a(j)$ and $R_i^{\mathrm{CB}}(j)$,

$$R_i(j) = C_i(j)R_i^a(j) + (1 - C_i(j))R_i^{\mathrm{CB}}(j),$$

where the $C_i(j)$'s are the coefficients to be determined. In particular, for the $n-$th nearest neighbors of atom i, we let

$$\begin{aligned} R_i(i \pm n) &= C_i^{\pm}(n) R_i^{\mathrm{a}}(i \pm n) + (1 - C_i^{\pm}(n)) R_i^{\mathrm{CB}}(i \pm n) \\ &= C_i^{\pm}(n)(y_{i\pm n} - y_i)/\epsilon + n(1 - C_i^{\pm}(n))(y_{i\pm 1} - y_i)/\epsilon. \end{aligned} \tag{4.2}$$

The original QC method and the quasi-nonlocal approach correspond to the case when $C_i(j)$ equals to either 0 or 1. We further require that away from the interface, in the local region, $C_i(j) = 0$ in accordance with the CB rule and in the nonlocal region, $C_i(j) = 1$ in accordance with the atomistic reconstruction. Using these constraints, we can solve the linear system (4.1) to determine the coefficients $C_i(j)$. Tables of coefficient for different crystal structures have been provided in [7]. Throughout this paper, we assume that

$$0 \le C_i^{+}(2), C_i^{-}(2) \le 1. \tag{4.3}$$

As was shown in [7], as long as a reconstruction scheme is *geometrically consistent*, there are no *ghost forces* at the local-nonlocal interface. In addition, geometric consistency is also a necessary condition for local uniform first order accuracy at the local/nonlocal interface, see [7, Proposition 5].

The quasi-nonlocal approach is a special case of geometrically consistent reconstruction schemes. The quasi-nonlocal reconstruction scheme uses the positions of the nearest neighbor atoms to reconstruct the relative position of other atoms. Therefore, the method is limited to cases for which, along each line, the interaction only involves the second nearest neighbors. If the interaction range is larger, for example if it involves the third nearest neighbors along a line, the condition (4.1) in the quasi-nonlocal approach is violated. In Fig. 3.1, the reconstruction of atom 3 starting from atom 0 will use the position of atom 1. However, the reconstruction of atom 0 from atom 3 does not involve atom 1, since it is not the nearest neighbor of atom 3.

5. Error Estimates for the Geometrically Consistent Quasicontinuum Method. In this section, we study the geometrically consistent QC method for the one-dimensional chain with a pairwise potential V_0 and Dirichlet boundary condition (3.2). It will be clear from the presentation that similar analysis carries over to the case of any finite range interaction (see [11] for details). We refer to [19, 8, 9, 1, 2, 20, 4, 26] for related work on the analysis of the QC method.

5.1. Analysis of the one-dimensional chain. The problem we need to solve is

$$\boldsymbol{y}^{\epsilon} \in \operatorname*{argmin}_{\boldsymbol{w} \in \mathcal{S}} \left\{ E^{\mathrm{tot}}(\boldsymbol{w}) - \langle \boldsymbol{f}, \boldsymbol{w} \rangle \right\},$$

where E^{tot} is the same as (3.1) with a general pairwise potential V_0. The local minimizer $\boldsymbol{y}^{\epsilon} \in \mathcal{S}$ satisfies the equilibrium equation:

$$\mathcal{L}_{\mathrm{at}}^{\epsilon}(\boldsymbol{y}^{\epsilon}) = \boldsymbol{f}. \tag{5.1}$$

We write (5.1) in component form as: for $i = -N, \ldots, N$,

$$-\frac{1}{\epsilon}\left\{ V'\left(D^{-} y_i\right) + V'\left(2\widehat{D} y_{i-1}\right) + V'\left(-D^{+} y_i\right) + V'\left(-2\widehat{D} y_{i+1}\right) \right\} = f_i. \tag{5.2}$$

Using the fact that V' is an odd function, we write (5.2) into a more compact form:

$$D^- V'\left(D^+ y_i\right) + 2\widehat{D} V'\left(2\widehat{D} y_i\right) = f_i. \tag{5.3}$$

From now on, we assume that there exists a smooth function

$$f(x) : I \equiv [-1/2, 1/2] \to \mathbb{R}$$

such that

$$f(x_i) = f_i \qquad i = -N, \ldots, N. \tag{5.4}$$

To begin with, we need to establish the existence results for the atomistic model (5.1) and derive a priori estimates for its solution, see Theorem 5.6. The proof is based on a systematic asymptotic analysis of the solution. We view the atomistic model as a singular perturbation of the macroscopic model obtained from Cauchy-Born rule [3]. Asymptotic expansions are used to construct approximate solution that satisfies the macroscopic equations to high-order accuracy. Finally, using linear stability results for the atomistic model and implicit functional theorem, we obtain the desired existence results. Such ideas have been used by Strang [32] in the context of nonlinear finite difference schemes. A general approach for constructing such higher order approximation for the atomistic model has been introduced in [10, §5]. Here, for the one-dimensional chain, the construction can be made quite explicit.

Define

$$\widetilde{y}_i = \begin{cases} x_i + u_{\rm cb}(x_i) + \epsilon^2 u_2(x_i), & \text{if } i = -N, \ldots, N, \\ x_i, & \text{if } i = -N-2, -N-1, N+1, N+2, \end{cases} \tag{5.5}$$

where $u_{\rm cb}$ satisfies

$$\begin{cases} \mathcal{L}_0(u_{\rm cb}(x)) = f(x), \quad \text{in} \quad I, \\ u_{\rm cb}(-1/2) = u_{\rm cb}(1/2) = 0, \end{cases} \tag{5.6}$$

and

$$\mathcal{L}_0(u_{\rm cb}) = -\frac{\mathrm{d}}{\mathrm{d}\,x}\left\{ V'\left(1 + \frac{\mathrm{d}u_{\rm cb}}{\mathrm{d}\,x}\right) + 2V'\left(2 + 2\frac{\mathrm{d}u_{\rm cb}}{\mathrm{d}\,x}\right)\right\}.$$

Moreover, u_2 satisfies

$$\begin{cases} \mathcal{L}_{\rm lin}(u_{\rm cb}(x))u_2(x) = -\mathcal{L}_2(u_{\rm cb}(x)), \quad \text{in} \quad I, \\ u_2(-1/2) = u_2(1/2) = 0, \end{cases} \tag{5.7}$$

where $\mathcal{L}_{\rm lin}(u_{\rm cb})$ is the linearized operator of $\mathcal{L}_0$ at $u_{\rm cb}$, which takes the form

$$\mathcal{L}_{\rm lin}(u_{\rm cb})u_2 = -\frac{\mathrm{d}}{\mathrm{d}\,x}\left\{\left[V''\left(1 + \frac{\mathrm{d}u_{\rm cb}}{\mathrm{d}\,x}\right) + 4V''\left(2 + 2\frac{\mathrm{d}u_{\rm cb}}{\mathrm{d}\,x}\right)\right]\frac{\mathrm{d}u_2}{\mathrm{d}\,x}\right\},$$

and

$$\begin{aligned}\mathcal{L}_2(u_{\rm cb}) = {} & \frac{1}{12}\frac{\mathrm{d}}{\mathrm{d}\,x}\left\{\left[V''\left(1 + \frac{\mathrm{d}u_{\rm cb}}{\mathrm{d}\,x}\right) + 16V''\left(2 + 2\frac{\mathrm{d}u_{\rm cb}}{\mathrm{d}\,x}\right)\right]\frac{\mathrm{d}^3 u_{\rm cb}}{\mathrm{d}\,x^3}\right\} \\ & + \frac{1}{24}\frac{\mathrm{d}}{\mathrm{d}\,x}\left\{\left[V''\left(1 + \frac{\mathrm{d}u_{\rm cb}}{\mathrm{d}\,x}\right) + 16V''\left(2 + 2\frac{\mathrm{d}u_{\rm cb}}{\mathrm{d}\,x}\right)\right]\left(\frac{\mathrm{d}^2 u_{\rm cb}}{\mathrm{d}\,x^2}\right)^2\right\}.\end{aligned}$$

It is easy to verify that $\widetilde{\boldsymbol{y}} \in \mathcal{S}$. We may also view $\widetilde{\boldsymbol{y}}$ as a function of x, which is denoted by $\widetilde{y}$ and defined as

$$\widetilde{y}(x) = x + u_{\rm cb}(x) + \epsilon^2 u_2(x), \quad x \in I.$$

We need to show that the problems (5.6) and (5.7) are solvable. Obviously, u_2 exists provided that $\mathcal{L}_{\rm lin}$ is coercive at $u_{\rm cb}$, and u_2 is smooth as long as $u_{\rm cb}$ is smooth. More precisely, we have the following regularity estimate for u_2:

$$\|u_2\|_{W^{2,p}(I)} \le C\|u_{\rm cb}\|_{W^{4,p}(I)}, \quad p \ge 1. \tag{5.8}$$

The case when $p \ge 2$ can be found in [12], and the case when $1 \le p < 2$ is quite elementary for this one-dimensional problem. The existence of $u_{\rm cb}$ is implied by the following lemma.

LEMMA 5.1. *There exist two constants ρ_1 and ρ_2 such that for any $m \ge 0$ and $p \ge 1$, for all $f \in W^{m,p}(I)$ with $\|f\|_{W^{m,p}(I)} \le \rho_1$, there exists a locally unique solution $u_{cb} \in W_0^{m+2,p}(I)$ that satisfies* (5.6) *and $\|u_{cb}\|_{W^{m+2,p}(I)} \le \rho_2$. Moreover, there exists a constant $\Lambda > 0$ such that*

$$\langle\, \mathcal{L}_{lin}(u_{cb})v, v\rangle \ge \Lambda\|v\|^2_{H^1(I)}, \qquad \text{for any} \quad v \in H_0^1(I), \tag{5.9}$$

where, $\langle\cdot,\cdot\rangle$ denotes the dual pair between $H_0^1(I)$ and $H^{-1}(I)$.

The proof of the above lemma follows essentially the same argument as in [38, Chapter IV, Theorem 5.3].

LEMMA 5.2. *There exists a constant ρ_1, if $\|f\|_{W^{4,p}(I)} \le \rho_1$ with $p \ge 1$, then there exists a $\widetilde{\boldsymbol{y}} \in \mathcal{S}$ such that*

$$\|\mathcal{L}^{\epsilon}_{at}(\widetilde{\boldsymbol{y}}) - \boldsymbol{f}\|_\infty \le C\epsilon^4, \tag{5.10}$$

where C depends on ρ_1.

Proof. Using the Taylor expansion, we obtain, for any $i = -N, \ldots, N$,

$$\big|\, \mathcal{L}^{\epsilon}_{\rm at}(\widetilde{\boldsymbol{y}})_i - [\mathcal{L}_0(\widetilde{y}(x) - x) + \epsilon^2\mathcal{L}_2(\widetilde{y}(x) - x)]|_{x=x_i} \,\big| \le C\epsilon^4,$$

where C depends on $\|u_{\rm cb}\|_{W^{5,\infty}(I)}$.

By the definition of $\widetilde{y}$ (5.5), using (5.6) and (5.7), we get, for any $i = -N, \ldots, N$,

$$\big|\, [\mathcal{L}_0(\widetilde{y} - x) + \epsilon^2\mathcal{L}_2(\widetilde{y} - x)]|_{x=x_i} - f_i \,\big| \le C\epsilon^4,$$

where C depends on $\|u_{\rm cb}\|_{W^{4,\infty}(I)}$. Combining the above two inequalities and using Lemma 5.1, we obtain (5.10). ∎

REMARK 5.3. *The estimate* (5.10) *improves the result in [10, Corollary 5.1] for the case when $d = 1$.*

Next, we give a direct proof of the coercivity of the linearized operator of the atomistic model. Define the Hessian matrix $\mathcal{H} \in \mathbb{R}^{(2N+1)^2}$ of the total energy as

$$\mathcal{H}_{ij}(\boldsymbol{w}) = \frac{\partial^2 E^{\rm tot}}{\partial w_i \partial w_j}(\boldsymbol{w}), \quad i, j = -N, \ldots, N. \tag{5.11}$$

We have the following coercivity inequality for $\mathcal{H}(\boldsymbol{w})$ at $\boldsymbol{w} = \boldsymbol{x}$.

LEMMA 5.4.

$$\langle\, \mathcal{H}(\boldsymbol{x})\boldsymbol{z}, \boldsymbol{z}\rangle \ge (V''(1) - 4|V''(2)|)\|\, \boldsymbol{z}\,\|_d^2 \qquad \text{for} \quad \boldsymbol{z} \in \mathbb{R}^{2N+1}. \tag{5.12}$$

Proof. A direct calculation gives

$$\begin{aligned}\epsilon^2 \langle \mathcal{H}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle &= \big(V''(1)+V''(2)\big)(z_{-N}^2+z_N^2)+V''(2)\left(z_{-N+1}^2+z_{N-1}^2\right)\\ &\quad + V''(1)\sum_{i=-N}^{N-1}(z_i-z_{i+1})^2+V''(2)\sum_{i=-N}^{N-2}(z_i-z_{i+2})^2.\end{aligned}\tag{5.13}$$

If $V''(2)<0$, then by the Cauchy-Schwartz inequality:

$$|z_i-z_{i+2}|^2\le 2(|z_i-z_{i+1}|^2+|z_{i+1}-z_{i+2}|^2),$$

we write (5.13) as

$$\begin{aligned}\epsilon^2 \langle \mathcal{H}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle &\ge [V''(1)+4V''(2)]\sum_{i=-N+1}^{N-2}(z_i-z_{i+1})^2\\ &\quad + [V''(1)+V''(2)](z_{-N}^2+z_N^2)+V''(2)\left(z_{-N+1}^2+z_{N-1}^2\right)\\ &\quad + [V''(1)+2V''(2)]\big((z_{-N}-z_{-N+1})^2+(z_N-z_{N-1})^2\big).\end{aligned}$$

For $i=N, j=N-1$ and $i=-N, j=-N+1$, we have

$$\begin{aligned}&[V''(1)+V''(2)]z_i^2+V''(2)\,z_j^2+[V''(1)+2V''(2)](z_i-z_j)^2\\ &\quad = [V''(1)+4V''(2)](z_i^2+(z_i-z_j)^2)+(-V''(2))[z_i^2+(2z_i-z_j)^2].\end{aligned}\tag{5.14}$$

Combining the above two inequality gives (5.12) for the case when $V''(2)<0$.

If $V''(2)\ge 0$, then we get (5.12) from (5.13). ∎

The next lemma is a perturbation result of (5.12) that follows exactly the same way as [10, Lemma 6.7], we omit the proof.

LEMMA 5.5. *If*

$$\langle \mathcal{H}(\boldsymbol{y}_1)\boldsymbol{z},\boldsymbol{z}\rangle \ge \kappa\|\,\boldsymbol{z}\,\|_d^2,$$

then there exists a constant $\delta>0$, such that if $\|D^+(\boldsymbol{y}_1-\boldsymbol{y}_2)\|_\infty\le\delta$, we have

$$\langle \mathcal{H}(\boldsymbol{y}_2)\boldsymbol{z},\boldsymbol{z}\rangle \ge (\kappa/2)\|\,\boldsymbol{z}\,\|_d^2.\tag{5.15}$$

Based on the above higher-order approximation result, we prove the interior regularity for the solution of the atomistic model that is the main result of this subsection.

THEOREM 5.6. *For $p\ge 1$, there exists a constant ρ_3 such that if $\|f\|_{W^{4,p}(I)}\le\rho_3$, then the problem* (5.1) *has a locally unique solution $\boldsymbol{y}^\epsilon\in\mathcal{S}$ satisfying*

$$\|D^+(\boldsymbol{y}^\epsilon-\widetilde{\boldsymbol{y}})\|_\infty\le C\epsilon^4.\tag{5.16}$$

Moreover,

$$\max_{-N+2\le i\le N-3}|(D^+)^3y_i^\epsilon|\le C,\qquad \max_{-N+2\le i\le N-2}\sum_{k=1}^{2}|(D^+)^k y_i^\epsilon|\le C.\tag{5.17}$$

Proof. The existence of $\boldsymbol{y}^\epsilon$ follows from [10, Theorem 2.2]. By [10, Lemma 6.8], the solution $\boldsymbol{y}^\epsilon$ satisfies

$$\| \boldsymbol{y}^\epsilon - \widetilde{\boldsymbol{y}} \|_d \le C\epsilon^4,$$

which immediately implies (5.16).

Moreover, for $i = -N+2, \dots, N-3$, the quantity $(D^+)^3 y_i^\epsilon$ is well-defined and we have

$$\begin{aligned}
|(D^+)^3 y_i^\epsilon| &\le |(D^+)^3 (y^\epsilon - \widetilde{y}_i)| + |(D^+)^3 \widetilde{y}_i| \\
&\le 3\epsilon^{-2} \| D^+(\boldsymbol{y}^\epsilon - \widetilde{\boldsymbol{y}}) \|_\infty + |(D^+)^3 \widetilde{y}_i| \\
&\le 3\epsilon^{-2} \| D^+(\boldsymbol{y}^\epsilon - \widetilde{\boldsymbol{y}}) \|_\infty + |(D^+)^3 u_{\rm cb}(x_i)| + 3|D^+ u_2(x_i)| \\
&\le C\epsilon^2 + C\|u_{\rm cb}\|_{W^{3,\infty}(I)} + C\|u_2\|_{W^{1,\infty}(I)} \\
&\le C\epsilon^2 + C\|u_{\rm cb}\|_{W^{4,p}(I)} + C\|u_2\|_{W^{2,p}(I)} \\
&\le C\epsilon^2 + C\|u_{\rm cb}\|_{W^{4,p}(I)} \\
&\le C,
\end{aligned}$$

where C depends on ρ_1. This leads to the first inequality in (5.17). Similar estimate holds for $|(D^+)^k y_i^\epsilon|$ with $k = 1, 2$. □

5.2. Convergence analysis of the geometrically consistent QC method. The problem we need to solve is: find the local minimizer $\boldsymbol{y}_{\rm qc} \in \mathcal{S}$ that satisfies

$$\boldsymbol{y}_{\rm qc} \in \operatorname*{argmin}_{\boldsymbol{w}\in\mathcal{S}} \big\{ E^{\rm gcs}(\boldsymbol{w}) - \langle \boldsymbol{f}, \boldsymbol{w} \rangle \big\},$$

where

$$E^{\rm gcs}(\boldsymbol{w}) = \sum_{i=-N-1}^{N} V(R_i(i+1)) + \sum_{i=-N-2}^{N} V(R_i(i+2)).$$

We write the equilibrium equations for the above problem as: find $\boldsymbol{y}_{\rm qc} \in \mathcal{S}$ such that

$$\mathcal{L}^\epsilon_{\rm gcs}(\boldsymbol{y}_{\rm qc})_i = f_i, \quad i = -N, \dots, N, \tag{5.18}$$

where

$$\begin{aligned}
\mathcal{L}^\epsilon_{\rm gcs}(\boldsymbol{z})_i = {} & D^- V'\left(D^+ z_i\right) \\
& - \frac{1}{2\epsilon}\big[C^-_{i+2}(2) V'\left(R_{i+2}(i)\right) + (C^-_i(2) - 2) V'\left(R_i(i-2)\right) \\
& \qquad + 2(1 - C^-_{i+1}(2)) V'\left(R_{i+1}(i-1)\right)\big] \\
& - \frac{1}{2\epsilon}\big[C^+_{i-2}(2) V'\left(R_{i-2}(i)\right) + (C^+_i(2) - 2) V'\left(R_i(i+2)\right) \\
& \qquad + 2(1 - C^+_{i-1}(2)) V'\left(R_{i-1}(i+1)\right)\big],
\end{aligned}$$

where $R_i(i \pm n)$ is defined the same as (4.2) with y replaced by z. To avoid the influence of the boundary condition on the accuracy of the method; cf., [37], we assume that

$$\mathcal{L}^\epsilon_{\rm gcs}(\boldsymbol{z})_i = \mathcal{L}^\epsilon_{\rm at}(\boldsymbol{z})_i, \qquad i = N, N-1. \tag{5.19}$$

TABLE 5.1
coefficients for 1D chain with next nearest neighbor interaction

Atom	-5	-4	-3	-2	-1	0	1	2	3	4	5
$C^+(2)$	1	α_1	α_2	α_3	α_4	α_5	α_6	α_7	0	0	0
$C^-(2)$	1	1	1	α_1	α_2	α_3	α_4	α_5	α_6	α_7	0

We make the following assumption on the coefficients:

$$\begin{aligned} &C_i^+(2) = 1, \quad i \le -5; \qquad C_i^+(2) = 0, \quad i \ge 3, \\ &C_i^-(2) = 1, \quad i \le -3; \qquad C_i^-(2) = 0, \quad i \ge 5. \end{aligned} \tag{5.20}$$

That leaves a sufficiently wide transition region for interactions that involves up to the next nearest neighbors.

The geometrically consistent condition (4.1) can be written in a more explicit form:

$$\begin{aligned} &C_{i-2}^+(2) - C_i^+(2) + 2[C_i^+(2) - C_{i-1}^+(2)] \\ &\qquad = C_{i+2}^-(2) - C_i^-(2) + 2[C_i^-(2) - C_{i+1}^-(2)] \end{aligned} \tag{5.21}$$

for any i-th atom with next nearest neighbor interaction.

To analyze the geometrically consistent QC method, we follow the strategy of Strang for the finite difference scheme [32]. Therefore, we need to study the stability and the consistency error of the method. The stability of the linearized operator of $\mathcal{L}_{\rm gcs}^\epsilon$ may be proven as in Lemma 5.4, which will be shown in Lemma 5.12 below. To analyze the consistency error, we firstly illuminate the geometrically consistent condition (5.21).

LEMMA 5.7. *For $i = -5, \ldots, 3$, if the geometrically consistent condition* (5.21) *and the assumption* (5.20) *hold, then*

$$C_i^+(2) = C_{i+2}^-(2). \tag{5.22}$$

Proof. For $i = -6, \ldots, 3$, denote by $d_i = C_i^+(2) - C_{i+2}^-(2)$. By (5.20) we get $d_{-5} = d_{-6} = 0$. Moreover, it follows from (5.21) that

$$d_i = 2d_{i-1} - d_{i-2},$$

which immediately implies

$$d_i - d_{i-1} = d_{i-1} - d_{i-2} = \cdots = d_{-5} - d_{-6} = 0.$$

Therefore $d_i = d_{i-1} = \cdots = d_{-6} = 0$, which leads to (5.22). ∎

By (5.22), we get Table 5.1 for the coefficients $C_i^+(2)$ and $C_i^-(2)$ with $i = -4, \ldots, 4$. If we take $\alpha_1 = \cdots = \alpha_4 = 1$ and $\alpha_5 = \alpha_6 = \alpha_7 = 0$ in Table 5.1, then the geometrically consistent QC method changes to the quasi-nonlocal QC method as shown in [7].

Next we define the truncation error functional as:

DEFINITION 5.8. *Let $\boldsymbol{y}^\epsilon \in \mathcal{S}$ be the solution of* (5.1). *The truncation error functional $\boldsymbol{F} \in \mathbb{R}^{2N+1}$ is defined as*

$$F_i = (\mathcal{L}_{at}^\epsilon - \mathcal{L}_{gcs}^\epsilon)(\boldsymbol{y}^\epsilon)_i, \qquad i = -N, \ldots, N.$$

A direct calculations gives $\boldsymbol{F} = \mathcal{O}(1)$ (see [11, Lemma 4.6] for a proof), which seems to suggest that this scheme does not converge. However, we will see that the truncation error functional has some structure that can be exploited, due to the translation invariance of the potential function [15] and the periodicity of the underlying lattice structure [27].

It is easy to see that $F_i = 0$ for $i = -N, \ldots, -5, N-1, N$. Using the assumption (5.20), we have, for $i = 5, \ldots, N-2$,

$$\begin{aligned} &F_i = D^+ Q_i, \\ &Q_i = V'\left(2\widehat{D} y_i\right) + V'\left(2\widehat{D} y_{i-1}\right) - 2V'\left(2D^+ y_{i-1}\right). \end{aligned} \tag{5.23}$$

Summing by parts for the first term in the right-hand side of (5.3), we obtain, for any $\boldsymbol{w} \in \mathbb{R}^9$,

$$\begin{aligned} \sum_{i=-4}^{4} \mathcal{L}^{\epsilon}_{\mathrm{at}}(\boldsymbol{z})_i w_i = {} & 2\sum_{i=-4}^{2} V'\left(R^a_{i+2}(i)\right) \widehat{D} w_{i+1} - \sum_{i=-4}^{4} D^- V'\left(D^+ y_i\right) w_i \\ & - V'\left(R^a_6(4)\right) \frac{w_4}{\epsilon} - V'\left(R^a_5(3)\right) \frac{w_3}{\epsilon} \\ & - V'\left(R^a_{\bar{6}}(\bar{4})\right) \frac{w_{\bar{4}}}{\epsilon} - V'\left(R^a_{\bar{5}}(\bar{3})\right) \frac{w_{\bar{3}}}{\epsilon}. \end{aligned} \tag{5.24}$$

Using the explicit expression of $\mathcal{L}^{\epsilon}_{\mathrm{gcs}}$ and summation by parts, we get

Lemma 5.9. *If* (5.20) *is true, then for any* $\boldsymbol{w} \in \mathbb{R}^9$*, we have*

$$\begin{aligned} \sum_{k=-4}^{4} \mathcal{L}^{\epsilon}_{gcs}(\boldsymbol{z})_i w_i = {} & -\sum_{i=-4}^{4} D^- V'\left(D^+ y_i\right) w_i \\ & + \frac{1}{2}\sum_{i=-4}^{2} \Big\{ \Big[(2 - C^-_{i+2}(2)) V'\left(R_{i+2}(i)\right) - C^+_i(2) V'\left(R_i(i+2)\right) \Big] D^+ w_{i+1} \\ & \qquad + \Big[C^-_{i+2}(2) V'\left(R_{i+2}(i)\right) - (2 - C^+_i(2)) V'\left(R_i(i+2)\right) \Big] D^+ w_i \Big\} \\ & - V'\left(R^{CB}_3(5)\right) D^+ w_3 + \left[V'\left(R^{CB}_4(6)\right) - V'\left(R^{CB}_5(3)\right) \right] \frac{w_4}{\epsilon} \\ & - V'\left(R^a_{\bar{5}}(\bar{3})\right) \frac{w_{\bar{3}}}{\epsilon} - V'\left(R^a_{\bar{6}}(\bar{4})\right) \frac{w_{\bar{4}}}{\epsilon}. \end{aligned} \tag{5.25}$$

Proof. Denote the second and the third terms of the expression of $\mathcal{L}^{\epsilon}_{\mathrm{gcs}}$ by I_1 and I_2, respectively, summation by parts, and using (5.20) we obtain

$$\begin{aligned} I_1 = {} & \frac{1}{2}\sum_{i=-4}^{2} V'\left(R_{i+2}(i)\right) \left[(2 - C^-_{i+2}(2)) D^+ w_{i+1} + C^-_{i+2}(2) D^+ w_i \right] \\ & - \frac{1}{2\epsilon} \left[-V'\left(R^a_{\bar{4}}(\bar{6})\right) w_{\bar{4}} - V'\left(R^a_{\bar{3}}(\bar{5})\right) w_{\bar{3}} + 2V'\left(R^{\mathrm{CB}}_5(3)\right) w_4 \right], \end{aligned}$$

and

$$I_2 = -\frac{1}{2}\sum_{i=-4}^{2} V'\left(R_i(i+2)\right)\left[C_i^+(2)D^+w_{i+1} + (2-C_i^+(2))D^+w_i\right]$$
$$-\frac{1}{2\epsilon}[V'\left(R_{\bar{6}}^a(\bar{4})\right)w_{\bar{4}} + V'\left(R_{\bar{5}}^a(\bar{3})\right)w_{\bar{3}} - 2V'\left(R_4^{\mathrm{CB}}(6)\right)w_4] - V'\left(R_3^{\mathrm{CB}}(5)\right)D^+w_3.$$

Combining the above two equations, we get (5.25). □

Combining the above three identities (5.23), (5.24) and (5.25), and using the fact that $2\widehat{D} = D^+ + D^-$, we obtain the following identity for $\boldsymbol{F}$.

LEMMA 5.10. *If* (5.20) *is true, then for any* $\boldsymbol{w} \in \mathbb{R}^{2N+1}$*, we have*

$$\begin{aligned}
&\langle \boldsymbol{F}, \boldsymbol{w}\rangle \\
&= \sum_{i=-4}^{2}\left[\left(\frac{C_{i+2}^-(2)}{2} - 1\right)V'\left(R_{i+2}(i)\right) + \frac{C_i^+(2)}{2}V'\left(R_i(i+2)\right) + V'\left(R_{i+2}^a(i)\right)\right]D^+w_{i+1} \\
&\quad + \sum_{i=-4}^{2}\left[V'\left(R_{i+2}^a(i)\right) - \frac{C_{i+2}^-(2)}{2}V'\left(R_{i+2}(i)\right) + \left(1 - \frac{C_i^+(2)}{2}\right)V'\left(R_i(i+2)\right)\right]D^+w_i \\
&\quad - \sum_{i=4}^{N-3} Q_{i+1}D^+w_i - \left[V'\left(R_3^a(5)\right) - V'\left(R_3^{CB}(5)\right)\right]D^+w_3 + Q_{N-1}\frac{w_{N-2}}{\epsilon}.
\end{aligned}$$

A remarkable aspect of the above lemma is that it is valid *without* assuming the geometrically consistent condition (5.21). Given this condition, using the a priori estimates for the atomistic solution $\boldsymbol{y}^\epsilon$, we can prove that the truncation error of the geometrically consistent QC method is small in a weak norm.

LEMMA 5.11. *Let* $\boldsymbol{y}^\epsilon \in \mathcal{S}$ *be the solution of the atomistic model* (5.1)*. Under the same conditions in Theorem 5.6 and if the geometrically consistent condition* (4.1) *and the assumption* (5.20) *are valid, then there exists a constant* C *such that*

$$|\langle \boldsymbol{F}, \boldsymbol{w}\rangle| \le C\epsilon\|\boldsymbol{w}\|_d, \qquad \forall \boldsymbol{w} \in \mathbb{R}^{2N+1}. \tag{5.26}$$

Proof. We start with the expression of $\langle \boldsymbol{F}, \boldsymbol{w}\rangle$ in Lemma 5.10. Denote the right-hand side of $\langle \boldsymbol{F}, \boldsymbol{w}\rangle$ by $I_1, \ldots, I_5$ and let $C_i^+(2) = C_{i+2}^-(2) = \alpha$. By (5.22) and Taylor expansion, we obtain

$$\begin{aligned}
&\left(-1 + \frac{1}{2}C_{i+2}^-(2)\right)V'\left(R_{i+2}(i)\right) + \frac{1}{2}C_i^+(2)V'\left(R_i(i+2)\right) + V'\left(R_{i+2}^a(i)\right) \\
&= (1-\alpha/2)\left[V'\left(R_{i+2}^a(i)\right) - V'\left(R_{i+2}(i)\right)\right] + \frac{\alpha}{2}\left[V'\left(R_{i+2}^a(i)\right) - V'\left(R_i(i+2)\right)\right] \\
&= (1-\alpha)\epsilon\Big[(1-\alpha/2)\int_0^1 V''\left(tR_{i+2}^a(i) + (1-t)R_{i+2}(i)\right)\,\mathrm{d}t \\
&\qquad\qquad - (\alpha/2)\int_0^1 V''\left(tR_{i+2}^a(i) + (1-t)R_i(i+2)\right)\,\mathrm{d}t\Big](D^+)^2y_i^\epsilon.
\end{aligned}$$

Proceeding along the same line, we get

$$\begin{aligned}
&V'\left(R^a_{i+2}(i)\right) + \left(1 - \frac{1}{2}C^-_{i+2}(2)\right) V'\left(R_i(i+2)\right) - \frac{1}{2}C^+_i(2)V'\left(R_{i+2}(i)\right) \\
&= (1-\alpha/2)\big[V'\left(R^a_{i+2}(i)\right) - V'\left(-R_i(i+2)\right)\big] + \frac{\alpha}{2}\big[V'\left(R^a_{i+2}(i)\right) - V'\left(R_{i+2}(i)\right)\big] \\
&= (1-\alpha)\epsilon\Big[(\alpha/2-1)\int_0^1 V''\left(tR^a_{i+2}(i) - (1-t)R_i(i+2)\right)\,\mathrm{d}t \\
&\qquad\qquad + (\alpha/2)\int_0^1 V''\left(tR^a_{i+2}(i) + (1-t)R_{i+2}(i)\right)\,\mathrm{d}t\Big](D^+)^2 y^\epsilon_i.
\end{aligned}$$

Using the a priori estimates (5.17) for y^ϵ_i with $i = -4, \ldots, 2$, we bound I_1 and I_2 as

$$|I_1| + |I_2| \le C\epsilon \sum_{i=-4}^{2} |D^+ w_{i+1}| \le C\epsilon \| \boldsymbol{w} \|_d.$$

Using a Taylor expansion, we can write Q_i for $i = 1, \ldots, N-1$ as

$$\begin{aligned}
Q_i &= \epsilon\left[\int_0^1 V''\left((1+t)D^+ y^\epsilon_{i-1} + (1-t)D^+ y^\epsilon_i\right)\,\mathrm{d}t\right](D^+)^2 y^\epsilon_{i-1} \\
&\quad - \epsilon\left[\int_0^1 V''\left((1+t)D^+ y^\epsilon_{i-1} + (1-t)D^+ y^\epsilon_{i-2}\right)\,\mathrm{d}t\right](D^+)^2 y^\epsilon_{i-2} \\
&= \epsilon^2\left[\int_0^1 V''\left((1+t)D^+ y^\epsilon_{i-1} + (1-t)D^+ y^\epsilon_i\right)\,\mathrm{d}t\right](D^+)^3 y^\epsilon_{i-2} \\
&\quad - \epsilon^2\left[\int_0^1\int_0^1 V'''\left((1+t)D^+ y^\epsilon_{i-1} + (1-t)D^+(sy^\epsilon_i + (1-s)y^\epsilon_{i-2})\right)\,\mathrm{d}s\,(1-t)\,\mathrm{d}t\right] \\
&\qquad \times (D^+)^2(y^\epsilon_{i-2} + y^\epsilon_{i-1})(D^+)^2 y^\epsilon_{i-2}.
\end{aligned}$$

Using (5.17) once again, we have

$$|Q_i| \le C\epsilon^2 \qquad \text{for} \quad i = 1, \ldots, N-1,$$

which immediately implies

$$|I_3| \le C\epsilon^2 \sum_{i=4}^{N-2} |D^+ w_i| \le C\epsilon^2 N \left(\sum_{i=4}^{N-2} |D^+ w_i|^2\right)^{1/2} \le C\epsilon^{3/2} \| \boldsymbol{w} \|_d.$$

A direct calculation gives

$$R^a_3(5) - R^{\mathrm{CB}}_3(5) = \epsilon (D^+)^2 y^\epsilon_3.$$

Therefore, we obtain

$$V'\left(R^a_3(5)\right) - V'\left(R^{\mathrm{CB}}_3(5)\right) = \epsilon \int_0^1 V''\left(tR^a_3(5) + (1-t)R^{\mathrm{CB}}_3(5)\right)\,\mathrm{d}t\,(D^+)^2 y^\epsilon_3,$$

which yields

$$|I_4| \le C\epsilon |D^+ w_3| \le C\epsilon \| \boldsymbol{w} \|_d.$$

By (3.29) and the above estimate for Q_{N-1}, we get

$$|I_5| \le C\epsilon |w_{N-2}| \le C\epsilon^2 \| \boldsymbol{w} \|_d.$$

Combing the above estimates for $I_1, \ldots, I_5$, we get (5.26). □

Given any $\boldsymbol{F} \in \mathbb{R}^{2N+1}$, define

$$\|\boldsymbol{F}\|_{-d} = \sup_{\boldsymbol{w} \in \mathbb{R}^{2N+1}} \frac{\langle \boldsymbol{F}, \boldsymbol{w} \rangle}{\| \boldsymbol{w} \|_d}. \tag{5.27}$$

This norm is the so-called Spijker norm [36, 31]. By Lemma 5.11, we obtain

$$\|\boldsymbol{F}\|_{-d} \le C\epsilon.$$

This suggests that the local truncation error of the geometrically consistent scheme is *small* measured in Spijker norm.

Next, we prove the stability of the geometrically consistent QC method. The proof follows the same line as for (5.12). Since we modify the equilibrium equations for the boundary atoms, cf., (5.19), there is no well-defined energy functional. Therefore, the Hessian matrix is defined as

$$(\mathcal{H}_{\rm QC})_{ij} = -\frac{\partial (\mathcal{L}^\epsilon_{\rm gcs})_i}{\partial w_j}(\boldsymbol{w}),$$

where $(\mathcal{L}^\epsilon_{\rm gcs})_i$ is regarded as a function of $\boldsymbol{w}$. We may use $\mathcal{H}$ to replace $\mathcal{H}_{\rm QC}$ when there is no confusion occurs.

LEMMA 5.12. *If the assumptions* (5.20) *is valid for* $i = -4, \ldots, 4$ *and the geometrically consistent condition* (4.1) *holds true, then, for all* $\boldsymbol{z} \in \mathbb{R}^{2N+1}$,

$$\langle \mathcal{H}_{QC}(\boldsymbol{x})\boldsymbol{z}, \boldsymbol{z} \rangle \ge [V''(1) - 6|V''(2)|] \| \boldsymbol{z} \|_d^2, \quad N \ge 4. \tag{5.28}$$

Proof. By (5.20), and the elementary identity:

$$a^2 - ab = \frac{1}{2}(a-b)^2 + \frac{1}{2}(a^2 - b^2), \quad a, b \in \mathbb{R},$$

a direct calculation gives, for any $\boldsymbol{z} \in \mathbb{R}^{2N+1}$,

$$\begin{aligned}
\epsilon^2 \langle \mathcal{H}_{\rm QC}(\boldsymbol{x})\boldsymbol{z}, \boldsymbol{z} \rangle &= [V''(1) + V''(2)] z_{-N}^2 + V''(2)\, z_{-N+1}^2 + \left(V''(1) + \frac{3}{2} V''(2) \right) z_N^2 \\
&\quad + \frac{V''(2)}{2}(3z_{N-2}^2 - z_{N-1}^2 - z_{N-3}^2) \\
&\quad + \sum_{i=-N}^{N-3} \big(-\epsilon^2 \mathcal{H}_{i,i+1}\big)(z_i - z_{i+1})^2 + \sum_{i=-N}^{N-4} \big(-\epsilon^2 \mathcal{H}_{i,i+2}\big)(z_i - z_{i+2})^2 \\
&\quad + [V''(1) + 2V''(2)](z_{N-2} - z_{N-1})^2 + V''(1)\,(z_{N-1} - z_N)^2 \\
&\quad + \frac{V''(2)}{2} \left((z_{N-3} - z_{N-1})^2 + (z_{N-2} - z_N)^2 \right).
\end{aligned} \tag{5.29}$$

A direct calculation gives

$$\begin{aligned}
\epsilon^2 \mathcal{H}_{i,i+1} &= -V''(1) + \big[(C_i^+(2) - 2)(1 - C_i^+(2)) + (1 - C_{i-1}^+(2)) C_{i-1}^+(2) \big] V''(2) \\
&\quad + \big[(1 - C_{i+2}^-(2)) C_{i+2}^-(2) + (C_{i+1}^-(2) - 2)(1 - C_{i+1}^-(2)) \big] V''(2), \\
\epsilon^2 \mathcal{H}_{i,i+2} &= -\frac{1}{2} \big[C_i^+(2)(2 - C_i^+(2)) + C_{i+2}^-(2)(2 - C_{i+2}^-(2)) \big] V''(2),
\end{aligned}$$

which together with the geometrically consistent condition (5.22) leads to

$$\begin{aligned}-\epsilon^2(\mathcal{H}_{i,i+1}+2\mathcal{H}_{i,i+2}+2\mathcal{H}_{i-1,i+1}) &= V''(1)\\ &\quad+\big[4-C_i^+(2)+C_{i+2}^-(2)+C_{i-1}^+(2)-C_{i+1}^-(2)\big]V''(2)\\ &= V''(1)+4V''(2)\,.\end{aligned}\tag{5.30}$$

Using (5.20), we get

$$\begin{cases}-\epsilon^2(\mathcal{H}_{-N,-N+1}+2\mathcal{H}_{-N,-N+2}) = V''(1)+2V''(2)\,,\\ -\epsilon^2(\mathcal{H}_{N-3,N-2}+2\mathcal{H}_{N-4,N-2}) = V''(1)+4V''(2)\,.\end{cases}\tag{5.31}$$

If $V''(2)<0$, then by the Cauchy-Schwartz inequality

$$|z_i-z_{i+2}|^2\le 2(|z_i-z_{i+1}|^2+|z_{i+1}-z_{i+2}|^2),$$

the equations (5.30) and (5.31), we obtain

$$\begin{aligned}\epsilon^2\langle\mathcal{H}_{\rm QC}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle &\ge [V''(1)+4V''(2)]\sum_{i=-N}^{N-4}(z_i-z_{i+1})^2\\ &+[V''(1)+5V''(2)](z_{N-3}-z_{N-2})^2+[V''(1)+4V''(2)](z_{N-2}-z_{N-1})^2\\ &+[V''(1)+V''(2)](z_{N-1}-z_N)^2\\ &+\Big\{[V''(1)+V''(2)]z_{-N}^2+V''(2)\,z_{-N+1}^2+[V''(1)+2V''(2)](z_{-N}-z_{-N+1})^2\Big\}\\ &+\left(V''(1)+\frac{3}{2}V''(2)\right)z_N^2+\frac{V''(2)}{2}(3z_{N-2}^2-z_{N-1}^2-z_{N-3}^2).\end{aligned}$$

Invoking (5.14) once again we obtain

$$\epsilon^2\langle\mathcal{H}_{\rm QC}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle\ge[V''(1)+5V''(2)]\|\boldsymbol{z}\|_d^2+\frac{3V''(2)}{2}z_{N-2}^2.$$

By (3.29) and $N\ge 4$, we get

$$\begin{aligned}\epsilon^2\langle\mathcal{H}_{\rm QC}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle &\ge\left(V''(1)+5V''(2)+\frac{9V''(2)}{2}\epsilon^2\right)\|\boldsymbol{z}\|_d^2\\ &\ge[V''(1)+6V''(2)]\|\boldsymbol{z}\|_d^2.\end{aligned}$$

On the other hand, if $V''(2)\ge 0$, then we have

$$\epsilon^2\langle\mathcal{H}_{\rm QC}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle\ge\big(V''(1)-3V''(2)\,\epsilon^2\big)\|\boldsymbol{z}\|_d^2\ge[V''(1)-3V''(2)]\|\boldsymbol{z}\|_d^2.$$

Combining the above two inequalities leads to (5.12). □

We are ready to prove the main theorem of this paper.

THEOREM 5.13. *Assume that the geometrically consistent condition* (4.1)*, the conditions* (4.3) *and* (5.20) *hold. Assume that* $p\ge 1, m\ge 4$*. There exists a constant* κ_1 *such that if* $\|f\|_{W^{m,p}(I)}\le\kappa_1$*, then the problem* (5.18) *has a locally unique solution* $\boldsymbol{y}_{qc}$ *that satisfies*

$$\|D^+(\boldsymbol{y}_{qc}-\boldsymbol{y}^\epsilon)\|_\infty\le C\epsilon.\tag{5.32}$$

Proof. Write

$$\mathcal{L}^{\epsilon}_{\mathrm{gcs}}(\boldsymbol{y}) - \mathcal{L}^{\epsilon}_{\mathrm{gcs}}(\boldsymbol{y}^{\epsilon}) = \int_0^1 \mathcal{H}_{\mathrm{QC}}(t\boldsymbol{y} + (1-t)\boldsymbol{y}^{\epsilon})\,\mathrm{d}t \cdot (\boldsymbol{y} - \boldsymbol{y}^{\epsilon}).$$

Hence $\boldsymbol{y} \in \mathcal{S}$ is a solution of (5.18) if and only if

$$\int_0^1 \mathcal{H}_{\mathrm{QC}}(t\boldsymbol{y} + (1-t)\boldsymbol{y}^{\epsilon})\,\mathrm{d}t \cdot (\boldsymbol{y} - \boldsymbol{y}^{\epsilon}) = \boldsymbol{F},$$

since

$$\mathcal{L}^{\epsilon}_{\mathrm{gcs}}(\boldsymbol{y}) - \mathcal{L}^{\epsilon}_{\mathrm{gcs}}(\boldsymbol{y}^{\epsilon}) = \mathcal{L}^{\epsilon}_{\mathrm{gcs}}(\boldsymbol{y}) - \mathcal{L}^{\epsilon}_{\mathrm{at}}(\boldsymbol{y}^{\epsilon}) + \mathcal{L}^{\epsilon}_{\mathrm{at}}(\boldsymbol{y}^{\epsilon}) - \mathcal{L}^{\epsilon}_{\mathrm{gcs}}(\boldsymbol{y}^{\epsilon}) = (\mathcal{L}^{\epsilon}_{\mathrm{at}} - \mathcal{L}^{\epsilon}_{\mathrm{gcs}})(\boldsymbol{y}^{\epsilon}).$$

Next define

$$\mathcal{S}_1 = \{\, \boldsymbol{y} \in \mathcal{S} \mid \|D^+(\boldsymbol{y} - \boldsymbol{y}^{\epsilon})\|_{\infty} < \sqrt{\epsilon}\,\}.$$

Let $\widehat{T} : \mathcal{S}_1 \to \mathcal{S}_1$, and $\hat{T}(\boldsymbol{y})$ be the solution of the following linear system:

$$\int_0^1 \mathcal{H}_{\mathrm{QC}}(t\boldsymbol{y} + (1-t)\boldsymbol{y}^{\epsilon})\,\mathrm{d}t \cdot (\hat{T}(\boldsymbol{y}) - \boldsymbol{y}^{\epsilon}) = \boldsymbol{F}.$$

Define $\boldsymbol{w} \equiv \widehat{T}(\boldsymbol{y}) - \boldsymbol{y}^{\epsilon}$, using (5.16), we obtain

$$\begin{aligned}
\|D^+(t\boldsymbol{y} + (1-t)\boldsymbol{y}^{\epsilon} - \boldsymbol{x})\|_{\infty} &\le t\|D^+(\boldsymbol{y} - \boldsymbol{y}^{\epsilon})\|_{\infty} + \|D^+(\boldsymbol{y}^{\epsilon} - \widetilde{\boldsymbol{y}})\|_{\infty} + \|D^+(\widetilde{\boldsymbol{y}} - \boldsymbol{x})\|_{\infty} \\
&\le \sqrt{\epsilon} + C\epsilon^{5/2} + |u_{\mathrm{cb}}|_{W^{1,\infty}(I)} + C\epsilon^2|u_2|_{W^{1,\infty}(I)} \\
&\le (\sqrt{\epsilon} + C\epsilon^{5/2} + C_I\epsilon^2|u_2|_{W^{2,p}(I)}) + C_I\|u_{\mathrm{cb}}\|_{W^{2,p}(I)}, \qquad (5.33)
\end{aligned}$$

where C_I is the imbedding constant. By the regularity estimate (5.8), we have, for sufficiently small ϵ, we get

$$\sqrt{\epsilon} + C\epsilon^{5/2} + C\epsilon^2\|u_2\|_{W^{2,p}(I)} \le \sqrt{\epsilon} + C\epsilon^{5/2} + C\rho_2\epsilon^2 < \delta/2.$$

Moreover, there exists a constant ρ_3 such that if $\|f\|_{L^p(I)} \le \rho_3$, then

$$C_1\|u_{\mathrm{cb}}\|_{W^{2,p}(I)} \le \delta/2.$$

Substituting the above two inequalities into (5.33) leads to

$$\|\, D^+(t\boldsymbol{y} + (1-t)\boldsymbol{y}^{\epsilon} - \boldsymbol{x})\,\|_{\infty} < \delta.$$

Therefore, using Lemma 5.5 and Lemma 5.12, we get

$$\left\langle \int_0^1 \mathcal{H}_{\mathrm{QC}}(t\boldsymbol{y} + (1-t)\boldsymbol{y}^{\epsilon})\,\mathrm{d}t\boldsymbol{w}, \boldsymbol{w} \right\rangle \ge \frac{\kappa'}{2}\|\,\boldsymbol{w}\,\|_d^2. \qquad (5.34)$$

Using (5.26) and (5.34), we obtain

$$\|\,\boldsymbol{w}\,\|_d \le C\epsilon.$$

By the definition of $\|\cdot\|_d$, the above inequality immediately implies

$$\|\, D^+(\widehat{T}(\boldsymbol{y}) - \boldsymbol{y}^{\epsilon})\,\|_{\infty} = \|\, D^+\boldsymbol{w}\,\|_{\infty} \le \|\,\boldsymbol{w}\,\|_d \le C\epsilon. \qquad (5.35)$$

Therefore, for sufficiently small ϵ, we have

$$\|D^+\boldsymbol{w}\|_\infty < \sqrt{\epsilon}.$$

Thus, we conclude that $\widehat{T}(\boldsymbol{y}) \in \mathcal{S}_1$. By the fixed point theorem, there exists a solution of the geometrically consistent QC method. The solution is locally unique since the Hessian matrix

$$\int_0^1 \mathcal{H}_{\rm QC}(t\boldsymbol{y} + (1-t)\boldsymbol{y}^\epsilon)\,{\rm d}t$$

is non-degenerate for small f.

The error estimate (5.32) follows from (5.35). □

A direct consequence of the above theorem is

COROLLARY 5.14. *If $p \geq 1, m \geq 4$, then there exists a constant ρ such that for all $\|f\|_{W^{m,p}(I)} \leq \rho$, the quasi-nonlocal QC method has a locally unique solution $\boldsymbol{y}_{qc} \in \mathcal{S}$ that satisfies*

$$\|D^+(\boldsymbol{y}_{qc} - \boldsymbol{y}^\epsilon)\|_\infty \leq C\epsilon.$$

The uniform first order convergence of the geometrically consistent QC method may seem quite unexpected since the pointwise local truncation error of such schemes is of $\mathcal{O}(1)$. The origin of the above result lies in the *supra-convergence* phenomenon [17, 35, 36] as shown in Lemma 5.11.

The analysis presented above can be extended to high dimension, when the interface between the local and nonlocal regions is planar, i.e., there are no corners along the interface. To do so, we have to establish the stability result and the consistent analysis in high dimensions. The stability results, namely, Lemma 5.4 and Lemma 5.12 can be easily extended to high dimensions by combining the argument in [10] and in the proof of Lemma 5.4. As for the consistency analysis, there are two main ingredients. One is the analysis of the local truncation error that is guaranteed by the geometrically consistent condition. The other is the structure of the consistency error, i.e., (5.26). This is also due to the symmetry of the lattice and the potential function. Even though the main ideas for the analysis in high dimensions are quite clear, the technicalities are quite involved. We shall present the detailed analysis in a separate paper [23].

5.3. Stability condition. In the remaining part we verify the stability condition

$$V''(1) > 6|V''(2)| \tag{5.36}$$

for several pairwise potentials.

First we consider the Lennard-Jones potential [18]:

$$V_0(r) = 4\big((\sigma/r)^{12} - (\sigma/r)^6\big),$$

where σ is some atomic length scale parameter. The equilibrium bond length $\epsilon = (2/K)^{1/6}\sigma$ with $K = (1+2^{-6})/(1+2^{-12}) > 1$. A direct calculation gives

$$V''(2) < 0 \quad \text{and} \quad V''(1) - 6|V''(2)| = V''(1) + 6V''(2) > 72K > 0.$$

This verifies (5.36).

TABLE 5.2
Parameters for various metals; data for ar_0 adopted from [13, Table I]

Metal	Rb	Cs	Na	K	Ba	Fe	Cr
ar_0	1.206	1.260	1.267	1.293	1.650	1.988	2.260
M	1.452	1.597	1.615	1.678	1.191	.96	.903
$\operatorname{sgn}(V''(2))$	+	+	+	+	−	−	−

The next example is the Morse potential [25] mentioned before:

$$V_0(r) = e^{-a(r-r_0)} - 2e^{-a(r-r_0)}.$$

Let ϵ be the equilibrium bond length and denote by $s = e^{ar_0}$ and $t = e^{-a\epsilon}$, we find that t satisfies

$$2st^3 + (s-2)t - 1 = 0. \tag{5.37}$$

It is clear to see that there exists a unique solution $t \in (0,1)$, denoted by t_0, a direct calculation gives

$$V''(1) - 6|V''(2)| = 2a^2\epsilon^2 st_0(2st_0 - 1 - 6|1 + t_0 - st_0|).$$

Let $M \equiv 2st_0 - 1 - 6|1 + t_0 - st_0|$. For the cubic metals listed in [13], e.g., Rb, Cs, Na, K, Ba, Fe, Cr, et al., see Table 5.2 for the corresponding values of M.

6. Conclusion. The analysis presented here is done for one-dimensional models, which demonstrates that

1. the deformation gradient may have $\mathcal{O}(1)$ error;
2. the geometrically consistent QC method is uniformly accurate, even near the interface.

The main limitation of the analysis in this paper is the assumption that every atom is treated as a representative atom. The motivation comes from the fact that we are mainly interested in the local-nonlocal interface. To understand the QC method fully, we also need to analyze the coarsening procedure, in particular, the transition between atom-based summation and element-based summation [7]. As was pointed in [7], this is where difficulty associated with corners comes from. At the present time, there is no clean solution to this problem.

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Appendix A. Auxiliary Results and Estimates of the Green's Difference Function.

We prove some auxiliary results in §3 in this part.

Proof of (3.17) *and* (3.16) Adding the 3rd row to the 1st row and 2nd row to the 4th row, and subtracting respectively (-2) times the 2nd row and 3rd row from 1st row and 4th row, using the relation $(3.14)_2$, we get

$$\det A = \begin{vmatrix} -5\omega_1^{N+i} & -5\omega_2^{N+i} & 5\omega_1^{N-i} & 5\omega_2^{N-i} \\ F_{N+i}(\omega_1) & F_{N+i}(\omega_2) & -F_{N-i}(\omega_1) & -F_{N-i}(\omega_2) \\ F_{N+i+1}(\omega_1) & F_{N+i+1}(\omega_2) & -F_{N-i-1}(\omega_1) & -F_{N-i-1}(\omega_2) \\ -5\omega_1^{N+i+1} & -5\omega_2^{N+i+1} & 5\omega_1^{N-i-1} & 5\omega_2^{N-i-1} \end{vmatrix}.$$

Multiplying the first row by $-\omega_1$ and adding to the 4th row we obtain

$$\det A = \begin{vmatrix} -5\omega_1^{N+i} & -5\omega_2^{N+i} & 5\omega_1^{N-i} & 5\omega_2^{N-i} \\ F_{N+i}(\omega_1) & F_{N+i}(\omega_2) & -F_{N-i}(\omega_1) & -F_{N-i}(\omega_2) \\ F_{N+i+1}(\omega_1) & F_{N+i+1}(\omega_2) & -F_{N-i-1}(\omega_1) & -F_{N-i-1}(\omega_2) \\ 0 & 5\omega_2^{N+i+1}(\omega_1^2-1) & 5\omega_1^{N-i-1}(1-\omega_1^2) & 0 \end{vmatrix}.$$

Multiplying the 4th row by $\omega_1/(\omega_1^2-1)$ and adding to the 1st row we obtain

$$\det A = \begin{vmatrix} -5\omega_1^{N+i} & 0 & 0 & 5\omega_2^{N-i} \\ F_{N+i}(\omega_1) & F_{N+i}(\omega_2) & -F_{N-i}(\omega_1) & -F_{N-i}(\omega_2) \\ F_{N+i+1}(\omega_1) & F_{N+i+1}(\omega_2) & -F_{N-i-1}(\omega_1) & -F_{N-i-1}(\omega_2) \\ 0 & 5\omega_2^{N+i+1}(\omega_1^2-1) & 5\omega_1^{N-i-1}(1-\omega_1^2) & 0 \end{vmatrix}.$$

Multiplying the 1st column by ω_2^{2N} and adding to the 4th column, and the 2nd column by ω_1^{2N} and adding to the 3rd column, respectively, we obtain

$$\begin{aligned}\det A = 25(\omega_2-\omega_1)\big[&\big(\omega_1^{2N}F_{N+i}(\omega_2)-F_{N-i}(\omega_1)\big)\big(\omega_2^{2N}F_{N+i+1}(\omega_1)-F_{N-i-1}(\omega_2)\big) \\ &-\big(\omega_1^{2N}F_{N+i+1}(\omega_2)-F_{N-i-1}(\omega_1)\big)\big(\omega_2^{2N}F_{N+i}(\omega_1)-F_{N-i}(\omega_2)\big)\big].\end{aligned}$$

A straightforward calculation gives

$$\begin{aligned}\det A &= 25(\omega_1-\omega_2)[\omega_1^N g(\omega_2)+\omega_2^N g(\omega_1)] \\ &\quad\times[\omega_2^N(F_{N-i-1}+F_{N+i+1})(\omega_1)-\omega_1^N(F_{N-i-1}+F_{N+i+1})(\omega_2)].\end{aligned}$$

Using the expression of $F_m(z)$, we get (3.17).

We only calculate γ_i and δ_i in (3.13) since $\mathcal{G}$ is symmetric. By definition,

$$\gamma_i = (\operatorname{cof} A)_{43}/\det A, \qquad \delta_i = (\operatorname{cof} A)_{44}/\det A.$$

Moreover, we only calculate γ_i since $(\operatorname{cof} A)_{44}(\omega_1,\omega_2) = (\operatorname{cof} A)_{43}(\omega_2,\omega_1)$. By (3.14), a direct calculation gives

$$\begin{aligned}\gamma_i(\omega_1,\omega_2) &= 5\omega_2^N\Big[[\omega_1^N g(\omega_2)+\omega_2^N g(\omega_1)][\omega_1^{N+i}F_{N+i+1}(\omega_2)-\omega_2^{N+i}F_{N+i+1}(\omega_1)] \\ &\quad+[\omega_1-\omega_2+g(\omega_1)\omega_2^{N+i}-g(\omega_2)\omega_1^{N+i}][\omega_2^N F_{N+i+1}(\omega_1)-\omega_1^N F_{N-i-1}(\omega_2)]\Big]/\det A.\end{aligned}$$

Substituting $F_m(z)$ into the above equation, we obtain (3.16). □

Proof of Lemma 3.7 The upper bound in $(3.18)_1$ immediately follows from (3.15) and Lemma 3.6, while the lower bound follows from the fact that $\mathcal{G}$ is monotone [40].

Using (3.15) and (3.16), a direct calculation gives

$$D_1D_2\mathcal{G}_{i,j} = D^+\gamma_i(\omega_1,\omega_2)D^+F_{N-j}(\omega_1) + D^+\gamma_i(\omega_2,\omega_1)D^+F_{N-j}(\omega_2), \tag{A.1}$$

where $D^+F_{N-j}(z) = [-g(z)+z^{N-j-1}(1-z)]/\epsilon, z=\omega_1,\omega_2$ and

$$\begin{aligned}D^+\gamma_i(\omega_1,\omega_2) = \Big[&\frac{5}{\epsilon}(\omega_1-\omega_2)[\omega_2^{2N}g(\omega_1)+g(\omega_2)] \\ &+5D^+\omega_1^{N+i}[\omega_2^{2N}(\omega_1-\omega_2)+2f(\omega_2)g(\omega_2)+2Ng^2(\omega_2)] \\ &-5D^+\omega_2^{N+i}[f(\omega_1)g(\omega_2)+f(\omega_2)g(\omega_1)+2Ng(\omega_1)g(\omega_2)]\Big]/\det A,\end{aligned}$$

where we have used $f(\omega_2)g(\omega_1) - f(\omega_1)g(\omega_2) = \omega_1 - \omega_2$. By

$$f(\omega_1)g(\omega_2) + f(\omega_2)g(\omega_1) = 15, \quad g(\omega_1)g(\omega_2) = 5,$$

we write $D^+\gamma_i$ as

$$D^+\gamma_i(\omega_1,\omega_2) = \Big[\frac{5}{\epsilon}(\omega_1-\omega_2)[\omega_2^{2N}g(\omega_1)+g(\omega_2)] - 5(10N+15)D^+\omega_2^{N+i} + 5D^+\omega_1^{N+i}[\omega_2^{2N}(\omega_1-\omega_2)+2f(\omega_2)g(\omega_2)+2Ng^2(\omega_2)]\Big]/\det A.$$

Using (3.17), we get

$$\det A = \mathcal{O}(\epsilon^{-1}|\omega_2|^{2N}),$$

which together with the above expression of $D^+\gamma_i$ leads to

$$D^+\gamma_i(\omega_1,\omega_2) = \mathcal{O}(1), \quad D^+\gamma_i(\omega_2,\omega_1) = \mathcal{O}(\epsilon^{-1}|\omega_1|^{N-i-1}).$$

Substituting the above estimate into (A.1), we obtain

$$|D_1D_2\mathcal{G}_{i,j}| \le C(\epsilon^{-1}+\epsilon^{-1}|\omega_1|^{N-j-1}+\epsilon^{-2}|\omega_1|^{j-i}) \le C\epsilon^{-2}(\epsilon+|\omega_1|^{j-i}),$$

which together with the facts that $j \ge i$ and the symmetry of $\mathcal{G}$, we obtain (3.18) for $i = -N+2,\dots,N-2$.

Using Lemma 3.6 and proceeding along the same line, we find that the estimate (3.18) remains true for the cases when $i = -N, -N+1, N-1, N$. This finishes the proof. □

Appendix B. A-priori Estimate for the Solution of (3.5)**.** Define $\widehat{\boldsymbol{y}}^{\,\epsilon} \equiv \boldsymbol{y}_{\rm qc} - \boldsymbol{x}$, by (3.5), $\widehat{\boldsymbol{y}}^{\,\epsilon}$ satisfies

$$\widehat{\mathcal{A}}\widehat{\boldsymbol{y}}^{\,\epsilon} = \boldsymbol{f}. \tag{B.1}$$

LEMMA B.1. *For $\widehat{\boldsymbol{y}}^{\,\epsilon}$ the solution of* (B.1)*, we have*

$$|\widehat{y}^{\,\epsilon}_{-N}|, |\widehat{y}^{\,\epsilon}_{-N+1}| \le \frac{(N+1)\epsilon^2}{2}\|\boldsymbol{f}\|_\infty. \tag{B.2}$$

Proof. Note that $\widehat{\mathcal{A}}$ is an irreducible diagonally dominant matrix. Therefore, $\widehat{\mathcal{A}}$ is monotone [40], i.e., each entry of $\widehat{\mathcal{A}}^{-1}$ is nonnegative. Define $\boldsymbol{g} = \epsilon^2\boldsymbol{e}$ with $\boldsymbol{e} = (1,\dots,1) \in \mathbb{R}^{2N+1}$. A direct calculation gives

$$(\widehat{\mathcal{A}}\boldsymbol{g})_{-N} = (\widehat{\mathcal{A}}\boldsymbol{g})_N = 2, (\widehat{\mathcal{A}}\boldsymbol{g})_{-N+1} = (\widehat{\mathcal{A}}\boldsymbol{g})_{N-1} = 1, \quad \text{and } (\mathcal{A}\boldsymbol{g})_i = 0 \text{ otherwise.}$$

Hence,

$$g_i = (\widehat{\mathcal{A}}^{-1}\widehat{\mathcal{A}}\boldsymbol{g})_i = \sum_{j=-N}^{N}(\widehat{\mathcal{A}}^{-1})_{ij}(\widehat{\mathcal{A}}\boldsymbol{g})_j \ge 2[(\mathcal{A}^{-1})_{i,-N} + (\widehat{\mathcal{A}}^{-1})_{i,N}].$$

Therefore,

$$0 \le (\widehat{\mathcal{A}}^{-1})_{i,-N} + (\widehat{\mathcal{A}}^{-1})_{i,N} \le \epsilon^2/2. \tag{B.3}$$

Next we let $\boldsymbol{g} \in \mathbb{R}^{2N+1}$ with $g_i = (N+1+i)(N+1-i)\epsilon^2, i = -N, \ldots, N$. Using the relation

$$g_{i-2} + g_{i+2} = 2g_i - 8 \qquad \text{and} \qquad g_{i-1} + g_{i+1} = 2g_i - 2,$$

we obtain $(\widehat{\mathcal{A}}\boldsymbol{g})_{-N} = (\widehat{\mathcal{A}}\boldsymbol{g})_N = 7 - 2N$ and $(\widehat{\mathcal{A}}\boldsymbol{g})_i = 10$ otherwise. Therefore,

$$g_i = (\widehat{\mathcal{A}}^{-1}\widehat{\mathcal{A}}\boldsymbol{g})_i = (7-2N)[(\widehat{\mathcal{A}}^{-1})_{i,-N} + (\widehat{\mathcal{A}}^{-1})_{i,N}] + 10 \sum_{j=-N+1}^{N-1} (\widehat{\mathcal{A}}^{-1})_{ij},$$

which together with (B.3) leads to

$$(\widehat{\mathcal{A}}^{-1}\boldsymbol{e})_i = \frac{g_i}{10} + \frac{2N+3}{10}[(\widehat{\mathcal{A}}^{-1})_{i,-N} + (\widehat{\mathcal{A}}^{-1})_{i,N}] \le \frac{g_i}{10} + \frac{2N+3}{20}\epsilon^2,$$

using the above identity with $i = -N$ and $-N+1$ we get (B.2). □

Next we prove (3.11). Denote by $\boldsymbol{t} = (D^+ y_{-N}, \ldots, D^+ y_0) \in \mathbb{R}^{N+1}$ that satisfies

$$\hat{\mathcal{C}}\boldsymbol{t} = \boldsymbol{g}, \tag{B.4}$$

where

$$\hat{\mathcal{C}} = \begin{pmatrix} 2 & 1 & \ldots & \ldots & \ldots & 0 \\ -1 & 2 & 1 & \ldots & \ldots & 0 \\ -1 & -2 & 2 & 1 & \ldots & 0 \\ & \ddots & \ddots & \ddots & \ddots & \\ \ldots & -1 & -2 & 2 & 1 & \ldots \\ \ldots & \ldots & -1 & -2 & 3/2 & 1/2 \\ \ldots & \ldots & \ldots & -1 & 2 & 5 \end{pmatrix},$$

and

$$g_1 = -\epsilon f_1 + \frac{2}{\epsilon}\widehat{y}^{\,\epsilon}_{-N}, \quad g_2 = -\epsilon f_2 + \frac{1}{\epsilon}\widehat{y}^{\,\epsilon}_{-N+1}, \quad g_i = -\epsilon f_i \quad \text{for } i = 3, \ldots, N+1.$$

Proof of (3.11) Denote the $(N+1)$-th row of $\hat{\mathcal{C}}^{-1}$ by $(x_1, \ldots, x_{N+1})$. It is easy to verify that

$$\begin{cases} 2x_1 - x_2 - x_3 = 0, \\ x_{i-1} + 2x_i - 2x_{i+1} - x_{i+2} = 0, \quad i = 2, \ldots, N-1, \\ x_{N-1} + (3/2)x_N - 2x_{N+1} = 0, \\ (1/2)x_N + 5x_{N+1} = 1. \end{cases}$$

By standard theory of recurrence equation, we get

$$x_i = a + b(\omega_1^{i-1} + \omega_2^{i-1}), \qquad a = \frac{6[\psi(\omega_1) + \psi(\omega_2)]}{\phi(\omega_1) + \phi(\omega_2)}, \quad b = -\frac{1}{\phi(\omega_1) + \phi(\omega_2)},$$
$$\phi(z) = z^{N-2}(97z + 38), \quad \psi(z) = z^{N-2}(5z/2 + 1).$$

Using the fact that $a = \mathcal{O}(1)$ and $b = \mathcal{O}(|\omega_1|^N)$, we get

$$|x_1| + |x_2| \le 2|a| + 5|b| \le C,$$

and

$$\sum_{i=1}^{N+1}|x_i| \le |a|(N+1)+|b|\left(\frac{1}{1-|\omega_1|}+\frac{|\omega_2|^{N+1}-1}{|\omega_2|-1}\right) \le CN,$$

which together with (B.2) leads to

$$|D^+\widehat{y}_0^{\epsilon}| \le \frac{2}{\epsilon}(|x_1|+|x_2|)(|\widehat{y}_{-N}^{\epsilon}|+|\widehat{y}_{-N+1}^{\epsilon}|)+\epsilon\left(\sum_{i=1}^{N+1}|x_i|\right)\|\boldsymbol{f}\|_\infty \le C\|\boldsymbol{f}\|_\infty,$$

Using the triangle inequality, we obtain the estimate (3.11) for D^+y_0. Proceeding along the same line, we get the estimate for $D^+y_{\bar{1}}$. □

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