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SHARP STABILITY ESTIMATES FOR THE FORCE-BASED QUASICONTINUUM APPROXIMATION OF HOMOGENEOUS TENSILE DEFORMATION*

M. DOBSON†, M. LUSKIN‡, AND C. ORTNER§

Abstract. The accuracy of atomistic-to-continuum hybrid methods can be guaranteed only for deformations where the lattice configuration is stable for both the atomistic energy and the hybrid energy. For this reason, a sharp stability analysis of atomistic-to-continuum coupling methods is essential for evaluating their capabilities for predicting the formation of lattice defects. We formulate a simple one-dimensional model problem and give a detailed analysis of the linear stability of the force-based quasicontinuum (QCF) method at homogeneous deformations. The focus of the analysis is the question of whether the QCF method is able to predict a critical load at which fracture occurs. Numerical experiments show that the spectrum of a linearized QCF operator is identical to the spectrum of a linearized energy-based quasi-nonlocal quasicontinuum (QNL) operator, which we know from our previous analyses to be positive below the critical load. However, the QCF operator is nonnormal, and it turns out that it is not generally positive definite, even when all of its eigenvalues are positive. Using a combination of rigorous analysis and numerical experiments, we investigate in detail for which choices of "function spaces" the QCF operator is stable, uniformly in the size of the atomistic system.

Key words. atomistic-to-continuum coupling, quasicontinuum method, sharp stability estimates

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1. Introduction.

Low energy equilibria for crystalline materials are typically characterized by localized defects that interact with their environment through long-range elastic fields. Atomistic-to-continuum coupling methods seek to make the accurate computation of such problems possible by using the accuracy of atomistic modeling only in the neighborhood of defects where the deformation is highly nonuniform. At some distance from the defects, sufficient accuracy can be obtained by the use of continuum models, which facilitate the reduction of degrees of freedom. The accuracy of the atomistic model at the defect combined with the efficiency of a continuum model for the far field enables, in principle, the reliable simulation of systems that are inaccessible to pure atomistic or pure continuum models.

Typical test problems for atomistic-to-continuum coupling methods have been

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†CERMICS - ENPC, 6 et 8 avenue Blaise Pascal, Cité Descartes - Champs sur Marne, 77455 Marne la Vallée Cedex 2, France (dobsonm@cermics.enpc.fr). This author's research was supported in part by the University of Minnesota Doctoral Dissertation Fellowship, the NSF Mathematical Sciences Postdoctoral Research Fellowship, DMS-0757355, DMS-0811039, the Department of Energy under Award number DE-FG02-05ER25706, the Institute for Mathematics and Its Applications, and the University of Minnesota Supercomputing Institute.

‡School of Mathematics, University of Minnesota, 206 Church St. SE, Minneapolis, MN 55455 (luskin@umn.edu). This author's research was supported in part by DMS-0757355, DMS-0811039, the Department of Energy under Award number DE-FG02-05ER25706, the Institute for Mathematics and Its Applications, and the University of Minnesota Supercomputing Institute.

§Mathematical Institute, University of Oxford, St. Giles' 24–29, Oxford OX1 3LB, UK (ortner@maths.ox.ac.uk). This author's research was supported in part by the EPSRC critical mass programme "New Frontiers in the Mathematics of Solids."

dislocation formation under an indenter, crack tip deformation, and deformation and fracture of grain boundaries [17]. In each of these problems, the crystal deforms quasistatically until the equilibrium equations become singular, for example, when a dislocation is formed or moves or when a crack tip advances. Depending on the nature of the singularity, the crystal will then generally undergo a dynamic process when further loaded.

The quasicontinuum (QC) method, one such atomistic-to-continuum coupling scheme, models the continuum region by constructing an energy density that equals the atomistic energy density for any uniform strain (the Cauchy–Born rule). During the past several years, many variants of the QC approximation have been proposed that differ in the coupling between the atomistic and continuum regions [3, 5, 11, 13, 17, 19, 23, 25, 26]. Analyses of QC approximations have been given in [7, 12, 15, 16, 18, 20]. We refer the reader to [8] for a detailed review of the formulation and analysis, relevant to the present work, of different QC methods. Other coupling models are analyzed in [1, 21, 22].

In [8], we have begun to investigate whether the QC method can reliably predict the formation of defects. The main ingredient to establish whether or not this is the case is a sharp analysis to predict under which conditions the QC method is "stable." More precisely, we ask whether there exist "stable" solutions of the QC method *up to a critical load* for the atomistic energy. We have begun to investigate this question in some depth for the most common energy-based QC formulations in [8]. In the present paper, we present a corresponding sharp stability analysis for the force-based quasicontinuum (QCF) method [4, 5, 23].

We focus on a homogeneous one-dimensional periodic chain with next-nearest neighbor pair interactions, which is introduced in section 2.1. For this model, the homogeneous configuration ceases to be stable for the atomistic energy when the applied tensile strain reaches a critical value (fracture).

For the atomistic model and for energy-based QC formulations, coercivity (positivity) of the second variation evaluated at the equilibrium solution provides the natural notion of stability. However, the QCF method, which we describe in sections 2.3 and 2.5, leads to nonconservative equilibrium equations, and therefore positivity of the linearized QCF operator may be an inappropriate notion of stability. Indeed, we prove in section 4.1 that, generically, the linearized QCF operator is indefinite.

As a consequence, we consider two further notions of stability. First, we investigate for which choices of discrete function spaces (that is, for which choices of topologies) does the linearized QCF operator have an inverse that is bounded uniformly in the size of the atomistic system. In section 4.2, we present several sharp stability results as well as interesting counterexamples. However, these operator stability results do not necessarily correspond to any physical notion of stability. Hence, in section 4.4, we propose the notion of *dynamical stability*, which can be reduced to certain properties of the eigenvalues. Our notion of *dynamical stability* is meant only as a methodology to determine stability, not as a method to actually approximate the Hamiltonian dynamics of the exact atomistic system. A careful numerical study suggests that the spectrum of the linearized QCF operator and that of the linearized quasi-nonlocal QC (QNL) operator (see [25] and section 4.3) are identical. Combined with our previous results [8], this indicates that the QCF method is *dynamically stable* up to the critical load for fracture of the atomistic energy.

2. The force-based QC method.

2.1. The atomistic model problem. We consider deformations from the reference lattice $\varepsilon\mathbb{Z}$, where $\varepsilon > 0$ is a scaling that we will fix below. To avoid technical difficulties caused by infinite domains or by boundary layers, we admit only deformations that are periodic displacements from the homogeneous lattice $y_F = F\varepsilon\mathbb{Z} = (F\varepsilon\ell)_{\ell\in\mathbb{Z}}$; that is, we admit deformations from the space

$$\begin{aligned} \mathcal{Y}_F &= \; y_F + \mathcal{U}, \qquad \text{where} \\ \mathcal{U} &= \; \left\{ u \in \mathbb{R}^{\mathbb{Z}} : u_{\ell+2N} = u_\ell \text{ for } \ell \in \mathbb{Z}, \text{ and } \sum_{\ell=-N+1}^{N} u_\ell = 0 \right\}. \end{aligned}$$

We call F the *macroscopic deformation gradient*, and we set $\varepsilon = 1/N$ throughout. Although the energies and forces are defined for general $2N$-periodic displacements, we admit only those with zero mean, as is common for continuum problems with periodic boundary conditions, in order to obtain unique solutions to the equilibrium equations.

We consider only nearest neighbor and next-nearest neighbor pair interactions so that the *scaled potential energy per period* of a deformation $y \in \mathcal{Y}_F$ is given by

$$\mathcal{E}_{\mathrm{a}}(y) = \varepsilon \sum_{\ell=-N+1}^{N} \big(\phi(y'_\ell) + \phi(y'_\ell + y'_{\ell+1}) \big),$$

where ϕ is a Lennard-Jones-type interaction potential such that

(i) $\phi \in \mathrm{C}^3((0,+\infty);\mathbb{R})$,

(ii) there exists $r_* > 0$ such that ϕ is convex in $(0, r_*)$ and concave in $(r_*, +\infty)$,

(iii) $\phi^{(k)}(r) \to 0$ rapidly as $r \nearrow \infty$ for $k = 0, \ldots, 3$,

and where y' denotes the discrete backward difference

$$y'_\ell = \varepsilon^{-1}(y_\ell - y_{\ell-1}).$$

For future use, we additionally define the centered second difference

$$y''_\ell = \varepsilon^{-2}(y_{\ell+1} - 2y_\ell + y_{\ell-1}).$$

Assumption (iii) on the interaction potential is not strictly necessary for our analysis but serves to motivate that next-nearest neighbor interactions are typically dominated by nearest neighbor terms.

We assume that the atomistic system is subject to $2N$-periodic external forces $(f_\ell)_{\ell\in\mathbb{Z}}$ with zero mean, i.e., $f \in \mathcal{U}$, so that the *total energy per period* takes the form

$$\mathcal{E}_a^{tot}(y) = \mathcal{E}_a(y) - \varepsilon \sum_{\ell=-N+1}^{N} f_\ell y_\ell.$$

Equilibria $y \in \mathcal{Y}_F$ of the atomistic total energy are solutions to the equilibrium equations

$$\mathcal{F}_{\mathrm{a},\ell}(y) + f_\ell = 0, \qquad -\infty < \ell < \infty, \tag{2.1}$$

where the (scaled) atomistic forces $\mathcal{F}_{\mathrm{a}} : \mathcal{Y}_F \to \mathcal{U}^*$ are defined by

$$\mathcal{F}_{\mathrm{a},\ell}(y) := -\frac{1}{\varepsilon}\frac{\partial \mathcal{E}_{\mathrm{a}}(y)}{\partial y_\ell}, \qquad -\infty < \ell < \infty,$$

and where $\mathcal{U}^*$ is the space of linear functionals on $\mathcal{U}$. We remark that the translational invariance of the atomistic energy implies that $\mathcal{F}_{\mathrm{a},\ell}(y)$ has zero mean,

$$\sum_{\ell=-N+1}^{N} \mathcal{F}_{\mathrm{a},\ell}(y) = \frac{d}{ds}\mathcal{E}_{\mathrm{a}}\left(y - \frac{s}{\varepsilon}e\right)\Big|_{s=0} = 0, \tag{2.2}$$

where $e = (1)_{\ell\in\mathbb{Z}}$ is the unit translation vector. Thus, we see that choosing f to have zero mean is necessary for the existence of solutions.

We note, moreover, that y_F is an equilibrium of the atomistic energy, that is,

$$\mathcal{F}_{\mathrm{a},\ell}(y_F) = 0, \qquad -\infty < \ell < \infty \qquad \forall\, F > 0.$$

The question which we will investigate in this paper, beginning in section 3, is for which F is y_F a *stable equilibrium* and whether the force-based QC method is able to predict the stability of y_F.

2.2. The local QC approximation. We begin by observing that the atomistic energy can be rewritten as a sum over the contributions from each atom:

$$\begin{aligned} \mathcal{E}_{\mathrm{a}}(y) =&\ \varepsilon \sum_{\ell=-N+1}^{N} E^{\mathrm{a}}_\ell(y), \qquad \text{where} \\ E^{\mathrm{a}}_\ell(y) =&\ \tfrac{1}{2}\big[\phi(y'_\ell) + \phi(y'_{\ell+1}) + \phi(y'_{\ell-1}+y'_\ell) + \phi(y'_{\ell+1}+y'_{\ell+2})\big]. \end{aligned} \tag{2.3}$$

If y is "smooth," that is, if y'_ℓ varies slowly, then the atomistic energy can be accurately approximated by the Cauchy–Born or *local QC* energy

$$\begin{aligned} \mathcal{E}_{\mathrm{qcl}}(y) =&\ \varepsilon \sum_{\ell=-N+1}^{N} E^{\mathrm{c}}_\ell(y), \qquad \text{where} \\ E^{\mathrm{c}}_\ell(y) =&\ \tfrac{1}{2}\big[\phi(y'_\ell) + \phi(y'_{\ell+1}) + \phi(2y'_\ell) + \phi(2y'_{\ell+1})\big] = \tfrac{1}{2}\big[\phi_{\mathrm{cb}}(y'_\ell) + \phi_{\mathrm{cb}}(y'_{\ell+1})\big], \end{aligned} \tag{2.4}$$

where $\phi_{\mathrm{cb}}(r) = \phi(r) + \phi(2r)$ is the Cauchy–Born stored energy function.

In this approximation we have replaced the next-nearest neighbor interactions by nearest neighbor interactions to obtain a model with *stronger locality*. This makes it possible to coarsen the model (to remove degrees of freedom), which eventually leads to significant gains in efficiency [5, 17]. However, in the present work we will not consider this additional step.

An equilibrium $y \in \mathcal{Y}_F$ of the local QC energy is a solution to the equilibrium equations

$$\mathcal{F}_{\mathrm{c},\ell}(y) + f_\ell = 0, \qquad -\infty < \ell < \infty, \tag{2.5}$$

where the (scaled) local QC forces $\mathcal{F}_{\mathrm{c}} : \mathcal{Y}_F \to \mathcal{U}^*$ are defined by

$$\mathcal{F}_{\mathrm{c},\ell}(y) := -\frac{1}{\varepsilon}\frac{\partial \mathcal{E}_{\mathrm{a}}(y)}{\partial y_\ell}, \qquad -\infty < \ell < \infty.$$

As in (2.2) it follows that the vector $\mathcal{F}_{\mathrm{c}}(y)$ has zero mean.

2.3. The force-based QC approximation. If a deformation y is "smooth" except in a small region of the domain, then it is desirable to couple the accurate atomistic description with the efficient continuum description. The force-based quasicontinuum (QCF) approximation achieves this by mixing the equilibrium equations of the atomistic model with those of the continuum model without any interface or transition region.

Suppose that y is "smooth" except in a region $\mathcal{A} := \{-K, \dots, K\}$, where $K > 1$. We call $\mathcal{A}$ the *atomistic region* and $\mathcal{C} = \{-N+1, \dots, N\} \backslash \mathcal{A}$ the *continuum region*. The force-based QC approximation is obtained by evaluating the forces in the atomistic region by the full atomistic model (2.1) and the forces in the continuum region by the local QC model (2.5). This yields the QCF operator for the (scaled) forces $\mathcal{F}_{\mathrm{qcf}} : \mathcal{Y}_F \to \mathcal{U}^*$, defined by

$$\mathcal{F}_{\mathrm{qcf},\ell}(y) := \begin{cases} \mathcal{F}_{\mathrm{a},\ell}(y) & \text{if } \ell \in \mathcal{A}, \\ \mathcal{F}_{\mathrm{c},\ell}(y) & \text{if } \ell \in \mathcal{C}. \end{cases} \tag{2.6}$$

Force-based coupling methods such as (2.6) are trivially consistent (provided the continuum model is consistent with the atomistic model) and are therefore a natural remedy for the inconsistencies one observes when formulating simple energy-based coupling methods such as the original QC method [19]. Similar constructions have appeared in the literature under several different names and for various applications (e.g., FeAt [14], CADD [24], or *brutal force mixing* [2]). The force-based QC method arose out of the desire to correct ghost forces present in the original QC method [23], and QCF was identified to be the underlying model of the proposed *ghost-force correction* method in [4, 5]. A rate of convergence and basin of attraction for the convergence of the ghost-force correction iteration to the force-based QC method were given in [5]. Sharp stability estimates for the ghost-force correction iteration are given in [9].

Unfortunately, the forces generated by the QCF method are nonconservative and hence cannot be associated with an energy. Moreover, even though both the atomistic forces $\mathcal{F}_{\mathrm{a}}(y)$ and the local QC forces $\mathcal{F}_{\mathrm{c}}(y)$ have zero mean, it turns out that this is false for the mixed forces $\mathcal{F}_{\mathrm{qcf}}(y)$. A straightforward computation shows that

$$\begin{aligned} \sum_{\ell=-N+1}^{N} \mathcal{F}_{\mathrm{qcf},\ell}(y) = {} & \varepsilon^{-1}[2\phi'(2y'_{-K}) - \phi'(y'_{-K} + y'_{-K-1}) - \phi'(y'_{-K+1} + y'_{-K})] \\ & - \varepsilon^{-1}[2\phi'(2y'_{K+1}) - \phi'(y'_{K+2} + y'_{K+1}) - \phi'(y'_{K+1} + y'_{K})], \end{aligned}$$

which is in general nonzero. After introducing the necessary notation, we will overcome this difficulty by defining a variational form of the QCF method, which effectively projects the QCF forces onto the correct range.

2.4. Norms and variational notation. We recall the backward first difference $v'_\ell = \varepsilon^{-1}(v_\ell - v_{\ell-1})$ and the centered second difference $v''_\ell = \varepsilon^{-2}(v_{\ell+1} - 2v_\ell + v_{\ell-1})$.

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

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

and we let $\mathcal{U}^{0,p}$ denote the space $\mathcal{U}$ equipped with the ℓ^p_ε norm. We further define the $\mathcal{U}^{1,p}$ norm

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

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.

The inner product associated with the ℓ^2_ε 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 have defined the norms $\|\cdot\|_{\ell^p_\varepsilon}$ and the inner product $\langle\cdot,\cdot\rangle$ on $\mathcal{U}$, though we will also apply them for arbitrary vectors from $\mathbb{R}^{2N}$.

The external force $f = (f_\ell)_{\ell\in\mathbb{Z}}$ is a zero mean $2N$-periodic vector, and we have seen that the atomistic forces and the forces in the QCL method are also zero mean $2N$-periodic vectors. Using the inner product, we can view f_ℓ as a linear functional on $\mathcal{U}$. We recall that the space of linear functionals on $\mathcal{U}$ is denoted by $\mathcal{U}^*$, and we note that each such $T \in \mathcal{U}^*$ has a unique representation as a zero mean $2N$-periodic vector $g_T \in \mathcal{U}$:

$$T[v] = \langle g_T, v\rangle \qquad \forall\, v \in \mathcal{U}. \tag{2.7}$$

We will normally not make a distinction between these representations. For example, an external force vector f may be equally interpreted as a linear functional (i.e., $f \in \mathcal{U}^*$) or identified with its Riesz representation (i.e., $f \in \mathcal{U}$).

For $g \in \mathcal{U}^*$, $s = 0, 1$, and $1 \le p \le \infty$, we define the negative norms $\|g\|_{\mathcal{U}^{-s,p}}$ as follows:

$$\|g\|_{\mathcal{U}^{-s,p}} := \sup_{\substack{v\in\mathcal{U}\\ \|v\|_{\mathcal{U}^{s,q}}=1}} \langle g, v\rangle, \tag{2.8}$$

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

Since we can identify elements of $\mathcal{U}^*$ with elements of $\mathcal{U}$, we can investigate the relationship between the $\mathcal{U}^{-0,p}$ and $\mathcal{U}^{0,p}$ norms. This will be useful later on in our analysis. It turns out that $\|\cdot\|_{\mathcal{U}^{-0,p}} \ne \|\cdot\|_{\mathcal{U}^{0,p}}$ in general but that the following equivalence relation holds:

$$\|u\|_{\mathcal{U}^{-0,p}} \le \|u\|_{\mathcal{U}^{0,p}} \le 2\|u\|_{\mathcal{U}^{-0,p}} \qquad \forall\, u \in \mathcal{U}. \tag{2.9}$$

To see this, we note that the inequality $\|u\|_{\mathcal{U}^{-0,p}} \le \|u\|_{\mathcal{U}^{0,p}}$ follows from (2.8) and Hölder's inequality. To prove the second inequality, we use that fact that, for $u \in \mathcal{U}$,

$$\|u\|_{\mathcal{U}^{0,p}} = \sup_{\substack{v\in\mathbb{R}^{2N}\\ \|v\|_{\ell^q_\varepsilon}=1}} \langle u, v\rangle = \sup_{\substack{v\in\mathbb{R}^{2N}\\ \|v\|_{\ell^q_\varepsilon}=1}} \langle u, v - \bar{v}\rangle,$$

where $\bar{v} = \frac{1}{2N}\sum_{j=-N+1}^{N} v_j$. Thus, we can estimate

$$\|u\|_{\mathcal{U}^{0,p}} \le \|u\|_{\mathcal{U}^{-0,p}} \sup_{\substack{v\in\mathbb{R}^{2N}\\ \|v\|_{\ell^q_\varepsilon}=1}} \|v - \bar{v}\|_{\ell^q_\varepsilon} \le 2\|u\|_{\mathcal{U}^{-0,p}},$$

where we also used the fact that, by Hölder's inequality, $\|\bar{v}\|_{\ell^q_\varepsilon} \le \|v\|_{\ell^q_\varepsilon}$ for any $v \in \mathbb{R}^{2N}$.

2.5. Projection of nonconservative forces. If we interpret forces as elements of $\mathcal{U}^*$, then it is natural to consider the following variational formulation of the QCF method:

$$\big\langle \mathcal{F}_{\rm qcf}(y) + f, u \big\rangle = 0 \qquad \forall\, u \in \mathcal{U}. \tag{2.10}$$

In other words, (2.10) requires that $\mathcal{F}_{\rm qcf}(y) + f = 0$ as a functional in $\mathcal{U}^*$. This formulation guarantees that the QCF operator has the correct range.

To obtain an atom-based description of the equilibrium equations, we explicitly compute the representation of $\mathcal{F}_{\rm qcf}(y) \in \mathcal{U}^*$ as an element of $\mathcal{U}$ (see also (2.7)), that is, as a zero mean $2N$-periodic vector $\mathcal{P}_{\mathcal{U}}\mathcal{F}_{\rm qcf}(y)$, where $\mathcal{P}_{\mathcal{U}}$ is defined by

$$\big(\mathcal{P}_{\mathcal{U}} v\big)_\ell = v_\ell - \frac{1}{2N}\sum_{j=-N+1}^{N} v_j.$$

With this notation, the variational equilibrium equations can be understood as *projected* equilibrium equations in atom-based form:

$$\big(\mathcal{P}_{\mathcal{U}}\mathcal{F}_{\rm qcf}(y)\big)_\ell + f_\ell = 0, \qquad -\infty < \ell < \infty. \tag{2.11}$$

The equivalent formulations (2.10) and (2.11) define the correct force-based QC method for the periodic model problem defined in section 2.1.

Remark. The projection of the QCF equilibrium system is, in some sense, an artifact of the periodic boundary conditions. For the displacement boundary conditions that we analyzed in [10], or for the mixed boundary conditions that are considered in [6], this projection is not necessary.

3. Stability of homogeneous deformations. It is easy to see that, in the absence of external forces, the homogeneous lattice $y = y_F$ is an equilibrium of the atomistic energy as well as the local QC energy, that is,

$$\mathcal{F}_{\rm a}(y_F) = 0 \quad \text{and} \quad \mathcal{F}_{\rm c}(y_F) = 0 \qquad \forall\, F > 0.$$

For some values of F, this equilibrium will be stable, by which we mean that the second variation

$$\mathcal{E}_a''(y_F)[u,v] = \varepsilon \sum_{\ell=-N+1}^{N} \big\{ \phi_F'' u_\ell' v_\ell' + \phi_{2F}''(u_\ell' + u_{\ell+1}')(v_\ell' + v_{\ell+1}') \big\} \qquad \text{for } u \in \mathcal{U},$$

where

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

is positive definite, that is,

$$\mathcal{E}_{\rm a}''(y_F)[u,u] > 0 \qquad \forall\, u \in \mathcal{U}\setminus\{0\}.$$

(We note that a second variation, e.g., $\mathcal{E}_{\rm a}''(y_F)$, may be understood either as a bilinear form on $\mathcal{U}$ or a linear operator from $\mathcal{U}$ to $\mathcal{U}^*$. It can also be expressed as a Hessian matrix with respect to a given basis for the vector space $\mathcal{U}$.)

In order to avoid having to distinguish several cases, we will assume throughout our analysis that $F \geq r_*/2$, which implies by property (ii) of the interaction potential that $\phi''_{2F} \le 0$. This assumption holds for most realistic interaction potentials so long as the chain is not under extreme compression.

As above, we can evaluate the second variation of the local QC energy at $y = y_F$,

$$\mathcal{E}''_{\rm qcl}(y_F)[u,v] = \varepsilon \sum_{\ell=-N+1}^{N} A_F u'_\ell v'_\ell,$$

where A_F is the *elastic modulus* of the continuum model:

$$A_F := \phi''_{\rm cb}(F) = \phi''_F + 4\phi''_{2F}.$$

Thus, we say that y_F is stable for the local QC approximation if $\mathcal{E}''_{\rm qcl}(y_F)[u,u] > 0$ for all $u \in \mathcal{U} \setminus \{0\}$.

In [8], we have given explicit characterizations for which F the equilibrium y_F is stable in the atomistic model and in several energy-based QC models. The results for the atomistic and the local QC models are summarized in the following proposition.

PROPOSITION 3.1 (cf. Props. 1 and 2 in [8]). *Let $F \ge r_*/2$; then the second variations $\mathcal{E}''_{\rm a}(y_F)$, respectively, $\mathcal{E}''_{\rm qcl}(y_F)$, are positive definite if and only if*

$$A_F - \lambda_N^2 \varepsilon^2 \phi''_{2F} > 0, \quad \textit{respectively, if} \quad A_F > 0,$$

where $2 \le \lambda_N \le \pi$.

If we denote the critical strains which divide the regions of stability for the atomistic and QCL models, respectively, by $F^*_{\rm a}$ and $F^*_{\rm c}$, then a relatively straightforward error analysis [8, sec. 5] shows that $F^*_{\rm a} = F^*_{\rm c} + O(\varepsilon^2)$; that is, the QCL model accurately reproduces the onset of a fracture instability. In the following section, we investigate whether or not the QCF method has a similar property.

4. Sharp stability of the force-based QC method. A trivial consequence of the definition of $\mathcal{F}_{\rm qcf}$ in (2.6) is that $y = y_F$ is also a solution of the QCF equilibrium equations (2.11):

$$\mathcal{F}_{\rm qcf}(y_F) = 0 \qquad \forall\, F > 0.$$

(As a matter of fact, this means that the QCF method is consistent; though this is not the focus of the present work.)

To investigate the stability of the QCF method we define the linearized QCF operator $L_{{\rm qcf},F} := -\mathcal{F}'_{\rm qcf}(y_F) : \mathcal{U} \to \mathcal{U}^*$ by

$$\langle L_{{\rm qcf},F} u, v\rangle := -\langle \mathcal{F}'_{\rm qcf}(y_F)[u], v\rangle \qquad \forall\, u,\, v \in \mathcal{U}.$$

The equilibrium equations for the linearized force-based approximation are then given by $u \in \mathcal{U}$ satisfying

$$\langle L_{{\rm qcf},F} u, v\rangle = \langle f, v\rangle \qquad \forall\, v \in \mathcal{U},$$

or in functional form

$$\mathcal{P}_{\mathcal{U}} L_{{\rm qcf},F} u = f,$$

where

$$(L_{{\rm qcf},F} u)_\ell = \begin{cases} \phi''_F u''_\ell + \phi''_{2F}(u''_{\ell-1} + 2u''_\ell + u''_{\ell+1}), & \ell \in \mathcal{A}, \\ (\phi''_F + 4\phi''_{2F}) u''_\ell, & \ell \in \mathcal{C}. \end{cases} \tag{4.1}$$

We remark that, while $L_{{\rm qcf},F} \in L(\mathcal{U}, \mathcal{U}^*)$, the projected operator $\mathcal{P}_{\mathcal{U}} L_{{\rm qcf},F}$ may be interpreted as a map from $\mathcal{U}$ to $\mathcal{U}$.

4.1. Lack of coercivity. Since the force field $\mathcal{F}_{\mathrm{qcf}}(y)$ is nonconservative and the linearized QCF operator $L_{\mathrm{qcf},F}$ is not the second variation of an energy functional, positivity (or coercivity) of $L_{\mathrm{qcf},F}$ may be the incorrect notion of stability for the QCF model. Indeed, it turns out that if N is large, then $L_{\mathrm{qcf},F}$ cannot be positive definite.

THEOREM 4.1. *Let $\phi''_F > 0$ and $\phi''_{2F} \neq 0$; then there exist constants $C_1, C_2 > 0$, which may depend on ϕ''_F and ϕ''_{2F}, such that, for N sufficiently large and for $2 \leq K \leq N/2$,*

$$-C_1 N^{1/2} \leq \inf_{\substack{u \in \mathcal{U} \\ \|u'\|_{\ell^2_\varepsilon}=1}} \langle L_{\mathrm{qcf},F} u, u\rangle \leq -C_2 N^{1/2}.$$

In [10], we have established this result for a Dirichlet boundary value problem. The proof carries over from the Dirichlet case almost verbatim and is therefore omitted. As a matter of fact, the test function which we explicitly constructed in the proof of Lemma 4.1 in [10] is already periodic and, after shifting it to have zero mean, can therefore be used again to prove Theorem 4.1.

Theorem 4.1 forces us to consider alternative notions of stability. For example, one could understand $L_{\mathrm{qcf},F}$ as a linear operator between appropriately chosen discrete function spaces, determine for which values of F it is bijective, and estimate the norm of its inverse. Physically, this measures the magnitude of the response of the equilibrium configuration to perturbations in external forces. In section 4.2 we attempt to find the largest interval surrounding $F = 1$ for which $L_{\mathrm{qcf},F}$ is bijective and consider this region to be the approximation of the stable region given by operator stability of $L_{\mathrm{qcf},F}$. However, an operator can be bijective and its inverse can have bounded norm even when it has negative eigenvalues, so for a general equilibrium state such as y_F, invertibility alone is not a suitable criterion for determining the "physical" stability. To be able to decide whether a stable equilibrium of the QCF equations is also stable in a physical sense, we propose a notion of dynamical stability in section 4.4.

4.2. Stability as a linear operator. Since $\mathcal{U}$ is a finite-dimensional linear space, the choice of topology with which we equip it is unimportant to the question of whether $L_{\mathrm{qcf},F}$ is invertible. However, it has significant repercussions when we analyze an operator norm of the inverse, that is, $\|L^{-1}_{\mathrm{qcf},F}\|$, in the limit as $N \to \infty$.

Our strongest and simplest result is obtained when we view $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F}$ as a map from $\mathcal{U}^{2,\infty}$ to $\mathcal{U}^{0,\infty}$.

THEOREM 4.2. *If $|\phi''_F| - (4 + 2\varepsilon)|\phi''_{2F}| > 0$, then $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F} : \mathcal{U} \to \mathcal{U}$ is bijective and*

$$\big\|(\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F})^{-1}\big\|_{L(\mathcal{U}^{0,\infty},\, \mathcal{U}^{2,\infty})} \leq \frac{1}{|\phi''_F| - (4 + 2\varepsilon)|\phi''_{2F}|}.$$

Proof. By (4.1) we can rewrite $L_{\mathrm{qcf},F}$ in the form

$$\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F} = \phi''_F L_1 + \phi''_{2F} \mathcal{P}_{\mathcal{U}} \tilde{L}_2,$$

where L_1 and $\tilde{L}_2$ are given by

$$\begin{aligned}
(L_1 u)_\ell &= -\varepsilon^{-2}(u_{\ell+1} - 2u_\ell + u_{\ell-1}) \quad \text{and} \\
(\tilde{L}_2 u)_\ell &= \begin{cases} -\varepsilon^{-2}(u_{\ell+2} - 2u_\ell + u_{\ell-2}), & \ell = -K, \dots, K, \\ -4\varepsilon^{-2}(u_{\ell+1} - 2u_\ell + u_{\ell-1}) & \text{otherwise.} \end{cases}
\end{aligned}$$

We note that $\mathcal{P}_\mathcal{U} L_1 = L_1$, which is why we have included the projection only in the second-neighbor operator.

The projection of $\tilde{L}_2$ given by $\mathcal{P}_\mathcal{U}\tilde{L}_2$ is

$$(\mathcal{P}_\mathcal{U}\tilde{L}_2 u)_\ell = (\tilde{L}_2 u)_\ell - \frac{\varepsilon}{2}\sum_{j=-N+1}^{N} (\tilde{L}_2 u)_j.$$

We will prove below that

$$\|\mathcal{P}_\mathcal{U}\tilde{L}_2\|_{L(\mathcal{U}^{2,\infty},\, \mathcal{U}^{0,\infty})} \le 4 + 2\varepsilon. \tag{4.2}$$

Assuming that this bound is established, we obtain

$$\begin{aligned}\|\mathcal{P}_\mathcal{U} L_{\mathrm{qcf,F}} u\|_{\ell^\infty} \ge{}& |\phi''_F|\|L_1 u\|_{\ell^\infty} - |\phi''_{2F}|\|\mathcal{P}_\mathcal{U}\tilde{L}_2 u\|_{\ell^\infty}\\ \ge{}& (|\phi''_F| - (4+2\varepsilon)|\phi''_{2F}|)\|u''\|_{\ell^\infty},\end{aligned}$$

which is equivalent to the statement of the theorem.

To prove (4.2), we note that, for $\ell = -K, \dots, K$, we have

$$(\tilde{L}_2 u)_\ell = -(u''_{\ell+1} + 2u''_\ell + u''_{\ell-1}) = -4u''_\ell - (u''_{\ell+1} - 2u''_\ell + u''_{\ell-1}).$$

Using the first representation of $(\tilde{L}_2 u)_\ell$ above, we immediately see that (for ℓ from the continuum region this statement is trivial)

$$\big|(\tilde{L}_2 u)_\ell\big| \le 4\|u''\|_{\ell^\infty} \qquad \text{for } \ell = -N+1, \dots, N.$$

From the second representation of $(\tilde{L}_2 u)_\ell$, we obtain

$$\begin{aligned}\sum_{\ell=-N+1}^{N} (\tilde{L}_2 u)_\ell ={}& -4\sum_{\ell=-N+1}^{N} u''_\ell - \sum_{\ell=-K}^{K} (u''_{\ell+1} - 2u''_\ell + u''_{\ell-1})\\ ={}& -u''_{K+1} + u''_K + u''_{-K} - u''_{-K-1},\end{aligned}$$

and hence

$$\begin{aligned}\big|(\mathcal{P}_\mathcal{U}\tilde{L}_2 u)_\ell\big| \le{}& \big|(\tilde{L}_2 u)_\ell\big| + \left|\frac{\varepsilon}{2}\sum_{j=-N+1}^{N}(\tilde{L}_2 u)_j\right|\\ \le{}& 4\|u''\|_{\ell^\infty} + \frac{\varepsilon}{2}\big(|u''_{K+1}| + |u''_K| + |u''_{-K-1}| + |u''_{-K}|\big)\\ \le{}& (4+2\varepsilon)\|u''\|_{\ell^\infty}.\end{aligned}$$

This establishes (4.2) and thus concludes the proof of the theorem. ∎

Remark. With a small modification, Theorem 4.2 remains true for an arbitrary choice of the atomistic region $\mathcal{A}$. The correction 2ε then needs to be replaced by $n_i\varepsilon$, where n_i is the number of interfaces between the atomistic and the continuum region.

Remark. Theorem 4.2 also holds in the case of the artificial Dirichlet boundary conditions analyzed in [10]. In that case, the projection $\mathcal{P}_\mathcal{U}$ is not required, and therefore the correction 2ε does not occur at all.

Theorem 4.2 is, in many respects, a very satisfactory result. It shows that, except for a small error, QCF is stable whenever the atomistic model is. However, the choice of function space $\mathcal{U}^{2,\infty}$ is somewhat unusual, and it is highly unlikely that such a result would remain true in higher dimensions, as it requires a regularity that is not normally exhibited by linear elliptic systems.

It is therefore also interesting to analyze the QCF operator as a map from $\mathcal{U}^{1,p}$ to $\mathcal{U}^{-1,p} = (\mathcal{U}^{1,q})^*$, where $1 \le p \le \infty$. However, we saw in [10, Thm. 7.1] for a Dirichlet problem that, for $1 \le p < \infty$, the stability of $L_{\mathrm{qcf},F}$ is not uniform in N. The following theorem, whose proof is contained in Appendix B, establishes the same result for the periodic model we consider in the present paper.

THEOREM 4.3. *Suppose that $\phi''_F > 0$, $\phi''_{2F} \in \mathbb{R} \setminus \{0\}$, and $1 \le p < \infty$. Then there exists a constant $C > 0$, depending on ϕ''_F and ϕ''_{2F}, such that, for $2 \le K < N - 2$,*

$$\|L^{-1}_{\mathrm{qcf},F}\|_{L(\mathcal{U}^{-1,p},\ \mathcal{U}^{1,p})} \ge CN^{1/p}.$$

It remains to investigate the case $p = \infty$. The following result is an extension of [10, Thm. 5.1] to periodic boundary conditions. Its proof is contained in Appendix A.

THEOREM 4.4. *If $F \ge r_*/2$ and $\phi''_F + 8\phi''_{2F} > 0$, then*

$$\|L^{-1}_{\mathrm{qcf},F}\|_{L(\mathcal{U}^{-1,\infty},\ \mathcal{U}^{1,\infty})} \le \frac{2}{\phi''_F + 8\phi''_{2F}}.$$

Theorem 4.4 establishes *operator stability* of the $L_{\mathrm{qcf},F}$ operator, uniformly in N, provided that $\phi''_F + 8\phi''_{2F} > 0$. Compared with Proposition 3.1 this result predicts a significantly smaller stability region than either the atomistic model or the continuum model. We employ numerical experiments to see whether the condition $\phi''_F + 8\phi''_{2F} > 0$ is sharp.

The norm $\|L^{-1}_{\mathrm{qcf},F}\|_{L(\mathcal{U}^{-1,\infty},\ \mathcal{U}^{1,\infty})}$ is difficult to calculate explicitly, so we will estimate it in terms of the ℓ^∞-operator norm of a related matrix. To that end, we note that, according to Lemma A.1, $L_{\mathrm{qcf},F}$ can be represented in terms of a conjugate operator, $E_{\mathrm{qcf},F}$, by

$$\langle L_{\mathrm{qcf},F} u, v\rangle = \langle E_{\mathrm{qcf},F} u', v'\rangle \qquad \forall u, v \in \mathcal{U}.$$

The explicit matrix representation of $E_{\mathrm{qcf},F}$ provided in formula (A.4) is such that $E_{\mathrm{qcf},F} e = A_F e$, where $e = (1, \dots, 1)^T$, and where we recall that $A_F = \phi''_F + 4\phi''_{2F}$. It thus follows that the projected operator $\mathcal{P}_{\mathcal{U}} E_{\mathrm{qcf},F} : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$ satisfies

$$\mathcal{P}_{\mathcal{U}} E_{\mathrm{qcf},F} : \mathcal{U} \to \mathcal{U} \quad \text{and} \quad \mathcal{P}_{\mathcal{U}} E_{\mathrm{qcf},F} e = 0.$$

Here, and for the remainder of the section, we identify $\mathcal{U}$ with the subspace of $\mathbb{R}^{2N}$ of zero mean vectors. After these preliminary remarks, we establish the following result.

PROPOSITION 4.5. *The QCF operator $L_{\mathrm{qcf},F} : \mathcal{U} \to \mathcal{U}^*$ is invertible if and only if $(\mathcal{P}_{\mathcal{U}} E_{\mathrm{qcf},F} + e \otimes e) \in \mathbb{R}^{2N \times 2N}$ is invertible, and*

$$\tfrac{1}{2}\|T\|_\infty \le \|L^{-1}_{\mathrm{qcf},F}\|_{L(\mathcal{U}^{-1,\infty},\ \mathcal{U}^{1,\infty})} \le 2\|T\|_\infty,$$

where

$$T = \mathcal{P}_{\mathcal{U}} (\mathcal{P}_{\mathcal{U}} E_{\mathrm{qcf},F} + e \otimes e)^{-1} \mathcal{P}_{\mathcal{U}},$$

and where $\|T\|_\infty$ denotes the ℓ^∞-operator norm of T.

Proof. The first statement follows from the discussion above.

To prove the upper and lower bounds for $\|L^{-1}_{\mathrm{qcf},F}\|_{L(\mathcal{U}^{-1,\infty},\mathcal{U}^{1,\infty})}$, we first note that, by definition of T, it follows that

$$T\mathcal{P}_{\mathcal{U}} E_{\mathrm{qcf},F} f = \mathcal{P}_{\mathcal{U}} E_{\mathrm{qcf},F} T f = f \qquad \forall\, f \in \mathcal{U};$$

that is, $T = (\mathcal{P}_{\mathcal{U}} E_{\mathrm{qcf},F})^{-1}$ on $\mathcal{U}$. In addition, we also have $Te = 0$.

Next, we note that

$$\frac{1}{\|L_{\mathrm{qcf},F}^{-1}\|_{L(\mathcal{U}^{-1,\infty},\,\mathcal{U}^{1,\infty})}} = \inf_{\substack{v\in\mathcal{U}\\ \|v'\|_{\ell_\varepsilon^\infty}=1}} \sup_{\substack{w\in\mathcal{U}\\ \|w'\|_{\ell_\varepsilon^1}=1}} \langle L_{\mathrm{qcf},F} v,\, w\rangle$$

$$= \inf_{\substack{v\in\mathcal{U}\\ \|v'\|_{\ell_\varepsilon^\infty}=1}} \sup_{\substack{w\in\mathcal{U}\\ \|w'\|_{\ell_\varepsilon^1}=1}} \langle E_{\mathrm{qcf},F} v',\, w'\rangle = \frac{1}{\|E_{\mathrm{qcf},F}^{-1}\|_{L(\mathcal{U}^{-0,\infty},\,\mathcal{U}^{0,\infty})}}.$$

Since $T = (\mathcal{P}_{\mathcal{U}} E_{\mathrm{qcf},F})^{-1}$ on $\mathcal{U}$, it follows that

$$\|L_{\mathrm{qcf},F}^{-1}\|_{L(\mathcal{U}^{-1,\infty},\,\mathcal{U}^{1,\infty})} = \|T\|_{L(\mathcal{U}^{-0,\infty},\,\mathcal{U}^{0,\infty})}.$$

To prove the upper bound, we use (2.9) to estimate

$$\|T\|_{L(\mathcal{U}^{-0,\infty},\,\mathcal{U}^{0,\infty})} = \sup_{\substack{f\in\mathcal{U}\\ f\neq 0}} \frac{\|Tf\|_{\mathcal{U}^{0,\infty}}}{\|f\|_{\mathcal{U}^{-0,\infty}}} \le \sup_{\substack{f\in\mathcal{U}\\ f\neq 0}} \frac{\|Tf\|_{\ell_\varepsilon^\infty}}{\frac{1}{2}\|f\|_{\ell_\varepsilon^\infty}} \le 2 \sup_{\substack{f\in\mathbb{R}^{2N}\\ f\neq 0}} \frac{\|Tf\|_{\ell_\varepsilon^\infty}}{\|f\|_{\ell_\varepsilon^\infty}} = 2\|T\|_\infty.$$

To prove the lower bound, we first note that $T\mathcal{P}_{\mathcal{U}} = T$. We will also use the fact that $\|\mathcal{P}_{\mathcal{U}} f\|_{\ell_\varepsilon^\infty} \le 2\|f\|_{\ell_\varepsilon^\infty}$ for all $f \in \mathbb{R}^{2N}$. Employing also (2.9) again, we can deduce that

$$\|T\|_{L(\mathcal{U}^{-0,\infty},\,\mathcal{U}^{0,\infty})} = \sup_{\substack{f\in\mathbb{R}^{2N}\\ \mathcal{P}_{\mathcal{U}} f\neq 0}} \frac{\|T\mathcal{P}_{\mathcal{U}} f\|_{\mathcal{U}^{0,\infty}}}{\|\mathcal{P}_{\mathcal{U}} f\|_{\mathcal{U}^{-0,\infty}}} \ge \sup_{\substack{f\in\mathbb{R}^{2N}\\ \mathcal{P}_{\mathcal{U}} f\neq 0}} \frac{\|T\mathcal{P}_{\mathcal{U}} f\|_{\mathcal{U}^{0,\infty}}}{\|\mathcal{P}_{\mathcal{U}} f\|_{\mathcal{U}^{0,\infty}}} = \sup_{\substack{f\in\mathbb{R}^{2N}\\ \mathcal{P}_{\mathcal{U}} f\neq 0}} \frac{\|Tf\|_{\ell_\varepsilon^\infty}}{\|\mathcal{P}_{\mathcal{U}} f\|_{\ell_\varepsilon^\infty}}$$

$$\ge \sup_{\substack{f\in\mathbb{R}^{2N}\\ \mathcal{P}_{\mathcal{U}} f\neq 0}} \frac{\|Tf\|_{\ell_\varepsilon^\infty}}{2\|f\|_{\ell_\varepsilon^\infty}} = \frac{1}{2} \sup_{\substack{f\in\mathbb{R}^{2N}\\ f\neq 0}} \frac{\|Tf\|_{\ell_\varepsilon^\infty}}{\|f\|_{\ell_\varepsilon^\infty}} = \tfrac{1}{2}\|T\|_\infty.$$

The penultimate equality holds because $\mathcal{P}_{\mathcal{U}} f = 0$ implies that $Tf = 0$. ◻

In Proposition 4.5 we have reduced the estimation of the operator norm of $L_{\mathrm{qcf},F}^{-1}$ to the computation of the ℓ^∞-operator norm (which is simply the largest row sum of the absolute value of the entries) of a matrix $T \in \mathbb{R}^{2N\times 2N}$, which is explicitly available (note that $\mathcal{P}_{\mathcal{U}} = I - \frac{1}{2} e \otimes e \in \mathbb{R}^{2N\times 2N}$).

In Figure 4.1, we plot the norm of T as a function of $A_F/\phi''_F = 1 + 4\phi''_{2F}/\phi''_F$. We clearly observe that $L_{\mathrm{qcf},F}$ is in fact stable for all macroscopic gradients F for which $A_F > 0$; that is, the bound required in Theorem 4.4 is not sharp. Moreover, the numerical experiments shown in Figure 4.1 support the following conjecture.

CONJECTURE 1. *If $\phi''_F + 4\phi''_{2F} > 0$, then $L_{\mathrm{qcf},F}$ is invertible. Furthermore, there exists a positive, real-valued function $\eta(r) : \mathbb{R}_{>0} \to \mathbb{R}_{>0}$ independent of N, K, ϕ''_F, and ϕ''_{2F}, such that whenever $\phi''_F + 4\phi''_{2F} > 0$,*

$$\|L_{\mathrm{qcf},F}^{-1}\|_{L(\mathcal{U}^{-1,\infty},\,\mathcal{U}^{1,\infty})} \le \tfrac{1}{\phi''_F}\,\eta\Big(1 + 4\tfrac{\phi''_{2F}}{\phi''_F}\Big).$$

We note that $\eta(1 + 4\frac{\phi''_{2F}}{\phi''_F}) \to \infty$ as $1 + 4\frac{\phi''_{2F}}{\phi''_F} \to 0$. In fact, the numerical experiments suggest that $\|L_{\mathrm{qcf},F}^{-1}\|_{L(\mathcal{U}^{-1,\infty},\,\mathcal{U}^{1,\infty})}$ grows faster than $\frac{1}{\phi''_F + 4\phi''_{2F}}$, which would imply that an estimate such as the one in Theorem 4.4, but with the constant 8 replaced by 4, would be false.

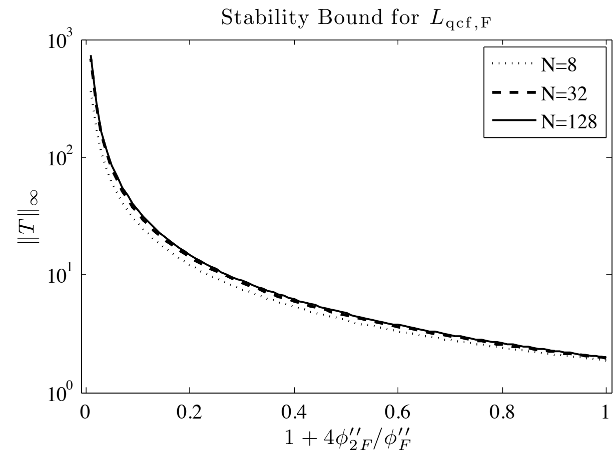

FIG. 4.1. *Computation of* $\|T\|_\infty$*, where* $T = \mathcal{P}_\mathcal{U}(\mathcal{P}_\mathcal{U} E_{\mathrm{qcf},F} + e\otimes e)^{-1}\mathcal{P}_\mathcal{U}$*, which gives lower and upper bounds for* $\|L^{-1}_{\mathrm{qcf},F}\|_{L(\mathcal{U}^{-1,\infty},\, \mathcal{U}^{1,\infty})}$ *(cf. Proposition* 4.5*). The graphs indicate that* $L_{\mathrm{qcf},F}$ *is stable as an operator from* $\mathcal{U}^{1,\infty}$ *to* $\mathcal{U}^{-1,\infty}$*, uniformly in* N*, for all macroscopic strains* F *up to the critical strain for QCL and QNL.*

4.3. The quasi-nonlocal coupling method. In preparation for the following section, where we introduce another notion of stability for the QCF method, we review a popular energy-based coupling method. In the next section, we will make numerical comparisons between this method and the QCF method.

The quasi-nonlocal quasicontinuum (QNL) approximation [25] was derived as a modification of the energy-based QC approximation [19] in order to correct the inconsistency at the atomistic-to-continuum interface [5, 23]. In the case of next-nearest neighbor pair interaction, the QNL method can be formulated as follows. Nearest neighbor interaction terms are left unchanged. A next-nearest neighbor interaction term $\phi(\varepsilon^{-1}(y_{\ell+1} - y_{\ell-1}))$ is left unchanged if atom ℓ belongs to the atomistic region but is replaced by a Cauchy–Born approximation

$$\phi(\varepsilon^{-1}(y_{\ell+1} - y_{\ell-1})) \approx \tfrac{1}{2}\big[\phi(2y'_\ell) + \phi(2y'_{\ell+1})\big] \quad \text{if } \ell \in \mathcal{C}.$$

This process yields the QNL energy functional

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

We remark that the QNL method is consistent for our next-nearest neighbor pair interaction model, and in particular, y_F is an equilibrium of the QNL energy functional in the absence of external forces. Moreover, in [8] we have established the following sharp stability result for the QNL method, which shows that the QNL method is predictive up to the limit load for fracture.

PROPOSITION 4.6 (Prop. 3 in [8]). *Suppose that* $F \geq r_*/2$ *and that* $K \leq N - 1$*; then* $\mathcal{E}''_{\mathrm{qnl}}(y_F)$ *is positive definite in* $\mathcal{U}$ *if and only if* $A_F > 0$.

4.4. Dynamical stability. We have pointed out in section 4.1 that operator stability for $L_{\mathrm{qcf},F}$ cannot guarantee that the equilibrium y_F is a stable equilibrium of the atomistic model (e.g., a local minimum). To obtain at least a theoretical methodology

TABLE 4.1

The spectra of $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F}$ and $\mathcal{E}''_{\mathrm{qnl}}(y_F)$ are computed for the tabulated values of N and K, as well as for $A_F = -0.5, -0.4, \ldots, 0.9, 1$ with $\phi''_F = 1$ fixed. In each case, the ℓ^∞ norm of the ordered vectors constructed from the difference of the eigenvalues is computed and the maximum over the different values of A_F is formed. The resulting number is displayed below. All entries are zero to numerical precision of the eigenvalue solver.

N	8	16	32	64	128
$K = 4$	6.54*e*-13	4.21*e*-12	1.82*e*-11	9.28*e*-11	4.66*e*-10
$K = \lfloor N^{1/2} \rfloor$	7.11*e*-13	4.21*e*-12	1.96*e*-11	8.73*e*-11	4.95*e*-10
$K = \lfloor N^{2/3} \rfloor$	8.24*e*-13	3.75*e*-12	2.41*e*-11	9.09*e*-11	4.37*e*-10
$K = N/2$	6.54*e*-13	3.75*e*-12	2.23*e*-11	8.55*e*-11	5.53*e*-10

to determine stability of y_F from the QCF operator alone, we propose the notion of *dynamical stability*. We stress that we do not propose the following dynamical system as an approximation to the exact Hamiltonian dynamics for the atomistic energy functional but only as a means to study the stability of the equilibrium $y = y_F$.

The dynamical system

$$\begin{aligned} &\ddot{u}(t) + \mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F} u(t) = 0, \\ &u(0) = u_0, \quad u'(0) = 0 \end{aligned} \tag{4.3}$$

has a unique solution $u \in \mathrm{C}^\infty([0, +\infty); \mathcal{U})$. We call this dynamical system *stable* if there exists a constant C, possibly dependent on N, such that

$$\|u(t)\|_{\ell^2_\varepsilon} \le C \|u_0\|_{\ell^2_\varepsilon} \qquad \forall t > 0, \quad \forall u_0 \in \mathcal{U}. \tag{4.4}$$

This condition can be best understood in terms of the spectrum of $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F}$. In numerical experiments, which are shown in Table 4.1, we have made the surprising observation that $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F}$ and $\mathcal{E}''_{\mathrm{qnl}}(y_F)$ appear to have the same spectrum. This has led us to make the following conjecture.

CONJECTURE 2. *For all $N \ge 4$, and $F > 0$, the operator $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F}$ is diagonalizable and its spectrum is identical to the spectrum of $\mathcal{E}''_{\mathrm{qnl}}(y_F)$.*

Since $\mathcal{E}''_{\mathrm{qnl}}(y_F)$ is positive if and only if $A_F > 0$ (cf. Proposition 4.6), the validity of the conjecture would imply that $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F}$ has positive real eigenvalues if and only if $A_F > 0$.

To see how this observation implies dynamical stability (4.4) for $A_F > 0$, let V denote the matrix whose columns are the eigenvectors for $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F}$. Then V has full rank and $V^{-1} \mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F} V$ is a diagonal matrix with the eigenvalues of $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F}$ on its diagonal. If we define $z(t) = V^{-1} u(t)$, then

$$\begin{aligned} \ddot{z}(t) + V^{-1} \mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F} V z(t) &= 0, \\ z(0) = V^{-1} u_0, \quad z'(0) &= 0. \end{aligned}$$

The solution to the above system of equations is $z_j(t) = z_j(0) \cos(\sqrt{\lambda_j} t)$, which clearly satisfies the bound $\|z(t)\|_{\ell^2_\varepsilon} \le \|V^{-1} u_0\|_{\ell^2_\varepsilon}$ for all t. Thus, we can estimate

$$\begin{aligned} \|u(t)\|_{\ell^2_\varepsilon} &\le \|V\|_{L(\ell^2_\varepsilon, \ell^2_\varepsilon)} \|V^{-1} u(t)\|_{\ell^2_\varepsilon} \\ &\le \|V\|_{L(\ell^2_\varepsilon, \ell^2_\varepsilon)} \|V^{-1} u_0\|_{\ell^2_\varepsilon} \\ &\le \mathrm{cond}(V) \|u_0\|_{\ell^2_\varepsilon}, \end{aligned}$$

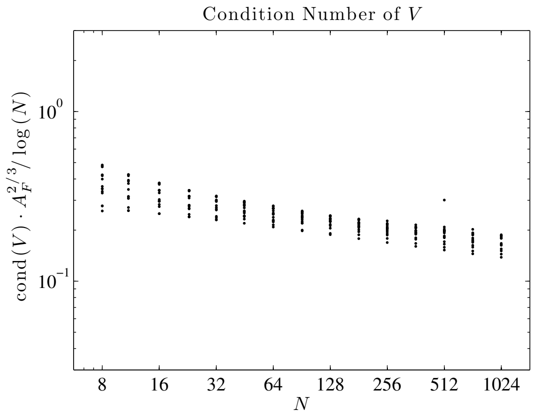

FIG. 4.2. *For each value of* N*, data points are plotted which represent* $\mathrm{cond}\,(V)\cdot A_F^{2/3}/\log(N)$ *for* $K = 4, N^{1/2}, N^{2/3}, N/2$ *and* $A_F = 1/2, 1/4, 1/8$*. Here,* $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F} = V\Lambda^{\mathrm{qcf}} V^{-1}$ *is the spectral decomposition of* $\mathcal{P}_{\mathcal{U}} L_{\mathrm{qcf},F}$*. We note the outlier at* $N = 512$*,* $K = 256$*, and* $A_F = 1/4$*, which is likely due to numerical instability in the computation of* $\mathrm{cond}(V)$ *when a gap between eigenvalues of* $L_{\mathrm{qcf},F}$ *is sufficiently small.*

where the condition number of V is defined as usual by $\mathrm{cond}(V) = \|V\|\,\|V^{-1}\|$. Hence, we see that, subject to the validity of Conjecture 2, the dynamical system (4.3) is indeed stable for $A_F > 0$.

Remark. We present numerical experiments in Figure 4.2 showing that $\mathrm{cond}(V)$ grows very slowly with increasing N. It appears that $\mathrm{cond}(V)$ grows like $\mathrm{O}(\log N)$, although the convergence of $\mathrm{cond}\,(V)\cdot A_F^{2/3}/\log(N)$ for large N was violated for some values of N, K, and A_F. The existence of these special values of N, K, and A_F can possibly be explained by a numerical instability in the computation of $\mathrm{cond}(V)$ when a gap between eigenvalues of $L_{\mathrm{qcf},F}$ is sufficiently small.

Conclusion. We propose that a sharp stability analysis of atomistic-to-continuum coupling methods is an essential ingredient for the evaluation of their predictive capability, as important as a sharp consistency analysis. In the present paper, we have established such a sharp stability analysis for the force-based QC method applied to the problem of tensile loading. We have analyzed three notions of stability:

(i) *Positivity* (coercivity) is generically not satisfied.

(ii) *Operator stability*, uniformly in the size of the atomistic system, holds only with an appropriate choice of function spaces. It does not hold for several natural choices.

(iii) *Dynamical stability* is satisfied up to the critical load. This result is based on the numerical observation that the spectra of the QCF and QNL operators coincide.

Positivity and dynamical stability are equivalent for energy-based methods, and under suitable conditions and choices of function spaces they imply operator stability. However, the fact that the QCF method is nonconservative and gives rise to nonnormal operators leads to a much richer mathematical structure.

Appendix A. Proof of Theorem 4.4: Stability of $L_{\mathrm{qcf},F}$. Theorem 4.4 states that if $\phi_F'' + 8\phi_{2F}'' > 0$, then $L_{\mathrm{qcf},F}$ is stable as an operator from $\mathcal{U}^{1,\infty}$ to $\mathcal{U}^{-1,\infty}$, uniformly in N.

The proof of this statement uses a variational representation for the QCF operator, which we derived in [10], and which is also valid for periodic boundary conditions:

$$L_{\mathrm{qcf},\,F} = \phi''_F L_1 + \phi''_{2F}(L_2^{\mathrm{reg}} + L_2^{\mathrm{sng}}),$$

where the three operators $L_1, L_2^{\mathrm{reg}}, L_2^{\mathrm{sng}} : \mathcal{U} \to \mathcal{U}^*$ are given by

$$\begin{aligned}
\langle L_1 u, v\rangle &= \langle u', v'\rangle, \\
\langle L_2^{\mathrm{reg}} u, v\rangle &= \varepsilon \sum_{\ell=-N+1}^{-K} 4u'_\ell v'_\ell + \varepsilon \sum_{\ell=-K+1}^{K} (u'_{\ell-1} + 2u'_\ell + u'_{\ell+1})v'_\ell + \varepsilon \sum_{\ell=K+1}^{N} 4u'_\ell v'_\ell, \\
\langle L_2^{\mathrm{sng}} u, v\rangle &= (u'_{-K+1} - 2u'_{-K} + u'_{-K-1})v_{-K} - (u'_{K+2} - 2u'_{K+1} + u'_K)v_K.
\end{aligned}$$

We omit the proof of this representation, which is a straightforward summation by parts argument and carries over verbatim from [10]. Upon defining

$$\sigma_\ell(u') = \begin{cases} \phi''_F u'_\ell + \phi''_{2F}(u'_{\ell-1} + 2u'_\ell + u'_{\ell+1}), & \ell = -K+1, \dots, K, \\ (\phi''_F + 4\phi''_{2F})u'_\ell & \text{otherwise,} \end{cases}$$

as well as

$$\begin{aligned}
\alpha_K(u') &= \phi''_{2F}(u'_{K+2} - 2u'_{K+1} + u'_K) \quad \text{and} \\
\alpha_{-K}(u') &= \phi''_{2F}(u'_{-K+1} - 2u'_{-K} + u'_{-K-1}),
\end{aligned} \tag{A.1}$$

we can rewrite this representation as

$$\langle L_{\mathrm{qcf},\,F} u, v\rangle = \langle \sigma(u'), v'\rangle + \alpha_{-K}(u')v_{-K} - \alpha_K(u')v_K.$$

Using the periodic Heaviside function $h \in \mathcal{U}$, given by

$$h_\ell = \begin{cases} \frac{1}{2}(1 - \varepsilon\ell) - \frac{\varepsilon}{4}, & \ell \ge 0, \\ -\frac{1}{2}(1 + \varepsilon\ell) - \frac{\varepsilon}{4}, & \ell < 0, \end{cases} \tag{A.2}$$

and setting $\tilde{h}_\ell = h_{\ell-1}$, the point evaluation functional $v \mapsto v_0$, $v \in \mathcal{U}$, can be represented by

$$v_0 = \langle h', v\rangle = -\langle \tilde{h}, v'\rangle \qquad \forall\, v \in \mathcal{U}.$$

Combining these observations, we obtain the following result.

LEMMA A.1. *The operator $L_{\mathrm{qcf},F}$ can be written as*

$$\langle L_{\mathrm{qcf},F} u, v\rangle = \langle E_{\mathrm{qcf},F} u', v'\rangle \qquad \forall\, u, v \in \mathcal{U}, \tag{A.3}$$

where

$$(E_{\mathrm{qcf},F} u')_\ell = \sigma_\ell(u') - \alpha_{-K}(u') h_{\ell+K-1} + \alpha_K(u') h_{\ell-K-1}, \tag{A.4}$$

for σ, h, and $\alpha_{\pm K}$ as defined above.

Even though the variational representations of the Dirichlet case and the periodic case are the same, we cannot translate the proof for inf-sup stability that we used in [10], as it required a matrix representation that is unavailable for periodic boundary conditions. Instead, we will compute a fairly explicit characterization of $L_{\mathrm{qcf},\,F}^{-1}$ to estimate its norm directly. It is most convenient to do so if we define an equivalent norm on $\mathcal{U}^{-1,\infty}$. Note that $L_1 : \mathcal{U} \to \mathcal{U}^*$ is bijective, and hence we can define

$$\|g\|_{\tilde{\mathcal{U}}^{-1,\infty}} = \|L_1^{-1} g\|_{\mathcal{U}^{1,\infty}} \qquad \text{for } g \in \mathcal{U}^*.$$

LEMMA A.2. *For all $g \in \mathcal{U}^*$, it holds that*

$$\frac{1}{2}\|g\|_{\tilde{\mathcal{U}}^{-1,\infty}} \le \|g\|_{\mathcal{U}^{-1,\infty}} \le \|g\|_{\tilde{\mathcal{U}}^{-1,\infty}}.$$

Proof. Let $z = L_1^{-1} g$, that is,

$$\langle z', v' \rangle = \langle g, v \rangle \qquad \forall v \in \mathcal{U}.$$

Taking the supremum over v with $\|v'\|_{\ell^1_\varepsilon} = 1$ and applying Hölder's inequality, we obtain the upper bound

$$\|g\|_{\mathcal{U}^{-1,\infty}} \le \|z'\|_{\ell^\infty_\varepsilon} = \|g\|_{\tilde{\mathcal{U}}^{-1,\infty}}.$$

The lower bound follows from the fact, which is proved below, that

$$\tfrac{1}{2}\|z'\|_{\ell^\infty_\varepsilon} \le \sup_{\substack{v \in \mathcal{U} \\ \|v'\|_{\ell^1_\varepsilon} = 1}} \langle z', v' \rangle \qquad \forall z \in \mathcal{U}. \tag{A.5}$$

Namely, this implies that

$$\tfrac{1}{2}\|g\|_{\tilde{\mathcal{U}}^{-1,\infty}} = \tfrac{1}{2}\|z'\|_{\ell^\infty_\varepsilon} \le \sup_{\substack{v \in \mathcal{U} \\ \|v'\|_{\ell^1_\varepsilon} = 1}} \langle z', v' \rangle = \sup_{\substack{v \in \mathcal{U} \\ \|v'\|_{\ell^1_\varepsilon} = 1}} \langle g, v \rangle = \|g\|_{\mathcal{U}^{-1,\infty}}.$$

To prove (A.5), we fix $z \in \mathcal{U}$ and let ℓ_1, ℓ_2 be such that $z'_{\ell_1} = \|z'\|_{\ell^\infty_\varepsilon}$ and $z'_{\ell_2} < 0$. (A similar argument can be used if $z'_{\ell_1} = -\|z'\|_{\ell^\infty_\varepsilon}$.) We obtain (A.5) from the fact that $\frac{1}{2}\|z'\|_{\ell^\infty_\varepsilon} \le \langle z', v' \rangle$, where $v \in \mathcal{U}$ is defined by

$$v'_\ell = \begin{cases} \frac{1}{2\varepsilon} & \text{if } \ell = \ell_1, \\ -\frac{1}{2\varepsilon} & \text{if } \ell = \ell_2, \\ 0 & \text{otherwise.} \end{cases} \qquad \square$$

COROLLARY A.3. *Suppose that F is such that $L_{\mathrm{qcf},F} : \mathcal{U} \to \mathcal{U}^*$ is invertible; then*

$$\begin{aligned} \|(L_1^{-1} L_{\mathrm{qcf},F})^{-1}\|_{L(\mathcal{U}^{1,\infty},\, \mathcal{U}^{1,\infty})} &\le \|L_{\mathrm{qcf},F}^{-1}\|_{L(\mathcal{U}^{-1,\infty},\, \mathcal{U}^{1,\infty})} \\ &\le 2\|(L_1^{-1} L_{\mathrm{qcf},F})^{-1}\|_{L(\mathcal{U}^{1,\infty},\, \mathcal{U}^{1,\infty})}. \end{aligned}$$

Proof. Using Lemma A.2, we can prove the following bound:

$$\begin{aligned} \frac{1}{\|(L_1^{-1} L_{\mathrm{qcf},F})^{-1}\|_{L(\mathcal{U}^{1,\infty},\, \mathcal{U}^{1,\infty})}} &= \inf_{\substack{u \in \mathcal{U} \\ \|u\|_{\mathcal{U}^{1,\infty}} = 1}} \|L_1^{-1} L_{\mathrm{qcf},F} u\|_{\mathcal{U}^{1,\infty}} \\ &\ge \inf_{\substack{u \in \mathcal{U} \\ \|u\|_{\mathcal{U}^{1,\infty}} = 1}} \|L_{\mathrm{qcf},F} u\|_{\mathcal{U}^{-1,\infty}} = \frac{1}{\|L_{\mathrm{qcf},F}^{-1}\|_{L(\mathcal{U}^{-1,\infty},\, \mathcal{U}^{1,\infty})}}, \end{aligned}$$

which gives the first stated inequality. The second inequality follows from a similar argument. $\square$

Corollary A.3 shows that we can bound the operator norm $\|L_{\mathrm{qcf},\,F}^{-1}\|_{L(\mathcal{U}^{-1,\infty},\, \mathcal{U}^{1,\infty})}$ in terms of $\|(L_1^{-1} L_{\mathrm{qcf},\,F})^{-1}\|_{L(\mathcal{U}^{1,\infty},\, \mathcal{U}^{1,\infty})}$. The latter operator norm can be computed using the formula

$$\|(L_1^{-1} L_{\mathrm{qcf},F})^{-1}\|_{L(\mathcal{U}^{1,\infty},\, \mathcal{U}^{1,\infty})} = \left\{ \inf_{\substack{u \in \mathcal{U} \\ \|u'\|_{\ell^\infty_\varepsilon} = 1}} \left\|(L_1^{-1} L_{\mathrm{qcf},F} u)'\right\|_{\ell^\infty_\varepsilon} \right\}^{-1}. \tag{A.6}$$

In the next lemma, we establish an explicit representation of $L_1^{-1}L_{\mathrm{qcf},\,F}$ which will subsequently allow us to construct upper and lower bounds for (A.6).

LEMMA A.4. *Let $z = L_1^{-1}L_{\mathrm{qcf},\,F}u$; then*

$$\begin{aligned} z'_\ell = \ & \sigma_\ell(u') - \frac{\varepsilon}{2}\phi''_{2F}\{u'_{-K} - u'_{-K+1} - u'_K + u'_{K+1}\} \\ & - \alpha_{-K}(u')h_{\ell+K-1} + \alpha_K(u')h_{\ell-K-1}, \end{aligned}$$

where σ, h, and $\alpha_{\pm K}$ are as defined above.

Remark. We note that the term $\frac{1}{2}\varepsilon\{u'_{-K} - u'_{-K+1} - u'_K + u'_{K+1}\}$ is the average of σ, and the function h is a periodic Heaviside function defined in (A.2).

Proof of Lemma A.4. The function z is the solution of the variational principle

$$\langle z', v'\rangle = \langle L_{\mathrm{qcf},\,F}u, v\rangle = \langle E_{\mathrm{qcf},F}u', v'\rangle,$$

where $E_{\mathrm{qcf},F}$ is defined in (A.4), and is given by

$$(E_{\mathrm{qcf},F}u')_\ell = \sigma_\ell(u') - \alpha_{-K}(u')h_{\ell+K-1} + \alpha_K(u')h_{\ell-K-1}.$$

We note that a function $w \in \mathbb{R}^{2N}$ is a gradient, that is, $w = v'$ for some $v \in \mathcal{U}$, if and only if $\sum_{\ell=-N+1}^N w_\ell = 0$. Hence, we obtain $z' = E_{\mathrm{qcf},F}u' - \overline{E_{\mathrm{qcf},F}u'}$, where $\overline{E_{\mathrm{qcf},F}u'} := \frac{1}{2}\varepsilon\sum_{\ell=-N+1}^N (E_{\mathrm{qcf},F}u')_\ell$. Since h has zero mean, we need only to compute $\bar\sigma$:

$$\bar\sigma := \frac{1}{2N}\sum_{\ell=-N+1}^N \sigma_\ell = \frac{A_F}{2N}\sum_{\ell=-N+1}^N u'_\ell + \frac{\phi''_{2F}}{2N}\sum_{\ell=-K+1}^K (u'_{\ell-1} - 2u'_\ell + u'_{\ell+1}).$$

Since u is periodic, u' has zero mean, and hence the first sum on the right-hand side vanishes. The second sum has telescope structure, and we obtain

$$\overline{E_{\mathrm{qcf},F}u'} = \bar\sigma = \frac{\varepsilon}{2}\phi''_{2F}(u'_{-K} - u'_{-K+1} - u'_K + u'_{K+1}).$$

This concludes the proof of the lemma. ∎

We are now ready to conclude the proof of Theorem 4.4.

Proof of Theorem 4.4. We set $z = L_1^{-1}L_{\mathrm{qcf},\,F}u$ and use Lemma A.4 to deduce the bound

$$\begin{aligned} \|z'\|_{\ell^\infty_\varepsilon} \geq \ & \|\sigma(u')\|_{\ell^\infty_\varepsilon} - 2\varepsilon|\phi''_{2F}|\|u'\|_{\ell^\infty_\varepsilon} \\ & - \max(|\alpha_{-K}(u')|, |\alpha_K(u')|)\max_\ell(|h_{\ell+K-1}| + |h_{\ell-K-1}|). \end{aligned} \tag{A.7}$$

To bound the first term on the right-hand side, we note that

$$|\sigma_\ell(u')| \geq \phi''_F|u'_\ell| + 4\phi''_{2F}\|u'\|_{\ell^\infty_\varepsilon},$$

which immediately implies that

$$\|\sigma(u')\|_{\ell^\infty_\varepsilon} \geq A_F\|u'\|_{\ell^\infty_\varepsilon}. \tag{A.8}$$

To bound the third term on the right-hand side of (A.7), we crudely estimate

$$\max_{\ell=-N+1,\dots,N}(|h_{\ell+K-1}| + |h_{\ell-K-1}|) \leq 1 - \tfrac{1}{2}\varepsilon,$$

which is true whenever $K \geq 1$, and deduce from (A.1) that

$$\max(|\alpha_{-K}(u')|, |\alpha_K(u')|) \leq 4|\phi''_{2F}|.$$

The additional term $-\frac{1}{2}\varepsilon$ cancels the second term on the right-hand side of (A.7), so that we obtain

$$\|z'\|_{\ell^\infty_\varepsilon} \geq (\phi''_F + 8\phi''_{2F})\|u'\|_{\ell^\infty_\varepsilon}.$$

Employing Corollary A.3 and formula (A.6), we obtain Theorem 4.4. $\square$

Appendix B. Proof of Theorem 4.3: Instability of $L_{\mathrm{qcf},F}$. We now prove Theorem 4.3 on the instability of $L_{\mathrm{qcf},F}$ as an operator acting between $\mathcal{U}^{1,p}$ and $\mathcal{U}^{-1,p}$, $1 \leq p < \infty$. The bound $\|L^{-1}_{\mathrm{qcf},F}\|_{L(\mathcal{U}^{-1,p},\mathcal{U}^{1,p})} \geq CN^{1/p}$ follows from the following lemma.

LEMMA B.1. *Suppose that $\phi''_F > 0$, $\phi''_{2F} \in \mathbb{R}\backslash\{0\}$, and $p, q \in \mathbb{R}$ satisfy $1 \leq p < \infty$, $1 < q \leq \infty$, and $\frac{1}{p} + \frac{1}{q} = 1$. Then there exists a constant $C > 0$ such that*

$$\inf_{\substack{v \in \mathcal{U} \\ \|v'\|_{\ell^p_\varepsilon}=1}} \sup_{\substack{w \in \mathcal{U} \\ \|w'\|_{\ell^p_\varepsilon}=1}} \langle L_{\mathrm{qcf},F} v,\, w\rangle \leq CN^{-1/p}.$$

Proof. We recall from Lemma A.4 that we can represent $L_{\mathrm{qcf},F}v$ in the form

$$\langle L_{\mathrm{qcf},F} v, w\rangle = \langle E_{\mathrm{qcf},F} v', w'\rangle \qquad \forall w \in \mathcal{U}, \tag{B.1}$$

where

$$(E_{\mathrm{qcf},F} v')_\ell = \sigma_\ell(v') - \alpha_{-K}(v')h_{\ell+K-1} + \alpha_K(v')h_{\ell-K-1},$$

and where

$$\begin{aligned}
\sigma_\ell(v') &= \begin{cases} \phi''_F v'_\ell + \phi''_{2F}(v'_{\ell-1} + 2v'_\ell + v'_{\ell+1}), & \ell = -K+1, \ldots, K, \\ (\phi''_F + 4\phi''_{2F})v'_\ell & \text{otherwise}, \end{cases} \\
\alpha_K(v') &= \phi''_{2F}(v'_{K+2} - 2v'_{K+1} + v'_K), \\
\alpha_{-K}(v') &= \phi''_{2F}(v'_{-K+1} - 2v'_{-K} + v'_{-K-1}), \\
h_\ell &= \begin{cases} \frac{1}{2}(1 - \varepsilon\ell) - \frac{\varepsilon}{4}, & \ell \geq 0, \\ -\frac{1}{2}(1 + \varepsilon\ell) - \frac{\varepsilon}{4}, & \ell < 0. \end{cases}
\end{aligned}$$

We choose $v \in \mathcal{U}$ with the derivative given by

$$v'_\ell = \begin{cases} 0, & \ell = K-1, \\ -\frac{A_F}{6\phi''_{2F}}, & \ell = K, \\ \frac{A_F}{3\phi''_{2F}}, & \ell = K+1, \\ -\frac{A_F}{6\phi''_{2F}}, & \ell = K+2, \\ h_{\ell-K-1} & \text{otherwise}. \end{cases}$$

Such a representation is possible if and only if the vector $(v'_\ell)_{\ell=-N+1}^N$ defined above has zero mean. To see that this holds, we use the symmetry of h_ℓ to calculate

$$\sum_{\ell=-N+1}^{N} v'_\ell = \sum_{\ell \neq K-1,\, K,\, K+1,\, K+2} h_{\ell-K-1} = 0.$$

If we insert v into the equations above, we find that

$$\alpha_{-K}(v') = 0, \quad \alpha_K(v') = -A_F,$$

and

$$\sigma_\ell(v') = \begin{cases} (\phi''_F + 2\phi''_{2F})h_{-3} + \phi''_{2F}h_{-4}, & \ell = K-2, \\ \phi''_{2F}h_{-3} - \frac{1}{6}A_F, & \ell = K-1, \\ -\frac{\phi''_F A_F}{6\phi''_{2F}}, & \ell = K, \\ \frac{A_F^2}{3\phi''_{2F}}, & \ell = K+1, \\ -\frac{A_F^2}{6\phi''_{2F}}, & \ell = K+2, \\ A_F h_{\ell-K-1} & \text{otherwise}, \end{cases}$$

which implies that

$$(E_{\mathrm{qcf},F}v')_\ell = \begin{cases} -2\phi''_{2F}h_{-3} + \phi''_{2F}h_{-4}, & \ell = K-2, \\ \phi''_{2F}h_{-3} - \frac{1}{6}A_F - A_F h_{-2}, & \ell = K-1, \\ -\frac{\phi''_F A_F}{6\phi''_{2F}} - A_F h_{-1}, & \ell = K, \\ \frac{A_F^2}{3\phi''_{2F}} - A_F h_0, & \ell = K+1, \\ -\frac{A_F^2}{6\phi''_{2F}} - A_F h_1, & \ell = K+2, \\ 0 & \text{otherwise}. \end{cases}$$

Note that all the terms above are bounded in absolute value, independently of N and K.

Inserting these formulas into (B.1), applying Hölder's inequality, and using the fact that $(E_{\mathrm{qcf},F}v)'_\ell$ is nonzero for only five indices, we obtain

$$\begin{aligned} \langle L_{\mathrm{qcf},F}v, w\rangle &= \langle E_{\mathrm{qcf},F}v', w'\rangle \\ &\le \big\|E_{\mathrm{qcf},F}v'\big\|_{\ell^p_\varepsilon}\|w'\|_{\ell^q_\varepsilon} \\ &\le \varepsilon^{1/p}\Big[5\big\|E_{\mathrm{qcf},F}v'\big\|^p_{\ell^\infty_\varepsilon}\Big]^{1/p}\|w'\|_{\ell^q_\varepsilon} \\ &\le C\varepsilon^{1/p}\|w'\|_{\ell^q_\varepsilon}. \end{aligned}$$

It remains to show that $\|v'\|_{\ell^p_\varepsilon}$ is bounded below as $N \to \infty$. As a matter of fact, it can be seen from the definition of v'_ℓ that

$$|v'_\ell| \ge \tfrac{1}{4} \qquad \text{for } \ell = K+1-\frac{N}{2}, \dots, K-2,$$

which gives

$$\|v'\|_{\ell^p_\varepsilon} \ge \Bigg[\sum_{\ell=K+1-N/2}^{K-2} \varepsilon\big(\tfrac{1}{4}\big)^p\Bigg]^{1/p} = \tfrac{1}{4}\left[\left(\frac{N}{2}-3\right)\varepsilon\right]^{1/p}.$$

Thus, replacing v by $v/\|v'\|_{\ell^p_\varepsilon}$ gives the desired result. ∎

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