

A Γ -CONVERGENCE ANALYSIS OF THE QUASICONTINUUM METHOD*

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Abstract. We present a Γ -convergence analysis of the quasicontinuum method focused on the behavior of the approximate energy functionals in the continuum limit of a harmonic and defect-free crystal. The analysis shows that, under general conditions of stability and boundedness of the energy, the continuum limit is attained provided that the continuum—e.g., finite-element—approximation spaces are strongly dense in an appropriate topology and provided that the lattice size converges to zero more rapidly than the mesh size. The equicoercivity of the quasicontinuum energy functionals is likewise established with broad generality, which, in conjunction with Γ -convergence, ensures the convergence of the minimizers. We also show under rather general conditions that, for interatomic energies having a clusterwise additive structure, summation or quadrature rules that suitably approximate the local element energies do not affect the continuum limit. Finally, we propose a discrete patch test that provides a practical means of assessing the convergence of quasicontinuum approximations. We demonstrate the utility of the discrete patch test by means of selected examples of application.

Key words. quasicontinuum method, atomistic-to-continuum models, Γ -convergence

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1. Introduction. The quasicontinuum method of Tadmor, Phillips, and Ortiz [59, 60] was originally conceived as an approximation scheme for zero-temperature molecular statics consisting of: (i) adaptive interpolation constraints on the motion of the atoms aimed at eliminating degrees of freedom in regions where the displacement field is nearly affine, and (ii) summation or quadrature rules for purposes of avoiding full lattice sums. The initial development of the method was application-driven, with primary emphasis given to probing multiscale phenomena straddling the atomistic and continuum scales. Examples of such applications include: dislocations and plasticity [44, 50, 61]; nanoindentation [58, 31, 32]; nanovoid growth [40, 41]; fracture [43, 45, 44]; grain boundaries [56]; and others. Extensions to finite-temperature, be it at equilibrium [22, 55, 42, 62], or with heat conduction accounted for [33, 3, 6], greatly extend the range of applicability of the method.

The mathematical analysis of the quasicontinuum method is comparatively more

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recent and starts in earnest with the work of Lin [34, 35]. In particular, the analysis of summation or quadrature rules has attracted considerable interest and has led to significant improvements over the early implementations of the method. For instance, Gunzburger and Zhang [28, 64] have proposed quadrature rules that are based on both force and energy formulations, and have performed error analyses for monatomic chains. Luskin and Ortner [37] and Dobson, Luskin, and Ortner [19, 20, 18, 21] have extensively investigated node-based cluster summation rules for both force-based and energy-based formulations and performed a systematic error and stability analyses. For more recent work in the development and analysis of quasicontinuum methods in higher dimensions, see [23, 29, 36, 38, 48, 49, 53, 54].

While the mathematical work mentioned above is mostly based in error analysis, in the present work we present an analysis of the quasicontinuum method based on Γ -convergence (cf., e.g., [15]), a notion of variational convergence for general energy-minimization problems that, in particular, implies convergence of solutions. In view of the strongly nonlinear and multiscale character of the typical problems of interest, and the proclivity of such problems to involve fine microstructure, the application of Γ -convergence tools to their analysis indeed suggests itself naturally. Specifically, we seek to ascertain the convergence of quasicontinuum approximations in the *continuum* or *long wavelength limit*. These limits are attained by allowing the lattice parameter to become vanishingly small or by considering displacement fields of increasingly slow variation on the scale of the lattice, respectively. Discrete-to-continuum limits of this type have been investigated by Γ -convergence in a number of areas of application (cf., e.g., [46, 2, 8]). A natural first notion of convergence, and the basis for the analysis presented in this paper, is to require that approximation schemes become exact in the continuum limit, i.e., that approximation of the interatomic energy does not “spoil” the continuum limit. For simplicity, we focus our attention on a harmonic and defect-free crystal occupying a finite domain Ω and deforming under all-around Dirichlet boundary conditions. A similar analytical approach in the context of fracture mechanics is currently being investigated by Schäffner and Schlömerkemper [52].

Our analysis shows that, when full lattice sums are performed, density of the continuum approximating spaces, e.g., finite-element spaces, in $H_0^1(\Omega)$ essentially ensures the convergence of the corresponding quasicontinuum approximations, provided that the lattice parameter vanishes more rapidly than the mesh size. The equicoercivity of the quasicontinuum energy functionals is likewise established with broad generality, which, in conjunction with Γ -convergence, ensures the convergence of the minimizers. The analysis also shows that, when the interatomic energy is short-ranged and has an additive structure, the convergence of the quasicontinuum method is not affected when suitably defined summation rules are employed.

The notion of convergence adopted in this work, namely, the attainment by the approximate interatomic energy of the exact continuum limit, may be thought of as a discrete *patch test* (cf., e.g., [30, 65]). Thus, as in the conventional patch test, the present notion of convergence concerns the exactness of the approximation scheme when the displacement field is ostensibly affine. As a practical application of our convergence analysis, we describe an implementation of the discrete patch test that can be applied to general interatomic potentials. The discrete patch test concerns a periodic unit cell and does not require mesh refinement. Instead, a sequence of rescaled external force fields of increasingly slow variation is applied over the periodic unit cell. We then verify that, as the applied force field is rescaled, the quasicontinuum solution converges in energy to the continuum limit of the interatomic energy. We report numerical examples of applications that illustrate the implementation of the

proposed discrete patch test and demonstrate the type of convergence expected from the theoretical analysis.

2. Harmonic lattices. We regard an *infinite crystal* as a point set spanning a *simple Bravais lattice* of coordinates

$$(2.1) \quad x(l) = \sum_{i=1}^n l^i a_i,$$

where n is the spatial dimension, $l \equiv (l^1, \dots, l^n) \in \mathbb{Z}^n$ are integer lattice coordinates, and $\{a_i, i = 1, \dots, n\}$ is a basis for the Bravais lattice. We denote by $\{a^i, i = 1, \dots, n\}$ the *dual* basis, defined by the property $a^i \cdot a_j = \delta^i_j$, and recall that $2\pi a^i$ is the basis of the *reciprocal lattice*. A deformation of an infinite crystal is a mapping $y: \mathbb{Z}^n \rightarrow \mathbb{R}^n$ such that $y(l)$ is the position of the point l in the deformed configuration of the crystal. We shall assume that the total potential energy of the deformed crystal can be written as a function of the general form

$$(2.2) \quad F(y) = E(y) - \langle f, y \rangle,$$

where E is the interatomic energy, $f: \mathbb{Z}^n \rightarrow \mathbb{R}^n$ is an applied force field, and we write

$$(2.3) \quad \langle f, y \rangle = V \sum_{l \in \mathbb{Z}^n} \langle f(l), y(l) \rangle,$$

where V is the atomic volume. On physical grounds, the interatomic energy $E(y)$ is required to be invariant under superposed translations and infinitesimal rotations. The problem of interest is to find the stable equilibrium configurations of the crystal lattice, i.e., the potential energy minimizers, under the action of applied force fields.

The interatomic energy E is often expressed in terms of so-called interatomic potentials (cf., e.g., [26]). However, the energy landscape defined by general interatomic potentials is typically of great complexity and exhibits numerous energy wells, or conformations, e.g., corresponding to lattice-invariant deformations. We shall, therefore, restrict our analysis to *harmonic crystals*, i.e., crystals whose interatomic energy is quadratic in the displacement field $u(l) = y(l) - x(l)$. The harmonic approximation of a general interatomic energy may be obtained formally by expanding the energy $E(x + u)$ in Taylor series of u about some reference equilibrium configuration. If the reference configuration takes the form of a Bravais lattice (2.1), the resulting harmonic interatomic energy takes the form (cf., e.g., [4])

$$(2.4) \quad E(u) = \sum_{l \in \mathbb{Z}^n} \frac{1}{2} \langle (\Phi * u)(l), u(l) \rangle,$$

where Φ is the force-constant field of the lattice and $*$ denotes the discrete convolution (cf. Appendix A). From invariance of the interatomic energy $E(y)$ under superposed translations and rotations, it follows that the harmonic interatomic energy $E(u)$ is invariant under superposed linearized translations and rotations. The corresponding potential energy is

$$(2.5) \quad F(u) = E(u) - \langle f, u \rangle.$$

Again, the problem of interest is to find the stable equilibrium displacements of the crystal lattice under the action of applied force fields.

Harmonic models suffice to describe crystal acoustics and, in particular, the dispersion relations of crystals, which can exhibit a good deal of structure (cf., e.g., [47]). More generally, the harmonic model is found to adequately describe the thermodynamics of perfect crystals at low temperatures (cf., e.g., [63]). Harmonic models can also be extended to account for lattice defects, such as dislocations, by recourse to the method of eigendeformations [4]. The fidelity of this latter approach, e.g., as regards the prediction of defect core energies and low-energy defect structures, has been assessed in detail elsewhere [51, 5].

In view of the periodicity of the lattice and the convolution form of the harmonic interatomic energy (2.4), it is natural to resort to the discrete Fourier representation of the displacement field (cf. Appendix A)

$$(2.6) \quad \hat{u}(k) = V \sum_{l \in \mathbb{Z}^n} u(l) e^{-ik \cdot x(l)}, \quad k \in B,$$

with inverse

$$(2.7) \quad u(l) = \frac{1}{(2\pi)^n} \int_B \hat{u}(k) e^{ik \cdot x(l)} dk,$$

where B is the Brillouin zone of the reciprocal lattice. An application of the discrete Parseval's identity and convolution theorems (cf. Appendix A) additionally yields the representation

$$(2.8) \quad F(u) = \frac{1}{(2\pi)^n} \int_B \frac{1}{2} \langle D(k) \hat{u}(k), \hat{u}^*(k) \rangle dk - \frac{1}{(2\pi)^n} \int_B \langle \hat{f}(k), \hat{u}(k) \rangle dk$$

of the potential energy, where $\hat{u}(k)$ and $\hat{f}(k)$ are the discrete Fourier transforms of $u(l)$ and $f(l)$, respectively, and

$$(2.9) \quad D(k) = \frac{1}{V^2} \hat{\Phi}(k) = \frac{1}{V} \sum_{l \in \mathbb{Z}^n} \Phi(l) e^{-ik \cdot x(l)}, \quad k \in B,$$

is the dynamical matrix of the lattice (cf., e.g., [4]). Many interatomic potentials are short-ranged, in which case the sum (2.9) is finite and the function $D(k)$ is C^∞ . It additionally follows from reciprocity, centrosymmetry, and translation invariance that $D(k)$ is real, symmetric, even, and $D(0) = 0$. From these properties, a Taylor expansion of $D(k)$ about the origin gives the *long-wavelength limit* of the dynamical matrix as

$$(2.10) \quad (D_0)_{ik}(k) \equiv \lim_{\varepsilon \rightarrow 0} \varepsilon^{-2} D_{ik}(\varepsilon k) = \lim_{\varepsilon \rightarrow 0} \varepsilon^{-2} \frac{1}{V} \sum_{l \in \mathbb{Z}^n} \Phi_{ik}(l) e^{-i\varepsilon k \cdot x(l)} = c_{ijkl} k_j k_l,$$

where

$$(2.11) \quad c_{ijkl} = -\frac{1}{2V} \sum_{l \in \mathbb{Z}^n} \Phi_{ik}(l) x_j(l) x_l(l)$$

are the elastic moduli of the lattice. The major and minor symmetries

$$(2.12) \quad c_{ijkl} = c_{klij} = c_{jikl} = c_{ijlk}$$

are a direct consequence of reciprocity and invariance under superposed rotations, respectively.

3. The continuum limit. In ascertaining the convergence of approximations of the interatomic energy (2.4), it is natural to investigate their behavior in the *continuum* or *long wavelength limit*, i.e., the limiting behavior of the energy as the lattice parameter is allowed to become vanishingly small. Indeed, in the present setting a natural notion of convergence, and the basis for subsequent analyses, is to require that approximation schemes become exact in the continuum limit. We specifically seek to characterize the continuum limit of the energy in the sense of Γ -convergence. As is well-known, Γ -convergence of the energy function also guarantees convergence of the energy minimizers under rather general conditions (cf., e.g., [15]). The investigation of the continuum limit has the additional benefit of setting the functional framework—and supplying useful tools—for the analysis of approximation schemes.

3.1. Formulation of the continuum limit. A convenient definition of the continuum limit that lends itself to analysis by Γ -convergence may be formulated as follows. Consider a function $f \in C_0^\infty(\mathbb{R}^n, \mathbb{R}^n)$, the space of C^∞ functions from \mathbb{R}^n to \mathbb{R}^n with compact support, and the corresponding sequence of rescaled functions

$$(3.1) \quad f_\varepsilon(x) = \varepsilon^2 f(\varepsilon x),$$

of decreasing variation on the scale of the lattice. The sequence (f_ε) in turn defines the sequence of lattice functions

$$(3.2) \quad g_\varepsilon(l) = \frac{1}{(2\pi)^n} \int_B \hat{f}_\varepsilon(k) e^{ik \cdot x(l)} dk,$$

where $\hat{f}_\varepsilon(k) = \varepsilon^{2-n} \hat{f}(k/\varepsilon)$. Consider now the corresponding sequence of scaled potential energies

$$(3.3) \quad F_\varepsilon(u) = \varepsilon^{n-2} (E(u) - \langle g_\varepsilon, u \rangle),$$

where the factor ε^{n-2} accounts for the expected linear-elastic scaling of the energy and is introduced in order to obtain a well-defined limit. The sequence (F_ε) represents the potential energies of a fixed crystal deforming under the action of applied force fields g_ε of increasingly slow spatial variation relative to the crystal lattice, or *long wavelength* limit. We may alternatively rewrite the rescaled potential energy in the form

$$(3.4) \quad \begin{aligned} F_\varepsilon(u) &= \varepsilon^{n-2} \left(\frac{1}{(2\pi)^n} \int_B \frac{1}{2} \langle D(k) \hat{u}(k), \hat{u}^*(k) \rangle dk - \frac{1}{(2\pi)^n} \int_B \langle \varepsilon^{2-n} \hat{f}(k/\varepsilon), \hat{u}(k) \rangle dk \right) \\ &= \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \frac{1}{2} \langle \varepsilon^{-2} D(\varepsilon\xi) \varepsilon^n \hat{u}(\varepsilon\xi), \varepsilon^n \hat{u}^*(\varepsilon\xi) \rangle d\xi - \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \langle \hat{f}(\xi), \varepsilon^n \hat{u}(\varepsilon\xi) \rangle d\xi \\ &= \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \frac{1}{2} \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}_\varepsilon(\xi), \hat{u}_\varepsilon^*(\xi) \rangle d\xi - \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \langle \hat{f}(\xi), \hat{u}_\varepsilon(\xi) \rangle d\xi, \end{aligned}$$

where

$$(3.5) \quad \hat{u}_\varepsilon(\xi) = \varepsilon^n \hat{u}(\varepsilon\xi)$$

are rescaled displacements over the ε -lattice, i.e., over the retraction of the original lattice by ε . In this representation, the sequence (F_ε) may be regarded as the potential

energies of a sequence of increasingly fine crystals deforming under the action of a fixed applied force field, or *continuum limit*.

The preceding scaling argument leads to the consideration of the sequence of rescaled potential energies

$$(3.6) \quad F_\varepsilon(u_\varepsilon) = E_\varepsilon(u_\varepsilon) - \langle f, u_\varepsilon \rangle,$$

where

$$(3.7) \quad E_\varepsilon(u_\varepsilon) = \sum_{l \in \mathbb{Z}^n} \frac{1}{2} \langle (\varepsilon^{n-2} \Phi * u_\varepsilon)(l), u_\varepsilon(l) \rangle = \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \frac{1}{2} \langle \varepsilon^{-2} D(\varepsilon \xi) \hat{u}_\varepsilon(\xi), \hat{u}_\varepsilon^*(\xi) \rangle d\xi$$

is the rescaled interatomic energy of the crystal, and

$$(3.8) \quad \langle f, u_\varepsilon \rangle = \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \langle \hat{f}(\xi), \hat{u}_\varepsilon(\xi) \rangle d\xi$$

is the rescaled potential energy of the applied force field. Specifically, we wish to ascertain the Γ -limit of the sequence (F_ε) in an appropriate topological vector space. We expect the external potential energy $\langle f, \cdot \rangle$ to be continuous in that topology and, hence, to go through to the Γ -limit (cf., e.g., [15]). In anticipation of this property, in what follows we restrict our attention to the Γ -limit of the interatomic energy E_ε . Continuity of the forcing term will be established in (3.46).

3.2. Linear elasticity. We expect the limiting energy functional of the crystal to be the linear elastic energy [4]

$$(3.9) \quad E_0(u) = \int_{\mathbb{R}^n} \frac{1}{2} \langle c \nabla u(x), \nabla u(x) \rangle dx = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \frac{1}{2} \langle D_0(k) \hat{u}(k), \hat{u}^*(k) \rangle dk,$$

where c denotes the elastic moduli tensor (2.11) and $D_0(k)$ is the corresponding continuum dynamical matrix (2.10). Suppose that the elastic moduli have the stability and boundedness properties

$$(3.10) \quad \alpha |e|^2 \leq \langle ce, e \rangle \leq \beta |e|^2$$

for some constants $0 < \alpha \leq \beta$ and all symmetric matrices e . Then, it follows that

$$(3.11) \quad E_0(u) \leq \beta \|e(u)\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)}^2 \leq \beta \|\nabla u\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)}^2 \leq \beta \|u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2,$$

where

$$(3.12) \quad e(u) = \frac{1}{2} (\nabla u + \nabla u^T)$$

is the *strain operator*. This elementary estimate shows that the linear elastic energy of an infinite body is well-defined over the Hilbert space $H^1(\mathbb{R}^n, \mathbb{R}^n)$ (cf., e.g., [1], for background on Lebesgue and Sobolev spaces), i.e., it may be regarded as a functional $E_0: H^1(\mathbb{R}^n, \mathbb{R}^n) \rightarrow \mathbb{R}$.

However, the linear elastic energy of an infinite elastic body fails to be coercive, and the corresponding minimum problem is ill-posed in general. We recall that a function $F: X \rightarrow \bar{\mathbb{R}}$ over a reflexive and separable Banach space X is *sequentially coercive* in the weak topology of X if and only if $F(u)$ tends to $+\infty$ as $\|u\|_X$ tends

to $+\infty$. Thus, whereas Korn's inequality ensures energy control of $\|\nabla u\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)} \equiv |u|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}$, it does not follow, in general, that the H^1 -seminorm $|u|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}$ in turn controls $\|u\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)}$ for arbitrary $u \in H^1(\mathbb{R}^n, \mathbb{R}^n)$. Indeed, Poincaré's inequality fails over \mathbb{R}^n . In typical applications, this failure of compactness is resolved in a number of ways, e.g., by restriction to certain domains $\Omega \subset \mathbb{R}^n$, not necessarily bounded, [1], by restriction to periodicity (cf., section 5), by appending potentials defined by *capacity measures* [11], by working on quotient spaces [49], and others.

In the present work, we ensure compactness simply by considering linear elastic bodies of finite extent, i.e., bodies occupying bounded domains $\Omega \subset \mathbb{R}^n$, and by enforcing zero-displacement boundary conditions, in the sense of traces, on its entire boundary $\partial\Omega$.

The corresponding equilibrium problem consists of minimizing the restriction of linear elastic energy E_0 to $H_0^1(\Omega, \mathbb{R}^n)$. General displacement boundary conditions can likewise be enforced simply by translation [15]. The case of periodic boundary conditions is also amenable to an altogether similar analysis. We shall assume throughout that Ω is a bounded Lipschitz domain. We recall that domains satisfying a strong local Lipschitz condition have the *approximation property*, i.e., they admit a total extension operator [1].

However, in order to place the linear elastic energy (3.9) and the interatomic energies for crystals (2.4) on a common functional footing, we formally extend the bounded linear elastic problem to all of \mathbb{R}^n by *exterior extension*. We recall that \tilde{u} is the *zero or trivial exterior extension* of a function $u \in H_0^1(\Omega, \mathbb{R}^n)$ if

$$(3.13) \quad \tilde{u}(x) = \begin{cases} u(x) & \text{almost everywhere (a.e.) in } \Omega, \\ 0 & \text{otherwise.} \end{cases}$$

We also recall that, if Ω has the segment property [1], then a function u on Ω belongs to $H_0^1(\Omega, \mathbb{R}^n)$ if and only if the zero exterior extension \tilde{u} of u belongs to $H^1(\mathbb{R}^n, \mathbb{R}^n)$ and that the extension operator is continuous [1]. Let X_0 denote the closed subspace of $H^1(\mathbb{R}^n, \mathbb{R}^n)$ consisting of displacement fields such that $u = \tilde{u}|_\Omega$, i.e., which vanish outside Ω , where $u|_\Omega$ denotes the *restriction* of u to Ω . Evidently, X_0 is isometrically isomorphic to $H_0^1(\Omega, \mathbb{R}^n)$. We can now define an extended linear elastic energy $E_0: H^1(\mathbb{R}^n, \mathbb{R}^n) \rightarrow \bar{\mathbb{R}}$ over Ω as

$$(3.14) \quad E_0(u) = \begin{cases} \int_{\mathbb{R}^n} \frac{1}{2} \langle c \nabla u(x), \nabla u(x) \rangle dx & \text{if } u \in X_0, \\ +\infty & \text{otherwise.} \end{cases}$$

Given $f \in H_0^1(\Omega, \mathbb{R}^n)^*$, we define the potential energy $F_0: H^1(\mathbb{R}^n, \mathbb{R}^n) \rightarrow \bar{\mathbb{R}}$ as

$$(3.15) \quad F_0(u) = E_0(u) - \langle f, u \rangle,$$

where

$$(3.16) \quad \langle f, u \rangle = f(u|_\Omega).$$

The weak sequential coercivity of F_0 is a direct consequence of Korn's inequality and Poincaré's inequality (cf., e.g., [13]). The weak sequentially lower-semicontinuity of F_0 follows simply from convexity and the weak closedness of $H_0^1(\Omega, \mathbb{R}^n)$ (cf., e.g., [25]). Finally, the existence of minimizers of F_0 in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ follows as a direct consequence of Tonelli's theorem [15].

3.3. The continuum limit as a Γ-limit. In order to define a proper Γ-limit we proceed to redefine the discrete interatomic energies (3.7) as a sequence of functionals over $H^1(\mathbb{R}^n, \mathbb{R}^n)$. To this end, recall that the L^2 -function v_ε whose ordinary Fourier transform \hat{v}_ε is supported in B/ε , wherein it coincides with the discrete Fourier transform of a square-summable ε -lattice function u_ε , is known as the *Whittaker–Shannon interpolation* of u_ε (cf., e.g., [39]). Thus,

$$(3.17) \quad \hat{v}_\varepsilon(\xi) = \begin{cases} \hat{u}_\varepsilon(\xi) & \text{if } \xi \in B/\varepsilon, \\ 0 & \text{otherwise.} \end{cases}$$

Recall, in addition, that the Whittaker–Shannon interpolation defines an isometric isomorphism between the space of square-summable ε -lattice functions and the space of L^2 -functions that are *band-limited*, i.e., whose ordinary Fourier transform is supported in B/ε (cf., e.g., [39]). This isometric isomorphism supplies a representation of square-summable ε -lattice functions in terms of *band-limited* L^2 -functions. If u_ε is a square-summable ε -lattice displacement field with Whittaker–Shannon interpolation v_ε , then we have

$$(3.18) \quad E_\varepsilon(u_\varepsilon) = \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \frac{1}{2} \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{v}_\varepsilon(\xi), \hat{v}_\varepsilon(\xi) \rangle d\xi,$$

which supplies the corresponding representation of the interatomic energy in terms of *band-limited* L^2 -functions.

We shall additionally understand an ε -lattice vector-valued function over Ω to be a function of the form $u_\varepsilon: \{l \in \mathbb{Z}^n \text{ such that } x_\varepsilon(l) \in \Omega\} \rightarrow \mathbb{R}^n$. Given an ε -lattice vector-valued function u_ε , its *restriction* to Ω is denoted by $u_{\varepsilon|\Omega}$. Thus, $u_{\varepsilon|\Omega}$ over Ω is the ε -lattice vector-valued function over Ω such that $u_{\varepsilon|\Omega}(l) = u_\varepsilon(l)$ for all $l \in \mathbb{Z}^n$ with $x_\varepsilon(l) \in \Omega$. Finally, the *zero or trivial exterior extension* to \mathbb{R}^n of an ε -lattice vector-valued function u_ε over Ω is the ε -lattice vector-valued function

$$(3.19) \quad \tilde{u}_\varepsilon(l) = \begin{cases} u_\varepsilon(l) & \text{if } x_\varepsilon(l) \in \Omega, \\ 0 & \text{otherwise.} \end{cases}$$

Based on these considerations, we may extend the rescaled interatomic energies E_ε to functionals $E_\varepsilon: H^1(\mathbb{R}^n, \mathbb{R}^n) \rightarrow \bar{\mathbb{R}}$ (not renamed) as follows. For fixed $\Omega \subset \mathbb{R}^n$, let X_ε denote the closed subspace of $H^1(\mathbb{R}^n, \mathbb{R}^n)$ consisting of band-limited displacements, i.e., displacements whose Fourier transform is supported in B/ε , such that their corresponding ε -lattice functions vanish outside Ω ,

$$(3.20) \quad X_\varepsilon = \{u \in H^1(\mathbb{R}^n, \mathbb{R}^n) : \text{supp } \hat{u} \subset B/\varepsilon \text{ and } u = 0 \text{ on } \varepsilon\mathbb{Z}^n \setminus \Omega\}.$$

Then we set

$$(3.21) \quad E_\varepsilon(u) = \begin{cases} \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \frac{1}{2} \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}^*(\xi) \rangle d\xi & \text{if } u \in X_\varepsilon, \\ +\infty & \text{otherwise.} \end{cases}$$

Evidently, $X_\varepsilon = \{E_\varepsilon < +\infty\}$ and, if $u_\varepsilon \in X_\varepsilon$, the finite value of $E_\varepsilon(u_\varepsilon)$ coincides with the interatomic energy of the ε -lattice displacement whose Whittaker–Shannon interpolation is u_ε .

In order to ascertain the continuum limit of the sequence (E_ε) , we begin by establishing a key density property of the spaces (X_ε) . To this end, if $u \in C(\mathbb{R}^n, \mathbb{R}^n)$, we

denote by $P_\varepsilon u$ the Whittaker–Shannon interpolation of the sampled function $u(x_\varepsilon(l))$. Thus, the Fourier transform of $P_\varepsilon u$ is given by the *Poisson summation formula*

$$(3.22) \quad \widehat{P_\varepsilon u}(\xi) = \begin{cases} \sum_{m \in \mathbb{Z}^n} \hat{u}(\xi + 2\pi m_i a^i / \varepsilon) & \text{if } \xi \in B/\varepsilon, \\ 0 & \text{otherwise,} \end{cases}$$

provided that \hat{u} decays sufficiently fast.

The density property of the sequence of subspaces X_ε is established by the following proposition.

PROPOSITION 3.1. *Let $u_0 \in X_0$. Then, there exists a sequence (u_ε) in $H^1(\mathbb{R}^n, \mathbb{R}^n)$, with $u_\varepsilon \in X_\varepsilon$, such that $u_\varepsilon \rightarrow u_0$.*

Proof. Let $u_0 \in X_0$. Let (u_δ) be a sequence in $C_0^\infty(\Omega, \mathbb{R}^n)$ converging to u_0 such that

$$(3.23) \quad |u_\delta|_{H^\alpha(\mathbb{R}^n, \mathbb{R}^n)} \leq C\delta^{1-\alpha} |u_0|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}$$

for some $\alpha \geq 1$ chosen below (cf. [1, sect. 5.33]). We then have the bound

$$(3.24) \quad \begin{aligned} |k|^\alpha |\hat{u}_\delta(k)| &\leq \|D^\alpha u_\delta\|_{L^1(\mathbb{R}^n, \mathbb{R}^n)} \\ &\leq |\Omega|^{1/2} \|D^\alpha u_\delta\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)} \leq C|\Omega|^{1/2} \delta^{1-\alpha} |u_0|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}, \end{aligned}$$

where we have made use of Hölder's inequality and the boundedness of Ω . Equivalently, we have

$$(3.25) \quad |\hat{u}_\delta(k)| \leq \frac{C|\Omega|^{1/2}}{\delta^{\alpha-1}|k|^\alpha} |u_0|_{H^1(\mathbb{R}^n, \mathbb{R}^n)},$$

which shows that $\hat{u}_\delta(k)$ decays as $|k|^{-\alpha}$. Let $u_{\delta,\varepsilon} = P_\varepsilon u_\delta$. Since $u_\delta \in C_0^\infty(\Omega, \mathbb{R}^n)$, it follows that $u_{\delta,\varepsilon}$ vanishes on ε -lattice points outside Ω and, hence, $u_{\delta,\varepsilon} \in X_\varepsilon$. In addition, by the decay property of $\hat{u}_\delta(k)$ and Poisson's summation formula (3.22) we have, for $\alpha > n$,

$$(3.26) \quad \begin{aligned} \|u_{\delta,\varepsilon} - u_\delta\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2 &= \frac{1}{(2\pi)^n} \int_{B/\varepsilon} (1 + |\xi|^2) \left| \sum_{m \in \mathbb{Z}^n \setminus \{0\}} \hat{u}_\delta(\xi + 2\pi m_i a^i / \varepsilon) \right|^2 d\xi \\ &+ \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n \setminus B/\varepsilon} (1 + |\xi|^2) |\hat{u}_\delta(\xi)|^2 d\xi \\ &\leq \frac{C\varepsilon^{2\alpha-2-n}}{\delta^{2(\alpha-1)}} |u_0|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2. \end{aligned}$$

Choosing $\alpha = n + 1$, the preceding estimate specializes to

$$(3.27) \quad \|u_{\delta,\varepsilon} - u_\delta\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2 \leq \frac{C\varepsilon^n}{\delta^{2n}} |u_0|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2.$$

In addition, by the triangular inequality we have

$$(3.28) \quad \begin{aligned} \|u_{\delta,\varepsilon} - u_0\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} &\leq \|u_{\delta,\varepsilon} - u_\delta\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} + \|u_\delta - u_0\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} \\ &\leq \frac{C\varepsilon^{n/2}}{\delta^n} |u_0|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} + \|u_\delta - u_0\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}. \end{aligned}$$

Let $\eta > 0$. Choose δ such that $\|u_\delta - u_0\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} < \eta/2$ and then ε_δ such that $\frac{C\varepsilon_\delta^{n/2}}{\delta^n} |u_0|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} < \eta/2$, whereupon,

$$(3.29) \quad \|u_{\delta,\varepsilon_\delta} - u_0\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} < \eta,$$

and the sequence $(u_{\delta,\varepsilon_\delta})$ converges to u_0 in $H^1(\mathbb{R}^n, \mathbb{R}^n)$. \square

We note that the sequence of subspaces (X_ε) is not contained in X_0 in general, as the displacements in X_ε need not vanish identically outside Ω or even on the boundary $\partial\Omega$. Thus, if the space X_0 is regarded as a *constraint set*, in the sense of constraining displacements from $H^1(\mathbb{R}^n, \mathbb{R}^n)$ to X_0 , then the sequence (X_ε) does not provide an *interior approximation* to X_0 in the terminology of constrained minimization problems (cf., e.g., [10]).

We are now set to investigate the limiting behavior of the sequence of discrete interatomic energies (E_ε) . In this regard, the equicoercivity of the sequence warrants special attention in view of the central role that it plays in the convergence of minimizers. We recall (cf., e.g., [15]) that a subset K of a topological space is *sequentially compact* if every sequence in K has a subsequence that converges to a point of K . We also recall that a sequence (F_i) of functionals over a topological space is *sequentially equicoercive* if for every $t \in \mathbb{R}$ there exists a closed sequentially compact K_t such that $\{F_i \leq t\} \subset K_t$ for every $i \in \mathbb{N}$.

We begin with an auxiliary lemma.

LEMMA 3.2. *Let $K \subset \mathbb{R}^n$ be a set disjoint from $\overline{\Omega}$. Then, for every $u_\varepsilon \in X_\varepsilon$ and $\varepsilon \leq c \operatorname{dist}(\Omega, K)$,*

$$(3.30) \quad \|u_\varepsilon\|_{L^2(K, \mathbb{R}^n)} \leq C\varepsilon \|Du_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{n^2})},$$

where the two constants depend only on the space dimension n and on the lattice basis (a_i) .

Proof. We choose $p \in (1, 2)$ and an integer k not larger than n such that $\alpha = k - n/p \in (0, 1)$. This is always possible, for example, by taking $k = n$ and $p = 2n/(2n - 1)$. Let Q_ε be a parallelepiped defined by the Bravais basis $(k\varepsilon a_i)$ and contained in the complement of Ω . By the Sobolev–Morrey embedding there is a polynomial $q: \mathbb{R}^n \rightarrow \mathbb{R}^n$ of degree less than k such that

$$(3.31) \quad \|u_\varepsilon - q\|_{C^\alpha(Q_\varepsilon, \mathbb{R}^n)} \leq C \|D^k u_\varepsilon\|_{L^p(Q_\varepsilon, \mathbb{R}^{n^{k+1}})}.$$

Since u_ε vanishes on the lattice, the same estimate holds pointwise for q on the $(k+1)^n$ lattice points contained in the closure of Q_ε . Since this set contains $k + 1$ points in each coordinate direction, and the degree of q is less than k , the estimate holds for q pointwise in Q_ε , and therefore

$$(3.32) \quad \|u_\varepsilon\|_{C^\alpha(Q_\varepsilon, \mathbb{R}^n)} \leq C \|D^k u_\varepsilon\|_{L^p(Q_\varepsilon, \mathbb{R}^{n^{k+1}})}.$$

From Hölder’s inequality we additionally obtain

$$(3.33) \quad \|u_\varepsilon\|_{L^\infty(Q_\varepsilon, \mathbb{R}^n)} \leq C\varepsilon^\alpha \|D^k u_\varepsilon\|_{L^p(Q_\varepsilon, \mathbb{R}^{n^{k+1}})} \leq C\varepsilon^\alpha \varepsilon^{\frac{n}{p} - \frac{n}{2}} \|D^k u_\varepsilon\|_{L^2(Q_\varepsilon, \mathbb{R}^{n^{k+1}})}$$

and

$$(3.34) \quad \|u_\varepsilon\|_{L^2(Q_\varepsilon, \mathbb{R}^n)}^2 \leq C\varepsilon^{2\alpha} \varepsilon^{\frac{2n}{p}} \|D^k u_\varepsilon\|_{L^2(Q_\varepsilon, \mathbb{R}^{n^{k+1}})}^2.$$

If the constant c in the statement is chosen as the inverse of the diameter of the scaled parallelepiped Q_1 , then no parallelepiped of the form of Q_ε can intersect both $\overline{\Omega}$ and K , and therefore the set K can be covered by ε -lattice parallelepipeds such as Q_ε that do not intersect Ω . Therefore,

$$(3.35) \quad \|u_\varepsilon\|_{L^2(K, \mathbb{R}^n)}^2 \leq C\varepsilon^{2\alpha} \varepsilon^{\frac{2n}{p}} \|D^k u_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{n^{k+1}})}^2.$$

Since u_ε is band-limited and, therefore, its Fourier transform is supported in B/ε , we have

$$(3.36) \quad \|D^k u_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{k+1})} \leq \frac{C}{\varepsilon^{k-1}} \|Du_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{n^2})}.$$

Combining the preceding two estimates and inserting the definition of α we obtain

$$(3.37) \quad \|u_\varepsilon\|_{L^2(K, \mathbb{R}^n)} \leq C\varepsilon \|Du_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{n^2})},$$

which concludes the proof. \square

COROLLARY 3.3. *Let (u_ε) be a sequence in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ such that $u_\varepsilon \in X_\varepsilon$. Suppose that (u_ε) converges weakly to $u_0 \in H^1(\mathbb{R}^n, \mathbb{R}^n)$. Then $u_0 \in X_0$.*

Proof. Let K be a closed set disjoint from $\overline{\Omega}$. From Lemma 3.2 we have

$$(3.38) \quad \|u_\varepsilon\|_{L^2(K, \mathbb{R}^n)} \leq C\varepsilon \|Du_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{n^2})}$$

for all ε sufficiently small. Therefore, $u_\varepsilon \rightarrow 0$ in $L^2(K, \mathbb{R}^n)$. By assumption, $u_\varepsilon \rightharpoonup u_0$ in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ and, therefore, also in $L^2(K, \mathbb{R}^n)$. By the uniqueness of the weak limit, the restriction of u_0 to K is 0 as an element of $L^2(K, \mathbb{R}^n)$, and hence, $u_0 = 0$ a.e. in K . Since K is an arbitrary compact subset of the complement of the closure of Ω , it follows that $u_0 = 0$ a.e. in that complement. \square

COROLLARY 3.4. *There is a real number $C > 0$ such that*

$$(3.39) \quad \|u_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)} \leq C|u_\varepsilon|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}$$

for every $u_\varepsilon \in X_\varepsilon$ and ε sufficiently small.

Proof. Let B_R be a ball which contains Ω . Let $K = \overline{B_{R+2}} \setminus B_{R+1}$. From Lemma 3.2 we have, for ε sufficiently small,

$$(3.40) \quad \|u_\varepsilon\|_{L^2(K; \mathbb{R}^n)} \leq C \|Du_\varepsilon\|_{L^2(\mathbb{R}^n; \mathbb{R}^{n \times n})}.$$

In addition, Poincaré's inequality applied to the set B_{R+2} shows that there is $u_* \in \mathbb{R}^n$ such that

$$(3.41) \quad \|u_\varepsilon - u_*\|_{L^2(B_{R+2}; \mathbb{R}^n)} \leq C \|Du_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{n \times n})}.$$

The constant depends on R and, therefore, on Ω , but not on ε . Combining these two equations we conclude

$$(3.42) \quad |u_*| |K|^{1/2} = \|u_*\|_{L^2(K, \mathbb{R}^n)} \leq C \|Du_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{n \times n})},$$

and therefore

$$(3.43) \quad \|u_\varepsilon\|_{L^2(B_{R+2}; \mathbb{R}^n)} \leq C \|Du_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{n \times n})},$$

with a constant which only depends on the domain. An application of Lemma 3.2 to the set $K' = \mathbb{R}^n \setminus B_{R+2}$ then gives

$$(3.44) \quad \|u_\varepsilon\|_{L^2(\mathbb{R}^n \setminus B_{R+2}; \mathbb{R}^n)} \leq C \|Du_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^{n \times n})}.$$

The sum of the last two equations concludes the proof. \square

The equicoercivity of the sequence (E_ε) with respect to weak convergence in H^1 may be established as follows.

THEOREM 3.5 (equicoercivity). *Let $E_\varepsilon : H^1(\mathbb{R}^n, \mathbb{R}^n) \rightarrow \bar{\mathbb{R}}$ be defined by (3.21). Suppose that there is a positive constant C_L such that*

$$(3.45) \quad C_L |\xi|^2 |\zeta|^2 \leq \langle \varepsilon^{-2} D(\varepsilon \xi) \zeta, \zeta \rangle.$$

Then, the sequence (E_ε) is weakly sequentially equicoercive in $H^1(\mathbb{R}^n, \mathbb{R}^n)$. In addition, all of the accumulation points of sequences of bounded energy belong to X_0 .

This result shows that sequences of bounded energy have subsequences which are weakly convergent in $H^1(\mathbb{R}^n, \mathbb{R}^n)$, and implies that this is the concept of convergence we should adopt in studying the limiting energy. In particular, we can now make precise the continuity of the forcing term. For any choice of the external forces $f \in H^{-1}(\mathbb{R}^n, \mathbb{R}^n)$, and for any sequence (u_ε) which converges weakly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ to some u_0 , one has

$$(3.46) \quad \lim_{\varepsilon \rightarrow 0} \langle f, u_\varepsilon \rangle = \langle f, u_0 \rangle.$$

Proof. Let (u_ε) in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ be such that the sequence $(E_\varepsilon(u_\varepsilon))$ is bounded. Then, necessarily, $u_\varepsilon \in X_\varepsilon$. In addition, by (3.45) we have

$$(3.47) \quad \begin{aligned} E_\varepsilon(u_\varepsilon) &= \frac{1}{(2\pi)^n} \int \frac{1}{2} \langle \varepsilon^{-2} D(\varepsilon \xi) \hat{u}_\varepsilon(\xi), \hat{u}_\varepsilon^*(\xi) \rangle d\xi \\ &\geq \frac{C_L}{(2\pi)^n} \int \frac{1}{2} |\xi|^2 |\hat{u}_\varepsilon(\xi)|^2 d\xi = C_L |u_\varepsilon|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2, \end{aligned}$$

and, by Corollary 3.4, the sequence $(\|u_\varepsilon\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)})$ is bounded. Therefore, there is a subsequence of (u_ε) that converges weakly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ to $u_0 \in H^1(\mathbb{R}^n, \mathbb{R}^n)$. By Corollary 3.3, $u_0 \in X_0$. \square

The continuum limit of harmonic crystals is now established by the following theorem.

THEOREM 3.6 (continuum limit). *Let $E_\varepsilon : H^1(\mathbb{R}^n, \mathbb{R}^n) \rightarrow \bar{\mathbb{R}}$ and $E_0 : H^1(\mathbb{R}^n, \mathbb{R}^n) \rightarrow \bar{\mathbb{R}}$ be defined by (3.21) and (3.14), respectively. Suppose the following:*

- (i) *For every $\zeta \in \mathbb{C}^n$ the function $\langle D(\cdot)\zeta, \zeta \rangle$ is measurable on B .*
- (ii) *There are positive constants $C_U \geq C_L > 0$ such that*

$$(3.48) \quad C_L |k|^2 |\zeta|^2 \leq \langle D(k)\zeta, \zeta \rangle \leq C_U |k|^2 |\zeta|^2$$

for a.e. $k \in B$ and for every $\zeta \in \mathbb{C}^n$.

- (iii) *The sequence $\varepsilon^{-2} D(\varepsilon \xi)$ converges pointwise to $D_0(\xi)$ in \mathbb{R}^n .*
- Then $\Gamma\text{-}\lim_{\varepsilon \rightarrow 0} E_\varepsilon = E_0$ in the weak topology of $H^1(\mathbb{R}^n, \mathbb{R}^n)$.*

In order to better illustrate the structure of the proof, we subdivide it into several partial results. We remark that Γ -convergence holds both in the strong and in the weak topology of $H^1(\mathbb{R}^n, \mathbb{R}^n)$, whereas the coercivity statement in Theorem 3.5 holds only in the weak topology.

LEMMA 3.7. *Let X be a metric space and let $I_\varepsilon : X \rightarrow \mathbb{R}$, $\varepsilon > 0$, a family of functionals which converge pointwise to I_0 , in the sense that $I_\varepsilon(u) \rightarrow I_0(u)$ for all $u \in X$, and are strongly continuous in X , uniformly in ε , in the sense that for all $u \in X$ one has*

$$(3.49) \quad \limsup_{\delta \rightarrow 0} \{ |I_\varepsilon(u) - I_\varepsilon(v)| : \varepsilon > 0, v \in B_\delta(u) \} = 0.$$

If a sequence (u_ε) is given with $u_\varepsilon \rightarrow u_0$, $u_0 \in X$, then

$$(3.50) \quad \lim_{\varepsilon \rightarrow 0} I_\varepsilon(u_\varepsilon) = I_0(u_0).$$

Proof. We denote by $\omega(\delta)$ the supremum in (3.49). Condition (3.49) then states that $\lim_{\delta \rightarrow 0} \omega(\delta) = 0$. Let $u_\varepsilon \rightarrow u$. Then

$$(3.51) \quad |I_0(u) - I_\varepsilon(u_\varepsilon)| \leq |I_0(u) - I_\varepsilon(u)| + |I_\varepsilon(u) - I_\varepsilon(u_\varepsilon)| \leq |I_0(u) - I_\varepsilon(u)| + \omega(\|u - u_\varepsilon\|_X).$$

The first term converges to zero by the pointwise convergence, the second by the uniform continuity. \square

We now show that the functionals of interest for Theorem 3.6 obey the assumptions of Lemma 3.7, after the restriction to X_ε is removed.

LEMMA 3.8. *Under the assumptions of Theorem 3.6, the functional*

$$(3.52) \quad I_\varepsilon(u) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \chi_{B/\varepsilon}(\xi) \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}^*(\xi) \rangle d\xi$$

is strongly continuous in $H^1(\mathbb{R}^n; \mathbb{R}^n)$, uniformly in ε (in the sense of (3.49)), and converges pointwise to

$$(3.53) \quad I_0(u) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \langle D_0(\xi) \hat{u}(\xi), \hat{u}^*(\xi) \rangle d\xi.$$

Proof. Let $u \in H^1(\mathbb{R}^n; \mathbb{R}^n)$. By (3.48) and dominated convergence,

$$(3.54) \quad \begin{aligned} \lim_{\varepsilon \rightarrow 0} \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \chi_{B/\varepsilon}(\xi) \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}^*(\xi) \rangle d\xi \\ = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \langle D_0(\varepsilon\xi) \hat{u}(\xi), \hat{u}^*(\xi) \rangle d\xi = E_0(u). \end{aligned}$$

This proves the pointwise convergence. For $u, v \in H^1(\mathbb{R}^n; \mathbb{R}^n)$ we compute

$$(3.55) \quad \begin{aligned} I_\varepsilon(u) - I_\varepsilon(v) &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \chi_{B/\varepsilon}(\xi) \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}^*(\xi) - \hat{v}^*(\xi) \rangle d\xi \\ &\quad + \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \chi_{B/\varepsilon}(\xi) \langle \varepsilon^{-2} D(\varepsilon\xi) (\hat{u}(\xi) - \hat{v}(\xi)), \hat{v}^*(\xi) \rangle d\xi. \end{aligned}$$

By (3.48) and Hölder's inequality applied to both terms we obtain

$$(3.56) \quad |I_\varepsilon(u) - I_\varepsilon(v)| \leq C_U (\|u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} + \|v\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}) \|u - v\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)},$$

with a constant which does not depend on ε . For $\|u - v\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} < \delta$ we obtain

$$(3.57) \quad |I_\varepsilon(u) - I_\varepsilon(v)| \leq C_U (2\|u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} + \delta) \delta$$

for all $\varepsilon > 0$, and uniform continuity is proven. \square

Proof of Theorem 3.6. We recall that E_ε Γ -converges to E_0 weakly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ if: (a) For every $u \in H^1(\mathbb{R}^n, \mathbb{R}^n)$, there exists a sequence (u_ε) converging weakly to u in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ such that $\lim_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon) = E_0(u)$, and (b) for every sequence (u_ε) converging weakly to u in $H^1(\mathbb{R}^n, \mathbb{R}^n)$, $\liminf_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon) \geq E_0(u)$.

We proceed to prove (a). Let $u \in H^1(\mathbb{R}^n, \mathbb{R}^n)$. If $u \notin X_0$, then $E_0(u) = \infty$ and we can take a constant sequence $u_\varepsilon = u_0$. By Corollary 3.3 one has $u_\varepsilon \notin X_\varepsilon$ for ε sufficiently small, hence $E_\varepsilon(u_\varepsilon) = \infty$ and the proof is concluded. If $u \in X_0$, by Proposition 3.1, there is a sequence (u_ε) , with $u_\varepsilon \in X_\varepsilon$, converging strongly (hence

weakly) to u in $H^1(\mathbb{R}^n, \mathbb{R}^n)$. By Lemma 3.8 we can apply Lemma 3.7 to this sequence and obtain $I_\varepsilon(u_\varepsilon) \rightarrow I_0(u)$. Since $E_\varepsilon = I_\varepsilon$ on X_ε , and $E_0 = I_0$ on X_0 , we have

$$(3.58) \quad \lim_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon) = \lim_{\varepsilon \rightarrow 0} I_\varepsilon(u_\varepsilon) = I_0(u) = E_0(u).$$

This concludes the proof of (a).

Next we proceed to prove (b). Suppose now that $u_\varepsilon \rightharpoonup u$ in $H^1(\mathbb{R}^n, \mathbb{R}^n)$. Suppose, in addition, that $\liminf_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon) < +\infty$, otherwise there is nothing to prove. Pass to a subsequence, again denoted by (u_ε) , that gives the lim inf as a limit. By (3.54), it suffices to prove that

$$(3.59) \quad \lim_{\varepsilon \rightarrow 0} \frac{1}{(2\pi)^n} \int_{B/\varepsilon} (\langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}_\varepsilon(\xi), \hat{u}_\varepsilon^*(\xi) \rangle - \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}^*(\xi) \rangle) d\xi \geq 0.$$

To this end, consider the identity

$$(3.60) \quad \begin{aligned} & \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}_\varepsilon(\xi), \hat{u}_\varepsilon^*(\xi) \rangle - \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}^*(\xi) \rangle \\ &= \langle \varepsilon^{-2} D(\varepsilon\xi) (\hat{u}_\varepsilon(\xi) - \hat{u}(\xi)), \hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi) \rangle + 2 \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi) \rangle. \end{aligned}$$

Furthermore,

$$(3.61) \quad \begin{aligned} & \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi) \rangle \\ &= \langle (\varepsilon^{-2} D(\varepsilon\xi) - D_0(\xi)) \hat{u}(\xi), \hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi) \rangle + \langle D_0(\xi) \hat{u}(\xi), \hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi) \rangle. \end{aligned}$$

By weak convergence,

$$(3.62) \quad \lim_{\varepsilon \rightarrow 0} \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \chi_{B/\varepsilon}(\xi) \langle D_0(\xi) \hat{u}(\xi), \hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi) \rangle d\xi = 0.$$

In addition, by Hölder,

$$(3.63) \quad \begin{aligned} & \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \langle (\varepsilon^{-2} D(\varepsilon\xi) - D_0(\xi)) \hat{u}(\xi), \hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi) \rangle d\xi \\ &= \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \langle |\xi|^{-1} (\varepsilon^{-2} D(\varepsilon\xi) - D_0(\xi)) \hat{u}(\xi), |\xi| (\hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi)) \rangle d\xi \\ &\leq \left(\frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \chi_{B/\varepsilon}(\xi) |\xi|^{-1} |\varepsilon^{-2} D(\varepsilon\xi) - D_0(\xi)|^2 |\hat{u}(\xi)|^2 d\xi \right)^{1/2} \|u_\varepsilon - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}, \end{aligned}$$

where the first factor converges to 0 by dominated convergence. Therefore,

$$(3.64) \quad \lim_{\varepsilon \rightarrow 0} \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi) \rangle d\xi = 0,$$

and

$$(3.65) \quad \begin{aligned} & \lim_{\varepsilon \rightarrow 0} \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}_\varepsilon(\xi), \hat{u}_\varepsilon^*(\xi) \rangle - \langle \varepsilon^{-2} D(\varepsilon\xi) \hat{u}(\xi), \hat{u}^*(\xi) \rangle d\xi \\ &= \lim_{\varepsilon \rightarrow 0} \frac{1}{(2\pi)^n} \int_{B/\varepsilon} \langle \varepsilon^{-2} D(\varepsilon\xi) (\hat{u}_\varepsilon(\xi) - \hat{u}(\xi)), \hat{u}_\varepsilon^*(\xi) - \hat{u}^*(\xi) \rangle d\xi \geq 0, \end{aligned}$$

as required. \square

We recall that the convergence of minimizers follows from Γ -convergence and the equicoercivity of the sequence (E_ε) (cf., e.g., [15]). More precisely, the weak sequential equicoercivity of the sequence (E_ε) implies that the minimizers of E_0 are accumulation points of minimizing sequences, i.e., if $E_\varepsilon(u_\varepsilon) = \inf E_\varepsilon$, then the sequence u_ε has a subsequence that converges weakly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ to a minimizer of E_0 .

4. Approximation: The quasicontinuum method. In the framework of molecular statics, the quasicontinuum method (cf., e.g., [59, 60, 31]) is an approximation scheme that consists of: (i) placing interpolation constraints, possibly adaptively, on the motion of the atoms with a view to eliminating degrees of freedom in regions where the displacement field is nearly affine, and (ii) using summation rules to avoid full lattice sums. We proceed by recounting the salient aspects of the method that are relevant to the present analysis.

4.1. Quasicontinuum with full lattice sums. When full lattice sums are allowed, i.e., in the absence of summation rules, the quasicontinuum method reduces to constrained minimization of the energy. Thus, suppose that we can identify a sequence (Y_ε) of subspaces of X_ε , representing “coarse-grained” displacements of the ε -lattice. Define the coarse-grained, or *reduced*, lattice elastic energy

$$(4.1) \quad J_\varepsilon(u) = \begin{cases} E_\varepsilon(u) & \text{if } u \in Y_\varepsilon, \\ +\infty & \text{otherwise.} \end{cases}$$

Note that, in general, the real-space evaluation of J_ε entails the computation of full lattice sums, which is likely to entail prohibitive computational expense. The practical implementation of the method thus requires an additional approximation step in the form of summation rules, to be treated in section 4.2.

For fully-summed coarse-grained energies we can easily extend the convergence result of Theorem 3.6. We also recall that, by Proposition 3.1, the sequence (X_ε) itself has the density property.

THEOREM 4.1. *Assume that a sequence of subspaces (Y_ε) is given such that $Y_\varepsilon \subset X_\varepsilon$, and that (Y_ε) is (strongly) dense on X_0 in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ in the sense that for every $u \in X_0$ there exists a sequence (u_ε) such that $u_\varepsilon \in Y_\varepsilon$ and $u_\varepsilon \rightarrow u$ strongly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$. Assume that J_ε is defined as above, including the assumptions of Theorem 3.6 on the interaction kernel. Then*

$$(4.2) \quad E_0 = \Gamma\text{-}\lim_{\varepsilon \rightarrow 0} J_\varepsilon$$

weakly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ and (J_ε) is weakly equicoercive in $H^1(\mathbb{R}^n, \mathbb{R}^n)$.

Proof. The proof follows closely to that of Theorem 3.6.

(a) Let $u \in H^1(\mathbb{R}^n, \mathbb{R}^n)$. By assumption there is a sequence (u_ε) with $u_\varepsilon \in Y_\varepsilon$ and $u_\varepsilon \rightarrow u$. As in part (a) of the proof of Theorem 3.6 we apply Lemmas 3.8 and 3.7 to obtain (recalling that $Y_\varepsilon \subset X_\varepsilon$)

$$(4.3) \quad \lim_{\varepsilon \rightarrow 0} J_\varepsilon(u_\varepsilon) = \lim_{\varepsilon \rightarrow 0} I_\varepsilon(u_\varepsilon) = I_0(u) = E_0(u).$$

(b) Assume now that $u_\varepsilon \rightarrow u$. Using first $Y_\varepsilon \subset X_\varepsilon$ and then Theorem 3.6, we obtain

$$(4.4) \quad \liminf_{\varepsilon \rightarrow 0} J_\varepsilon(u_\varepsilon) \geq \liminf_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon) \geq E_0(u).$$

(c) Correspondingly, the equicoercivity of (J_ε) , and hence the convergence of minimizers, follows immediately from the equicoercivity of (E_ε) and the ordering $J_\varepsilon \geq E_\varepsilon$. \square

The preceding theorem provides general conditions under which coarse-graining of the lattice displacements does not “spoil” the continuum limit. This invariance of the continuum limit under coarse-graining provides a natural notion of convergence of quasicontinuum approximations.

In practice, the challenge is to construct coarse-graining approximations that are convergent, in the sense of Theorem 4.1, and lend themselves to efficient computational implementations. The most common implementation of the quasicontinuum method to date consists of direct sampling of the continuum interpolations at the atoms of the lattice. Thus, as before, suppose that (X_h) is a sequence of approximating subspaces that is dense in X_0 , such as finite-element spaces. We note that the assumption that the approximating spaces are contained in X_0 may place restrictions on the domains Ω that can be considered, e.g., polyhedral domains. Then, we consider the projection of $u_h \in X_h$ to band-limited functions,

$$(4.5) \quad u_{\varepsilon,h} = P_\varepsilon u_h,$$

where P_ε was defined above (3.22). Thus, $u_{\varepsilon,h}$ is obtained by sampling u_h on the ε -lattice and subsequently applying Whittaker–Shannon interpolation. Alternatively, the discrete Fourier transform of $u_{\varepsilon,h}$ is related to the ordinary Fourier transform of u_h through Poisson’s summation formula (3.22). Correspondingly, we define the sequence of subspaces

$$(4.6) \quad X_{\varepsilon,h} = \{P_\varepsilon u_h : u_h \in X_h\}.$$

Define now $Y_\varepsilon = X_{\varepsilon,h_\varepsilon}$ for some sequence (h_ε) such that $h_\varepsilon \rightarrow 0$. Evidently, Y_ε is a subspace of X_ε for all $\varepsilon > 0$. We proceed to verify that the sequence Y_ε has the density property. To this end, we begin by recalling the following lemma.

LEMMA 4.2 (Bramble and Hilbert [9]). *Let $u \in H^2(\mathbb{R}^n, \mathbb{R}^n)$. Then there exists a constant C independent of ε and u such that*

$$(4.7) \quad \|P_\varepsilon u - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} \leq C\varepsilon \|u\|_{H^2(\mathbb{R}^n, \mathbb{R}^n)}.$$

The density of Y_ε is now established by the following proposition.

PROPOSITION 4.3. *Let $u \in H^1(\mathbb{R}^n, \mathbb{R}^n)$, and let $u_h \in X_h$ be a sequence such that $u_h \rightarrow u$ strongly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$. Let ρ_δ be a mollifier and set $u_\varepsilon = P_\varepsilon(\rho_{\delta_\varepsilon} * u_{h_\varepsilon})$, with $h_\varepsilon \rightarrow 0$, $\delta_\varepsilon \rightarrow 0$, and $\varepsilon/\delta_\varepsilon \rightarrow 0$. Then u_ε converges to u strongly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$.*

Proof. We have

$$(4.8) \quad \begin{aligned} \|u_\varepsilon - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} &= \|P_\varepsilon(\rho_{\delta_\varepsilon} * u_{h_\varepsilon}) - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} \\ &\leq \|P_\varepsilon(\rho_{\delta_\varepsilon} * u_{h_\varepsilon}) - \rho_{\delta_\varepsilon} * u_{h_\varepsilon}\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} + \|\rho_{\delta_\varepsilon} * u_{h_\varepsilon} - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} \\ &\leq \|P_\varepsilon(\rho_{\delta_\varepsilon} * u_{h_\varepsilon}) - \rho_{\delta_\varepsilon} * u_{h_\varepsilon}\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} \\ &\quad + \|\rho_{\delta_\varepsilon} * (u_{h_\varepsilon} - u)\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} + \|\rho_{\delta_\varepsilon} * u - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} \\ &\leq C\varepsilon \|\rho_{\delta_\varepsilon} * u_{h_\varepsilon}\|_{H^2(\mathbb{R}^n, \mathbb{R}^n)} + \|u_{h_\varepsilon} - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} + \|\rho_{\delta_\varepsilon} * u - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} \\ &\leq \frac{C\varepsilon}{\delta_\varepsilon} \|u_{h_\varepsilon}\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} + \|u_{h_\varepsilon} - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)} + \|\rho_{\delta_\varepsilon} * u - u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}, \end{aligned}$$

where we have made use of Lemma 4.2 and the properties of mollifiers. By the strong convergence of u_h and the convergence properties of mollifiers [1], the right-hand side of this inequality converges to 0 provided that $\varepsilon/\delta_\varepsilon \rightarrow 0$. \square

Hence, Theorem 4.1 applies and the corresponding sequence J_ε of coarse-grained energies Γ -converges to E_0 . Moreover, by equicoercivity the minimizers of J_ε converge (weakly) to minimizers of E_0 .

4.2. Summation rules and sundry variational crimes. The constrained-minimization—or Rayleigh–Ritz—scheme described previously effectively reduces the dimensionality of the solution spaces used in calculations to the dimension of the approximation spaces X_h . However, the evaluation of the reduced energy J_ε in real space still requires the computation of full lattice sums of the form (2.4), which detracts from the efficiency of the approach. In order to obtain an approximation scheme with overall complexity $O(\dim(X_h))$, it is therefore necessary to approximate full lattice sums by means of *summation rules* (cf., e.g., [59, 60, 31]). The net effect of this additional approximation is to *perturb* the reduced interatomic energy J_ε , equation (3.21), resulting in the *quasicontinuum* interatomic energy \tilde{J}_ε . In contrast to the fully integrated reduced energy functional J_ε , the quasicontinuum energy functional \tilde{J}_ε is no longer the restriction of the interatomic energy E_ε to a subspace Y_ε of X_ε . Thus, in the parlance of variational approximation methods (cf., e.g., [12, 10]), the summation rules constitute a *variational crime*. Another common variational crime is the perturbation of the domain Ω into a sequence of domains Ω_h resulting from meshing, but, as already mentioned, this additional source of error will not be considered in this paper (cf., e.g., [12] for an analysis of domain approximation errors). It may be expected from standard theory that, if the perturbation of the functional is uniformly small, then the variational crime does not compromise convergence (cf., e.g., [12, 10]). In the present context, we specifically wish to ascertain conditions on summation rules that ensure the convergence of the associated quasicontinuum scheme.

4.2.1. An abstract variational-crime framework. A general abstract framework for the analysis of perturbed energy functionals, or *variational crimes*, may be formulated as follows. We begin by defining the sequence of functionals

$$(4.9) \quad G_\varepsilon(u) = \begin{cases} \tilde{J}_\varepsilon(u) - J_\varepsilon(u) & \text{if } u \in Y_\varepsilon, \\ 0 & \text{otherwise,} \end{cases}$$

and write

$$(4.10) \quad \tilde{J}_\varepsilon = J_\varepsilon + G_\varepsilon.$$

Thus, G_ε represents the energy perturbation, or *energy error* incurred as a result of the summation rule.

The following theorem establishes general abstract conditions for the convergence of sequences of perturbed energy functionals.

THEOREM 4.4 (locally uniform convergence). *Suppose that the sequence (J_ε) Γ -converges to E_0 weakly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$. Assume that there exists a positive sequence (C_ε) converging to 0 such that*

$$(4.11) \quad |G_\varepsilon(u)| \leq C_\varepsilon \|u\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2$$

for all $u \in H^1(\mathbb{R}^n, \mathbb{R}^n)$. Then, $J_\varepsilon + G_\varepsilon$ Γ -converges to E_0 weakly in $H^1(\mathbb{R}^n, \mathbb{R}^n)$. Suppose, in addition, that

$$(4.12) \quad J_\varepsilon(u_\varepsilon) \geq C \|u_\varepsilon\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2.$$

Then the sequence $(J_\varepsilon + G_\varepsilon)$ is also weakly equicoercive in $H^1(\mathbb{R}^n, \mathbb{R}^n)$.

Proof. Let $u \in H^1(\mathbb{R}^n, \mathbb{R}^n)$, and let (u_ε) be a sequence in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ such that $u_\varepsilon \rightharpoonup u$ and $\lim_{\varepsilon \rightarrow 0} J_\varepsilon(u_\varepsilon) = E_0(u)$. Then,

$$(4.13) \quad \begin{aligned} |(J_\varepsilon + G_\varepsilon)(u_\varepsilon) - E_0(u)| &\leq |J_\varepsilon(u_\varepsilon) - E_0(u)| + |G_\varepsilon(u_\varepsilon)| \\ &\leq |J_\varepsilon(u_\varepsilon) - E_0(u)| + C_\varepsilon \|u_\varepsilon\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2. \end{aligned}$$

But, by weak convergence, the sequence $\|u_\varepsilon\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}$ is bounded and the right-hand side of the inequality converges to 0, whence it follows that $\lim_{\varepsilon \rightarrow 0} (J_\varepsilon + G_\varepsilon)(u_\varepsilon) = E_0(u)$, as required. Let $u \in H^1(\mathbb{R}^n, \mathbb{R}^n)$, and let (u_ε) be a sequence in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ such that $u_\varepsilon \rightharpoonup u$. Then, the sequence $\|u_\varepsilon\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}$ is bounded, and

$$(4.14) \quad |G_\varepsilon(u_\varepsilon)| \leq C_\varepsilon \|u_\varepsilon\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2,$$

where the right-hand side converges to 0. Hence,

$$(4.15) \quad \liminf_{\varepsilon \rightarrow 0} (J_\varepsilon + G_\varepsilon)(u_\varepsilon) = \liminf_{\varepsilon \rightarrow 0} J_\varepsilon(u_\varepsilon) \geq E_0(u),$$

as required. Consider now a sequence (u_ε) in $H^1(\mathbb{R}^n, \mathbb{R}^n)$ such that $(J_\varepsilon(u_\varepsilon) + G_\varepsilon(u_\varepsilon))$ is bounded. From $(J_\varepsilon + G_\varepsilon)(u_\varepsilon) \leq A < +\infty$ and the assumptions, we have

$$(4.16) \quad C \|u_\varepsilon\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2 \leq A + C_\varepsilon \|u_\varepsilon\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2.$$

For small ε , we have $C_\varepsilon < C/w$ and, therefore, $(C/2)\|u_\varepsilon\|_{H^1(\mathbb{R}^n, \mathbb{R}^n)}^2 \leq A$. \square

The preceding theorem is a simple adaptation of general results concerning the Γ -convergence of functionals under perturbations having locally uniform convergence [15]. In particular, Theorem 4.4 provides abstract conditions ensuring that a perturbation G_ε does not compromise convergence.

4.2.2. Summation rules based on elementwise Gaussian quadrature.

The challenge that remains is to devise specific summation rules that satisfy the conditions of Theorem 4.4 while reducing the overall complexity of the scheme to $O(\dim(X_h))$. A particular class of computationally efficient and convergent summation rules can be formulated by exploiting the *additive structure* of the interatomic energy and adapting the classical numerical quadrature rules for finite elements (cf., e.g., [59, 60, 31]).

We shall assume that the harmonic interatomic energy has a *clusterwise* additive structure of the form

$$(4.17) \quad E(u) = \sum_{\alpha \in I} E_\alpha(u),$$

where I indexes the clusters in the crystal, and

$$(4.18) \quad E_\alpha(u) = \frac{1}{2} \langle A_\alpha u, u \rangle$$

is a nonnegative quadratic energy for the α cluster expressed in terms of cluster force constants A_α . We also assume that E_α is translation invariant, i.e., invariant under superposed rigid translations. We shall say that cluster energy α is *short-ranged*, with *radius of interaction* r_α , if $E_\alpha(u) = E_\alpha(v)$ if $u = v$ in a certain ball of radius r_α . We shall say that the cluster energies are *uniformly short-ranged* if there exists r such that $r_\alpha < r$ for all α .

We recall that many interatomic potentials commonly used in practice, including pair potentials, Embedded Atom Method (EAM) potentials for metals [16], and the Stillinger–Weber and related potentials for covalent crystals [57], have indeed a clusterwise additive structure of the form (4.17). A simple example is furnished by the case of nearest-neighbor interactions, for which the energy takes the form

$$(4.19) \quad E_{\text{NN}}(u) = \sum_{\alpha \in I} \frac{1}{2} \langle B_{\alpha} du_{\alpha}, du_{\alpha} \rangle,$$

where I now indexes the atomic bonds in the crystal, du_{α} is the displacement difference between the end atoms of bond α , and B_{α} is a bondwise $n \times n$ matrix of force constants. Note that, by writing (4.19) in terms of discrete differentials du_{α} , the cluster energy is automatically translation invariant.

As in the previous section (cf. section 3), in order to define the continuum limit of the interatomic energy we consider a sequence of lattices of size rescaled by ε , and the sequence of rescaled interatomic energies

$$(4.20) \quad E_{\varepsilon}(u_{\varepsilon}) = \sum_{\alpha \in I_{\varepsilon}} \frac{1}{2} \langle A_{\varepsilon, \alpha} u_{\varepsilon}, u_{\varepsilon} \rangle \equiv \sum_{\alpha \in I_{\varepsilon}} E_{\varepsilon, \alpha}(u_{\varepsilon}),$$

where u_{ε} is an ε -lattice displacement, $E_{\varepsilon, \alpha}$ is the rescaled energy of cluster α , I_{ε} indexes clusters on the ε -lattice, and the $A_{\varepsilon, \alpha}$ are rescaled force constants. We note that, if the unscaled cluster energy E_{α} has finite range with radius of interaction r_{α} , then $E_{\varepsilon, \alpha}$ also has finite range with radius of interaction $r_{\varepsilon, \alpha} = \varepsilon r_{\alpha}$. Suppose now that the unscaled cluster energies are uniformly bounded, i.e.,

$$(4.21) \quad E_{\alpha}(u) \leq C \sum_{l \in \mathcal{C}_{\alpha}} |u(l)|^2$$

for some constant C independent of α . Here and subsequently, the set \mathcal{C}_{α} of lattice coordinates identifies the atoms contained in cluster α . Then, the rescaled cluster energies satisfy the bound

$$(4.22) \quad E_{\varepsilon}(u_{\varepsilon}) \leq C \varepsilon^{n-2} \sum_{l \in \mathcal{C}_{\varepsilon, \alpha}} |u_{\varepsilon}(l)|^2,$$

where C is independent of ε and α .

Recall (cf. section 4.1) that the fully-summed quasicontinuum energy J_{ε} is the restriction of the interatomic energy E_{ε} to subspaces of the form $Y_{\varepsilon} = X_{\varepsilon, h_{\varepsilon}}$, where (h_{ε}) is a sequence of positive numbers converging to zero, and $X_{\varepsilon, h_{\varepsilon}}$ is the space of band-limited functions obtained by sampling the approximation subspace $X_{h_{\varepsilon}}$ of X_0 , equation (4.5). We also recall that in effecting the continuum limit, Proposition 4.3, we assume that the element size h_{ε} vanishes more slowly than the lattice size ε , i.e., $\varepsilon/h_{\varepsilon} \rightarrow 0$. Therefore, if the interatomic interactions are short-ranged, then it follows that $r_{\varepsilon}/h_{\varepsilon} = r\varepsilon/h_{\varepsilon} \rightarrow 0$, i.e., the range of interaction is increasingly small relative to the element size.

Next we exploit this structure, in conjunction with the additivity of the energy, in order to define a sequence $(\tilde{J}_{\varepsilon})$ of *approximately summed* energies. Denote by $\mathcal{T}_{h_{\varepsilon}}$ the collection of elements in the mesh defining the finite-element approximation space $X_{h_{\varepsilon}}$. For every element $K_{\varepsilon} \in \mathcal{T}_{h_{\varepsilon}}$, we additionally denote by $\dot{I}_{K_{\varepsilon}}$ the index set of all the clusters that are fully contained in K_{ε} . Suppose that, for every $u_{\varepsilon} \in Y_{\varepsilon}$, the total

energy of the clusters in \dot{K}_ε is computed *exactly* by an *element summation rule* of the type

$$(4.23) \quad \sum_{\alpha \in \dot{I}_{K_\varepsilon}} E_{\varepsilon,\alpha}(u_\varepsilon) = \sum_{\alpha \in \tilde{I}_{K_\varepsilon}} \tilde{w}_{K_\varepsilon,\alpha} E_{\varepsilon,\alpha}(u_\varepsilon),$$

where $\tilde{I}_{K_\varepsilon}$ indexes a collection of *quadrature clusters* within K_ε and $\tilde{w}_{K_\varepsilon,\alpha}$ are the corresponding *quadrature weights*. For instance, if the approximation spaces X_{h_ε} are defined by piecewise linear interpolation over simplices, and if the energy is of the nearest-neighbor type, equation (4.19), then an element summation rule may be obtained by choosing $\tilde{I}_{K_\varepsilon}$ to consist of a single bond of each bond type in the element, with weights equal to the corresponding number of bonds (cf. [4] for classifications of bonds by type in common crystal lattices). Then, for every $u_\varepsilon \in Y_\varepsilon$ we set

$$(4.24) \quad \tilde{E}_\varepsilon(u_\varepsilon) = \sum_{K_\varepsilon \in \mathcal{T}_{h_\varepsilon}} \sum_{\alpha \in \tilde{I}_{K_\varepsilon}} \tilde{w}_{K_\varepsilon,\alpha} E_{\varepsilon,\alpha}(u_\varepsilon),$$

and, as previously,

$$(4.25) \quad \tilde{J}_\varepsilon(u) = \begin{cases} \tilde{E}_\varepsilon(u) & \text{if } u \in Y_\varepsilon, \\ +\infty & \text{otherwise.} \end{cases}$$

The corresponding error function is

$$(4.26) \quad G_\varepsilon(u) = \begin{cases} \tilde{E}_\varepsilon(u) - E_\varepsilon(u) & \text{if } u \in Y_\varepsilon, \\ 0 & \text{otherwise.} \end{cases}$$

In view of Theorem 4.4, the aim is now to determine conditions under which the locally uniform convergence condition (4.11) is satisfied.

We recall that the discrete differential du of a lattice field u is obtained by taking differences along the elementary atomic bonds of the lattice [4]. For present purposes, it suffices to tally differences over bonds defined by the Bravais basis vectors $(a_i, i = 1, \dots, n)$. We note that the collection of all bonds corresponding that are translates of one basis vector defines a Bravais lattice. Thus, the collection of all bonds in the lattice defines—and can be indexed as— n independent Bravais lattices. Specifically, we set

$$(4.27) \quad du(l, j) = u(l + e_j) - u(l),$$

with $l \in \mathbb{Z}^n$, $(e_j)_i = \delta_{ij}$. To each bond, we additionally assign a position

$$(4.28) \quad x(l, j) = \frac{1}{2}(x(l) + x(l + e_j)),$$

corresponding to the midpoint of the bond. The composite Bravais lattice structure of the lattice bonds enables the discrete Fourier representation of the discrete differential

$$(4.29) \quad \widehat{du}(k, j) = V \sum_{l \in \mathbb{Z}^n} e^{-ik \cdot x(l, j)} du(l, j).$$

A straightforward calculation gives, explicitly,

$$(4.30) \quad \widehat{du}(k, j) = 2 \sin \frac{k \cdot a_j}{2} \hat{u}(k).$$

We also recall that a sequence of triangulations \mathcal{T}_h of Ω is said to be *regular* if for every element $K_h \in \mathcal{T}_h$ there is a diffeomorphism $\varphi_{K_h} : \hat{K} \rightarrow K_h$ from a fixed reference domain \hat{K} and a constant σ independent of h such that

$$(4.31) \quad \|\nabla\varphi_{K_h}\|_{L^\infty(\hat{K}, \mathbb{R}^n)} \|\nabla\varphi_{K_h}^{-1}\|_{L^\infty(K_h, \mathbb{R}^n)} \leq \sigma$$

(cf., e.g., [12, 10]). For instance, if the elements in \mathcal{T}_h are affine-diffeomorphic to a reference domain \hat{K} , then we have

$$(4.32a) \quad \|\nabla\varphi_{K_h}\|_{L^\infty(\hat{K}, \mathbb{R}^n)} \leq \frac{\text{diam}(K_h)}{\rho(\hat{K})},$$

$$(4.32b) \quad \|\nabla\varphi_{K_h}^{-1}\|_{L^\infty(K_h, \mathbb{R}^n)} \leq \frac{\text{diam}(\hat{K})}{\rho(K_h)},$$

where $\rho(K) = \sup\{\text{diam}(S), S \text{ is a ball contained in } K\}$, and, therefore, \mathcal{T}_h is regular if

$$(4.33) \quad \sigma(K_h) \equiv \frac{\text{diam}(K_h)}{\rho(K_h)} \leq \sigma,$$

i.e., if the *aspect ratio* $\sigma(K_h)$ of the elements is uniformly bounded.

In order for lattice sampling within elements to be well-behaved, we additionally need to require that the local interpolants are free from fine oscillations. Indeed, the local finite-element interpolation schemes used in practice, e.g., interpolation by low-order polynomials, satisfy that property. We formalize this requirement as follows. Let \mathcal{T}_h be a triangulation of Ω . For every $K \in \mathcal{T}_h$ let $\mathcal{L}_\varepsilon(K)$ be the set of lattice coordinates $l \in \mathbb{Z}^n$ such that the bonds $(l, 1), \dots, (l, n)$ of the ε -lattice are contained in K . Let X_h be a finite-element approximation space defined on \mathcal{T}_h . We shall then say that the local interpolation is *taut* if there exist $\eta > 0$ and $C > 0$ such that

$$(4.34) \quad \|\nabla u_h\|_{L^2(K, \mathbb{R}^n)}^2 \leq V\varepsilon^{n-2} \sum_{l \in \mathcal{L}_\varepsilon(K)} \sum_{j=1}^n |du_{\varepsilon, h}(l, j)|^2$$

for every $u_h \in X_h$, $u_{\varepsilon, h}$ sampled from u_h on the ε -lattice, and $\varepsilon < \eta h$. Evidently, the tautness condition ensures that the local interpolants do not exhibit oscillations finer than an arbitrarily fine lattice, and that their gradient is controlled locally by the corresponding discrete differential over sufficiently fine lattices.

We begin with a lemma on the equivalence of discrete and continuous norms.

LEMMA 4.5. *Suppose that (X_{h_ε}) is a regular sequence of finite-element subspaces of X_0 , with $\varepsilon/h_\varepsilon \rightarrow 0$. Suppose that the local interpolation is taut. Let $u_\varepsilon \in Y_\varepsilon$ be sampled from $u_{h_\varepsilon} \in X_{h_\varepsilon}$. Then,*

$$(4.35) \quad \|\nabla u_{h_\varepsilon}\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)} \leq C \|\nabla u_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)}.$$

Proof. Let $u_\varepsilon \in Y_\varepsilon$ be sampled from $u_{h_\varepsilon} \in X_{h_\varepsilon}$ and suppose that $\varepsilon \ll h_\varepsilon$. We

have

$$\begin{aligned}
 \|\nabla u_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)}^2 &= \frac{1}{(2\pi)^n} \int_{B/\varepsilon} |\xi|^2 |\hat{u}_\varepsilon(\xi)|^2 d\xi \\
 &\geq \frac{C\varepsilon^{-2}}{(2\pi)^n} \int_{B/\varepsilon} \left(\sum_{j=1}^n 4 \sin^2 \frac{\xi \cdot (\varepsilon a_j)}{2} \right) |\hat{u}_\varepsilon(\xi)|^2 d\xi \\
 (4.36) \qquad &= V\varepsilon^{n-2} \sum_{l \in \mathbb{Z}^n} \sum_{j=1}^n |du_\varepsilon(l, j)|^2 \\
 &\geq V\varepsilon^{n-2} \sum_{K_\varepsilon \in \mathcal{T}_{h_\varepsilon}} \sum_{l \in \mathcal{L}_\varepsilon(K_\varepsilon)} \sum_{j=1}^n |du_\varepsilon(l, j)|^2.
 \end{aligned}$$

By the tautness of the local interpolation, for sufficiently large ε we have

$$\begin{aligned}
 (4.37) \qquad V\varepsilon^{n-2} \sum_{K_\varepsilon \in \mathcal{T}_{h_\varepsilon}} \sum_{l \in \mathcal{L}_{K_\varepsilon}} \sum_{j=1}^n |du_\varepsilon(l, j)|^2 \\
 \geq C \sum_{K_\varepsilon \in \mathcal{T}_{h_\varepsilon}} \|\nabla u_{h_\varepsilon}\|_{L^2(K_\varepsilon, \mathbb{R}^n)}^2 = C \|\nabla u_{h_\varepsilon}\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)},
 \end{aligned}$$

and (4.35) follows. \square

Conditions under which the locally uniform convergence condition (4.11) is satisfied by summation rules are provided by the following theorem.

THEOREM 4.6 (summation rules). *Suppose that the sequence (E_ε) of interatomic energies admits representation (4.17) in terms of translation-invariant, uniformly short-ranged nonnegative quadratic energies $E_{\varepsilon, \alpha}$ satisfying the uniform bound (4.22). Suppose that (X_{h_ε}) is a regular sequence of finite-element subspaces of X_0 , with $\varepsilon/h_\varepsilon \rightarrow 0$, and that the local interpolation is taut. Then, the sequence (4.26) of summation error functionals satisfies the locally uniform convergence condition (4.11).*

Proof. Consider an atomic cluster α . Let $\mathcal{T}_{h_\varepsilon, \alpha}$ be the collection of elements containing atoms in the cluster, and let $\Omega_{\varepsilon, \alpha} = \cup_{K_\varepsilon \in \mathcal{T}_{h_\varepsilon, \alpha}} K_\varepsilon$. Let $u_\varepsilon \in Y_\varepsilon$ be sampled from $u_{h_\varepsilon} \in X_{h_\varepsilon}$. Let $x_{\varepsilon, \alpha}$ be a reference point within the cluster. Then,

$$\begin{aligned}
 (4.38) \qquad E_{\varepsilon, \alpha}(u_\varepsilon) &\leq C\varepsilon^{n-2} \sum_{l \in \mathcal{C}_{\varepsilon, \alpha}} |u_\varepsilon(l) - u_{h_\varepsilon}(x_{\varepsilon, \alpha})|^2 \\
 &\leq C\varepsilon^{n-2} \sum_{l \in \mathcal{C}_{\varepsilon, \alpha}} |u_{h_\varepsilon}(x_\varepsilon(l)) - u_{h_\varepsilon}(x_{\varepsilon, \alpha})|^2.
 \end{aligned}$$

But, for every $l \in \mathcal{C}_{\varepsilon, \alpha}$,

$$\begin{aligned}
 (4.39) \qquad |u_{h_\varepsilon}(x_\varepsilon(l)) - u_{h_\varepsilon}(x_{\varepsilon, \alpha})| &\leq C|x_\varepsilon(l) - x_{\varepsilon, \alpha}| \|\nabla u_{h_\varepsilon}\|_{L^\infty(\Omega_{\varepsilon, \alpha}, \mathbb{R}^n)} \\
 &\leq C\varepsilon \|\nabla u_{h_\varepsilon}\|_{L^\infty(\Omega_{\varepsilon, \alpha}, \mathbb{R}^n)}.
 \end{aligned}$$

Therefore,

$$(4.40) \qquad E_{\varepsilon, \alpha}(u_\varepsilon) \leq C\varepsilon^n \|\nabla u_{h_\varepsilon}\|_{L^\infty(\Omega_{\varepsilon, \alpha}, \mathbb{R}^n)}^2.$$

But, since all norms on a finite-dimensional space are equivalent, we have

$$(4.41) \qquad \|\nabla u_{h_\varepsilon}\|_{L^\infty(\Omega_{\varepsilon, \alpha}, \mathbb{R}^n)} \leq Ch_\varepsilon^{-n/2} \|\nabla u_{h_\varepsilon}\|_{L^2(\Omega_{\varepsilon, \alpha}, \mathbb{R}^n)},$$

where, by the regularity of $\mathcal{T}_{h_\varepsilon}$ and the clusters, the constant C can be chosen independent of ε and α . Therefore,

$$(4.42) \quad E_{\varepsilon,\alpha}(u_\varepsilon) \leq C \frac{\varepsilon^n}{h_\varepsilon^n} \|\nabla u_{h_\varepsilon}\|_{L^2(\Omega_{\varepsilon,\alpha}, \mathbb{R}^n)}^2.$$

Let $\dot{I}_\varepsilon = \cup_{K_\varepsilon \in \mathcal{T}_{h_\varepsilon}} \dot{I}_{K_\varepsilon}$ be the index set of all the clusters fully contained within elements. From the fundamental property (4.23), we have

$$(4.43) \quad \tilde{E}_\varepsilon(u_\varepsilon) - E_\varepsilon(u_\varepsilon) = - \sum_{\alpha \in I_\varepsilon \setminus \dot{I}_\varepsilon} E_{\varepsilon,\alpha}(u_\varepsilon).$$

From the preceding estimates, we additionally have

$$(4.44) \quad \sum_{\alpha \in I_\varepsilon \setminus \dot{I}_\varepsilon} E_{\varepsilon,\alpha}(u_\varepsilon) \leq C \frac{\varepsilon^n}{h_\varepsilon^n} \sum_{K_\varepsilon \in \mathcal{T}_{h_\varepsilon}} N(K_\varepsilon) \|\nabla u_{h_\varepsilon}\|_{L^2(K_\varepsilon, \mathbb{R}^n)}^2,$$

where $N(K_\varepsilon)$ is the number of clusters that intersect the element K_ε and are not fully contained within it. But, appealing again to the regularity of $\mathcal{T}_{h_\varepsilon}$, we have

$$(4.45) \quad N(K_\varepsilon) \leq C \frac{h_\varepsilon^{n-1}}{\varepsilon^{n-1}}.$$

Therefore,

$$(4.46) \quad \sum_{\alpha \in I_\varepsilon \setminus \dot{I}_\varepsilon} E_{\varepsilon,\alpha}(u_\varepsilon) \leq C \frac{\varepsilon}{h_\varepsilon} \sum_{K_\varepsilon \in \mathcal{T}_{h_\varepsilon}} \|\nabla u_{h_\varepsilon}\|_{L^2(K_\varepsilon, \mathbb{R}^n)}^2 = C \frac{\varepsilon}{h_\varepsilon} \|\nabla u_{h_\varepsilon}\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)}^2$$

and

$$(4.47) \quad |\tilde{E}_\varepsilon(u_\varepsilon) - E_\varepsilon(u_\varepsilon)| \leq C \frac{\varepsilon}{h_\varepsilon} \|\nabla u_{h_\varepsilon}\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)}^2.$$

Finally, by Lemma 4.35 we have

$$(4.48) \quad |\tilde{E}_\varepsilon(u_\varepsilon) - E_\varepsilon(u_\varepsilon)| \leq C \frac{\varepsilon}{h_\varepsilon} \|\nabla u_\varepsilon\|_{L^2(\mathbb{R}^n, \mathbb{R}^n)}^2. \quad \square$$

The preceding theorem formalizes the expectation that, if the summation rule tallies exactly the energy of the interior clusters of the elements, and if the energy of the clusters is controlled by the local displacement gradient, then the summation error is concentrated over the boundaries of the elements and, therefore, becomes vanishingly small as $\varepsilon/h_\varepsilon \rightarrow 0$. Evidently, the same result should hold if the summation rules are not exact over the interior of the elements provided that the local summation errors are sufficiently small, but these extensions of the analysis will not be pursued here.

5. Numerical examples. The preceding Γ -convergence analysis sets forth necessary conditions for a quasicontinuum scheme to be admissible, in the sense of producing the right continuum limit. The analysis may thus be regarded as a first *screening test* of quasicontinuum schemes. Whereas the conditions of the convergence theorems can be verified directly on a case-by-case basis, it is nevertheless useful to formulate a numerical test that can be applied directly to implementations of particular schemes. Since the convergence test concerns the exactness of the approximation scheme when the displacement field is ostensibly affine, it may be regarded as *discrete patch test* (cf.,

e.g., [30, 65] for descriptions of the conventional patch test for finite-element analysis). As noted in section 3.1, the continuum and long-wavelength limits are equivalent up to the rescaling of the fields. We may exploit this equivalence in order to formulate a patch test that conveniently works with a fixed crystal lattice and a fixed mesh. In order to realize the long-wavelength limit of interest, we may consider a crystal in a periodic unit cell and subject to likewise periodic applied forces of increasing period. The test then consists of verifying that the resulting sequence of approximate energies approaches the limiting linear elastic energy of the crystal.

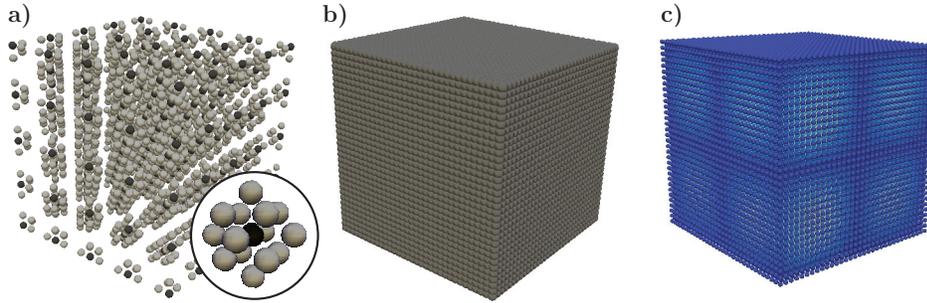


FIG. 5.1. Periodic unit cell employed in the discrete patch test. (a) Detail of the quasicontinuum model. Dark spheres represent representative atoms, light gray spheres indicate cluster atoms; the inset depicts one representative atom with its surrounding cluster atoms. (b) Fully atomistic periodic unit cell used to estimate the limiting energy E_0 . (c) Level plot of the applied forcing function $f_{\epsilon_2}(x)$.

As an example of application of the discrete patch test, we consider a defect-free three-dimensional body-centered cubic (bcc) vanadium crystal whose interatomic energy is characterized by the EAM [17], with extended Finnis–Sinclair multi-body potentials [14] for pure vanadium; see Figure 5.1. The crystal spans a cubic periodic unit cell (PUC) aligned with the cubic axes of the bcc lattice and with corners coincident with atomic positions in the undeformed lattice. The size of the PUC is $L = 40a_0$, where a_0 denotes the size of the undeformed bcc lattice, for a total of $N = 68,705$ atoms. In calculations, we consider representative atoms spaced at $h = 8a_0$, for a total of $N_h = 189$ representative atoms. The particular quasicontinuum implementation employed in calculations is based on meshfree local maximum-entropy (max-ent) interpolation [7]. We recall that the locality of the max-ent interpolation is controlled by a characteristic length $1/\sqrt{\beta}$ and that, in the limit $\beta \rightarrow \infty$, max-ent interpolation converges to piecewise affine interpolation supported on the Delaunay triangulation of the representative atoms, a scheme commonly used in early quasicontinuum implementations (cf., e.g., [59, 60]). In all calculations, we set $\beta h^2 = 0.1$. We additionally make use of an energy-based cluster-summation rule [24], with clusters centered at the representative atoms.

The PUC is subjected to the periodic forcing sequence

$$(5.1) \quad f_{\epsilon_m}(x) = \epsilon_m^2 \frac{f_0 L}{a_0} \left| \sin\left(\frac{\pi \epsilon_m x_1}{a_0}\right) \sin\left(\frac{\pi \epsilon_m x_2}{a_0}\right) \sin\left(\frac{\pi \epsilon_m x_3}{a_0}\right) \right|,$$

with $\epsilon_m = ma_0/L$ and $m = 1, \dots, L/a_0$, applied in one of the cubic directions. In calculations we set $f_0 = 0.01\text{eV}/\text{\AA}$, a forcing amplitude small enough to excite the harmonic response of the crystal only. Several elements of the forcing sequence are depicted in Figure 5.2. As is evident from the figure, the period of the forcing function $f_{\epsilon}(x)$ increases with decreasing ϵ . However, we note that the smallest value

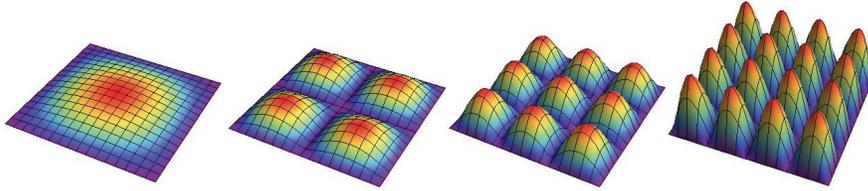


FIG. 5.2. Two-dimensional sections of the forcing functions f_{ϵ_1} , f_{ϵ_2} , f_{ϵ_3} , and f_{ϵ_4} .

of ϵ , $\epsilon_{\min} = a_0/L$, corresponding to the largest forcing period, is set by the PUC size L . Thus, the limit of interest can be approached ever more closely the larger the PUC size is, albeit at a concomitant increase in computational cost.

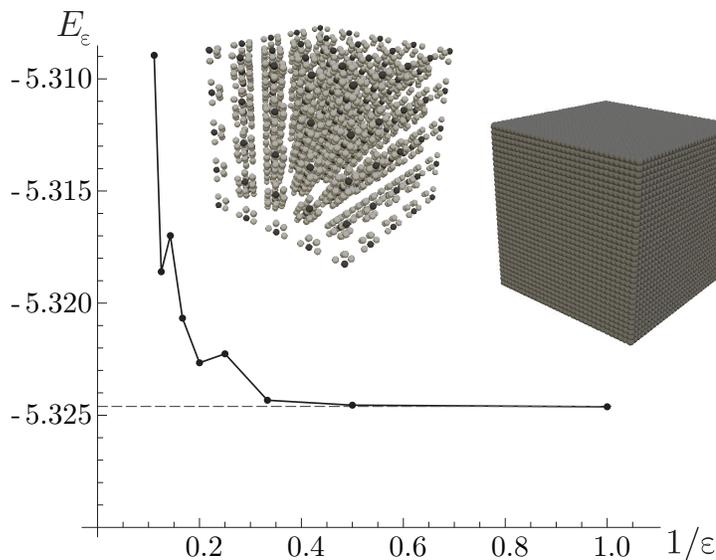


FIG. 5.3. Discrete patch test showing convergence of the approximate energies (per atom) E_ϵ towards the continuum limit E_0 .

We begin the execution of the test by estimating the limiting energy E_0 from a calculation at full atomistic resolution and $\epsilon = \epsilon_{\min}$. According to the preceding analysis, the sequence of approximate energies E_ϵ should converge to E_0 as ϵ decreases to zero. Figure 5.3 shows the sequence of approximate energies calculated using the quasicontinuum implementation, PUC and discretization size described in the foregoing. As may be seen from the figure, the approximate energies do indeed exhibit a clearly convergent trend, which in turn is suggestive of a convergent quasicontinuum scheme.

6. Summary, discussion, and concluding remarks. We have presented a Γ -convergence analysis of the quasicontinuum method focused on the behavior of the approximate energy functionals in the continuum limit. The analysis shows that, under general conditions of stability and boundedness of the energy, the continuum limit is attained provided that the finite-element spaces are strongly dense in an appropriate topology and provided that the lattice size converges to zero more rapidly than the mesh size. The equicoercivity of the quasicontinuum energy functionals is

likewise established with broad generality, which, in conjunction with Γ -convergence, ensures the convergence of the minimizers. We have also shown how summation or quadrature rules may be regarded as perturbations of the reduced fully-summed energy, or *variational crimes*. We show under rather general conditions that, for interatomic energies having a clusterwise additive structure, summation or quadrature rules that suitably approximate local element energies do not affect the continuum limit. Finally, we have proposed a discrete patch test that provides a practical means of assessing the convergence of quasicontinuum approximations, and demonstrated its utility through selected examples of application.

For definiteness, we have restricted our analysis to harmonic energies over defect-free lattices on bounded domains, whose continuum limit is linear elasticity. This particular focus has the beneficial effect of setting a simple and convenient functional framework for the analysis, namely, Sobolev spaces endowed with their strong and weak topologies, and of facilitating the characterization of the continuum limit. However, it should be carefully noted that most of the analysis makes scant or no use of the harmonicity of the energy. Indeed, a strength of Γ -convergence analysis is that it applies broadly to general classes of energies. The value of Γ -convergence as a tool for analyzing quasicontinuum approximating schemes may therefore be expected to extend well beyond harmonic crystals to general energies representing a broad range of material behaviors, including material failure and microstructure.

We also note that we have restricted our analysis to defect-free lattices and focused on the continuum limit of the energy, namely, the behavior of increasingly fine lattices deforming under a *fixed* applied force field f . In harmonic lattices, lattice defects such as dislocations can be described by the method of eigendeformations, or, equivalently, by appropriate force multipoles applied to the lattice [27, 4]. However, as the continuum limit is approached, such force multipoles scale with the lattice, in turn giving rise to a sequence of rescaled force fields f_ε . The quasicontinuum method was designed from its inception to provide adaptively full atomistic resolution near the core of defects, grain boundaries, and other structures on the scale of the lattice. Under such conditions, it is not longer possible to assume that the lattice parameter is uniformly small compared to the mesh size, with the result that the present analysis fails to apply and needs to be extended and generalized. In addition, we note that, even within the harmonic approximation, the characterization of the continuum limit of defective lattices remains a largely open problem to date.

Appendix A. The discrete Fourier transform. The ordinary Fourier transform of continuum fields is most often expressed in terms of wave-numbers. In applications concerned with the passing to the continuum, it is therefore natural to adopt a wave-number vector representation of the discrete Fourier transform. In particular, this representation ensures that the discrete and ordinary Fourier transforms of physical fields of the same kind have matching units. The wave-number representation of the discrete Fourier transform of a lattice function $f: \mathbb{Z}^n \rightarrow \mathbb{R}$ is

$$(A.1) \quad \hat{f}(k) = V \sum_{l \in \mathbb{Z}^n} f(l) e^{-ik \cdot x(l)},$$

where $x(l) = l^i a_i$ are the coordinates of the vertices of the lattice. The inverse mapping is given by

$$(A.2) \quad f(l) = \frac{1}{(2\pi)^n} \int_B \hat{f}(k) e^{ik \cdot x(l)} dk.$$

In this representation the convolution of two lattice functions f and g is

$$(A.3) \quad (f * g)(l) = V \sum_{l' \in \mathbb{Z}^n} f(l - l')g(l'),$$

and the convolution theorem states that

$$(A.4) \quad \widehat{f * g} = \hat{f}\hat{g}.$$

In addition, the Parseval identity reads

$$(A.5) \quad V \sum_{l \in \mathbb{Z}^n} f(l)g^*(l) = \frac{1}{(2\pi)^n} \int_B \hat{f}(k)\hat{g}^*(k)dk,$$

which establishes an isometric isomorphism between l^2 and $L^2(B)$.

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