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LINEAR STATIONARY ITERATIVE METHODS FOR THE FORCE-BASED QUASICONTINUUM APPROXIMATION

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ABSTRACT. Force-based multiphysics coupling methods have become popular since they provide a simple and efficient coupling mechanism, avoiding the difficulties in formulating and implementing a consistent coupling energy. They are also the only known pointwise consistent methods for coupling a general atomistic model to a finite element continuum model. However, the development of efficient and reliable iterative solution methods for the force-based approximation presents a challenge due to the non-symmetric and indefinite structure of the linearized force-based quasicontinuum approximation, as well as to its unusual stability properties. In this paper, we present rigorous numerical analysis and computational experiments to systematically study the stability and convergence rate for a variety of linear stationary iterative methods.

1. INTRODUCTION

Low energy local minima of crystalline atomistic systems are characterized by highly localized defects such as vacancies, interstitials, dislocations, cracks, and grain boundaries separated by large regions where the atoms are slightly deformed from a lattice structure. The goal of atomistic-to-continuum coupling methods [1–4, 15, 16, 22, 26, 28, 32] is to approximate a fully atomistic model by maintaining the accuracy of the atomistic model in small neighbors surrounding the localized defects and using the efficiency of continuum coarse-grained models in the vast regions that are only mildly deformed from a lattice structure.

Force-based atomistic-to-continuum methods decompose a computational reference lattice into an *atomistic region* $\mathcal{A}$ and a *continuum region* $\mathcal{C}$, and assign forces to representative atoms according to the region they are located in. In the quasicontinuum method, the representative atoms are all atoms in the atomistic region and the nodes of a finite element approximation in the continuum region. The force-based approximation is thus given by [5, 6, 10–12, 32]

$$\mathcal{F}_j^{\mathrm{qcf}}(y) := \begin{cases} \mathcal{F}_j^{\mathrm{a}}(y) & \text{if } j \in \mathcal{A}, \\ \mathcal{F}_j^{\mathrm{c}}(y) & \text{if } j \in \mathcal{C}, \end{cases}$$

where y denotes the positions of the representative atoms which are indexed by j, $\mathcal{F}_j^{\mathrm{a}}(y)$ denotes the atomistic force at representative atom j, and $\mathcal{F}_j^{\mathrm{c}}(y)$ denotes a continuum force at representative atom j.

The force-based quasicontinuum method (QCF) uses a Cauchy-Born strain energy density for the continuum model to achieve a patch test consistent approximation [6, 11, 24]. We recall that a patch test consistent atomistic-to-continuum approximation exactly reproduces the zero net forces of uniformly strained lattices [19, 24, 27]. However, the recently discovered unusual stability properties of the linearized force-based quasicontinuum (QCF) approximation, especially its indefiniteness, present a challenge to the development of efficient and reliable iterative methods [12]. Energy-based quasicontinuum approximations have many attractive features such as more reliable solution methods, but practical patch test consistent, energy-based quasicontinuum approximations have yet to be developed for most problems of physical interest, such as three-dimensional problems with many-body interaction potentials [20, 21, 30].

Rather than attempt an analysis of linear stationary methods for the full nonlinear system, in this paper we restrict our focus to the linearization of a one-dimensional model problem about the uniform deformation y^F and consider linear stationary methods of the form

$$P\big(u^{(n+1)} - u^{(n)}\big) = \alpha r^{(n)}, \tag{1}$$

where P is a nonsingular preconditioning operator, the damping parameter $\alpha > 0$ is fixed throughout the iteration (that is, stationary), and the residual is defined as

$$r^{(n)} := f - L_F^{\mathrm{qcf}} u^{(n)}.$$

We will see below that our analysis of this simple model problem already allows us to observe many interesting and crucial features of the various methods. For example, we can distinguish which iterative methods converge up to the critical strain F_* (see (8) for a discussion of the critical strain), and we obtain first results on their convergence rates.

We begin in Sections 2 and 3 by introducing the most important quasicontinuum approximations and outlining their stability properties, which are mostly straightforward generalizations of results from [9–11, 13]. In Section 4, we review the basic properties of linear stationary iterative methods.

In Section 5, we give an analysis of the Richardson Iteration ($P = I$) and prove a contraction rate of order $1 - O(N^{-2})$ in the ℓ_ε^p norm (discrete Sobolev norms are defined in Section 2.1), where N is the size of the atomistic system.

In Section 6, we consider the iterative solution with preconditioner $P = L_F^{\mathrm{qcl}}$, where L_F^{qcl} is a standard second order elliptic operator, and show that the preconditioned iteration with an appropriately chosen damping parameter α is a contraction up to the critical strain F_* only in $\mathcal{U}^{2,\infty}$ among the common discrete Sobolev spaces. We show, however, that a rate of contraction in $\mathcal{U}^{2,\infty}$ independent of N can be achieved with the elliptic preconditioner L_F^{qcl} and an appropriate choice of the damping parameter α.

In Section 7, we consider the popular ghost force correction iteration (GFC) which is given by the preconditioner $P = L_F^{\mathrm{qce}}$, and we show that the GFC iteration ceases to be a contraction for any norm at strains less than the critical strain. This result and others presented in Section 7 imply that the GFC iteration might not always reliably

reproduce the stability of the atomistic system [9]. We did not find that the GFC method predicted an instability at a reduced strain in our benchmark tests [18] (see also [24]). To explain this, we note that our 1D analysis in this paper can be considered a good model for cleavage fracture, but not for the slip instabilities studied in [18, 24]. We are currently attempting to develop a 2D benchmark test for cleavage fracture to study the stability of the GFC method.

2. The QC Approximations and Their Stability

We give a review of the prototype QC approximations and their stability properties in this section. The reader can find more details in [9, 10].

2.1. Function Spaces and Norms.

We consider a one-dimensional atomistic chain whose $2N+1$ atoms have the reference positions $x_j = j\varepsilon$ for $\varepsilon = 1/N$. The displacement of the boundary atoms will be constrained, so the space of admissible displacements will be given by the *displacement space*

$$\mathcal{U} = \left\{ u \in \mathbb{R}^{2N+1} : u_{-N} = u_N = 0 \right\}.$$

We will use various norms on the space $\mathcal{U}$ which are discrete variants of the usual Sobolev norms that arise naturally in the analysis of elliptic PDEs.

For displacements $v \in \mathcal{U}$ and $1 \leq p \leq \infty$, we define the ℓ_ε^p norms,

$$\|v\|_{\ell_\varepsilon^p} := \begin{cases} \left(\varepsilon \sum_{\ell=-N+1}^N |v_\ell|^p \right)^{1/p}, & 1 \leq p < \infty, \\ \max_{\ell=-N+1,\ldots,N} |v_\ell|, & p = \infty, \end{cases}$$

and we denote by $\mathcal{U}^{0,p}$ the space $\mathcal{U}$ equipped with the ℓ_ε^p norm. The inner product associated with the ℓ_ε^2 norm is

$$\langle v, w \rangle := \varepsilon \sum_{\ell=-N+1}^N v_\ell w_\ell \qquad \text{for } v, w \in \mathcal{U}.$$

We will also use $\|f\|_{\ell_\varepsilon^p}$ and $\langle f, g \rangle$ to denote the ℓ_ε^p-norm and ℓ_ε^2-inner product for arbitrary vectors f, g which need not belong to $\mathcal{U}$. In particular, we further define the $\mathcal{U}^{1,p}$ norm

$$\|v\|_{\mathcal{U}^{1,p}} := \|v'\|_{\ell_\varepsilon^p},$$

where $(v')_\ell = v'_\ell = \varepsilon^{-1}(v_\ell - v_{\ell-1})$, $\ell = -N+1, \ldots, N$, and we let $\mathcal{U}^{1,p}$ denote the space $\mathcal{U}$ equipped with the $\mathcal{U}^{1,p}$ norm. Similarly, we define the space $\mathcal{U}^{2,p}$ and its associated $\mathcal{U}^{2,p}$ norm, based on the centered second difference $v''_\ell = \varepsilon^{-2}(v_{\ell+1} - 2v_\ell + v_{\ell-1})$ for $\ell = -N+1, \ldots, N-1$.

We have that $v' \in \mathbb{R}^{2N}$ for $v \in \mathcal{U}$ has mean zero $\sum_{j=-N+1}^N v'_j = 0$. We can thus obtain from [10, Equation 9] that

$$\max_{\substack{v \in \mathcal{U} \\ \|v'\|_{\ell_\varepsilon^q}=1}} \langle u', v' \rangle \leq \max_{\substack{\sigma \in \mathbb{R}^{2N} \\ \|\sigma\|_{\ell_\varepsilon^q}=1}} \langle u', \sigma \rangle = \|u\|_{\mathcal{U}^{1,p}} \leq 2 \max_{\substack{v \in \mathcal{U} \\ \|v'\|_{\ell_\varepsilon^q}=1}} \langle u', v' \rangle. \tag{2}$$

We denote the space of linear functionals on $\mathcal{U}$ by $\mathcal{U}^*$. For $g \in \mathcal{U}^*$, $s = 0, 1$, and $1 \leq p \leq \infty$, we define the negative norms $\|g\|_{\mathcal{U}^{-s,p}}$ by

$$\|g\|_{\mathcal{U}^{-s,p}} := \sup_{\substack{v \in \mathcal{U} \\ \|v\|_{\mathcal{U}^{s,q}} = 1}} \langle g, v \rangle,$$

where $1 \leq q \leq \infty$ satisfies $\frac{1}{p} + \frac{1}{q} = 1$. We let $\mathcal{U}^{-s,p}$ denote the dual space $\mathcal{U}^*$ equipped with the $\mathcal{U}^{-s,p}$ norm.

For a linear mapping $A : \mathcal{U}_1 \to \mathcal{U}_2$ where $\mathcal{U}_i$ are vector spaces equipped with the norms $\|\cdot\|_{\mathcal{U}_i}$, we denote the operator norm of A by

$$\|A\|_{L(\mathcal{U}_1, \, \mathcal{U}_2)} := \sup_{v \in \mathcal{U}, \, v \neq 0} \frac{\|Av\|_{\mathcal{U}_2}}{\|v\|_{\mathcal{U}_1}}.$$

If $\mathcal{U}_1 = \mathcal{U}_2$, then we use the more concise notation

$$\|A\|_{\mathcal{U}_1} := \|A\|_{L(\mathcal{U}_1, \, \mathcal{U}_1)}.$$

If $A : \mathcal{U}^{0,2} \to \mathcal{U}^{0,2}$ is invertible, then we can define the *condition number* by

$$\mathrm{cond}(A) = \|A\|_{\mathcal{U}^{0,2}} \cdot \|A^{-1}\|_{\mathcal{U}^{0,2}}.$$

When A is symmetric and positive definite, we have that

$$\mathrm{cond}(A) = \lambda^A_{2N-1} / \lambda^A_1$$

where the eigenvalues of A are $0 < \lambda^A_1 \leq \cdots \leq \lambda^A_{2N-1}$. If a linear mapping $A : \mathcal{U} \to \mathcal{U}$ is symmetric and positive definite, then we define the A-inner product and A-norm by

$$\langle v, w \rangle_A := \langle Av, w \rangle, \qquad \|v\|^2_A = \langle Av, v \rangle.$$

The operator $A : \mathcal{U}_1 \to \mathcal{U}_2$ is *operator stable* if the operator norm $\|A^{-1}\|_{L(\mathcal{U}_2, \, \mathcal{U}_1)}$ is finite, and a sequence of operators $A_j : \mathcal{U}_{1,j} \to \mathcal{U}_{2,j}$ is *operator stable* if the sequence $\|(A_j)^{-1}\|_{L(\mathcal{U}_{2,j}, \, \mathcal{U}_{1,j})}$ is uniformly bounded. A symmetric operator $A : \mathcal{U}^{0,2} \to \mathcal{U}^{0,2}$ is called *stable* if it is positive definite, and this implies operator stability. A sequence of positive definite, symmetric operators $A_j : \mathcal{U}^{0,2} \to \mathcal{U}^{0,2}$ is called *stable* if their smallest eigenvalues $\lambda^{A_j}_1$ are uniformly bounded away from zero.

2.2. **The atomistic model.**

We now consider a one-dimensional atomistic chain whose $2N + 3$ atoms have the reference positions $x_j = j\varepsilon$ for $\varepsilon = 1/N$, and interact only with their nearest and next-nearest neighbors.

We denote the deformed positions by y_j, $j = -N - 1, \ldots, N + 1$; and we constrain the boundary atoms and their next-nearest neighbors to match the uniformly deformed state, $y^F_j = Fj\varepsilon$, where $F > 0$ is a macroscopic strain, that is,

$$\begin{aligned} y_{-N-1} &= -F(N+1)\varepsilon, & y_{-N} &= -FN\varepsilon, \\ y_N &= FN\varepsilon, & y_{N+1} &= F(N+1)\varepsilon. \end{aligned} \tag{3}$$

We introduced the two additional atoms with indices $\pm(N + 1)$ so that $y = y^F$ is an equilibrium of the atomistic model. The total energy of a deformation $y \in \mathbb{R}^{2N+3}$ is now given by

$$\mathcal{E}^{\mathrm{a}}(y) - \sum_{j=-N}^{N} \varepsilon f_j y_j,$$

where

$$\mathcal{E}^{\mathrm{a}}(y) \sum_{j=-N}^{N+1} \varepsilon\phi\Big(\frac{y_j - y_{j-1}}{\varepsilon}\Big) = \sum_{j=-N}^{N+1} \varepsilon\phi(y_j') + \sum_{j=-N+1}^{N+1} \varepsilon\phi(y_j' + y_{j-1}'). \quad (4)$$

Here, ϕ is a scaled two-body interatomic potential (for example, the normalized Lennard-Jones potential, $\phi(r) = r^{-12} - 2r^{-6}$), and f_j, $j = -N, \ldots, N$, are external forces. The equilibrium equations are given by the force balance conditions at the unconstrained atoms,

$$\begin{aligned} -\mathcal{F}_j^{\mathrm{a}}(y^{\mathrm{a}}) &= f_j && \text{for} \quad j = -N+1, \ldots, N-1, \\ y_j^{\mathrm{a}} &= Fj\varepsilon && \text{for} \quad j = -N-1, -N, N, N+1, \end{aligned} \quad (5)$$

where the atomistic force (per lattice spacing ε) is given by

$$\begin{aligned} \mathcal{F}_j^{\mathrm{a}}(y) :&= -\frac{1}{\varepsilon}\frac{\partial \mathcal{E}^a(y)}{\partial y_j} \\ &= \frac{1}{\varepsilon}\Big\{ \big[\phi'(y_{j+1}') + \phi'(y_{j+2}' + y_{j+1}')\big] - \big[\phi'(y_j') + \phi'(y_j' + y_{j-1}')\big] \Big\}. \end{aligned} \quad (6)$$

We linearize (6) by letting $u \in \mathbb{R}^{2N+3}$, $u_{\pm N} = u_{\pm(N+1)} = 0$, be a "small" displacement from the uniformly deformed state $y_j^F = Fj\varepsilon$; that is, we define

$$u_j = y_j - y_j^F \quad \text{for } j = -N-1, \ldots, N+1.$$

We then linearize the atomistic equilibrium equations (5) about the uniformly deformed state y^F and obtain a linear system for the displacement u^a,

$$\begin{aligned} (L_F^{\mathrm{a}} u^{\mathrm{a}})_j &= f_j && \text{for} \quad j = -N+1, \ldots, N-1, \\ u_j^a &= 0 && \text{for} \quad j = -N-1, -N, N, N+1, \end{aligned}$$

where $(L_F^{\mathrm{a}} v)_j$ is given by

$$(L_F^{\mathrm{a}} v)_j := \phi_F'' \left[\frac{-v_{j+1} + 2v_j - v_{j-1}}{\varepsilon^2}\right] + \phi_{2F}'' \left[\frac{-v_{j+2} + 2v_j - v_{j-2}}{\varepsilon^2}\right].$$

Here and throughout we define

$$\phi_F'' := \phi''(F) \quad \text{and} \quad \phi_{2F}'' := \phi''(2F),$$

where ϕ is the interatomic potential in (4). We will always assume that $\phi_F'' > 0$ and $\phi_{2F}'' < 0$, which holds for typical pair potentials such as the Lennard-Jones potential under physically realistic deformations.

The stability properties of L_F^{a} can be understood by using a representation derived in [9],

$$\langle L_F^{\mathrm{a}} u, u \rangle = \varepsilon A_F \sum_{\ell=-N+1}^{N} |u_\ell'|^2 - \varepsilon^3 \phi_{2F}'' \sum_{\ell=-N}^{N} |u_\ell''|^2 = A_F \|u'\|_{\ell_\varepsilon^2}^2 - \varepsilon^2 \phi_{2F}'' \|u''\|_{\ell_\varepsilon^2}^2, \quad (7)$$

where A_F is the *continuum elastic modulus*

$$A_F = \phi_F'' + 4\phi_{2F}''.$$

We can obtain the following result from the argument in [9, Prop. 1] and [12].

Proposition 1. *If $\phi_{2F}'' \leq 0$, then*

$$\min_{\substack{u \in \mathbb{R}^{2N+3} \setminus \{0\} \\ u_{\pm N} = u_{\pm(N+1)} = 0}} \frac{\langle L_F^a u, u \rangle}{\|u'\|_{\ell_\varepsilon^2}^2} = A_F - \varepsilon^2 \nu_\varepsilon \phi_{2F}'',$$

where

$$\nu_\varepsilon := \min_{\substack{u \in \mathbb{R}^{2N+3} \setminus \{0\} \\ u_{\pm N} = u_{\pm(N+1)} = 0}} \frac{\|u''\|_{\ell_\varepsilon^2}^2}{\|u'\|_{\ell_\varepsilon^2}^2}.$$

satisfies $0 < \nu_\varepsilon \leq C$ for some universal constant C.

2.2.1. *The critical strain F_*.* The previous result shows that L_F^a is positive definite, uniformly as $N \to \infty$, if and only if $A_F > 0$. For realistic interaction potentials, L_F^a is positive definite in a ground state $F_0 > 0$. For simplicity, we assume that $F_0 = 1$, and we ask how far the system can be "stretched" by applying increasing macroscopic strains F until it loses its stability. In the limit as $N \to \infty$, this happens at the *critical strain F_**, which is the smallest number larger than F_0, solving the equation

$$A_{F_*} = \phi''(F_*) + 4\phi''(2F_*) = 0. \tag{8}$$

2.3. **The local QC approximation (QCL).** The local quasicontinuum (QCL) approximation uses the Cauchy-Born approximation to approximate the nonlocal atomistic model by a local continuum model [5, 23, 26]. For next-nearest neighbor interactions, the Cauchy-Born approximation reads

$$\phi\left(\varepsilon^{-1}(y_{\ell+1} - y_{\ell-1})\right) \approx \tfrac{1}{2}\left[\phi(2y_\ell') + \phi(2y_{\ell+1}')\right],$$

and results in the QCL energy, for $y \in \mathbb{R}^{2N+3}$ satisfying the boundary conditions (3),

$$\begin{aligned}
\mathcal{E}^{\mathrm{qcl}}(y) = \sum_{j=-N+1}^{N} &\varepsilon\left[\phi(y_j') + \phi(2y_j')\right] \\
&+ \varepsilon\left[\phi(y_{-N}') + \frac{1}{2}\phi(2y_{-N}') + \phi(y_{N+1}') + \frac{1}{2}\phi(2y_{N+1}')\right].
\end{aligned} \tag{9}$$

Imposing the artificial boundary conditions of zero displacement from the uniformly deformed state, $y_j^F = Fj\varepsilon$, we obtain the QCL equilibrium equations

$$\begin{aligned}
-\mathcal{F}_j^{\mathrm{qcl}}(y^{\mathrm{qcl}}) &= f_j \qquad \text{for} \quad j = -N+1, \ldots, N-1, \\
y_j^{\mathrm{qcl}} &= Fj\varepsilon \qquad \text{for} \quad j = -N, N,
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{F}_j^{\mathrm{qcl}}(y) :&= -\frac{1}{\varepsilon}\frac{\partial \mathcal{E}^{\mathrm{qcl}}(y)}{\partial y_j} \\
&= \frac{1}{\varepsilon}\left\{\left[\phi'(y_{j+1}') + 2\phi'(2y_{j+1}')\right] - \left[\phi'(y_j') + 2\phi'(2y_j')\right]\right\}.
\end{aligned} \tag{10}$$

We see from (10) that the QCL equilibrium equations are well-defined with only a single constraint at each boundary, and we can restrict our consideration to $y \in \mathbb{R}^{2N+1}$ with $y_{-N} = -F$ and $y_N = F$ as the boundary conditions.

Linearizing the QCL equilibrium equations (10) about y^F results in the system

$$(L_F^{\mathrm{qcl}} u^{\mathrm{qcl}})_j = f_j \qquad \text{for} \quad j = -N+1, \ldots, N-1,$$

$$u_j^{\mathrm{qcl}} = 0 \qquad \text{for} \quad j = -N, \, N,$$

where

$$L_F^{\mathrm{qcl}} = A_F L$$

and L is the discrete Laplacian, for $v \in \mathcal{U}$, given by

$$(Lv)_j := -v_j'' = \left[\frac{-v_{j+1} + 2v_j - v_{j-1}}{\varepsilon^2} \right], \quad j = -N+1, \ldots, N-1. \qquad (11)$$

The QCL operator is a scaled discrete Laplace operator, so

$$\langle L_F^{\mathrm{qcl}} u, u \rangle = A_F \|u'\|_{\ell_\varepsilon^2}^2 \qquad \text{for all } u \in \mathcal{U}.$$

In particular, it follows that L_F^{qcl} is stable if and only if $A_F > 0$, that is, if and only if $F < F_*$, where F_* is the critical strain defined in (8).

2.4. The force-based QC approximation (QCF).
The force-based quasicontinuum (QCF) method combines the accuracy of the atomistic model with the efficiency of the QCL approximation by decomposing the computational reference lattice into an *atomistic region* $\mathcal{A}$ and a *continuum region* $\mathcal{C}$, and assigns forces to atoms according to the region they are located in. The QCF operator is given by [5,6]

$$\mathcal{F}_j^{\mathrm{qcf}}(y) := \begin{cases} \mathcal{F}_j^{\mathrm{a}}(y) & \text{if } j \in \mathcal{A}, \\ \mathcal{F}_j^{\mathrm{qcl}}(y) & \text{if } j \in \mathcal{C}, \end{cases} \qquad (12)$$

and the QCF equilibrium equations are given by

$$-\mathcal{F}_j^{\mathrm{qcf}}(y^{\mathrm{qcf}}) = f_j \qquad \text{for} \quad j = -N+1, \ldots, N-1,$$

$$y_j^{\mathrm{qcf}} = Fj\varepsilon \qquad \text{for} \quad j = -N, \, N.$$

We note that, since atoms near the boundary belong to $\mathcal{C}$, only one boundary condition is required at each end.

For simplicity, we specify the atomistic and continuum regions as follows. We fix $K \in \mathbb{N}$, $1 \le K \le N-2$, and define

$$\mathcal{A} = \{-K, \ldots, K\} \quad \text{and} \quad \mathcal{C} = \{-N+1, \ldots, N-1\} \setminus \mathcal{A}.$$

Linearizing (12) about y^F, we obtain

$$(L_F^{\mathrm{qcf}} u^{\mathrm{qcf}})_j = f_j \qquad \text{for} \quad j = -N+1, \ldots, N-1,$$

$$u_j^{\mathrm{qcf}} = 0 \qquad \text{for} \quad j = -N, \, N, \qquad (13)$$

where the linearized force-based operator is given explicitly by

$$(L_F^{\mathrm{qcf}} v)_j := \begin{cases} (L_F^{\mathrm{qcl}} v)_j, & \text{for } j \in \mathcal{C}, \\ (L_F^{\mathrm{a}} v)_j, & \text{for } j \in \mathcal{A}. \end{cases}$$

The stability analysis of the QCF operator L_F^{qcf} is less straightforward [10, 11]; we will therefore treat it separately and postpone it to Section 3.

2.5. **The original energy-based QC approximation (QCE).** The original energy-based quasicontinuum (QCE) method [26] defines an energy functional by assigning atomistic energy contributions in the atomistic region and continuum energy contributions in the continuum region. For our model problem, we obtain

$$\mathcal{E}^{\text{qce}}(y) = \varepsilon \sum_{\ell \in \mathcal{A}} \mathcal{E}_\ell^a(y) + \varepsilon \sum_{\ell \in \mathcal{C}} \mathcal{E}_\ell^c(y) \quad \text{for } y \in \mathbb{R}^{2N+1},$$

where

$$\mathcal{E}_\ell^c(y) = \tfrac{1}{2}\big(\phi(2y_\ell') + \phi(y_\ell') + \phi(y_{\ell+1}') + \phi(2y_{\ell+1}')\big), \quad \text{and}$$
$$\mathcal{E}_\ell^a(y) = \tfrac{1}{2}\big(\phi(y_{\ell-1}' + y_\ell') + \phi(y_\ell') + \phi(y_{\ell+1}') + \phi(y_{\ell+1}' + y_{\ell+2}')\big).$$

The QCE method is patch tests inconsistent [7, 8, 25, 31], which can be seen from the existence of "ghost forces" at the interface, that is, $\nabla \mathcal{E}^{\text{qce}}(y^F) = g^F \neq 0$. Hence, the linearization of the QCE equilibrium equations about y^F takes the form (see [8, Section 2.4] and [7, Section 2.4] for more detail)

$$
\begin{aligned}
(L_F^{\text{qce}} u^{\text{qce}})_j - g_j^F &= f_j && \text{for} \quad j = -N+1, \dots, N-1, \\
u_j^{\text{qce}} &= 0 && \text{for} \quad j = -N,\, N,
\end{aligned}
\tag{14}
$$

where, for $0 \le j \le N-1$, we have

$$(L_F^{\text{qce}} v)_j = \phi_F'' \frac{-v_{j+1} + 2v_j - v_{j-1}}{\varepsilon^2}$$

$$
+ \phi_{2F}'' \begin{cases}
4\dfrac{-v_{j+2} + 2v_j - v_{j-2}}{4\varepsilon^2}, & 0 \le j \le K-2, \\[2ex]
4\dfrac{-v_{j+2} + 2v_j - v_{j-2}}{4\varepsilon^2} + \dfrac{1}{\varepsilon}\dfrac{v_{j+2} - v_j}{2\varepsilon}, & j = K-1, \\[2ex]
4\dfrac{-v_{j+2} + 2v_j - v_{j-2}}{4\varepsilon^2} - \dfrac{2}{\varepsilon}\dfrac{v_{j+1} - v_j}{\varepsilon} + \dfrac{1}{\varepsilon}\dfrac{v_{j+2} - v_j}{2\varepsilon}, & j = K, \\[2ex]
4\dfrac{-v_{j+1} + 2v_j - v_{j-1}}{\varepsilon^2} - \dfrac{2}{\varepsilon}\dfrac{v_j - v_{j-1}}{\varepsilon} + \dfrac{1}{\varepsilon}\dfrac{v_j - v_{j-2}}{2\varepsilon}, & j = K+1, \\[2ex]
4\dfrac{-v_{j+1} + 2v_j - v_{j-1}}{\varepsilon^2} + \dfrac{1}{\varepsilon}\dfrac{v_j - v_{j-2}}{2\varepsilon}, & j = K+2, \\[2ex]
4\dfrac{-v_{j+1} + 2v_j - v_{j-1}}{\varepsilon^2}, & K+3 \le j \le N-1,
\end{cases}
$$

and where the vector of "ghost forces," g, is defined by

$$
g_j^F = \begin{cases}
0, & 0 \le j \le K-2, \\
-\tfrac{1}{2\varepsilon}\phi_{2F}', & j = K-1, \\
\tfrac{1}{2\varepsilon}\phi_{2F}', & j = K, \\
\tfrac{1}{2\varepsilon}\phi_{2F}', & j = K+1, \\
-\tfrac{1}{2\varepsilon}\phi_{2F}', & j = K+2, \\
0, & K+3 \le j \le N-1.
\end{cases}
$$

The equations for $j = -N+1, \dots, -1$ follow from symmetry.

The following result is a new sharp stability estimate for the QCE operator L_F^{qce}. Its somewhat technical proof is given in Appendix 8.1.

Theorem 2. *If $K \geq 1$, $N \geq K + 2$, and $\phi_{2F}'' \leq 0$, then*

$$\inf_{\substack{u \in \mathcal{U} \\ \|u'\|_{\ell_\varepsilon^2}=1}} \langle L_F^{\text{qce}} u, u \rangle = A_F + \lambda_K \phi_{2F}'',$$

where $\frac{1}{2} \leq \lambda_K \leq 1$. Asymptotically, as $K \to \infty$, we have

$$\lambda_K \sim \lambda_* + O(e^{-cK}) \quad \text{where } \lambda_* \approx 0.6595 \text{ and } c \approx 1.5826.$$

2.6. **The quasi-nonlocal QC approximation (QNL).** The QCF method is the simplest idea to circumvent the interface inconsistency of the QCE method, but gives non-conservative equilibrium equations [5]. An alternative energy-based approach was suggested in [14, 33], which is based on a modification of the energy at the interface. The quasi-nonlocal approximation (QNL) is given by the energy functional

$$\mathcal{E}^{\text{qnl}}(y) := \varepsilon \sum_{\ell=-N+1}^{N} \phi(y_\ell') + \varepsilon \sum_{\ell \in \mathcal{A}} \phi(y_\ell' + y_{\ell+1}') + \varepsilon \sum_{\ell \in \mathcal{C}} \tfrac{1}{2}\big[\phi(2y_\ell') + \phi(2y_{\ell+1}')\big],$$

where we set $\phi(y_{-N}') = \phi(y_{N+1}') = 0$. The QNL approximation is patch test consistent; that is, $y = y^F$ is an equilibrium of the QNL energy functional.

The linearization of the QNL equilibrium equations about y^F is

$$(L_F^{\text{qnl}} u^{\text{qnl}})_j = f_j \qquad \text{for} \quad j = -N+1, \ldots, N-1,$$
$$u_j^{\text{qnl}} = 0 \qquad \text{for} \quad j = -N, \, N,$$

where

$$(L_F^{\text{qnl}} v)_j = \phi_F'' \frac{-v_{j+1} + 2v_j - v_{j-1}}{\varepsilon^2}$$

$$+ \phi_{2F}'' \begin{cases} 4\dfrac{-v_{j+2} + 2v_j - v_{j-2}}{4\varepsilon^2}, & 0 \leq j \leq K-1, \\[2mm] 4\dfrac{-v_{j+2} + 2v_j - v_{j-2}}{4\varepsilon^2} - \dfrac{-v_{j+2} + 2v_{j+1} - v_j}{\varepsilon^2}, & j = K, \\[2mm] 4\dfrac{-v_{j+1} + 2v_j - v_{j-1}}{\varepsilon^2} + \dfrac{-v_j + 2v_{j-1} - v_{j-2}}{\varepsilon^2}, & j = K+1, \\[2mm] 4\dfrac{-v_{j+1} + 2v_j - v_{j-1}}{\varepsilon^2}, & K+2 \leq j \leq N-1. \end{cases} \quad (15)$$

We can repeat our stability analysis for the periodic QNL operator in [9, Sec. 3.3] verbatim to obtain the following result.

Proposition 3. *If $K < N - 1$, and $\phi_{2F} \leq 0$, then*

$$\inf_{\substack{u \in \mathcal{U} \\ \|u'\|_{\ell_\varepsilon^2}=1}} \langle L_F^{\text{qnl}} u, u \rangle = A_F.$$

Remark 1. Since $\phi_{2F}'' = (A_F - \phi_F'')/4$, the linearized operators $(\phi_F'')^{-1}L_F^{\mathrm{a}}$, $(\phi_F'')^{-1}L_F^{\mathrm{qcl}}$, $(\phi_F'')^{-1}L_F^{\mathrm{qcf}}$, $(\phi_F'')^{-1}L_F^{\mathrm{qce}}$, and $(\phi_F'')^{-1}L_F^{\mathrm{qnl}}$ depend only on A_F/ϕ_F'', N and K. $\qquad\square$

3. Stability and Spectrum of the QCF operator

In this section, we give various properties of the linearized QCF operator, most of which are variants of our results in [10,11]. We first give a result for the non-coercivity of the QCF operator which lies at the heart of many of the difficulties one encounters in analyzing the QCF method.

Theorem 4 (Theorem 1, [11]). *If $\phi_F'' > 0$ and $\phi_{2F}'' \in \mathbb{R} \setminus \{0\}$ then, for sufficiently large N, the operator L_F^{qcf} is* not *positive-definite. More precisely, there exist $N_0 \in \mathbb{N}$ and $C_1 \geq C_2 > 0$ such that, for all $N \geq N_0$ and $2 \leq K \leq N/2$,*

$$-C_1 N^{1/2} \leq \inf_{\substack{v \in \mathcal{U} \\ \|v'\|_{\ell_\varepsilon^2}=1}} \left\langle L_F^{\mathrm{qcf}} v, v \right\rangle \leq -C_2 N^{1/2}.$$

The proof of Theorem 4 yields also the following asymptotic result on the operator norm of L_F^{qcf}. Its proof is a straightforward extension of [11, Lemma 2], which covers the case $p = 2$, and we therefore omit it.

Lemma 5. *Let $\phi_{2F}'' \neq 0$, then there exists a constant $C_3 > 0$ such that for sufficiently large N, and for $2 \leq K \leq N/2$,*

$$C_3^{-1} N^{1/p} \leq \left\| L_F^{\mathrm{qcf}} \right\|_{L(\mathcal{U}^{1,p},\, \mathcal{U}^{-1,p})} \leq C_3 N^{1/p}.$$

As a consequence of Theorem 4 and Lemma 5, we analyzed the stability of L_F^{qcf} in alternative norms. By following the proof of [10, Theorem 3] verbatim (see also [10, Remark 3]), we can obtain the following sharp stability result.

Proposition 6. *If $A_F > 0$ and $\phi_{2F}'' \leq 0$, then L_F^{qcf} is invertible with*

$$\left\| (L_F^{\mathrm{qcf}})^{-1} \right\|_{L(\mathcal{U}^{0,\infty},\, \mathcal{U}^{2,\infty})} \leq 1/A_F.$$

If $A_F = 0$, then L_F^{qcf} is singular.

This result shows that L_F^{qcf} is operator stable up to the critical strain F_* at which the atomistic model loses its stability as well (cf. Section 2.2).

3.1. **Spectral properties of L_F^{qcf} in $\mathcal{U}^{0,2} = \ell_\varepsilon^2$.** The spectral properties of the L_F^{qcf} operator are fundamental for the analysis of the performance of iterative methods in Hilbert spaces. The basis of our analysis of L_F^{qcf} in the Hilbert space $\mathcal{U}^{0,2}$ is the surprising observation that, even though L_F^{qcf} is non-normal, it is nevertheless diagonalizable and its spectrum is identical to that of L_F^{qnl}. We first observed this numerically in [10, Section 4.4] for the case of periodic boundary conditions. A proof has since been

given in [13, Section 3], which translates verbatim to the case of Dirichlet boundary conditions and yields the following result.

Lemma 7. *For all $N \geq 4$, $1 \leq K \leq N - 2$, we have the identity*

$$L_F^{\mathrm{qcf}} = L^{-1} L_F^{\mathrm{qnl}} L. \tag{16}$$

In particular, the operator L_F^{qcf} is diagonalizable and its spectrum is identical to the spectrum of L_F^{qnl}.

We denote the eigenvalues of L_F^{qnl} (and L_F^{qcf}) by

$$0 < \lambda_1^{\mathrm{qnl}} \leq ... \lambda_\ell^{\mathrm{qnl}} \leq ... \leq \lambda_{2N-1}^{\mathrm{qnl}}.$$

The following lemma gives a lower bound for λ_1^{qnl}, an upper bound for $\lambda_{2N-1}^{\mathrm{qnl}}$, and consequently an upper bound for $\mathrm{cond}(L_F^{\mathrm{qnl}}) = \lambda_{2N-1}^{\mathrm{qnl}} / \lambda_1^{\mathrm{qnl}}$.

Lemma 8. *If $K < N - 1$ and $\phi_{2F}'' \leq 0$, then*

$$\lambda_1^{\mathrm{qnl}} \geq 2 A_F, \qquad \lambda_{2N-1}^{\mathrm{qnl}} \leq (A_F - 4\phi_{2F}'') \varepsilon^{-2} = \phi_F'' \varepsilon^{-2}, \quad and$$

$$\mathrm{cond}(L_F^{\mathrm{qnl}}) = \frac{\lambda_{2N-1}^{\mathrm{qnl}}}{\lambda_1^{\mathrm{qnl}}} \leq \left(\frac{\phi_F''}{2 A_F} \right) \varepsilon^{-2}.$$

For the analysis of iterative methods, we are also interested in the condition number of a basis of eigenvectors of L_F^{qcf} as N tends to infinity. Employing Lemma 7, we can write $L_F^{\mathrm{qcf}} = L^{-1} \Lambda^{\mathrm{qcf}} L$ where L is the discrete Laplacian operator and Λ^{qcf} is diagonal. The columns of L^{-1} are poorly scaled; however, a simple rescaling was found in [13, Thm. 3.3] for periodic boundary conditions. The construction and proof translate again verbatim to the case of Dirichlet boundary conditions and yield the following result (note, in particular, that the main technical step, [13, Lemma 4.6] can be applied directly).

Lemma 9. *Let $A_F > 0$, then there exists a matrix V of eigenvectors for the force-based QC operator L_F^{qcf} such that $\mathrm{cond}(V)$ is bounded above by a constant that is independent of N.*

3.2. **Spectral properties of L_F^{qcf} in $\mathcal{U}^{1,2}$.** In our analysis below, particularly in Sections 6.1 and 6.2, we will see that the preconditioner $L_F^{\mathrm{qcl}} = A_F L$ is a promising candidate for the efficient solution of the QCF system. The operator $L^{1/2}$ can be understood as a basis transformation to an orthonormal basis in $\mathcal{U}^{1,2}$. Hence, it will be useful to study the spectral properties of L_F^{qcf} in that space. The relevant (generalized) eigenvalue problem is

$$L_F^{\mathrm{qcf}} v = \lambda L v, \qquad v \in \mathcal{U}, \tag{17}$$

which can, equivalently, be written as

$$L^{-1} L_F^{\mathrm{qcf}} v = \lambda v, \qquad v \in \mathcal{U}, \tag{18}$$

or as

$$L^{-1/2} L_F^{\mathrm{qcf}} L^{-1/2} w = \lambda w, \qquad w \in \mathcal{U}, \tag{19}$$

with the basis transform $w = L^{1/2}v$, in either case reducing it to a standard eigenvalue problem in ℓ_ε^2. Since L and $L^{1/2}$ commute, Lemma 7 immediately yields the following result.

Lemma 10. *For all $N \geq 4$, $1 \leq K \leq N - 2$ the operator $L^{-1}L_F^{\mathrm{qcf}}$ is diagonalizable and its spectrum is identical to the spectrum of $L^{-1}L_F^{\mathrm{qnl}}$.*

We gave a proof in [12] of the following lemma, which completely characterizes the spectrum of $L^{-1}L_F^{\mathrm{qnl}}$, and thereby also the spectrum of $L^{-1}L_F^{\mathrm{qcf}}$. We denote the spectrum of $L^{-1}L_F^{\mathrm{qnl}}$ (and $L^{-1}L_F^{\mathrm{qcf}}$) by $\{\mu_j^{\mathrm{qnl}} : j = 1, \ldots, 2N - 1\}$.

Lemma 11. *Let $K \leq N - 2$ and $A_F > 0$, then the (unordered) spectrum of $L^{-1}L_F^{\mathrm{qnl}}$ (that is, the $\mathcal{U}^{1,2}$-spectrum) is given by*

$$\mu_j^{\mathrm{qnl}} = \begin{cases} A_F - 4\phi_{2F}'' \sin^2\left(\frac{j\pi}{4K+4}\right), & j = 1, \ldots, 2K + 1, \\ A_F, & j = 2K + 2, \ldots, 2N - 1. \end{cases}$$

In particular, if $\phi_{2F}'' \leq 0$, then

$$\frac{\max_j \mu_j^{\mathrm{qnl}}}{\min_j \mu_j^{\mathrm{qnl}}} = 1 - \frac{4\phi_{2F}''}{A_F}\sin^2\left(\frac{(2K+1)\pi}{4K+4}\right) = \frac{\phi_F''}{A_F} + \frac{4\phi_{2F}''}{A_F}\sin^2\left(\frac{\pi}{4K+4}\right) = \frac{\phi_F''}{A_F} + O(K^{-2}).$$

We conclude this study by stating a result on the condition number of the matrix of eigenvectors for the eigenvalue problem (19). Letting $\tilde{V}$ be an orthogonal matrix of eigenvectors of $L^{-1/2}L_F^{\mathrm{qnl}}L^{-1/2}$ and $\tilde{\Lambda}$ the corresponding diagonal matrix, then Lemma 7 yields

$$L^{-1/2}L_F^{\mathrm{qcf}}L^{-1/2} = L^{-1}\big[L^{-1/2}L_F^{\mathrm{qnl}}L^{-1/2}\big]L$$
$$= (\tilde{V}^T L)^{-1}\tilde{\Lambda}(\tilde{V}^T L).$$

Clearly, $\mathrm{cond}(\tilde{V}^T L) = O(N^2)$, which gives the following result.

Lemma 12. *If $A_F > 0$, then there exists a matrix $\widetilde{W}$ of eigenvectors for the preconditioned force-based QC operator $L^{-1/2}L_F^{\mathrm{qcf}}L^{-1/2}$, such that $\mathrm{cond}(\widetilde{W}) = O(N^2)$ as $N \to \infty$.*

4. Linear Stationary Iterative Methods

In this section, we investigate linear stationary iterative methods to solve the linearized QCF equations (13). These are iterations of the form

$$P\big(u^{(n)} - u^{(n-1)}\big) = \alpha r^{(n-1)}, \tag{20}$$

where P is a nonsingular preconditioner, the step size parameter $\alpha > 0$ is constant (that is, stationary), and the residual is defined as

$$r^{(n)} := f - L_F^{\mathrm{qcf}}u^{(n)}.$$

The iteration error

$$e^{(n)} := u^{\mathrm{qcf}} - u^{(n)}$$

satisfies the recursion

$$Pe^{(n)} = (P - \alpha L_F^{\mathrm{qcf}})e^{(n-1)},$$

or equivalently,

$$e^{(n)} = (I - \alpha P^{-1} L_F^{\mathrm{qcf}})e^{(n-1)} =: Ge^{(n-1)}, \tag{21}$$

where the operator $G = I - \alpha P^{-1} L_F^{\mathrm{qcf}} : \mathcal{U} \to \mathcal{U}$ is called the *iteration matrix*. By iterating (21), we obtain that

$$e^{(n)} = (I - \alpha P^{-1} L_F^{\mathrm{qcf}})^n e^{(0)} = G^n e^{(0)}. \tag{22}$$

Before we investigate various preconditioners, we briefly review the classical theory of linear stationary iterative methods [29]. We see from (22) that the iterative method (20) converges for every initial guess $u^{(0)} \in \mathcal{U}$ if and only if $G^n \to 0$ as $n \to \infty$. For a given norm $\|v\|$, for $v \in \mathcal{U}$, we can see from (22) that the reduction in the error after n iterations is bounded above by

$$\|G^n\| = \sup_{e^{(0)} \in \mathcal{U}} \frac{\|e^{(n)}\|}{\|e^{(0)}\|}.$$

It can be shown [29] that the convergence of the iteration for every initial guess $u^{(0)} \in \mathcal{U}$ is equivalent to the condition $\rho(G) < 1$, where $\rho(G)$ is the *spectral radius* of G,

$$\rho(G) = \max\{|\lambda_i| : \lambda_i \text{ is an eigenvalue of } G\}.$$

In fact, the Spectral Radius Theorem [29] states that

$$\lim_{n \to \infty} \|G^n\|^{1/n} = \rho(G)$$

for any vector norm on $\mathcal{U}$. However, if $\rho(G) < 1$ and $\|G\| \geq 1$, the Spectral Radius Theorem does not give any information about how large n must be to obtain $\|G^n\| \leq 1$. On the other hand, if $\rho(G) < 1$, then there exists a norm $\|\cdot\|$ such that $\|G\| < 1$, so that G itself is a contraction [17]. In this case, we have the stronger contraction property that

$$\|e^{(n)}\| \leq \|G\| \|e^{(n-1)}\| \leq \|G\|^n \|e^{(0)}\|.$$

In the remainder of this section, we will analyze the norm of the iteration matrix, $\|G\|$, for several preconditioners P, using appropriate norms in each case.

5. The Richardson Iteration $(P = I)$

The simplest example of a linear iterative method is the Richardson iteration, where $P = I$. If follows from Lemma 9 that there exists a similarity transform S such that

$$L_F^{\mathrm{qcf}} = S^{-1} \Lambda^{\mathrm{qnl}} S, \tag{23}$$

where $\mathrm{cond}(S) \leq C$ (where C is independent of N), and Λ^{qnl} is the diagonal matrix of $\mathcal{U}^{0,2}$-eigenvalues $(\lambda_j^{\mathrm{qnl}})_{j=1}^{2N-1}$ of L_F^{qcf}. As an immediate consequence, we obtain the identity

$$G_{\mathrm{id}}(\alpha) = I - \alpha L_F^{\mathrm{qcf}} = S^{-1}(I - \alpha \Lambda^{\mathrm{qnl}})S,$$

where yields

$$\|G_{\mathrm{id}}(\alpha)\|_{\ell_\varepsilon^2} \leq \mathrm{cond}(S)\|I - \alpha \Lambda^{\mathrm{qnl}}\|_{\ell_\varepsilon^2} \leq C \max_{j=1,\dots,2N-1} |1 - \alpha \lambda_j^{\mathrm{qnl}}|. \tag{24}$$

If $A_F > 0$, then it follows from Proposition 3 that $\lambda_j^{\mathrm{qnl}} > 0$ for all j, and hence that the iteration matrix $G_{\mathrm{id}}(\alpha) := I - \alpha L_F^{\mathrm{qcf}}$ is a contraction in the $\|\cdot\|_{\ell_\varepsilon^2}$ norm if and only if $0 < \alpha < \alpha_{\max}^{\mathrm{id}} := 2/\lambda_{2N-1}^{\mathrm{qnl}}$. It follows from Lemma 8 that $\alpha_{\max}^{\mathrm{id}} \le (2\varepsilon^2)/\phi_F''$.

We can minimize the contraction constant for $G_{\mathrm{id}}(\alpha)$ in the $\|v\|_{S^T S}$ norm by choosing $\alpha = \alpha_{\mathrm{opt}}^{\mathrm{id}} := 2/(\lambda_1^{\mathrm{qnl}} + \lambda_{2N-1}^{\mathrm{qnl}})$, and in this case we obtain from Lemma 8 that

$$\left\| G_{\mathrm{id}}\big(\alpha_{\mathrm{opt}}^{\mathrm{id}}\big) \right\|_{\ell_\varepsilon^2} \le C \frac{\lambda_{2N-1}^{\mathrm{qnl}} - \lambda_1^{\mathrm{qnl}}}{\lambda_{2N-1}^{\mathrm{qnl}} + \lambda_1^{\mathrm{qnl}}} \le C\left(1 - \frac{2A_F\varepsilon^2}{\phi_F''} \right).$$

It thus follows that the contraction constant for $G_{\mathrm{id}}(\alpha)$ in the $\|\cdot\|_{\ell_\varepsilon^2}$ norm is only of the order $1 - O(\varepsilon^2)$, even with an optimal choice of α. This is the same generic behavior that is typically observed for Richardson iterations for discretized second-order elliptic differential operators.

5.1. **Numerical example for the Richardson Iteration.**

In Figure 1, we plot the error in the Richardson iteration against the iteration number. As a typical example, we use the right-hand side

$$f(x) = h(x)\cos(3\pi x) \quad \text{where} \quad h(x) = \begin{cases} 1, & x \ge 0, \\ -1, & x < 0, \end{cases} \tag{25}$$

which is smooth in the continuum region but has a discontinuity in the atomistic region. We choose $\phi_F'' = 1$, $A_F = 0.5$, and the optimal $\alpha = \alpha_{\mathrm{opt}}^{\mathrm{id}}$ discussed above (we note that $G_{\mathrm{id}}(\alpha_{\mathrm{opt}}^{\mathrm{id}})$ depends only on A_F/ϕ_F'' and N, but $e^{(0)}$ depends on A_F and ϕ_F'' independently) . We observe initially a much faster convergence rate than the one predicted because the initial residual for (25) has a large component in the eigenspaces corresponding to the intermediate eigenvalues λ_j^{qnl} for $1 < j < 2N - 1$. However, after a few iterations the convergence behavior approximates the predicted rate.

6. Preconditioning with QCL ($P = L_F^{\mathrm{qcl}} = A_F L$)

We have seen in Section 5 that the Richardson iteration with the trivial preconditioner $P = I$ converges slowly, and with a contraction rate of the order $1 - O(\varepsilon^2)$. The goal of a (quasi-)optimal preconditioner for large systems is to obtain a performance that is independent of the system size. We will show in the present section that the preconditioner $P = A_F L$ (the system matrix for the QCL method) has this desirable quality.

Of course, preconditioning with $P = A_F L$ comes at the cost of solving a large linear system at each iteration. However, the QCL operator is a standard elliptic operator for which efficient solution methods exist. For example, the preconditioner $P = A_F L$ could be replaced by a small number of multigrid iterations, which would lead to a solver with optimal complexity. Here, we will ignore these additional complications and assume that P is inverted exactly.

Throughout the present section, the iteration matrix is given by

$$G_{\mathrm{qcl}}(\alpha) := I - \alpha(L_F^{\mathrm{qcl}})^{-1} L_F^{\mathrm{qcf}} = I - \alpha(A_F L)^{-1} L_F^{\mathrm{qcf}}, \tag{26}$$
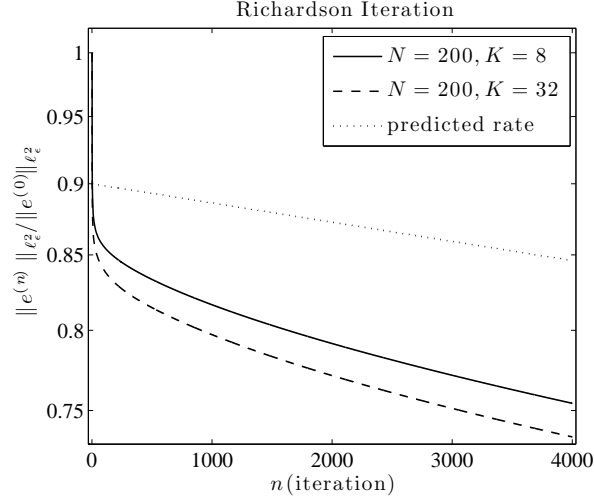
FIGURE 1. Normalized ℓ_ε^2-error of successive Richardson iterations for the linear QCF system with $N = 200, K = 8, 32, \phi_F'' = 1, A_F = 0.5$, optimal $\alpha = \alpha_{\mathrm{opt}}^{\mathrm{id}}$, right-hand side (25), and starting guess $u^{(0)} = 0$.

where $\alpha > 0$ and $A_F = \phi_F'' + 4\phi_{2F}'' > 0$. We will investigate whether, if $\mathcal{U}$ is equipped with a suitable topology, $G_{\mathrm{qcl}}(\alpha)$ becomes a contraction. To demonstrate that this is a non-trivial question, we first show that in the spaces $\mathcal{U}^{1,p}$, $1 \leq p < \infty$, which are natural choices for elliptic operators, this result does not hold.

Proposition 13. *If $2 \leq K \leq N/2$, $\phi_{2F}'' \neq 0$, and $p \in [1, \infty)$, then for any $\alpha > 0$ we have*
$$\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,p}} \sim N^{1/p} \qquad \text{as } N \to \infty.$$

Proof. We have from (2) and $q = p/(p-1)$ the inequality
$$\begin{aligned}
\left\|L^{-1}L_F^{\mathrm{qcf}}\right\|_{\mathcal{U}^{1,p}} &= \max_{\substack{u \in \mathcal{U} \\ \|u'\|_{\ell_\varepsilon^p}=1}} \left\|\left(L^{-1}L_F^{\mathrm{qcf}}u\right)'\right\|_{\ell_\varepsilon^p} \\
&\leq 2 \max_{\substack{u,v \in \mathcal{U} \\ \|u'\|_{\ell_\varepsilon^p}=1,\ \|v'\|_{\ell_\varepsilon^q}=1}} \left\langle \left(L^{-1}L_F^{\mathrm{qcf}}u\right)', v' \right\rangle \\
&= 2 \max_{\substack{u,v \in \mathcal{U} \\ \|u'\|_{\ell_\varepsilon^p}=1,\ \|v'\|_{\ell_\varepsilon^q}=1}} \left\langle L\left(L^{-1}L_F^{\mathrm{qcf}}u\right), v \right\rangle \\
&= 2 \max_{\substack{u,v \in \mathcal{U} \\ \|u'\|_{\ell_\varepsilon^p}=1,\ \|v'\|_{\ell_\varepsilon^q}=1}} \left\langle L_F^{\mathrm{qcf}}u, v \right\rangle \\
&= 2\left\|L_F^{\mathrm{qcf}}\right\|_{L(\mathcal{U}^{1,p},\ \mathcal{U}^{-1,p})}
\end{aligned}$$
as well as the reverse inequality
$$\left\|L_F^{\mathrm{qcf}}\right\|_{L(\mathcal{U}^{1,p},\ \mathcal{U}^{-1,p})} \leq \left\|L^{-1}L_F^{\mathrm{qcf}}\right\|_{\mathcal{U}^{1,p}}.$$

The result now follows from the definition of $G_{\mathrm{qcl}}(\alpha)$ in (26), Lemma 5, and the fact that $\alpha > 0$ and $A_F > 0$. $\qquad\square$

We will return to an analysis of the QCL preconditioner in the space $\mathcal{U}^{1,2}$ in Section 6.3, but will first attempt to prove convergence results in alternative norms.

6.1. **Analysis of the QCL preconditioner in $\mathcal{U}^{2,\infty}$.** We have found in our previous analyses of the QCF method [10, 11] that it has superior properties in the function spaces $\mathcal{U}^{1,\infty}$ and $\mathcal{U}^{2,\infty}$. Hence, we will now investigate whether α can be chosen such that $G_{\mathrm{qcl}}(\alpha)$ is a contraction, uniformly as $N \to \infty$. In [10], we have found that the analysis is easiest with the somewhat unusual choice $\mathcal{U}^{2,\infty}$. Hence we begin by analyzing $G_{\mathrm{qcl}}(\alpha)$ in this space.

To begin, we formulate a lemma in which we compute the operator norm of $G_{\mathrm{qcl}}(\alpha)$ explicitly. Its proof is slightly technical and is therefore postponed to Appendix 8.2.

Lemma 14. *If $N \geq 4$, then*

$$\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{2,\infty}} = \left|1 - \alpha\left(1 - \tfrac{2\phi''_{2F}}{A_F}\right)\right| + \alpha\left|\tfrac{2\phi''_{2F}}{A_F}\right|.$$

What is remarkable (though not necessarily surprising) about this result is that the operator norm of $G_{\mathrm{qcl}}(\alpha)$ is independent of N and K. This immediately puts us into a position where we can obtain contraction properties of the iteration matrix $G_{\mathrm{qcl}}(\alpha)$, that are uniform in N and K. It is worth noting, though, that the optimal contraction rate is not uniform as A_F approaches zero; that is, the preconditioner does not give uniform efficiency as the system approaches its stability limit.

Theorem 15. *Suppose that $N \geq 4$, $A_F > 0$, and $\phi''_{2F} \leq 0$, and define*

$$\alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty} := \frac{A_F}{A_F + 2|\phi''_{2F}|} = \frac{2A_F}{\phi''_F + A_F} \quad and \quad \alpha_{\max}^{\mathrm{qcl},2,\infty} := \frac{2A_F}{\phi''_F}.$$

Then $G_{\mathrm{qcl}}(\alpha)$ is a contraction of $\mathcal{U}^{2,\infty}$ if and only if $0 < \alpha < \alpha_{\max}^{\mathrm{qcl},2,\infty}$, and for any such choice the contraction rate is independent of N and K. The optimal choice is $\alpha = \alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}$, which gives the contraction rate

$$\left\|G_{\mathrm{qcl}}\left(\alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}\right)\right\|_{\mathcal{U}^{2,\infty}} = \frac{1 - \frac{A_F}{\phi''_F}}{1 + \frac{A_F}{\phi''_F}} < 1.$$

Proof. Note that $\alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty} = 1/\left(1 - \tfrac{2\phi''_{2F}}{A_F}\right)$. Hence, if we assume, first, that $0 < \alpha \leq \alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}$, then

$$\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{2,\infty}} = 1 - \alpha\left(1 - 2\tfrac{\phi''_{2F}}{A_F}\right) - 2\alpha\tfrac{\phi''_{2F}}{A_F} = 1 - \alpha =: m_1(\alpha).$$

The optimal choice is clearly $\alpha = \alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}$ which gives the contraction rate

$$\left\|G_{\mathrm{qcl}}\left(\alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}\right)\right\|_{\mathcal{U}^{2,\infty}} = \alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}\left|\tfrac{2\phi''_{2F}}{A_F}\right| = \frac{2|\phi''_{2F}|}{\phi''_F + 2\phi''_{2F}} = \frac{1 - \frac{A_F}{\phi''_F}}{1 + \frac{A_F}{\phi''_F}}.$$

Alternatively, if $\alpha \geq \alpha_{\text{opt}}^{\text{qcl},2,\infty}$, then

$$\left\|G_{\text{qcl}}(\alpha)\right\|_{\mathcal{U}^{2,\infty}} = \alpha\left(1 - \frac{4\phi_{2F}''}{A_F}\right) - 1 = \alpha\frac{\phi_F''}{A_F} - 1 =: m_2(\alpha).$$

This value is strictly increasing with α, hence the optimal choice is again $\alpha = \alpha_{\text{opt}}^{\text{qcl},2,\infty}$.

Moreover, we have $m_2(\alpha) < 1$ if and only if

$$\alpha < \frac{2A_F}{\phi_F''} = \alpha_{\max}^{\text{qcl},2,\infty}.$$

Since, for $\alpha = \alpha_{\text{opt}}^{\text{qcl},2,\infty}$ we have $m_1(\alpha) = m_2(\alpha) < 1$, it follows that $\alpha_{\max}^{\text{qcl},2,\infty} > \alpha_{\text{opt}}^{\text{qcl},2,\infty}$ (as a matter of fact, the condition $\alpha_{\max}^{\text{qcl},2,\infty} > \alpha_{\text{opt}}^{\text{qcl},2,\infty}$ is equivalent to $A_F > 0$). In conclusion, we have shown that $\|G_{\text{qcl}}(\alpha)\|_{\mathcal{U}^{2,\infty}}$ is independent of N and K and that it is strictly less than one if and only if $\alpha < \alpha_{\max}^{\text{qcl},2,\infty}$, with optimal value $\alpha = \alpha_{\text{opt}}^{\text{qcl},2,\infty}$. $\square$

As an immediate corollary, we obtain the following general convergence result.

Corollary 16. *Suppose that $N \geq 4$, $A_F > 0$, $\phi_{2F}'' \leq 0$, and suppose that $\|\cdot\|_X$ is a norm defined on $\mathcal{U}$ such that*

$$\|u\|_X \leq C\|u\|_{\mathcal{U}^{2,\infty}} \qquad \forall u \in \mathcal{U}.$$

Moreover, suppose that $0 < \alpha < \alpha_{\max}^{\text{qcl},2,\infty}$. Then, for any $u \in \mathcal{U}$,

$$\|G_{\text{qcl}}(\alpha)^n u\|_X \leq \hat{q}^n C\|u\|_{\mathcal{U}^{2,\infty}} \to 0 \quad \text{as } n \to \infty,$$

where $\hat{q} := \|G_{\text{qcl}}(\alpha)\|_{\mathcal{U}^{2,\infty}} < 1$.

In particular, the convergence is uniform among all N, K and all possible initial values $u \in \mathcal{U}$ for which a uniform bound on $\|u\|_{\mathcal{U}^{2,\infty}}$ holds.

Proof. We simply note that, according to Theorem 15, for $0 < \alpha < \alpha_{\max}^{\text{qcl},2,\infty}$, we have

$$\|G_{\text{qcl}}(\alpha)^n\|_{\mathcal{U}^{2,\infty}} \leq \hat{q}^n,$$

where $\hat{q} := \|G_{\text{qcl}}(\alpha)\|_{\mathcal{U}^{2,\infty}} < 1$ is a number that is independent of N and K. Hence, we have

$$\|G_{\text{qcl}}(\alpha)^n u\|_X \leq C\|G_{\text{qcl}}(\alpha)^n u\|_{\mathcal{U}^{2,\infty}} \leq C\hat{q}^n\|u\|_{\mathcal{U}^{2,\infty}}.$$

$\square$

Remark 2. Although we have seen in Theorem 15 and Corollary 16 that the linear stationary method with preconditioner $A_F L$ and with sufficiently small step size α is convergent, this convergence may still be quite slow if the initial data is "rough." Particularly in the context of defects, we may, for example, be interested in the convergence properties of this iteration when the initial residual is small or moderate in $\mathcal{U}^{1,p}$, for some $p \in [1,\infty]$, but possibly of order $O(N)$ in the $\mathcal{U}^{2,\infty}$-norm. We can see from the following Poincaré and inverse inequalities

$$\|u\|_{\mathcal{U}^{1,\infty}} \leq \frac{1}{2}\|u\|_{\mathcal{U}^{2,\infty}} \qquad \text{and} \qquad \|u\|_{\mathcal{U}^{2,\infty}} \leq 2N\|u\|_{\mathcal{U}^{1,\infty}} \qquad \text{for all } u \in \mathcal{U};$$

that the application of Corollary 16 to the case $X = \mathcal{U}^{1,\infty}$ gives the estimate

$$\|G_{\text{qcl}}(\alpha)^n u\|_{\mathcal{U}^{1,\infty}} \leq \hat{q}^n N\|u\|_{\mathcal{U}^{1,\infty}} \qquad \text{for all } u \in \mathcal{U}.$$

Similarly, with $X = \mathcal{U}^{1,2}$, we obtain

$$\|G_{\mathrm{qcl}}(\alpha)^n u\|_{\mathcal{U}^{1,2}} \leq \hat{q}^n N^{3/2} \|u\|_{\mathcal{U}^{1,2}} \qquad \text{for all } u \in \mathcal{U}. \tag{27}$$

We have seen in Proposition 13 that a direct convergence analysis in $\mathcal{U}^{1,p}$, $p < \infty$, may be difficult with analytical methods, hence we focus in the next section on the case $\mathcal{U}^{1,\infty}$. $\qquad \square$

6.2. **Analysis of the QCL preconditioner in $\mathcal{U}^{1,\infty}$.** As before, we first compute the operator norm of the iteration matrix explicitly. The proof of the following lemma is again postponed to the Appendix 8.2.

Lemma 17. *If $K \geq 3$, $N \geq \max(9, K + 3)$, and $\phi''_{2F} \leq 0$, then*

$$\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}} = \begin{cases} |1 - \alpha| + \alpha 4 \left| \frac{\phi''_{2F}}{A_F} \right| & \text{for } 0 \leq \alpha \leq \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}, \\ \left| 1 - \alpha \left(1 - 2\frac{\phi''_{2F}}{A_F} \right) \right| + \alpha(6 + 2\varepsilon - 4\varepsilon K) \left| \frac{\phi''_{2F}}{A_F} \right| & \text{for } \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty} \leq \alpha, \end{cases}$$

where

$$\alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty} := \left[1 + (2 + \varepsilon - 2\varepsilon K) \left| \frac{\phi''_{2F}}{A_F} \right| \right]^{-1}$$

satisfies $\alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty} \leq \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty} \leq 1$.

Again we note that the operator norm is independent, but now up to terms of order $\mathrm{O}(\varepsilon K)$, of the system size.

Theorem 18. *Suppose that $K \geq 3$, $N \geq \max(9, K + 3)$, and $\phi''_{2F} < 0$, then the following statements are true:*

(i) *If $\phi''_F + 8\phi''_{2F} \leq 0$, then $G_{\mathrm{qcl}}(\alpha)$ is not a contraction of $\mathcal{U}^{1,\infty}$, for any value of α.*

(ii) *If $\phi''_F + 8\phi''_{2F} > 0$, then $G_{\mathrm{qcl}}(\alpha)$ is a contraction for sufficiently small α. More precisely, setting*

$$\alpha_{\max}^{\mathrm{qcl},1,\infty} := \frac{2A_F}{A_F + (8 + 2\varepsilon - 4\varepsilon K)|\phi''_{2F}|},$$

we have that $G_{\mathrm{qcl}}(\alpha)$ is a contraction of $\mathcal{U}^{1,\infty}$ if and only if $0 < \alpha < \alpha_{\max}^{\mathrm{qcl},1,\infty}$. The operator norm $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}}$ is minimized by choosing $\alpha = \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}$ (cf. Lemma 17) and in this case

$$\left\| G_{\mathrm{qcl}}\left(\alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}\right) \right\|_{\mathcal{U}^{1,\infty}} = 1 - \frac{\phi''_F + 8\phi''_{2F}}{\phi''_F + (2 - \varepsilon + 2\varepsilon K)\phi''_{2F}} < 1.$$

Proof. Suppose, first, that $0 < \alpha \leq \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}$. Since $\alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty} \leq 1$ it follows that

$$\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}} = 1 - \alpha \frac{\phi''_F + 8\phi''_{2F}}{A_F},$$

and hence $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}} < 1$ if and only if $\phi''_F + 8\phi''_{2F} > 0$. In that case $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}}$ is strictly decreasing in $(0, \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}]$.

Since $\alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty} \geq \alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty} = (1 - 2\frac{\phi''_{2F}}{A_F})^{-1}$ we can see that $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}}$ is always strictly increasing in $[\alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}, +\infty)$ and hence if $\phi''_F + 8\phi''_{2F} > 0$, then $\alpha = \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}$ minimizes

the operator norm $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}}$. Moreover, straightforward computations show that $\alpha_{\max}^{\mathrm{qcl},1,\infty} > \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}$ and that $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}} < 1$ if and only if $0 < \alpha < \alpha_{\max}^{\mathrm{qcl},1,\infty}$. $\qquad\square$

We remark that the optimal value of α in $\mathcal{U}^{1,\infty}$, that is $\alpha = \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}$, is not the same as the optimal value, $\alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}$, in $\mathcal{U}^{2,\infty}$. However, it is easy to see that $\alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty} = \alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty} + O(\varepsilon K)$, and hence, even though $\alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}$ is not optimal in $\mathcal{U}^{1,\infty}$ it is still close to the optimal value. On the other hand, $\alpha_{\max}^{\mathrm{qcl},1,\infty}$ and $\alpha_{\max}^{\mathrm{qcl},2,\infty}$ are not close, since, if $4\varepsilon K - 2\varepsilon < 1$, then

$$\alpha_{\max}^{\mathrm{qcl},1,\infty} \leq \frac{2A_F}{\phi_F'' + 3|\phi_{2F}''|} < \frac{2A_F}{\phi_F''} = \alpha_{\max}^{\mathrm{qcl},2,\infty}.$$

In summary, we have seen that the contraction property of $G_{\mathrm{qcl}}(\alpha)$ in $\mathcal{U}^{1,\infty}$ is significantly more complicated than in $\mathcal{U}^{2,\infty}$, and that, in fact, $G_{\mathrm{qcl}}(\alpha)$ is *not* a contraction for all macroscopic strains F up to the critical strain F_*.

6.3. **Analysis of the QCL preconditioner in $\mathcal{U}^{1,2}$.** Even though we were able to prove uniform contraction properties for the QCL-preconditioned iterative method in $\mathcal{U}^{2,\infty}$, we have argued above that these are not entirely satisfactory in the presence of irregular solutions containing defects. Hence we analyzed the iteration matrix $G_{\mathrm{qcl}}(\alpha) = I - \alpha(A_F L)^{-1} L_F^{\mathrm{qcf}}$ in $\mathcal{U}^{1,\infty}$, but there we showed that it is not a contraction up to the critical load F_*. To conclude our results for the QCL preconditioner, we present a discussion of $G_{\mathrm{qcl}}(\alpha)$ in the space $\mathcal{U}^{1,2}$.

We begin by noting that it follows from (21) that

$$P^{1/2}e^{(n)} = P^{1/2}G_{\mathrm{qcl}}(\alpha)e^{(n-1)} = P^{1/2}\left(I - \alpha P^{-1}L_F^{\mathrm{qcf}}\right)P^{-1/2}\left(P^{1/2}e^{(n-1)}\right)$$

$$= \left(I - \alpha P^{-1/2}L_F^{\mathrm{qcf}}P^{-1/2}\right)\left(P^{1/2}e^{(n-1)}\right) =: \widetilde{G}_{\mathrm{qcl}}(\alpha)\left(P^{1/2}e^{(n-1)}\right).$$

Since $\|P^{1/2}v\|_{\ell_\varepsilon^2} = A_F^{1/2}\|v\|_{\mathcal{U}^{1,2}}$ for $v \in \mathcal{U}$, it follows that $G_{\mathrm{qcl}}(\alpha)$ is a contraction in $\mathcal{U}^{1,2}$ if and only if $\widetilde{G}_{\mathrm{qcl}}(\alpha)$ is a contraction in ℓ_ε^2. Unfortunately, we have shown in Proposition 13 that $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,2}} \sim N^{1/2}$ as $N \to \infty$. Hence, we will follow the idea used in Section 5 and try to find an alternative norm with respect to which $\widetilde{G}_{\mathrm{qcl}}(\alpha)$ is a contraction.

From Lemma 10 we deduce that there exists a similarity transform $\tilde{S}$ such that $\mathrm{cond}(\tilde{S}) \leq N^2$, and such that

$$L^{-1/2}L_F^{\mathrm{qcf}}L^{-1/2} = \tilde{S}^{-1}\widetilde{\Lambda}^{\mathrm{qnl}}\tilde{S},$$

where $\widetilde{\Lambda}^{\mathrm{qnl}}$ is the diagonal matrix of $\mathcal{U}^{1,2}$-eigenvalues $(\mu_j^{\mathrm{qnl}})_{j=1}^{2N-1}$ of L_F^{qnl}. As an immediate consequence we obtain

$$\widetilde{G}_{\mathrm{qcl}}(\alpha) = \tilde{S}^{-1}\left(I - \tfrac{\alpha}{A_F}\widetilde{\Lambda}^{\mathrm{qnl}}\right)\tilde{S}.$$

Proceeding as in Section 5, we would obtain that $\|\widetilde{G}_{\mathrm{qcl}}(\alpha)\|_{\ell_\varepsilon^2} \leq O(N^2)$. Instead, we observe that

$$\big\|G_{\mathrm{qcl}}(\alpha)u\big\|_{\tilde{S}^T\tilde{S}} = \big\|\tilde{S}\widetilde{G}_{\mathrm{qcl}}(\alpha)u\big\|_{\ell_\varepsilon^2} = \big\|(I - \tfrac{\alpha}{A_F}\widetilde{\Lambda}^{\mathrm{qnl}})\tilde{S}u\big\|_{\ell_\varepsilon^2}$$

$$\leq \big\|I - \tfrac{\alpha}{A_F}\widetilde{\Lambda}^{\mathrm{qnl}}\big\|_{\ell_\varepsilon^2}\|\tilde{S}u\|_{\ell_\varepsilon^2} = \max_{j=1,\ldots,2N-1}\big|1 - \tfrac{\alpha}{A_F}\mu_j^{\mathrm{qnl}}\big|\,\|u\|_{\tilde{S}^T\tilde{S}},$$

that is,

$$\big\|\widetilde{G}_{\mathrm{qcl}}(\alpha)\big\|_{\tilde{S}^T\tilde{S}} \leq \max_{j=1,\ldots,2N-1}\big|1 - \tfrac{\alpha}{A_F}\mu_j^{\mathrm{qnl}}\big|. \tag{28}$$

Thus, we can conclude that $\widetilde{G}_{\mathrm{qcl}}(\alpha)$ is a contraction in the $\|\cdot\|_{\tilde{S}^T\tilde{S}}$-norm if and only if $0 < \alpha < \alpha_{\max}^{\mathrm{qcl},1,2} := 2A_F/\mu_{2N-1}^{\mathrm{qnl}}$. Moreover, we obtain the error bound

$$\|e^{(n)}\|_{\mathcal{U}^{1,2}} \leq \mathrm{cond}(\tilde{S})\,\tilde{q}^n\|e^{(0)}\|_{\mathcal{U}^{1,2}} \leq N^2\tilde{q}^n\|e^{(0)}\|_{\mathcal{U}^{1,2}},$$

where $\tilde{q} := \big\|\widetilde{G}_{\mathrm{qcl}}(\alpha)\big\|_{\tilde{S}^T\tilde{S}}$. This is slightly worse in fact, than (27), however, we note that this large prefactor cannot be seen in the following numerical experiment.

Moreover, optimizing the contraction rate with respect to α leads to the choice $\alpha_{\mathrm{opt}}^{\mathrm{qcl},1,2} := 2A_F/(\mu_1^{\mathrm{qnl}} + \mu_{2N-1}^{\mathrm{qnl}})$, and in this case we obtain from Lemma 11 that

$$\tilde{q} = \tilde{q}_{\mathrm{opt}} := \big\|\widetilde{G}_{\mathrm{qcl}}\big(\alpha_{\mathrm{opt}}^{\mathrm{qcl},1,2}\big)\big\|_{\tilde{S}^T\tilde{S}} = \frac{\mu_{2N-1}^{\mathrm{qnl}} - \mu_1^{\mathrm{qnl}}}{\mu_{2N-1}^{\mathrm{qnl}} + \mu_1^{\mathrm{qnl}}} \leq \frac{1 - \frac{A_F}{\phi_F''}}{1 + \frac{A_F}{\phi_F''}},$$

where the upper bound is sharp in the limit $K \to \infty$. It is particularly interesting to note that the contraction rate obtained here is precisely the same as the one in $\mathcal{U}^{2,\infty}$ (cf. Theorem 15). Moreover, it can be easily seen from Lemma 11 that $\alpha_{\mathrm{opt}}^{\mathrm{qcl},1,2} \to \alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}$ as $K \to \infty$, which is the optimal stepsize according to Theorem 15. We further have that $\alpha_{\max}^{\mathrm{qcl},1,2} \to \alpha_{\max}^{\mathrm{qcl},2,\infty}$ as $K \to \infty$.

6.4. **Numerical example for QCL-preconditioning.**

We now apply the QCL-preconditioned stationary iterative method to the QCF system with right-hand side (25), $\phi_F'' = 1$, $A_F = 0.2$, and the optimal value $\alpha = \alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty}$ (we note that $G_{\mathrm{id}}(\alpha_{\mathrm{opt}}^{\mathrm{qcl},2,\infty})$ depends only on A_F/ϕ_F'' and N, but $e^{(0)}$ depends on A_F and ϕ_F'' independently). The error for successive iterations in the $\mathcal{U}^{1,2}$, $\mathcal{U}^{1,\infty}$ and $\mathcal{U}^{2,\infty}$-norms are displayed in Figure 2. Even though our theory, in this case, predicts a perfect contractive behavior only in $\mathcal{U}^{2,\infty}$ and (partially) in $\mathcal{U}^{1,2}$, we nevertheless observe perfect agreement with the optimal predicted rate also in the $\mathcal{U}^{1,\infty}$-norms. As a matter of fact, the parameters are chosen so that case (i) of Theorem 18 holds, that is, $G_{\mathrm{qcl}}(\alpha)$ is *not* a contraction of $\mathcal{U}^{1,\infty}$. A possible explanation why we still observe this perfect asymptotic behavior is that the norm of $G_{\mathrm{qcl}}(\alpha)$ is attained in a subspace that is never entered in this iterative process. This is also supported by the fact that the exact solution is uniformly bounded in $\mathcal{U}^{2,\infty}$ as $N, K \to \infty$, which is a simple consequence of Proposition 6.

7. Preconditioning with QCE ($P = L_F^{\mathrm{qce}}$): Ghost-Force Correction

We have shown in [5, 12] that the popular *ghost force correction method (GFC)* is equivalent to preconditioning the QCF equilibrium equations by the QCE equilibrium
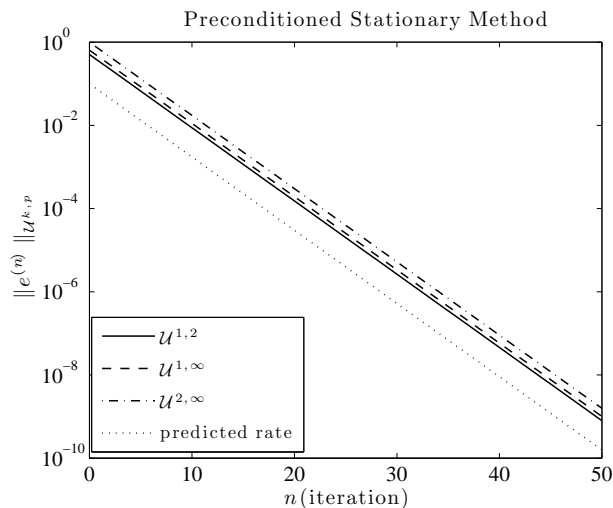
FIGURE 2. Error of the QCL-preconditioned linear stationary iterative method for the QCF system with $N = 800$, $K = 32$, $\phi''_F = 1$, $A_F = 0.2$, optimal value $\alpha = \alpha^{\mathrm{qcl},2,\infty}_{\mathrm{opt}}$, and right-hand side (25). In this case, the iteration matrix $G_{\mathrm{qcl}}(\alpha)$ is *not* a contraction of $\mathcal{U}^{1,\infty}$. Even though our theory predicts a perfect contractive behavior only in $\mathcal{U}^{2,\infty}$, we observe perfect agreement with the optimal predicted rate also in the $\mathcal{U}^{1,2}$ and $\mathcal{U}^{1,\infty}$-norms.

equations. The ghost force correction method in a quasi-static loading can thus be reduced to the question whether the iteration matrix

$$G_{\mathrm{qce}} := I - (L_F^{\mathrm{qce}})^{-1} L_F^{\mathrm{qcf}}$$

is a contraction. Due to the typical usage of the preconditioner L_F^{qce} in this case, we do not consider a step size α in this section. The purpose of the present section is (i) to investigate whether there exist function spaces in which G_{qce} is a contraction; and (ii) to identify the range of the macroscopic strains F where G_{qce} is a contraction.

We begin by recalling the fundamental stability result for the L_F^{qce} operator, Theorem 2:

$$\inf_{\substack{u \in \mathcal{U} \\ \|u'\|_{\ell_\varepsilon^2}=1}} \langle L_F^{\mathrm{qce}} u, u \rangle = A_F + \lambda_K \phi''_{2F},$$

where $\lambda_K \sim \lambda_* + O(e^{-cK})$ with $\lambda_* \approx 0.6595$. This result shows that the GFC iteration must necessarily run into instabilities before the deformation reaches the critical strain F_c^*. This is made precise in the following corollary which states that there is no norm with respect to which G_{qce} is a contraction up to the critical strain F_*.

Corollary 19. *Fix N and K, and let $\| \cdot \|_X$ be an arbitrary norm on the space $\mathcal{U}$, then, upon understanding G_{qce} as dependent on ϕ''_F and ϕ''_{2F}, we have*

$$\|G_{\mathrm{qce}}\|_X \to +\infty \quad as \quad A_F + \lambda_K \phi''_{2F} \to 0.$$

Despite this negative result, we may still be interested in the question of whether the GFC iteration is a contraction in "very stable regimes," that is, for macroscopic strains which are far away from the critical strain F_*. Naturally, we are particularly interested in the behavior as $N \to \infty$, that is, we will investigate in which function spaces the operator norm of G_{qce} remains bounded away from one as $N \to \infty$. Theorem 4 on the unboundedness of L_F^{qcf} immediately provides us with the following negative answer.

Proposition 20. *If $2 \leq K \leq N/2$, $\phi_{2F}'' \neq 0$, and $A_F + \lambda_K \phi_{2F}'' > 0$, then*

$$\|G_{\mathrm{qce}}\|_{\mathcal{U}^{1,2}} \sim N^{1/2} \qquad \text{as } N \to \infty.$$

Proof. It is an easy exercise to show that, if $A_F + \lambda_K \phi_{2F}'' > 0$, then the $\mathcal{U}^{1,2}$-norm is equivalent to the norm induced by L_F^{qce}, that is,

$$C^{-1}\|u\|_{\mathcal{U}^{1,2}} \leq \|u\|_{L_F^{\mathrm{qce}}} \leq C\|u\|_{\mathcal{U}^{1,2}}.$$

Hence, we have $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{1,2}} \approx \|G_{\mathrm{qce}}\|_{L_F^{\mathrm{qce}}}$ and by the same argument as in the proof of Proposition 13, and using again the uniform norm-equivalence, we can deduce that

$$\big\|G_{\mathrm{qce}}\big\|_{\mathcal{U}^{1,2}} \approx \big\|L_F^{\mathrm{qcf}}\big\|_{L(\mathcal{U}^{1,2},\ \mathcal{U}^{-1,2})} \pm 1 \sim N^{1/2} \quad \text{as } N \to \infty.$$

$\square$

Since the operator $(L_F^{\mathrm{qce}})^{-1} L_F^{\mathrm{qcf}}$ is more complicated than that of $(A_F L)^{-1} L_F^{\mathrm{qcf}}$, which we analyzed in the previous section, we continue to investigate the contraction properties of G_{qce} in various different norms in numerical experiments. In Figure 3, we plot the operator norm of G_{qce}, in the function spaces

$$\mathcal{U}^{k,p}, \quad k = 0, 1, 2, \quad p = 1, 2, \infty,$$

against the system size N (see Appendix 8.3 for a description of how we compute $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}}$). This experiment is performed for $A_F/\phi_F'' = 0.8$ which is at some distance from the singularity of L_F^{qce} (we note that G_{qce} depends only on A_F/ϕ_F'' and N since both $(\phi_F'')^{-1} L_F^{\mathrm{qcf}}$ and $(\phi_F'')^{-1} L_F^{\mathrm{qce}}$ depend only on A_F/ϕ_F'' and N). The experiments suggests clearly that $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}} \to \infty$ as $N \to \infty$ for all norms except for $\mathcal{U}^{1,\infty}$ and $\mathcal{U}^{2,1}$.

Hence, in a second experiment, we investigate how $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{1,\infty}}$ and $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{2,1}}$ behave, for fixed N and K, as $A_F + \lambda_K \phi_{2F}''$ approaches zero. The results of this experiment, which are are displayed in Figure 4, confirm the prediction of Corollary 19 that $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}} \to \infty$ as $A_F + \lambda_K \phi_{2F}''$ approaches zero. Indeed, they show that $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}} > 1$ already much earlier, namely around a strain F where $A_F \approx 0.52$ and $A_F + \lambda_K \phi_{2F}'' \approx 0.44$.

Our conclusion based on these analytical results and numerical experiments is that the GFC method is not universally reliable near the limit strain F_*, that is, under conditions near the formation or movement of a defect it can fail to converge to a stable solution of the QCF equilibrium equations as the quasi-static loading step tends to zero or the number of GFC iterations tends to infinity. Even though the simple model problem that we investigated here cannot, of course, provide a definite statement, it
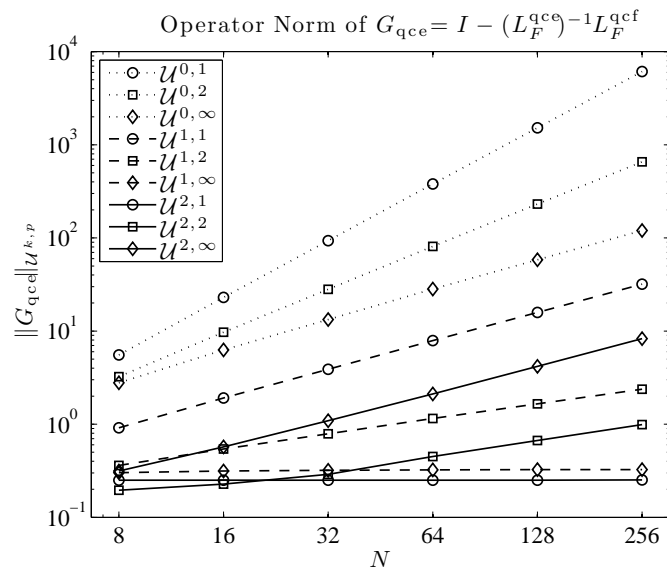
FIGURE 3. Graphs of the operator norm $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}}$, $k = 0, 1, 2$, $p = 1, 2, \infty$, plotted against the number of atoms, N, with atomistic region size $K = \lceil\sqrt{N}\rceil - 1$, and $A_F/\phi_F'' = 0.8$. (The graph for the $\mathcal{U}^{1,p}$-norms, $p = 1, \infty$, are only estimates up to a factor of $1/2$; cf. Appendix 8.3.) The graphs clearly indicate that $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}} \to \infty$ as $N \to \infty$ in all spaces except for $\mathcal{U}^{1,\infty}$ and $\mathcal{U}^{2,1}$.

shows at the very least that further investigations for more realistic model problems are required.

CONCLUSION

We proposed and studied linear stationary iterative solution methods for the QCF method with the goal of identifying iterative schemes that are efficient and reliable for all applied loads. We showed that, if the local QC operator is taken as the preconditioner, then the iteration is guaranteed to converge to the solution of the QCF system, up to the critical strain. What is interesting is that the choice of function space plays a crucial role in the efficiency of the iterative method. In $\mathcal{U}^{2,\infty}$, the convergence is always uniform in N and K, however, in $\mathcal{U}^{1,\infty}$ this is only true if the macroscopic strain is at some distance from the critical strain. This indicates that, in the presence of defects (that is, non-smooth solutions), the efficiency of a QCL-preconditioned method may be reduced. Further investigations for more realistic model problems are required to shed light on this issue.

We also showed that the popular GFC iteration must necessarily run into instabilities before the deformation reaches the critical strain F_c^*. Even for macroscopic strains that are far lower than the critical strain F_*, we show that $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{1,2}} \sim N^{1/2}$. We then give numerical experiments that suggest that $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}} \to \infty$ as $N \to \infty$ for all tested norms except for $\mathcal{U}^{1,\infty}$ and $\mathcal{U}^{2,1}$.

The results presented in this paper demonstrate the challenge for the development of reliable and efficient iterative methods for force-based approximation methods. Further analysis and numerical experiments for two and three dimensional problems are needed to more fully assess the implications of the results in this paper for realistic materials applications.
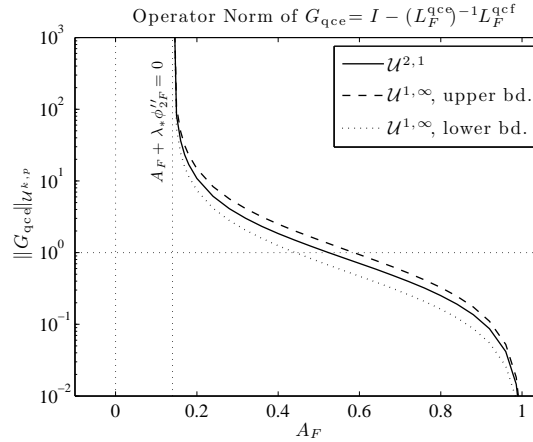
FIGURE 4. Graphs of the operator norm $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}}$, $(k,p) \in \{(1,\infty),(2,1)\}$, for fixed $N = 256, K = 15$, $\phi''_F = 1$, plotted against A_F. For the case $\mathcal{U}^{1,\infty}$ only estimates are available and upper and lower bounds are shown instead (cf. Appendix 8.3). The graphs confirm the result of Corollary 19 that $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}} \to \infty$ as $A_F + \lambda_K \phi''_{2F} \to 0$. Moreover, they clearly indicate that $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}} > 1$ already for strains F in the region $A_F \approx 0.5$, which are much lower than the critical strain at which L_F^{qce} becomes singular.

8. Appendix

8.1. **Proof of Theorem 2.** The purpose of this appendix is to prove the sharp stability result for the operator L_F^{qce}, formulated in Theorem 2. Using Formula (23) in [9] we obtain the following representation of L_F^{qce},

$$
\begin{aligned}
\left\langle L_F^{\mathrm{qce}}u, u\right\rangle = {} & \left\{ \sum_{\ell=-N+1}^{-K-2} \varepsilon A_F |u_\ell'|^2 + \sum_{\ell=K+3}^{N} \varepsilon A_F |u_\ell'|^2 \right\} \\
& + \left\{ \sum_{\ell=-K+2}^{K-1} \varepsilon \left(A_F |u_\ell'|^2 - \varepsilon^2 \phi_{2F}'' |u_\ell''|^2 \right) \right\} \\
& + \varepsilon \Big\{ (A_F - \phi_{2F}'')(|u_{-K+1}'|^2 + |u_K'|^2) + A_F(|u_{-K}'|^2 + |u_{K+1}'|^2) \\
& \qquad + (A_F + \phi_{2F}'')(|u_{-K-1}'|^2 + |u_{K+2}'|^2) \\
& \qquad - \tfrac{1}{2}\varepsilon^2 \phi_{2F}''(|u_{-K}''|^2 + |u_{-K-1}''|^2 + |u_K''|^2 + |u_{K+1}''|^2) \Big\}.
\end{aligned}
\tag{29}
$$

If $\phi_{2F}'' < 0$, then we can see from this decomposition that there is a loss of stability at the interaction between atoms $-K-2$ and $-K-1$ as well as between atoms $K+1$ and $K+2$. It is therefore natural to test this expression with a displacement $\hat{u}$ defined by

$$
\hat{u}_\ell' = \begin{cases} 1, & \ell = -K-1, \\ -1, & \ell = K+2, \\ 0, & \text{otherwise.} \end{cases}
$$

From (29), we easily obtain

$$
\left\langle L_F^{\mathrm{qce}}\hat{u}, \hat{u}\right\rangle = A_F + \tfrac{1}{2}\phi_{2F}''.
$$

In particular, we see that, if $A_F + \tfrac{1}{2}\phi_{2F}'' < 0$, then L_F^{qce} is indefinite. On the other hand, it was shown in [8] that L_F^{qce} is positive definite provided $A_F + \phi_{2F}'' > 0$. (As a matter of fact, the analysis in [8] is for periodic boundary conditions, however, since the Dirichlet displacement space is contained in the periodic displacement space the result is also valid for the present case.)

Thus, we have shown that

$$
\inf_{\substack{u \in \mathcal{U} \\ \|u'\|_{\ell_\varepsilon^2}=1}} \left\langle L_F^{\mathrm{qce}}u, u\right\rangle = A_F + \mu\phi_{2F}'', \quad \text{where } \tfrac{1}{2} \leq \mu \leq 1.
$$

To conclude the proof of Theorem 2, we need to show that μ depends only on K and that the stated asymptotic result holds.

From (29) it follows that L_F^{qce} can be written in the form

$$
\left\langle L_F^{\mathrm{qce}}u, u\right\rangle = (u')^T \mathcal{H} u',
$$

where we identify u' with the vector $u' = (u'_\ell)^N_{\ell=-N+1}$ and where $\mathcal{H} \in \mathbb{R}^{2N \times 2N}$. Writing $\mathcal{H} = \phi''_F \mathcal{H}_1 + \phi''_{2F} \mathcal{H}_2$, we can see that $\mathcal{H}_1 = \mathrm{Id}$ and that $\mathcal{H}_2$ has the entries

$$
\mathcal{H}_2 = \begin{pmatrix}
\ddots & \ddots & \ddots & & & & & \\
& 1 & 2 & 1 & & & & \\
& & 1 & 2 & 1 & & & \\
& & & 1 & 3/2 & 1/2 & & \\
& & & & 1/2 & 3 & 1/2 & \\
& & & & & 1/2 & 9/2 & 0 \\
& & & & & & 0 & 4 & 0 \\
& & & & & & & 0 & 4 & 0 \\
& & & & & & & & \ddots & \ddots & \ddots
\end{pmatrix}
$$

Here, the row with entries $[1, 3/2, 1/2]$ denotes the Kth row (in the coordinates u'_k). This form can be verified, for example, by appealing to (29). Let $\sigma(A)$ denote the spectrum of a matrix A. Since, by assumption, $\phi''_{2F} \leq 0$, the smallest eigenvalue of $\mathcal{H}$ is given by

$$
\min \sigma(\mathcal{H}) = \phi''_F + \phi''_{2F} \max \sigma(\mathcal{H}_2),
$$

that is, we need to compute the largest eigenvalue $\bar{\lambda}$ of $\mathcal{H}_2$. Since $\mathcal{H}_2 e_k = 4e_k$ for $k = K + 3, K + 4, \ldots$ and for $K = -K - 2, -K - 3, \ldots$, and since eigenvectors are orthogonal, we conclude that all other eigenvectors depend only on the submatrix describing the atomistic region and the interface. In particular, $\bar{\lambda}$ depends only on K but not on N. This proves the claim of Theorem 2 that λ_K depends indeed only on K.

We thus consider the $\{-K - 1, \ldots, K + 2\}$-submatrix $\bar{\mathcal{H}}_2$, which has the form

$$
\bar{\mathcal{H}}_2 = \begin{pmatrix}
9/2 & 1/2 & & & & & & \\
1/2 & 3 & 1/2 & & & & & \\
& 1/2 & 3/2 & 1 & & & & \\
& & 1 & 2 & 1 & & & \\
& & & \ddots & \ddots & \ddots & & \\
& & & & 1 & 2 & 1 & \\
& & & & & 1 & 3/2 & 1/2 \\
& & & & & & 1/2 & 3 & 1/2 \\
& & & & & & & 1/2 & 9/2
\end{pmatrix}.
$$

Letting $\bar{\mathcal{H}}_2 \psi = \lambda \psi$, then for $\ell = -K + 2, \ldots, K - 1$,

$$
\psi_{\ell-1} + 2\psi_\ell + \psi_{\ell+1} = \lambda \psi_\ell,
$$

and hence, ψ has the general form

$$
\psi_\ell = az^\ell + bz^{-\ell}, \qquad \ell = -K + 1, \ldots, K,
$$

leaving ψ_ℓ undefined for $\ell \in \{-K, -K - 1, K + 1, K + 2\}$ for now, and where $z, 1/z$ are the two roots of the polynomial

$$
z^2 + (2 - \lambda)z + 1 = 0.
$$

In particular, we have

$$
z = (\tfrac{1}{2}\lambda - 1) + \sqrt{(\tfrac{1}{2}\lambda - 1)^2 - 1} > 1. \tag{30}
$$

To determine the remaining degrees of freedom, we could now insert this general form into the eigenvalue equation and attempt to solve the resulting problem. This leads to a complicated system which we will try to simplify.

We first note that, for any eigenvector ψ, the vector $(\psi_{K-\ell})$ is also an eigenvector, and hence we can assume without loss of generality that ψ is skew-symmetric about $\ell = 1/2$. This implies that $a = -b$. Since the scaling is irrelevant for the eigenvalue problem, we therefore make the *ansatz* $\psi_\ell = z^\ell - z^{-\ell}$. Next, we notice that for K sufficiently large the term $z^{-\ell}$ is exponentially small and therefore does not contribute to the eigenvalue equation near the right interface. We may safely ignore it if we are only interested in the asymptotics of the eigenvalue $\bar{\lambda}$ as $K \to \infty$. Thus, letting $\hat{\psi}_\ell = z^\ell$, $\ell = 1, \ldots, K$ and $\hat{\psi}_\ell$ unknown, $\ell = K + 1, K + 2$, we obtain the system

$$z^{K-1} + \tfrac{3}{2}z^K + \tfrac{1}{2}\hat{\psi}_{K+1} = \hat{\lambda}z^K,$$

$$\tfrac{1}{2}z^K + 3\hat{\psi}_{K+1} + \tfrac{1}{2}\hat{\psi}_{K+2} = \hat{\lambda}\hat{\psi}_{K+1},$$

$$\tfrac{1}{2}\hat{\psi}_{K+1} + \tfrac{9}{2}\hat{\psi}_{K+2} = \hat{\lambda}\hat{\psi}_{K+2}.$$

The free parameters $\hat{\psi}_{K+1}, \hat{\psi}_{K+2}$ can be easily determined from the first two equations. From the final equation we can then compute $\hat{\lambda}$. Upon recalling from (30) that $\hat{z}$ can be expressed in terms of $\hat{\lambda}$, and conversely that $\hat{\lambda} = (\hat{z}^2 + 1)/\hat{z} + 2$, we obtain a polynomial equation of degree five for $\hat{z}$,

$$q(\hat{z}) := 4\hat{z}^5 - 12\hat{z}^4 + 9\hat{z}^3 - 3\hat{z}^2 - 4\hat{z} + 2 = 0.$$

Mathematica was unable to factorize q symbolically, hence we computed its roots numerically to twenty digits precision. It turns out that q has three real roots and two complex roots. The largest real root is at $\hat{z} \approx 2.206272296$ which gives the value

$$\hat{\lambda} = \frac{\hat{z}^2 + 1}{\hat{z}} + 2 \approx 4.659525505897.$$

The relative errors that we had previously neglected are in fact of order $\hat{z}^{-2K}$, and hence we obtain

$$\lambda_K = \lambda_* + O(e^{-cK}), \qquad \text{where} \quad \lambda_* \approx 0.6595 \quad \text{and} \quad c \approx 1.5826.$$

This concludes the proof of Theorem 2.

8.2. **Proofs of Lemmas 14 and 17.** In this appendix, we prove two technical lemmas from Section 6.1. Throughout, the iteration matrix $G_{\text{qcl}}(\alpha)$ is given by

$$G_{\text{qcl}}(\alpha) := I - \alpha(A_F L)^{-1}L_F^{\text{qcf}},$$

where $\alpha > 0$ and $A_F = \phi_F'' + 4\phi_{2F}'' > 0$. We begin with the proof of Lemma 14, which is more straightforward.

Proof of Lemma 14. Using the basic definition of the operator norm, and the fact that $Lz = -z''$, we obtain

$$\left\|G_{\text{qcl}}(\alpha)\right\|_{\mathcal{U}^{2,\infty}} = \max_{\substack{u \in \mathcal{U} \\ \|u''\|_{\ell_\varepsilon^\infty} = 1}} \left\|(G_{\text{qcl}}(\alpha)u)''\right\|_{\ell_\varepsilon^\infty} = \max_{\substack{u \in \mathcal{U} \\ \|u''\|_{\ell_\varepsilon^\infty} = 1}} \left\| - LG_{\text{qcl}}(\alpha)u\right\|_{\ell_\varepsilon^\infty}.$$

We write the operator $-LG_{\mathrm{qcl}}(\alpha) = -L + \frac{\alpha}{A_F}L_F^{\mathrm{qcf}}$ as follows:

$$\big[-LG_{\mathrm{qcl}}(\alpha)u\big]_\ell = \begin{cases} u''_\ell - \frac{\alpha}{A_F}\big(A_F u''_\ell\big), & \text{if } \ell \in \mathcal{C}, \\ u''_\ell - \frac{\alpha}{A_F}\big(\phi''_F u''_\ell + \phi''_{2F}(u''_{\ell-1} + 2u''_\ell + u''_{\ell+1})\big), & \text{if } \ell \in \mathcal{A}. \end{cases} \tag{31}$$

In the continuum region, we simply obtain

$$\big[-LG_{\mathrm{qcl}}(\alpha)u\big]_\ell = (1 - \alpha)u''_\ell \qquad \text{for } \ell \in \mathcal{C}.$$

If $\ell \in \mathcal{A}$, we manipulate (31), using the definition of $A_F = \phi''_F + 4\phi''_{2F}$, which yields

$$\begin{aligned}\big[-LG_{\mathrm{qcl}}(\alpha)u\big]_\ell &= \Big[1 - \tfrac{\alpha}{A_F}\big(\phi''_F + 2\phi''_{2F}\big)\Big]u''_\ell + \Big[-\tfrac{\alpha}{A_F}\phi''_{2F}\Big](u''_{\ell-1} + u''_{\ell+1}) \\ &= \Big[1 - \alpha\big(1 - \tfrac{2\phi''_{2F}}{A_F}\big)\Big]u''_\ell + \Big[-\alpha\tfrac{\phi''_{2F}}{A_F}\Big](u''_{\ell-1} + u''_{\ell+1}).\end{aligned}$$

In summary, we have obtained

$$\big[-LG_{\mathrm{qcl}}(\alpha)u\big]_\ell = \begin{cases} [1 - \alpha]u''_\ell, & \text{if } \ell \in \mathcal{C}, \\ \Big[1 - \alpha\big(1 - \tfrac{2\phi''_{2F}}{A_F}\big)\Big]u''_\ell + \Big[-\alpha\tfrac{\phi''_{2F}}{A_F}\Big](u''_{\ell-1} + u''_{\ell+1}) & \text{if } \ell \in \mathcal{A}. \end{cases}$$

It is now easy to see that

$$\|G_{\mathrm{qcl}}(\alpha)\|_{L(\mathcal{U}^{2,\infty},\,\mathcal{U}^{2,\infty})} \le \max\Big\{|1 - \alpha|, \big|1 - \alpha\big(1 - \tfrac{2\phi''_{2F}}{A_F}\big)\big| + \alpha\big|\tfrac{2\phi''_{2F}}{A_F}\big|\Big\}.$$

As a matter of fact, in view of the estimate

$$\big|1 - \alpha\big(1 - \tfrac{2\phi''_{2F}}{A_F}\big)\big| + \alpha\big|\tfrac{2\phi''_{2F}}{A_F}\big| \ge |1 - \alpha| - \alpha\big|\tfrac{2\phi''_{2F}}{A_F}\big| + \alpha\big|\tfrac{2\phi''_{2F}}{A_F}\big| = |1 - \alpha|,$$

the upper bound can be reduced to

$$\|G_{\mathrm{qcl}}(\alpha)\|_{L(\mathcal{U}^{2,\infty},\,\mathcal{U}^{2,\infty})} \le \big|1 - \alpha\big(1 - \tfrac{2\phi''_{2F}}{A_F}\big)\big| + \alpha\tfrac{2|\phi''_{2F}|}{A_F}. \tag{32}$$

To show that the bound is attained, we construct a suitable test function. We define $u \in \mathcal{U}$ via

$$u''_{-1} = u''_1 = \mathrm{sign}\Big[-\alpha\tfrac{2\phi''_{2F}}{A_F}\Big], \quad u''_0 = \mathrm{sign}\Big[1 - \alpha\big(1 - \tfrac{2\phi''_{2F}}{A_F}\big)\Big],$$

(note that $0 \in \mathcal{A}$ for any $K \ge 0$) and the remaining values of u''_ℓ in such a way that $\sum_{\ell=-N+1}^{N} u''_\ell = 0$. If $N \ge 4$, then there exists at least one function $u \in \mathcal{U}$ with these properties and it attains the bound (32). Thus, the bound in (32) is an equality, which concludes the proof of the lemma. $\square$

Before we prove Lemma 17, we recall an explicit representation of $L^{-1}L_F^{\mathrm{qcf}}$ that was useful in our analysis in [10]. The proof of the following result is completely analogous to that of [10, Lemma 14] and is therefore sketched only briefly. It is also convenient for the remainder of the section to define the following atomistic and continuum regions for the strains:

$$\mathcal{A}' = \big\{ -K + 1, \ldots, K\big\} \quad \text{and} \quad \mathcal{C}' = \big\{ -N + 1, \ldots, N\big\} \setminus \mathcal{A}'.$$

Lemma 21. *Let $u \in \mathcal{U}$ and $z = L^{-1}L_F^{\mathrm{qcf}}u$, then*

$$z'_\ell = \sigma(u')_\ell - \overline{\sigma(u')} + \phi''_{2F}\big(\tilde{\alpha}_{-K}(u')h_{-K,\ell} - \tilde{\alpha}_K(u')h_{K,\ell}\big),$$

where $\sigma(u')$, $h_{\pm K} \in \mathbb{R}^{2N}$ and $\overline{\sigma(u')}$, $\tilde{\alpha}_{\pm K}(u') \in \mathbb{R}$ are defined as follows:

$$\sigma(u')_\ell = \begin{cases} \phi_F'' u_\ell' + \phi_{2F}''(u_{\ell-1}' + 2u_\ell' + u_{\ell+1}'), & \ell \in \mathcal{A}', \\ (\phi_F'' + 4\phi_{2F}'')u_\ell', & \ell \in \mathcal{C}', \end{cases}$$

$$\overline{\sigma(u')} = \frac{1}{2N}\sum_{\ell=-N+1}^{N} \sigma(u')_\ell = \tfrac{\varepsilon}{2}\phi_{2F}''\big[u_{K+1}' - u_K' - u_{-K+1}' + u_{-K}'\big],$$

$$\tilde{\alpha}_{-K}(u') = u_{-K+1}' - 2u_{-K}' + u_{-K-1}', \quad \tilde{\alpha}_K(u') = u_{K+2}' - 2u_{K+1}' + u_K', \quad and$$

$$h_{\pm K,\ell} = \begin{cases} \tfrac{1}{2}(1 \mp \varepsilon K), & \ell = -N+1, \dots, \pm K, \\ \tfrac{1}{2}(-1 \mp \varepsilon K), & \ell = \pm K + 1, \dots, N. \end{cases}$$

Proof. In the notation introduced above, the variational representation of L_F^{qcf} from [10, Sec. 3] reads

$$\langle L_F^{\mathrm{qcf}} u, v \rangle = \langle \sigma(u'), v' \rangle + \phi_{2F}''\big[\tilde{\alpha}_{-K}(u')v_{-K} - \tilde{\alpha}_K(u')v_K\big] \qquad \forall u, v \in \mathcal{U}.$$

Using the fact that $v_{\pm N} = 0$ and $\sum_\ell v_\ell' = 0$, it is easy to see that the discrete delta-functions appearing in this representation can be rewritten as

$$v_{\pm K} = \langle h_{\pm K}, v' \rangle.$$

Hence, we deduce that the function $z = L^{-1}L_F^{\mathrm{qcf}}$ is given by

$$\langle z', v' \rangle = \langle L_F^{\mathrm{qcf}} u, v \rangle = \big\langle \sigma(u') + \phi_{2F}''[\tilde{\alpha}_{-K}(u')h_{-K} - \tilde{\alpha}_K(u')h_K], v' \big\rangle \quad \forall v \in \mathcal{U}.$$

In particular, it follows that

$$z' = \sigma(u') + \phi_{2F}''[\tilde{\alpha}_{-K}(u')h_{-K} - \tilde{\alpha}_K(u')h_K] + C,$$

where C is chosen so that $\sum_\ell z_\ell' = 0$. Since $h_{\pm K}$ are constructed so that $\sum_\ell h_{\pm K,\ell} = 0$, we only subtract the mean of $\sigma(u')$. Hence, $C = -\overline{\sigma(u')}$, for which the stated formula is quickly verified. $\qquad\square$

Proof of Lemma 17. Let $u \in \mathcal{U}$ with $\|u'\|_{\ell_\varepsilon^\infty} \le 1$. Setting $z = G_{\mathrm{qcl}}(\alpha)u$, and employing Lemma 21, we obtain

$$z_\ell' = u_\ell' - \frac{\alpha}{A_F}\Big[\sigma_\ell(u') - \overline{\sigma(u')} + \phi_{2F}''(\tilde{\alpha}_{-K}(u')h_{-K,\ell} - \tilde{\alpha}_K(u')h_{K,\ell})\Big]$$

$$= \Big[u_\ell' - \frac{\alpha}{A_F}\sigma_\ell(u')\Big] + \alpha\frac{\phi_{2F}''}{A_F}\Big[\tfrac{\varepsilon}{2}(u_{K+1}' - u_K' - u_{-K+1}' + u_{-K}')$$

$$- \tilde{\alpha}_{-K}(u')h_{-K,\ell} + \tilde{\alpha}_K(u')h_{K,\ell}\Big]$$

$$:= R_\ell + S_\ell.$$

We will estimate the terms R_ℓ and S_ℓ separately.

To estimate the first term, we distinguish whether $\ell \in \mathcal{C}'$ or $\ell \in \mathcal{A}'$. A quick computation shows that $R_\ell = (1 - \alpha)u_\ell'$ for $\ell \in \mathcal{C}'$. On the other hand, for $\ell \in \mathcal{A}'$ we

have

$$R_\ell = \left[1 - \tfrac{\alpha}{A_F}(\phi_F'' + 2\phi_{2F}'')\right]u_\ell' - \alpha\tfrac{\phi_{2F}''}{A_F}(u_{\ell-1}' + u_{\ell+1}')$$

$$= \left[1 - \alpha\left(1 - \tfrac{2\phi_{2F}''}{A_F}\right)\right]u_\ell' - \alpha\tfrac{\phi_{2F}''}{A_F}(u_{\ell-1}' + u_{\ell+1}') \qquad \forall \ell \in \mathcal{A}'.$$

Since $\|u'\|_{\ell_\varepsilon^\infty} \leq 1$, we can thus obtain

$$|R_\ell| \leq \begin{cases} |1 - \alpha|, & \ell \in \mathcal{C}', \\ \left|1 - \alpha\left(1 - \tfrac{2\phi_{2F}''}{A_F}\right)\right| + \alpha\left|\tfrac{2\phi_{2F}''}{A_F}\right|, & \ell \in \mathcal{A}'. \end{cases} \tag{33}$$

As a matter of fact, these bounds can be attained for certain ℓ, by choosing suitable test functions. For example, by choosing $u \in \mathcal{U}$ with $u_N' = \text{sign}(1 - \alpha)$ we obtain $R_N = |1 - \alpha|$, that is, R_N attains the bound (33). By choosing $u \in \mathcal{U}$ such that

$$u_0' = u_2' = \text{sign}\left(-\tfrac{\phi_{2F}''}{A_F}\right) = 1 \quad \text{and} \quad u_1' = \text{sign}\left(1 - \alpha\left(1 - \tfrac{2\phi_{2F}''}{A_F}\right)\right),$$

we obtain that R_1 attains the bound (33). In both cases one needs to choose the remaining free u_ℓ' so that $|u_\ell'| \leq 1$ and $\sum_\ell u_\ell' = 0$, which guarantees that such functions $u \in \mathcal{U}$ really exist. This can be done under the conditions imposed on N and K.

To estimate S_ℓ, we note that this term depends only on a small number of strains around the interface. We can therefore expand it in terms of these strains and their coefficients and then maximize over all possible interface contributions. Thus, we rewrite S_ℓ as follows:

$$S_\ell = \alpha\tfrac{\phi_{2F}''}{A_F}\Big\{ u_{-K-1}'[-h_{-K,\ell}] + u_{-K}'[2h_{-K,\ell} + \tfrac{\varepsilon}{2}] + u_{-K+1}'[-h_{-K,\ell} - \tfrac{\varepsilon}{2}]$$

$$u_K'[h_{K,\ell} - \tfrac{\varepsilon}{2}] + u_{K+1}'[-2h_{K,\ell} + \tfrac{\varepsilon}{2}] + u_{K+2}'[h_{K,\ell}]\Big\}.$$

This expression is maximized by taking u_ℓ' to be the sign of the respective coefficient (taking into account also the outer coefficient $\alpha\tfrac{\phi_{2F}''}{A_F}$), which yields

$$|S_\ell| \leq \alpha\left|\tfrac{\phi_{2F}''}{A_F}\right|\Big\{|h_{-K,\ell}| + |2h_{-K,\ell} + \tfrac{\varepsilon}{2}| + |h_{-K,\ell} + \tfrac{\varepsilon}{2}| + |h_{K,\ell} - \tfrac{\varepsilon}{2}| + |2h_{K,\ell} - \tfrac{\varepsilon}{2}| + |h_{K,\ell}|\Big\}$$

$$= \alpha\left|\tfrac{\phi_{2F}''}{A_F}\right|\Big\{|4h_{-K,\ell} + \varepsilon| + |4h_{K,\ell} - \varepsilon|\Big\}.$$

The equality of the first and second line holds because the terms $\pm\tfrac{\varepsilon}{2}$ do not change the signs of the terms inside the bars. Inserting the values for $h_{\pm K,\ell}$, we obtain the bound

$$|S_\ell| \leq \begin{cases} \alpha 4\left|\tfrac{\phi_{2F}''}{A_F}\right|, & \ell \in \mathcal{C}', \\ \alpha(4 + 2\varepsilon - 4\varepsilon K)\left|\tfrac{\phi_{2F}''}{A_F}\right|, & \ell \in \mathcal{A}', \end{cases}$$

and we note that this bound is attained if the values for u_ℓ', $\ell = -K-1, -K, -K+1, K, K+1, K+2$, are chosen as described above.

Combining the analyses of the terms R_ℓ and S_ℓ, it follows that

$$\|z'\|_{\ell_\varepsilon^\infty} \leq \max\Big\{ |1 - \alpha| + \alpha 4\left|\tfrac{\phi_{2F}''}{A_F}\right|,$$

$$\left|1 - \alpha\left(1 - \tfrac{2\phi_{2F}''}{A_F}\right)\right| + \alpha(6 + 2\varepsilon - 4\varepsilon K)\left|\tfrac{\phi_{2F}''}{A_F}\right|\Big\}.$$

To see that this bound is attained, we note that, under the condition that $K \geq 3$ and $N \geq K + 3$, the constructions at the interface to maximize S_ℓ and the constructions to maximize R_ℓ do not interfere. Moreover, under the additional condition $N \geq \max(9, K+3)$, sufficiently many free strains u'_ℓ remain to ensure that $\sum_\ell u'_\ell = 0$ for a test function $u \in \mathcal{U}$, $\|u'\|_{\ell_\varepsilon^\infty} = 1$, for which both R_ℓ and S_ℓ attain the stated bound. That is, we have shown that

$$\left\|G_{\mathrm{qcl}}(\alpha)\right\|_{\mathcal{U}^{1,\infty}} = \max\left\{|1 - \alpha| + \alpha 4 \frac{|\phi''_{2F}|}{A_F}, \right.$$
$$\left. \left|1 - \alpha\left(1 - \frac{2\phi''_{2F}}{A_F}\right)\right| + \alpha(6 + 2\varepsilon - 4\varepsilon K)\frac{|\phi''_{2F}|}{A_F}\right\}$$
$$=: \max\{m_{\mathcal{C}}(\alpha), m_{\mathcal{A}}(\alpha)\}.$$

To conclude the proof, we need to evaluate this maximum explicitly. To this end we first define $\alpha_1 = \left(1 - \frac{2\phi''_{2F}}{A_F}\right)^{-1} < 1$. For $0 \leq \alpha \leq \alpha_1$, we have

$$m_{\mathcal{A}}(\alpha) = 1 - \alpha + \alpha(4 + 2\varepsilon - 4\varepsilon K)\left|\frac{\phi''_{2F}}{A_F}\right|$$
$$\leq 1 - \alpha + \alpha 4 \left|\frac{\phi''_{2F}}{A_F}\right| = m_{\mathcal{C}}(\alpha),$$

that is, $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}} = m_{\mathcal{C}}(\alpha)$. Conversely, for $\alpha \geq 1$, we have

$$m_{\mathcal{A}}(\alpha) = \alpha\left(1 + (8 + 2\varepsilon - 4\varepsilon K)\frac{|\phi''_{2F}|}{A_F}\right) - 1$$
$$= m_{\mathcal{C}}(\alpha) + \alpha\left(4 + 2\varepsilon - 4\varepsilon K\right)\frac{|\phi''_{2F}|}{A_F}\right) \geq m_{\mathcal{C}}(\alpha),$$

that is, $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}} = m_{\mathcal{A}}(\alpha)$. Since, in $[\alpha_1, 1]$, $m_{\mathcal{C}}$ is strictly decreasing and $m_{\mathcal{A}}$ is strictly increasing, there exists a unique $\alpha_2 \in [\alpha_1, 1]$ such that $m_{\mathcal{C}}(\alpha_2) = m_{\mathcal{A}}(\alpha_2)$ and such that the stated formula for $\|G_{\mathrm{qcl}}(\alpha)\|_{\mathcal{U}^{1,\infty}}$ holds. A straightforward computation yields the value for $\alpha_2 = \alpha_{\mathrm{opt}}^{\mathrm{qcl},1,\infty}$ stated in the lemma. $\square$

8.3. Computation of $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}}$.

We have computed $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{k,p}}$ for $k = 0, 2, p = 1, 2, \infty$, from the standard formulas for the operator norm [17, 29] of the matrix G_{qce} and $LG_{\mathrm{qce}}L^{-1}$ with respect to ℓ_ε^p. For $k = 1$ and $p = 2$, the norm is also easy to obtain by solving a generalized eigenvalue problem.

The cases $k = 1$ and $p = 1, \infty$ are more difficult. In these cases, the operator norm of G_{qce} in $\mathcal{U}^{1,p}$ can be estimated in terms of the ℓ_ε^p-operator norm of the conjugate operator $\widehat{G} = I - (\widehat{L}_F^{\mathrm{qce}})^{-1}\widehat{L}_F^{\mathrm{qcf}} : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$ (see Lemma 11 for an analogous definition of the conjugate operator $\widehat{L}_F^{\mathrm{qnl}} : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$). It is not difficult to see that $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{1,p}} = \|\widetilde{G}\|_{\ell_\varepsilon^p, \mathbb{R}_*^{2N}}$ for $\widetilde{G} = I - (\widetilde{L}_F^{\mathrm{qce}})^{-1}\widetilde{L}_F^{\mathrm{qcf}} : \mathbb{R}_*^{2N} \to \mathbb{R}_*^{2N}$ where we recall that $\mathbb{R}_*^{2N} = \{\varphi \in \mathbb{R}^{2N} : \sum_\ell \varphi_\ell = 0\}$ (see Lemma 11 similarly for an analogous definition of the restricted conjugate operator $\widetilde{L}_F^{\mathrm{qnl}} : \mathbb{R}_*^{2N} \to \mathbb{R}_*^{2N}$), it follows from (2) that we have only computed $\|G_{\mathrm{qce}}\|_{\mathcal{U}^{1,p}}$ for $p = 1, \infty$ up to a factor of $1/2$. More precisely,

$$\|G_{\mathrm{qce}}\|_{\mathcal{U}^{1,p}} \leq \|\widehat{G}\|_{\ell_\varepsilon^p} \leq 2\|G_{\mathrm{qce}}\|_{\mathcal{U}^{1,p}}$$

Finally We note that we can obtain $\widehat{L}_F^{\mathrm{qcf}}$ from the representation given in Lemma 21 and that $\widehat{L}_F^{\mathrm{qce}}$ can be directly obtained from (14).

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