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SHARP UNIFORM CONVERGENCE RATE OF THE SUPERCELL APPROXIMATION OF A CRYSTALLINE DEFECT*

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Abstract. We consider the geometry relaxation of an isolated point defect embedded in a homogeneous crystalline solid, within an atomistic description. We prove a sharp convergence rate for a periodic supercell approximation with respect to uniform convergence of the discrete strains.

Key words. crystalline defect, supercell approximation, uniform convergence

AMS subject classifications. Primary, 65N12; Secondary, 65N15, 70C20, 74E15

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1. Introduction. The high computational cost of atomistic material models requires that the numerical geometry equilibration of crystalline defects is performed in small computational cells, employing "artificial boundary conditions" to emulate the crystalline far-field behavior. Aside from the model error (due to approximations in the potential energy surface) the main simulation error is therefore the error induced by the boundary condition. In [EOS16a] a framework was introduced to rigorously estimate these errors for a variety of defects and boundary conditions, including clamped and periodic, as well as to estimate approximation errors in atomistic/continuum and QM/MM multiscale schemes [LOSK16, OLOVK18, CO17]. All of these works control the error in the canonical energy norm.

In the present work we will prove the first sharp approximation error estimate for crystal defect equilibration in the *maximum norm* for the strains in dimension greater than one (see [OS08, DLO10] for examples of results in one dimension and [LM13] for a result in three but in the absence of defects). To highlight the main ideas required for this extension in a transparent setting, we have chosen to restrict this work to point defects embedded in an infinite homogeneous host crystal, under an interatomic potential interaction. This system is approximated using a supercell method with periodic boundary conditions, the most widely used scheme for simulating point defects.

Our main motivation for this work is [BDO18], where we require a sharp uniform convergence rate to obtain sharp convergence error estimates on the vibrational entropy of a point defect, as well as [BHO], where our new results significantly simplify the development of a multipole expansion theory for crystalline defects. However, our results are also of independent interest, namely in any scenario where the defect core geometry is of importance, but not the far-field, in which case the energy norm severely overestimates the simulation error. Concretely, the best-approximation error in the maximum norm is significantly smaller than in the energy norm, and moreover, there is ample numerical evidence that the best-approximation is indeed attained.

Unsurprisingly, and similarly as for maximum-norm error estimates for numerical approximation of PDEs [RS82, Dol99], our analysis relies on ideas from elliptic

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regularity theory, specifically sharp Green's function error estimates and a discrete Caccioppoli inequality.

Notably, our analysis applies not only to energy minimizers but to general equilibria, in particular saddle points, which are important objects in studying the mobility of crystalline defects. For these general equilibria, our energy-norm error estimates are new as well.

Outline. In section 2 we formulate the geometry equilibration problem, introduce the supercell approximation, state our main convergence results, and present numerical examples demonstrating that they are indeed sharp. In section 3 we present the proofs.

2. Results. Frequently used notation. We present a short overview of frequently used notation, some of which is discussed in more detail in the following sections.

- Λ, Λ^{hom}: atomistic lattice with and without defect.
- $\mathcal{R}_\ell \subset \Lambda - \ell$ is the (finite) interaction range and $\mathcal{R}_\ell = \mathcal{R}$ is independent of ℓ away from the defect or in the homogeneous case.
- $Du(\ell)$: matrix of discrete differences of u on $\mathcal{R}_\ell$; see (2.1). We write D^h instead of D in the homogeneous case using Λ^{hom} and $\mathcal{R}$.
- $\|u\|_{\ell^p(M)} := \big(\sum_M |u|^p\big)^{1/p}$, $\|u\|_{\ell^\infty(M)} := \sup_M |u|$, for a discrete set M. $\ell^p(M)$ also denotes the corresponding space of maps.
- $\dot{\mathcal{W}}^{1,2}(\Lambda)$: space of finite-energy displacements on Λ, i.e., all $u : \Lambda \to \mathbb{R}^m$ with $\|Du\|_{\ell^2(\Lambda)} < \infty$. And for short we will use $\dot{\mathcal{W}}^{1,2} := \dot{\mathcal{W}}^{1,2}(\Lambda)$, $\ell^2 = \ell^2(\Lambda)$.
- $\dot{\mathcal{W}}^{\mathrm{c}}$, $\mathcal{W}_N^{\mathrm{per}}$: space of displacements with compact support and with $2N\mathbb{Z}^d$-periodicity, respectively.
- T_R, T_N^{per}: truncation operator used for various purposes; see (3.3).
- $S_N^{\mathrm{hom}}, S_N^{\mathrm{def}}$: operators that convert maps on the defective lattice to maps on the homogeneous lattice and vice versa; compare (3.9).

2.1. Geometry equilibration of a point defect. The reference configuration of a point defect embedded in a d-dimensional homogeneous host crystal is given by a set $\Lambda \subset \mathbb{R}^d$, satisfying

(L) There exists $R_{\mathrm{def}} > 0$, $\mathsf{A} \in \mathbb{R}^{d\times d}$ invertible, such that
$\Lambda \cap B_{R_{\mathrm{def}}}$ is finite and $\Lambda \setminus B_{R_{\mathrm{def}}} = \mathsf{A}\mathbb{Z}^d \setminus B_{R_{\mathrm{def}}}$

We assume throughout that $d \geq 2$.

A lattice displacement is a function $u : \Lambda \to \mathbb{R}^m$, where $m \geq 1$ is the range dimension, typically $m = d$. Given an interaction cutoff radius $r_{\mathrm{cut}} > 0$, the *interaction range* at site ℓ is given by

$$\mathcal{R}_\ell := \{n - \ell \,|\, n \in \Lambda\} \cap B_{r_{\mathrm{cut}}}.$$

In particular, for $\ell > r_{\mathrm{cut}} + R_{\mathrm{def}}$ this is independent of ℓ and we write $\mathcal{R}_\ell = \mathcal{R}$. The associated finite difference gradient is given by

$$Du(\ell) := \big(D_\rho u(\ell)\big)_{\rho\in\mathcal{R}_\ell} := \big(u(\ell+\rho) - u(\ell)\big)_{\rho\in\mathcal{R}_\ell}. \tag{2.1}$$

We assume r_{cut} is large enough such that $\operatorname{span}\mathcal{R}_\ell = \mathbb{R}^d$ for all $\ell \in \Lambda$ and the graph with vertices Λ and edges $\{(\ell, \ell+\rho) : \ell \in \Lambda, \rho \in \mathcal{R}_\ell\}$ is connected.

Of particular interest are compact and finite-energy displacements described, respectively, by the spaces

$$\begin{aligned} \dot{\mathcal{W}}^{\mathrm{c}} &:= \dot{\mathcal{W}}^{\mathrm{c}}(\Lambda) := \big\{u : \Lambda \to \mathbb{R}^m \,\big|\, \operatorname{supp}(Du) \text{ is compact}\big\} \qquad \text{and} \\ \dot{\mathcal{W}}^{1,2} &:= \dot{\mathcal{W}}^{1,2}(\Lambda) := \big\{u : \Lambda \to \mathbb{R}^m \,\big|\, \|Du\|_{\ell^2(\Lambda)} < \infty\big\}, \end{aligned} \tag{2.2}$$

where

$$|Du(\ell)|^2 := \sum_{\rho\in\mathcal{R}_\ell} |D_\rho u(\ell)|^2 \qquad \text{and} \qquad \|Du\|_{\ell^2(\Lambda)} := \big\| \, |Du| \big\|_{\ell^2(\Lambda)}.$$

The latter defines a seminorm on both $\dot{\mathcal{W}}^{\mathrm{c}}$ and $\dot{\mathcal{W}}^{1,2}$.

The homogeneous background lattice is $\Lambda^{\mathrm{hom}} := \mathsf{A}\mathbb{Z}^d$, which of course satisfies all foregoing conditions. Since we will frequently convert between a defective lattice Λ and the associated homogeneous lattice Λ^{hom} we denote the associated finite-difference operator by $D^{\mathrm{h}}u(\ell) = (D_\rho u(\ell))_{\rho\in\mathcal{R}}$. We will normally identify $\dot{\mathcal{W}}^{\mathrm{c}} = \dot{\mathcal{W}}^{\mathrm{c}}(\Lambda)$, $\dot{\mathcal{W}}^{1,2} = \dot{\mathcal{W}}^{1,2}(\Lambda)$ but make the domains explicit in the case of the homogeneous system, $\dot{\mathcal{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}}), \dot{\mathcal{W}}^{1,2}(\Lambda^{\mathrm{hom}})$.

For each $\ell \in \Lambda$ let $V_\ell \in C^4((\mathbb{R}^m)^{\mathcal{R}_\ell})$, with $V_\ell(0) = 0$, be the site-energy associated with the lattice site ℓ; then the total potential energy difference is given by

$$\mathcal{E}(u) := \sum_{\ell\in\Lambda} V_\ell(Du(\ell)). \tag{2.3}$$

The renormalization $V_\ell(0) = 0$ is made for the sake of simplicity of notation and signals that $\mathcal{E}$ is in fact an energy difference. We assume that the interaction is homogeneous away from the defect, i.e., $V_\ell = V$ for all $|\ell| > r_{\mathrm{cut}} + R_{\mathrm{def}}$, and that V satisfies the natural point symmetry $V(A) = V((-A_{-\rho})_{\rho\in\mathcal{R}})$ for all $A \in (\mathbb{R}^m)^{\mathcal{R}}$.

$\mathcal{E}(u)$ is a priori only defined for $u \in \dot{\mathcal{W}}^{\mathrm{c}}$ or, slightly more generally, for $u : \Lambda \to \mathbb{R}^m$ with $|Du| \in \ell^1(\Lambda)$. To define it on $\dot{\mathcal{W}}^{1,2}$, it is proven in [EOS16a, Lemma 2.1] that $\mathcal{E} : \dot{\mathcal{W}}^{\mathrm{c}} \to \mathbb{R}$ is continuous with respect to the $\|D\cdot\|_{\ell^2}$-seminorm and that there exists a unique continuous extension to $\dot{\mathcal{W}}^{1,2}$. We still call this extension $\mathcal{E}$ and remark that, according to [EOS16a, Lemma 2.1], $\mathcal{E} \in C^3(\dot{\mathcal{W}}^{1,2})$. This is only to justify our notation as we will never in fact reference the energy itself in this paper but will work directly with its first variation,

$$\langle \delta\mathcal{E}(u), v\rangle = \sum_{\ell\in\Lambda} \nabla V_\ell(Du(\ell)) \cdot Dv(\ell) \qquad \text{for } v \in \dot{\mathcal{W}}^{\mathrm{c}}.$$

We are interested in equilibrium configurations, $\delta\mathcal{E}(\bar{u}) = 0$, or written as a variational formulation,

$$\big\langle \delta\mathcal{E}(\bar{u}), v\big\rangle = 0 \qquad \forall v \in \dot{\mathcal{W}}^{1,2}. \tag{2.4}$$

We say that $u \in \dot{\mathcal{W}}^{1,2}$ is *inf-sup stable* if $\delta^2\mathcal{E}(u) : \dot{\mathcal{W}}^{1,2} \to (\dot{\mathcal{W}}^{1,2})'$ is an isomorphism which can, for example, be quantified via

$$\inf_{\substack{v\in\dot{\mathcal{W}}^{1,2}\\ \|Dv\|_{\ell^2}=1}} \ \sup_{\substack{w\in\dot{\mathcal{W}}^{1,2}\\ \|Dw\|_{\ell^2}=1}} \big\langle \delta^2\mathcal{E}(u)v, w\big\rangle > 0. \tag{2.5}$$

Of particular interest is the stability of solutions $u = \bar{u}$.

In addition, our analysis requires stability of the homogeneous background crystal, a standard assumption in solid state physics known as *phonon stability* [Wal98], which in our notation can be written as

$$\sum_{\ell\in\Lambda^{\mathrm{hom}}} \nabla^2 V(0)\left[D^{\mathrm{h}}v(\ell), D^{\mathrm{h}}v(\ell)\right] \geq c_0 \left\|D^{\mathrm{h}}v\right\|^2_{\ell^2(\Lambda^{\mathrm{hom}})} \qquad \forall v \in \dot{\mathcal{W}}^{1,2}(\Lambda^{\mathrm{hom}}) \tag{2.6}$$

for some $c_0 > 0$. We assume throughout that (2.6) holds.

Under the lattice stability assumption (2.6), it is shown in [EOS16a, Theorem 1] that any solution $\bar{u} \in \dot{\mathcal{W}}^{1,2}$ to (2.4) satisfies

$$\big|D^j \bar{u}(\ell)\big| \lesssim |\ell|^{1-d-j} \qquad \text{for } j = 1, 2, 3; \quad |\ell| \text{ sufficiently large.} \tag{2.7}$$

2.2. Supercell approximation. We consider a finite-domain approximation to (2.4) with periodic boundary conditions, which we will call the *supercell approximation.* To that end, let $\mathsf{B} = (b_1, \ldots, b_d) \in \mathbb{R}^{d\times d}$ invertible such that $b_i \in \mathsf{A}\mathbb{Z}^d$. For each $N \in \mathbb{N}$, let

$$\Lambda_N := \Lambda \cap \mathsf{B}(-N, N]^d \qquad \text{and} \qquad \Lambda_N^{\text{per}} := \bigcup_{\alpha \in 2N\mathbb{Z}^d} \big(\mathsf{B}\alpha + \Lambda_N\big).$$

Then the space of periodic displacements is given by

$$\mathcal{W}_N^{\text{per}} := \mathcal{W}_N^{\text{per}}(\Lambda_N) := \left\{u : \Lambda_N^{\text{per}} \to \mathbb{R}^m \,\middle|\, u(\ell + \mathsf{B}\alpha) = u(\ell) \text{ for } \alpha \in 2N\mathbb{Z}^d\right\}.$$

For $u \in \mathcal{W}_N^{\text{per}}$ and for N sufficiently large, the periodic potential energy approximation is given by

$$\mathcal{E}_N(u) := \sum_{\ell \in \Lambda_N} V_\ell(Du(\ell))$$

and the resulting periodic supercell approximation to (2.4) by

$$\langle \delta\mathcal{E}_N(\bar{u}_N), v\rangle = 0 \qquad \forall v \in \mathcal{W}_N^{\text{per}}. \tag{2.8}$$

2.3. Sharp uniform convergence rate. While $\mathcal{W}_N^{\text{per}} \not\subset \dot{\mathcal{W}}^{1,2}$, we can still compare $D\bar{u}$ and $D\bar{u}_N$ pointwise.

THEOREM 2.1. *Let $\bar{u} \in \dot{\mathcal{W}}^{1,2}$ be an inf-sup stable solution to* (2.4)*; then there exists a $C > 0$ such that, for N sufficiently large, there are $\bar{u}_N \in \mathcal{W}_N^{\text{per}}$ satisfying* (2.8) *as well as*

$$\|D\bar{u}_N - D\bar{u}\|_{\ell^\infty(\Lambda_N)} \le CN^{-d}.$$

Remark 2.2. Since $\#\Lambda_N \approx N^d$, applying Hölder's inequality to Theorem 2.1 we obtain, for $p' = p/(p-1)$, $\|D\bar{u}_N - D\bar{u}\|_{\ell^p(\Lambda_N)} \le CN^{-d/p'}$.

2.4. Numerical tests. We implemented two numerical tests to confirm our analysis:

1. A vacancy in bulk W (bcc crystal structure), with interaction modeled by a Finnis–Sinclair (embedded atom) potential [WZLH13].
2. A self-interstitial in bulk Cu (fcc crystal structure), with interaction modeled by Morse pair-potential $\phi(r) = (e^{-2\alpha(r-1)} - 2e^{-\alpha(r-1)})\phi_{\text{cut}}(r)$ with stiffness parameter $\alpha = 4$ and cubic spline cut-off ϕ_{cut} on the interval $[1.5, 2.3]$.

In both cases, we choose a cubic computational cell: given the lattice parameter a_0 (side-length of the unit cell in equilibrium) the matrix B in section 2.2 is given by $\mathsf{B} = a_0 I$. The resulting equilibration problem (2.8) is then solved using a preconditioned nonlinear conjugate gradient algorithm [PKM+16]. To estimate the error a numerical comparison solution was computed with $N = \lceil 2.5N_{\max}\rceil$, where $N_{\max}$ denotes the largest N chosen for the test.

The results are shown in Figures 1 and 2. Although in both cases there is a mild preasymptotic behavior visible, the numerical errors follow closely the predicted rates. Note that we did not plot the errors on Λ with respect to the $\|D\cdot\|_{\ell^1}$-seminorm since they are theoretically infinite but in practice due to the finite domain of the comparison solution appear to converge very slowly.

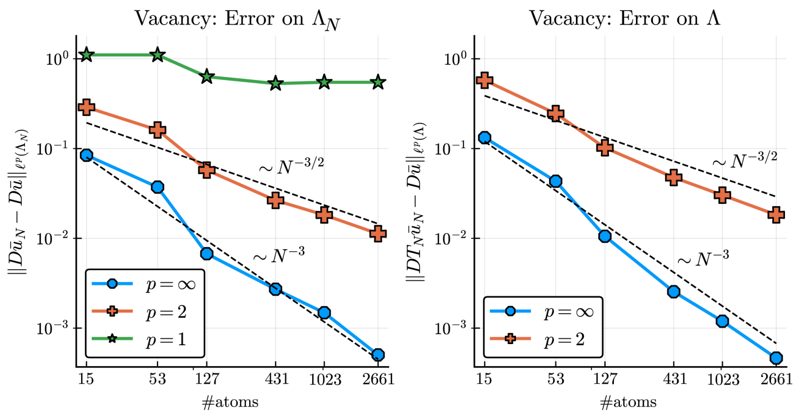

FIG. 1. *Numerical confirmation of the convergence rates predicted by Theorem* 2.1*: vacancy in bulk W (bcc), under EAM interaction.*

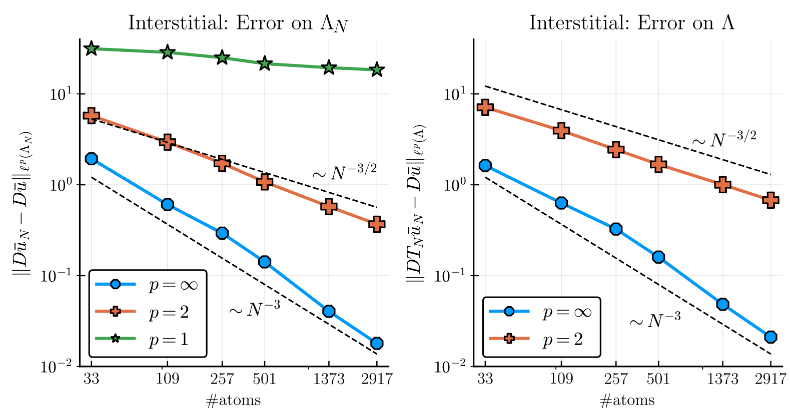

FIG. 2. *Numerical confirmation of the convergence rates predicted by Theorem* 2.1*: interstitial in bulk Cu (fcc), under Morse interaction.*

2.5. Conclusion. We haven given the first rigorous proofs of a sharp error estimate in the maximum norm (for strains) for the relaxation of a crystalline defect under artificial far-field boundary conditions.

Note that the current result is restricted to point defects with periodic boundary conditions. This simplifies one key aspect of the analysis: the sharp error estimates for the Green's function. Indeed, taking a broad view of the proof detailed in section 3, there are three fundamental ingredients in our analysis: (1) an inf-sup condition which allowed us to treat general equilibria instead of only minima; (2) a sharp error estimate for the Green's function (see Lemma 3.8); and (3) a Caccioppoli-type estimate (see Lemma 3.13). Our arguments for (1) and (3) seem to be generic and can likely be generalized to other situations, in particular to clamped boundary conditions for either point defects of dislocations. Extending our error estimate for the Green's function is likely difficult in general. However, whenever this can be achieved our results should be readily extendable.

3. Proofs. In sections 3.1–3.3, we establish auxiliary results, mostly adapting existing ideas to our setting. The proof of inf-sup stability of the periodic supercell approximation is given in section 3.4 and the proof of the sharp uniform convergence estimate in section 3.5.

3.1. Auxiliary results. An important technical tool that was used in [EOS16a] for the error analysis of the supercell approximation was a set of operators that enable us to convert functions defined in Λ to functions defined on Λ_N, and vice versa. The following results and their proofs are similar to those in [EOS16a].

Let $Q_R := \mathsf{B}(-R, R]^d$ and $\Lambda_R := \Lambda \cap Q_R$ for any $R \in \mathbb{N}$. For general $R > 0$ we define $Q_R := Q_{\lceil R \rceil}$ and $\Lambda_R = \Lambda_{\lceil R \rceil}$.

LEMMA 3.1 (discrete Poincaré inequality). *There exist $r_{\rm P}, R_{\rm P}, C_{\rm P} > 0$ such that for all $0 < R_1 < R_2$ with $R_1 \geq r_{\rm P}$, $R_2 - R_1 \geq r_{\rm P}$, $2 \leq p \leq \infty$, and $u : \Lambda_{R_2 + R_{\rm P}} \to \mathbb{R}^m$ we have*

$$\big\| u - \langle u \rangle_{\Lambda_{R_2} \setminus \Lambda_{R_1}} \big\|_{\ell^p(\Lambda_{R_2} \setminus \Lambda_{R_1})} \leq R_2 C_{\rm P} \| Du \|_{\ell^p(\Lambda_{R_2 + R_{\rm P}} \setminus \Lambda_{R_1 - R_{\rm P}})} \tag{3.1}$$

$$\textit{with} \qquad \langle u \rangle_{\Lambda'} = \frac{1}{|\Lambda'|} \sum_{\ell \in \Lambda'} u(\ell). \tag{3.2}$$

Proof. The restriction $R_1 \geq r_{\rm P}$ ensures that the defect region can be ignored. One can then apply [EOS16b, Lemma 7.1] and its proof verbatim to cubes instead of balls, which states that there exists $\tilde{a}$ such that

$$\| u - \tilde{a} \|_{\ell^2} \lesssim R_2 \| Du \|_{\ell^2(\Lambda_{R_2 + R_{\rm P}} \setminus \Lambda_{R_1 - R_{\rm P}})}.$$

Since $\tilde{a} = \langle u \rangle_{\Lambda_{R_2} \setminus \Lambda_{R_1}}$ minimizes the left-hand side, the stated result for $p = 2$ follows.

For $p = \infty$, the result is elementary. For $2 < p < \infty$ it follows from the Riesz–Thorin interpolation theorem. ∎

Let $\eta_R \in C^2(\mathbb{R}^d; [0, 1])$ be a cut-off function satisfying

- $\eta_R(x) = 1$ for $x \in Q_{4R/6}$,
- $\eta_R(x) = 0$ for $x \in \mathbb{R}^d \setminus Q_{5R/6}$,
- $|\nabla^j \eta_R| \leq C R^{-j}$ for $j = 1, 2$.

Let $A_R := \Lambda_{5R/6 + r_{\rm cut}} \setminus \Lambda_{4R/6 - r_{\rm cut}}$ be a lattice annulus; then for $u : \Lambda_R \to \mathbb{R}^m$ and $R \geq R_{\rm T} := \max\{2 r_{\rm P}, 6 R_{\rm P} + 6 r_{\rm cut}\}$ we can define the truncation $T_R u \in \dot{\mathcal{W}}^{\rm c}$ by

$$T_R u(\ell) := \begin{cases} \eta_R(\ell) \big(u(\ell) - \langle u \rangle_{A_R} \big), & \ell \in \Lambda_R, \\ 0 & \text{otherwise}. \end{cases} \tag{3.3}$$

For $R \leq N$ we can extend $T_R u$ periodically with respect to Λ_N, in which case we call it $T^{\rm per}_{N,R} u \in \mathcal{W}^{\rm per}_N$. Moreover, we set $T^{\rm per}_N := T^{\rm per}_{N,N}$. The following lemma, while formulated in terms of T_R, may also be applied to $T^{\rm per}_{N,R}$ and $T^{\rm per}_N$.

LEMMA 3.2. *There exists $C > 0$ such that, for R sufficiently large, $2 \leq p \leq \infty$, $u : \Lambda_R \to \mathbb{R}^m$,*

$$\| D T_R u \|_{\ell^p} \leq C \| Du \|_{\ell^p(\Lambda_R)}, \tag{3.4}$$

$$\| D T_R u - Du \|_{\ell^p(\Lambda_R)} \leq C \| Du \|_{\ell^p(\Lambda_R \setminus \Lambda_{R/2})}, \qquad \textit{and} \tag{3.5}$$

$$\| D^2 T_R u - D^2 u \|_{\ell^p(\Lambda_R)} \leq C \| D^2 u \|_{\ell^p(\Lambda_R \setminus \Lambda_{R/2})} + C R^{-1} \| Du \|_{\ell^2(\Lambda_R \setminus \Lambda_{R/2})}. \tag{3.6}$$

Proof. Since

$$D_\rho T_R u(\ell) = \eta_R(\ell + \rho) D_\rho u(\ell) + D_\rho \eta_R(\ell) \big(u(\ell) - \langle u \rangle_{A_R} \big),$$

we can use Lemma 3.1 and $R \geq R_{\mathrm{T}}$ to see that

$$\|DT_R u\|_{\ell^p} \lesssim \|Du\|_{\ell^p(\Lambda_R)} + \frac{1}{R}\|u - \langle u\rangle_{A_R}\|_{\ell^p(A_R)} \lesssim \|Du\|_{\ell^p(\Lambda_R)}.$$

Similarly,

$$D_\rho T_R u(\ell) - D_\rho u(\ell) = (\eta_R(\ell+\rho) - 1) D_\rho u(\ell) + D_\rho \eta_R(\ell)\big(u(\ell) - \langle u\rangle_{A_R}\big).$$

Now, $R \geq R_T$ ensures that $\eta_R(\ell+\rho) - 1 = 0$ for $\ell \in \Lambda_{R/2}$ as $R/2 + r_{\mathrm{cut}} \leq 4R/6$. Hence,

$$\|DT_R u - Du\|_{\ell^p(\Lambda_R)} \lesssim \|Du\|_{\ell^p(\Lambda_R\setminus\Lambda_{R/2})} + \frac{1}{R}\|u - \langle u\rangle_{A_R}\|_{\ell^p(A_R)} \lesssim \|Du\|_{\ell^p(\Lambda_R\setminus\Lambda_{R/2})}.$$

This establishes (3.4) and (3.5). The proof of (3.6) is analogous. ∎

As an immediate corollary of Lemma 3.2 we obtain pointwise estimates on $T_R\bar{u}$.

COROLLARY 3.3. *Let* $\bar{u} \in \dot{\mathcal{W}}^{1,2}$ *be a solution to* (2.4), *then there exists* $C > 0$ *such that for all* $R > 0, \ell \in \Lambda$ *and* $j = 1, 2$,

$$\big|D^j T_R \bar{u}(\ell)\big| \leq C(1+|\ell|)^{1-d-j}. \tag{3.7}$$

Proof. The case $j = 1$ is a straightforward consequence of (2.7) and (3.5) with $p = \infty$, where the right-hand side of (3.5) is estimated by $\|D\bar{u}\|_{\ell^\infty(\Lambda_R\setminus\Lambda_{R/2})} \lesssim (1+R/2)^{-d}$ for any R with $\ell \in \Lambda_R$. The case $j = 2$ follows from (2.7) and (3.6). ∎

3.2. The homogeneous problem. The proof of the sharp uniform convergence rates requires sharp estimates on the Green's function for the homogeneous supercell. In preparation for these, we first introduce some notation to effectively translate between the defective and homogeneous problems.

Recall from section 2 that $\Lambda^{\mathrm{hom}} = \mathsf{A}\mathbb{Z}^d$, and analogously let $\Lambda_N^{\mathrm{hom}} = Q_N \cap \Lambda^{\mathrm{hom}}$; then we define the associated potential energies by

$$\mathcal{E}^{\mathrm{hom}}(u) := \sum_{\ell\in\Lambda^{\mathrm{hom}}} V\left(D^{\mathrm{h}}u(\ell)\right) \qquad \text{and} \qquad \mathcal{E}_N^{\mathrm{hom}}(u) := \sum_{\ell\in\Lambda_N^{\mathrm{hom}}} V\left(D^{\mathrm{h}}u(\ell)\right)$$

for, respectively, $u \in \dot{\mathcal{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}})$ and $u \in \mathcal{W}_N^{\mathrm{per}}(\Lambda_N^{\mathrm{hom}})$. Of course, $\mathcal{E}^{\mathrm{hom}}, \mathcal{E}_N^{\mathrm{hom}}$ have the same regularity properties as $\mathcal{E}$, listed in section 2.1.

Moreover, phonon stability (2.6) can now be written as

$$\left\langle \delta^2\mathcal{E}^{\mathrm{hom}}(0)v, v\right\rangle \geq c_0 \left\|D^{\mathrm{h}}v\right\|^2_{\ell^2(\Lambda^{\mathrm{hom}})} \qquad \forall v \in \dot{\mathcal{W}}^{1,2}(\Lambda^{\mathrm{hom}}).$$

As a consequence there exists a *lattice Green's function.*

LEMMA 3.4. *There exists a* lattice Green's function $\mathcal{G} : \Lambda^{\mathrm{hom}} \to \mathbb{R}^{m\times m}$ *satisfying*

$$\begin{aligned} &\left\langle \delta^2\mathcal{E}^{\mathrm{hom}}(0)(\mathcal{G}e_i), v\right\rangle = v_i(0) \qquad \forall v \in \dot{\mathcal{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}}) \qquad \textit{and} \\ &\left|\left(D^{\mathrm{h}}\right)^j \mathcal{G}(\ell)\right| \leq C_j(1+|\ell|)^{2-d-j} \qquad \forall j \geq 1, \ell \in \Lambda^{\mathrm{hom}}. \end{aligned} \tag{3.8}$$

Furthermore, $\mathcal{G}(\ell) = \mathcal{G}(-\ell)$ *for all* $\ell \in \Lambda^{\mathrm{hom}}$.

Proof. The two claims in (3.8) are proven in [EOS16a, Lemma 12]. The point symmetry of $\mathcal{G}$ is an immediate consequence of the fact that the Fourier symbol satisfies $\hat{\mathcal{G}}(k) = \hat{\mathcal{G}}(-k)$. ∎

We remind the reader that the homogeneous and the defective lattice only differ on $B_{R_{\rm def}}$, i.e., $\Lambda^{\rm hom} \setminus B_{R_{\rm def}} = \Lambda \setminus B_{R_{\rm def}}$. To compare displacements u of the homogeneous and the defect problem, we can therefore define the linear operators $S_N^{\rm hom} : \mathcal{W}_N^{\rm per}(\Lambda_N) \to \mathcal{W}_N^{\rm per}(\Lambda_N^{\rm hom})$ and $S_N^{\rm def} : \mathcal{W}_N^{\rm per}(\Lambda_N^{\rm hom}) \to \mathcal{W}_N^{\rm per}(\Lambda_N)$ by fixing any $\ell_0 \in \Lambda \setminus B_{R_{\rm def}}$ and letting

$$S_N^{\rm hom} u(\ell) = \begin{cases} u(\ell), & \ell \in \Lambda^{\rm hom} \setminus B_{R_{\rm def}} \\ u(\ell_0), & \ell \in \Lambda^{\rm hom} \cap B_{R_{\rm def}} \end{cases} \qquad \text{for } u \in \mathcal{W}_N^{\rm per}(\Lambda_N), \text{ and}$$

$$S_N^{\rm def} u(\ell) = \begin{cases} u(\ell), & \ell \in \Lambda \setminus B_{R_{\rm def}} \\ u(\ell_0), & \ell \in \Lambda \cap B_{R_{\rm def}} \end{cases} \qquad \text{for } u \in \mathcal{W}_N^{\rm per}(\Lambda_N^{\rm hom}).$$

In particular, we have the following lemma as an immediate consequence of these definitions.

Lemma 3.5. *For some $R_{\rm S} \geq R_{\rm def} + r_{\rm cut}$ sufficiently large, we have $D^{\rm h} S_N^{\rm hom} u = Du$ and $D S_N^{\rm def} u = D^{\rm h} u$ for $|\ell| > R_{\rm def} + r_{\rm cut}$ as well as the estimates*

$$\big|D^{\rm h} S_N^{\rm hom} u(\ell)\big| \leq C \|Du\|_{\ell^\infty(B_{R_{\rm S}} \cap \Lambda_N)} \qquad \forall \ell \in \Lambda^{\rm hom} \cap B_{R_{\rm def}+r_{\rm cut}} \quad \textit{and}$$

$$\big|D S_N^{\rm def} u(\ell)\big| \leq C \|D^{\rm h} u\|_{\ell^\infty(B_{R_{\rm S}} \cap \Lambda_N^{\rm hom})} \qquad \forall \ell \in \Lambda \cap B_{R_{\rm def}+r_{\rm cut}}. \tag{3.9}$$

Remark 3.6. The operators $S_N^{\rm def}$ and $S_N^{\rm hom}$ are not "optimized" for practical purposes, which likely leads to poor constants in some of our estimates. However, we only use them as a technical tool in the proofs and are only concerned with rates. For specific defect structures, more natural operators $S_N^{\rm def}, S_N^{\rm hom}$ are easily constructed.

The definition and all properties in Lemma 3.5 directly translate to analogous operators $S^{\rm hom} : \dot{\mathcal{W}}^{1,2}(\Lambda) \to \dot{\mathcal{W}}^{1,2}(\Lambda^{\rm hom})$ and $S^{\rm def} : \dot{\mathcal{W}}^{1,2}(\Lambda^{\rm hom}) \to \dot{\mathcal{W}}^{1,2}(\Lambda)$ as well.

3.3. Periodic Green's function. We begin by recalling that phonon stability (2.6) also ensures the stability of the homogeneous periodic problem.

Lemma 3.7 (see [HO12, Theorem 3.6]). *For all $N > 0$ we have*

$$\big\langle \delta^2 \mathcal{E}_N^{\rm hom}(0) v, v \big\rangle \geq c_0 \|D^{\rm h} v\|^2_{\ell^2(\Lambda_N^{\rm hom})} \qquad \forall v \in \mathcal{W}_N^{\rm per}(\Lambda_N^{\rm hom}).$$

In particular, for every $f : \Lambda_N^{\rm hom} \to \mathbb{R}^m$ with $\sum_{\ell \in \Lambda_N^{\rm hom}} f(\ell) = 0$, there exists a unique $u \in \mathcal{W}_N^{\rm per}(\Lambda_N^{\rm hom})$ with $\sum_{\ell \in \Lambda_N^{\rm hom}} u(\ell) = 0$ such that

$$\big\langle \delta^2 \mathcal{E}_N^{\rm hom}(0) u, v \big\rangle = (f, v)_{\ell^2} \qquad \forall v \in \mathcal{W}_N^{\rm per}(\Lambda_N^{\rm hom}).$$

The *periodic Green's function* $\mathcal{G}_N : \Lambda_N^{\rm hom} \to \mathbb{R}^{m \times m}$ is then defined by the equation

$$\begin{aligned} \big\langle \delta^2 \mathcal{E}_N^{\rm hom}(0)(\mathcal{G}_N e_i), v \big\rangle &= v_i(0) - \frac{1}{|\Lambda_N^{\rm hom}|} \sum_{\ell \in \Lambda_N^{\rm hom}} v_i(\ell) \qquad \forall v \in \mathcal{W}_N^{\rm per}(\Lambda_N^{\rm hom}) \\ &=: \left(\delta_0 e_i - \frac{1}{|\Lambda_N^{\rm hom}|} \mathbf{1} e_i, v \right)_{\ell^2}. \end{aligned}$$

To estimate the decay of $\mathcal{G}_N$ we relate $\mathcal{G}$ and $\mathcal{G}_N$.

Lemma 3.8. *For every $j \geq 1$ there exist constants C_1, C_2, independent of N, such that*

$$\Big\| \left(D^{\rm h}\right)^j \mathcal{G} - \left(D^{\rm h}\right)^j \mathcal{G}_N \Big\|_{\ell^\infty(\Lambda_N^{\rm hom})} \leq C_1 N^{2-d-j}, \qquad \textit{and in particular}$$

$$\Big| \left(D^{\rm h}\right)^j \mathcal{G}_N(\ell) \Big| \leq C_2 \left(1 + \operatorname{dist}(\ell, 2N\mathsf{B}\mathbb{Z}^d)\right)^{2-d-j} \qquad \forall\, \ell \in \Lambda^{\rm hom}.$$

Proof. First, we note that

$$\sum_{\ell\in\Lambda^{\mathrm{hom}}} \left(D^{\mathrm{h}}\right)^j \mathcal{G}(\ell) = 0 \qquad \forall j \geq 3, \tag{3.10}$$

which is straightforward to prove due to the gradient structure. (For $j < 3$, $(D^{\mathrm{h}})^j\mathcal{G}(\ell)$ does not decay fast enough to even define this sum.)

Fix $i \in \{1, \dots, m\}$, and three interaction directions $\rho_1, \rho_2, \rho_3 \in \mathcal{R}$, and let

$$w(\ell) := \sum_{z\in\mathbb{Z}^d} D_{\rho_1}D_{\rho_2}D_{\rho_3}\mathcal{G}(\ell + 2N\mathsf{B}z)e_i \qquad \forall \ell \in \Lambda^{\mathrm{hom}}.$$

Due to the decay (3.8), the sum exists. Moreover, w is Λ_N^{hom}-periodic, satisfies

$$\left\langle \delta^2\mathcal{E}_N^{\mathrm{hom}}(0)w, v\right\rangle = (D_{\rho_1}D_{\rho_2}D_{\rho_3}\delta_0 e_i, v)_{\ell^2}$$

and according to (3.10) also $\sum_{\ell\in\Lambda_N^{\mathrm{hom}}} w(\ell) = 0$.

Since $D_{\rho_1}D_{\rho_2}D_{\rho_3}\mathcal{G}_N e_i$ solves the same equation and has average zero as well, we can therefore deduce that

$$\left(D^{\mathrm{h}}\right)^3 \mathcal{G}_N = \sum_{z\in\mathbb{Z}^d} \left(D^{\mathrm{h}}\right)^3 \mathcal{G}(\ell + 2N\mathsf{B}z).$$

Consequently, for $j \geq 3$ and $\ell \in \Lambda_N^{\mathrm{hom}}$,

$$\begin{aligned}
\left|\left(D^{\mathrm{h}}\right)^j \mathcal{G}(\ell) - \left(D^{\mathrm{h}}\right)^j \mathcal{G}_N(\ell)\right| &= \left|\sum_{z\in\mathbb{Z}^d\setminus\{0\}} \left(D^{\mathrm{h}}\right)^j \mathcal{G}(\ell + 2N\mathsf{B}z)\right| \\
&\lesssim \sum_{z\in\mathbb{Z}^d\setminus\{0\}} (1 + |\ell + 2N\mathsf{B}z|)^{2-d-j} \\
&\lesssim N^{2-d-j} \sum_{z\in\mathbb{Z}^d\setminus\{0\}} |\mathsf{B}^{-1}\ell/N + 2z|^{2-d-j} \\
&\lesssim N^{2-d-j},
\end{aligned}$$

where we used that the series converges due to $j \geq 3$ and the estimate is uniform due to the uniform lower bound $|\mathsf{B}^{-1}\ell/N + 2z| \geq 1$.

It remains to establish the estimate for $j = 1, 2$, which we will obtain from a discrete Poincaré inequality: For all $g : \Lambda_N^{\mathrm{hom}} \to \mathbb{R}^m$ we clearly have

$$|g(x) - g(y)| \leq CN \left\|D^{\mathrm{h}}g\right\|_{\ell^\infty(\Lambda_N^{\mathrm{hom}})} \qquad \forall x, y \in \Lambda_N^{\mathrm{hom}},$$

hence it immediately follows that

$$\|g - \langle g\rangle_{\Lambda_N^{\mathrm{hom}}}\|_{\ell^\infty(\Lambda_N^{\mathrm{hom}})} \leq CN \left\|D^{\mathrm{h}}g\right\|_{\ell^\infty(\Lambda_N^{\mathrm{hom}})}, \tag{3.11}$$

where $\langle g\rangle_{\Lambda_N^{\mathrm{hom}}} = |\Lambda_N^{\mathrm{hom}}|^{-1}\sum_{\ell\in\Lambda_N^{\mathrm{hom}}} g(\ell)$.

Fix $\rho, \sigma \in \mathcal{R}$ and let $K_N := \langle D_\rho D_\sigma\mathcal{G} - D_\rho D_\sigma\mathcal{G}_N\rangle_{\Lambda_N^{\mathrm{hom}}}$; then combining the estimate for $j = 3$ and (3.11) we obtain

$$\begin{aligned}
\|D_\rho D_\sigma\mathcal{G} - D_\rho D_\sigma\mathcal{G}_N\|_{\ell^\infty(\Lambda_N^{\mathrm{hom}})} &\leq \|D_\rho D_\sigma\mathcal{G} - D_\rho D_\sigma\mathcal{G}_N - K_N\|_{\ell^\infty(\Lambda_N^{\mathrm{hom}})} + |K_N| \\
&\lesssim N\|D^{\mathrm{h}}D_\rho D_\sigma\mathcal{G} - D^{\mathrm{h}}D_\rho D_\sigma\mathcal{G}_N\|_{\ell^\infty(\Lambda_N^{\mathrm{hom}})} + |K_N| \\
&\lesssim N^{-d} + \left|K_N\right|.
\end{aligned}$$

It thus remains to estimate K_N.

Periodicity of $\mathcal{G}_N$ implies that $\langle D_\rho D_\sigma \mathcal{G}_N \rangle_{\Lambda_N^{\rm hom}} = 0$, hence,

$$K_N = \left|\Lambda_N^{\rm hom}\right|^{-1} \sum_{\ell \in \Lambda_N^{\rm hom}} D_\rho D_\sigma \mathcal{G}(\ell).$$

Using discrete summation by parts we see that

$$\begin{aligned} |K_N| &= \left|\Lambda_N^{\rm hom}\right|^{-1} \left| \sum_{\ell \in (\Lambda_N^{\rm hom}+\rho)\setminus \Lambda_N^{\rm hom}} D_\sigma \mathcal{G}(\ell) - \sum_{\ell \in \Lambda_N^{\rm hom}\setminus(\Lambda_N^{\rm hom}+\rho)} D_\sigma \mathcal{G}(\ell) \right| \\ &\lesssim N^{-d} N^{d-1} N^{1-d} = N^{-d}, \end{aligned}$$

where we used $|\Lambda_N^{\rm hom} \setminus (\Lambda_N^{\rm hom}+\rho)| \lesssim N^{d-1}$ and the Green's function decay estimate (3.8). This establishes the result for $j = 2$.

To prove the estimate for $j = 1$, we can repeat the same argument on just $D_\rho \mathcal{G} - D_\rho \mathcal{G}_N$ to obtain

$$\|D_\rho \mathcal{G} - D_\rho \mathcal{G}_N\|_{\ell^\infty(\Lambda_N^{\rm hom})} \lesssim N^{1-d} + N^{-d} \left| \sum_{\ell \in \Lambda_N^{\rm hom}} D_\rho \mathcal{G}(\ell) \right|.$$

From here on, however, we need to argue differently and in particular exploit cancellations due to symmetries in the Green's function, to avoid logarithmic terms. To that end, we define the point symmetric extension

$$\Lambda_{s,N}^{\rm hom} = \Lambda^{\rm hom} \cap \mathsf{B}[-N,N]^d$$

of $\Lambda^{\rm hom}$ (i.e., $-\Lambda_{s,N}^{\rm hom} = \Lambda_{s,N}^{\rm hom}$) and use $\mathcal{G}(\ell) = \mathcal{G}(-\ell)$ to calculate

$$\begin{aligned} \left| \sum_{\ell \in \Lambda_N^{\rm hom}} D_\rho \mathcal{G}(\ell) \right| &\lesssim \left| \sum_{\ell \in \Lambda_{s,N}^{\rm hom}} D_\rho \mathcal{G}(\ell) \right| + N^{1-d} N^{d-1} \\ &= \left| \sum_{\ell \in \left(\Lambda_{s,N}^{\rm hom}+\rho\right)\setminus \Lambda_{s,N}^{\rm hom}} \mathcal{G}(\ell) - \sum_{\ell \in \Lambda_{s,N}^{\rm hom}\setminus\left(\Lambda_{s,N}^{\rm hom}+\rho\right)} \mathcal{G}(\ell) \right| + 1 \\ &= \left| \sum_{\ell \in \left(\Lambda_{s,N}^{\rm hom}+\rho\right)\setminus \Lambda_{s,N}^{\rm hom}} \mathcal{G}(-\ell) - \sum_{\ell \in \Lambda_{s,N}^{\rm hom}\setminus\left(\Lambda_{s,N}^{\rm hom}+\rho\right)} \mathcal{G}(\ell) \right| + 1 \\ &= \left| \sum_{\ell \in \left(\Lambda_{s,N}^{\rm hom}-\rho\right)\setminus \Lambda_{s,N}^{\rm hom}} \mathcal{G}(\ell) - \sum_{\ell \in \Lambda_{s,N}^{\rm hom}\setminus\left(\Lambda_{s,N}^{\rm hom}+\rho\right)} \mathcal{G}(\ell) \right| + 1 \\ &= \left| \sum_{\ell \in \left(\Lambda_{s,N}^{\rm hom}\right)\setminus\left(\Lambda_{s,N}^{\rm hom}+\rho\right)} \mathcal{G}(\ell-\rho) - \mathcal{G}(\ell) \right| + 1 \\ &\leq \sum_{\ell \in \left(\Lambda_{s,N}^{\rm hom}\right)\setminus\left(\Lambda_{s,N}^{\rm hom}+\rho\right)} |D\mathcal{G}(\ell)| + 1 \\ &\lesssim N^{d-1} N^{1-d} + 1 \\ &\lesssim 1. \end{aligned}$$

Hence, $\|D_\rho \mathcal{G} - D_\rho \mathcal{G}_N\|_{\ell^\infty(\Lambda_N^{\rm hom})} \lesssim N^{1-d}$. ∎

3.4. Inf-sup stability. The first step in the error analysis of the supercell approximation is to establish that it inherits inf-sup stability (2.5). This is a generalization of the result in [EOS16b, Theorem 7.7] that the supercell approximation inherits positivity of the Hessian operator, a more stringent notion of stability suitable only for minimizers.

In the stability analysis it is convenient to factor out constants from $\dot{\mathcal{W}}^{1,2}$ and $\mathcal{W}_N^{\rm per}$. Let $\mathcal{W}_0 \subset \dot{\mathcal{W}}^{1,2}$ and $\mathcal{W}_{N,0} \subset \mathcal{W}_N^{\rm per}$ denote the m-dimensional subspaces of all constant functions; then we define

$$\dot{W}^{1,2} := \dot{\mathcal{W}}^{1,2}/\mathcal{W}_0 \qquad \text{and} \qquad W_N^{\rm per} := \mathcal{W}_N^{\rm per}/\mathcal{W}_{N,0}.$$

The associated equivalence classes of a function $u \in \dot{\mathcal{W}}^{1,2}, \mathcal{W}_N^{\rm per}$ are denoted by $[u]$; however, whenever an expression is independent of constants, we will abuse notation and identify $[u] \equiv u$, for example, $D[u] = Du$. The inner products associated with $\dot{W}^{1,2}, W_N^{\rm per}$ are then defined by

$$(v, w)_{\dot{W}^{1,2}} = (Dv, Dw)_{\ell^2(\Lambda)} \qquad \text{and} \qquad (v, w)_{W_N^{\rm per}} = (Dv, Dw)_{\ell^2(\Lambda_N)}$$

and turn these factor spaces into Hilbert spaces.

For the proofs of the following results, recall that we made the standing assumption (2.6) that the homogeneous reference lattice is stable. Without this (standard) assumption the negative eigenspace identified in Lemma 3.9 need not be finite-dimensional, and this would make our strategy infeasible.

Lemma 3.9.

(i) *For all $u \in \dot{\mathcal{W}}^{1,2}$, there exists a subspace $\mathcal{W}_1 \subset \dot{\mathcal{W}}^{1,2}$ with finite co-dimension such that*

$$\left\langle \delta^2\mathcal{E}(u)v, v\right\rangle \geq \tfrac{1}{2}c_0\|Dv\|_{\ell^2}^2 \qquad \forall v \in \mathcal{W}_1.$$

(ii) *If, in addition, u is inf-sup stable* (2.5), *then there exists $c_1 > 0$ and an orthogonal decomposition $\dot{W}^{1,2} = W_- \oplus W_+$ with $\dim(W_-) = q$ finite and*

$$\pm\left\langle \delta^2\mathcal{E}(u)v, v\right\rangle \geq c_1\|Dv\|_{\ell^2}^2 \qquad \forall v \in W_\pm.$$

Moreover, we may choose $W_- = \operatorname{span}\{\psi_1, \ldots, \psi_q\}$, where ψ_j are eigenfunctions to negative eigenvalues of $\delta^2\mathcal{E}(u)$ in the $\dot{W}^{1,2}$ sense.

Proof.

(i) Recall that the operators $S^{\rm hom}, S^{\rm def}$ let us compare the homogeneous and the defect case by changing the displacements in $B_{R_{\rm def}}$. Let $\mathcal{W}_R := \{v \in \dot{\mathcal{W}}^{1,2} \,|\, Dv|_{B_R} = 0\}$; then for $v \in \mathcal{W}_R$, and for $R > R_{\rm def} + r_{\rm cut}$,

$$\begin{aligned}
&\left|\left\langle \delta^2\mathcal{E}(u)v, v\right\rangle - \left\langle \delta^2\mathcal{E}^{\rm hom}(0)S^{\rm hom}v, S^{\rm hom}v\right\rangle\right| \\
&\quad\lesssim \sum_{\ell \in \Lambda\setminus B_R} \left|\nabla^2 V(Du(\ell)) - \nabla^2 V(0)\right| |Dv(\ell)|^2 \\
&\quad\lesssim \|Du\|_{\ell^\infty(\Lambda\setminus B_R)}\|Dv\|_{\ell^2}^2 \lesssim \epsilon_R\|Dv\|_{\ell^2}^2,
\end{aligned}$$

where $\epsilon_R \to 0$ as $R \to \infty$ since $Du \in \ell^2$. Phonon stability (2.6) then implies that, for R sufficiently large,

$$\left\langle \delta^2\mathcal{E}(u)v, v\right\rangle \geq \tfrac{1}{2}c_0\|Dv\|_{\ell^2}^2.$$

Since the co-dimension of $\mathcal{W}_R$ is finite, statement (i) follows with $\mathcal{W}_1 = \mathcal{W}_R$.

(ii) Since $\delta^2\mathcal{E}(u)$ is a symmetric, continuous bilinear map on $\dot{W}^{1,2}$, there is a unique linear, self-adjoint, bounded operator $A(u)\in L(\dot{W}^{1,2})$ with $\langle\delta^2\mathcal{E}(u)v,w\rangle = (A(u)v,w)_{\dot{W}^{1,2}}$ for all $v,w \in \dot{W}^{1,2}$. Inf-sup stability (2.5) implies that $A(u)$ is an isomorphism. Thus, the spectrum of $A(u)$ is real, bounded, and bounded away from 0. In light of (i), the spectral subspace of the negative part of the spectrum is finite dimensional. The negative part of the spectrum thus consists of only finitely many eigenvalues (with multiplicity) $\lambda_1 \leq \cdots \leq \lambda_q$ and associated orthonormal eigenfunctions ψ_j, $1 \leq j \leq q$. Define $\mathcal{W}_- := \operatorname{span}\{\psi_1,\ldots,\psi_q\}$ to be that spectral subspace and $\mathcal{W}_+$ the orthogonal complement of $\mathcal{W}_-$; then (ii) follows. ∎

LEMMA 3.10. *Suppose that $u \in \dot{\mathcal{W}}^{1,2}$ is inf-sup stable* (2.5)*; then, for N sufficiently large,*

$$\inf_{\substack{v\in\mathcal{W}_N^{\rm per}\\ \|Dv\|_{\ell^2}=1}} \sup_{\substack{w\in\mathcal{W}_N^{\rm per}\\ \|Dw\|_{\ell^2}=1}} \left\langle \delta^2\mathcal{E}_N(T_N^{\rm per}u)v,w\right\rangle \geq \min(c_0/8, c_1/4), \tag{3.12}$$

where $T_N^{\rm per}$ is the truncation operator introduced and discussed in (3.3) *and thereafter.*

Proof. Let $u_N = T_N^{\rm per}u$, $H_N := \delta^2\mathcal{E}_N(u_N)$, and $H := \delta^2\mathcal{E}(u)$. We will consider the orthogonal decomposition $W_N^{\rm per} = W_{N,+}\oplus W_{N,-}$, where

$$W_{N,-} = \operatorname{span}\left\{T_{N,N/2}^{\rm per}\psi_j \,|\, j=1,\ldots,q\right\}$$

with ψ_j the negative eigenfunctions of H (cf. Lemma 3.9(ii)) and $W_{N,+}$ its orthogonal complement. We will prove that H_N is uniformly positive on $W_{N,+}$ and uniformly negative on $W_{N,-}$, which implies the stated inf-sup condition (3.12).

If $v_N \in W_{N,-}$, then $v_N = T_{N,N/2}^{\rm per}v$ for some $v \in W_-$. In particular, $Dv_N(\ell) = 0$ for $\ell \in \Lambda_N\setminus\Lambda_{N/2}$ and since also $Du_N(\ell) = Du(\ell)$ for all $\ell\in\Lambda_{N/2}$ we obtain

$$\begin{aligned}
\left\langle H_N T_{N,N/2}^{\rm per}v, T_{N,N/2}^{\rm per}v\right\rangle &= \sum_{\ell\in\Lambda_{N/2}} \nabla^2 V_\ell(Du_N(\ell))\left[DT_{N,N/2}^{\rm per}v, DT_{N,N/2}^{\rm per}v\right]\\
&= \sum_{\ell\in\Lambda_{N/2}} \nabla^2 V_\ell(Du(\ell))\big[DT_{N/2}v, DT_{N/2}v\big]\\
&= \big\langle HT_{N/2}v, T_{N/2}v\big\rangle\\
&= \big\langle Hv,v\big\rangle + \big\langle H\big(T_{N/2}v+v\big), T_{N/2}v - v\big\rangle\\
&\leq -c_1\|v\|^2_{\dot{W}^{1,2}} + C\|v\|_{\dot{W}^{1,2}}\|T_{N/2}v-v\|_{\dot{W}^{1,2}}.
\end{aligned}$$

Since $\|T_{N/2}\psi_j - \psi_j\|_{\dot{W}^{1,2}} \to 0$ for all $1\leq j\leq q$, for a given ϵ we obtain $\|T_{N/2}v - v\|_{\dot{W}^{1,2}} \leq \epsilon\|v\|_{\dot{W}^{1,2}}$ for all N large enough uniformly in $v\in W_-$. For ϵ small enough,

$$\langle H_N v_N, v_N\rangle \leq (-c_1 + C\epsilon)\|v\|^2_{\dot{W}^{1,2}} \leq \frac{-c_1+C\epsilon}{(1+\epsilon)^2}\|v_N\|^2_{W^{\rm per}} \leq -c_1/2\|v_N\|^2_{W^{\rm per}}. \tag{3.13}$$

Next we prove uniform positivity of H_N on $W_{N,+}$, the complement of $W_{N,-}$. This is a straightforward variation of the argument when $W_{N,-}=\{0\}$ treated in [EOS16b, Theorem 7.7]. First, we take an increasing sequence N_k such that

$$\lim_{k\to\infty} \min_{\substack{v\in W_{N_k,+}\\ \|v\|_{W_{N_k}^{\rm per}}=1}} \langle H_{N_k}v,v\rangle = \liminf_{N\to\infty} \min_{\substack{v\in W_{N,+}\\ \|v\|_{W_N^{\rm per}}=1}} \langle H_N v,v\rangle$$

and then choose

$$v_k \in \arg \min_{\substack{v \in W_{N_k,+} \\ \|v\|_{W^{\rm per}_{N_k}}=1}} \langle H_{N_k} v, v \rangle.$$

Next, we want to choose a second sequence $R_k \uparrow \infty$, $R_k \leq N_k/4$, and decompose

$$v_k = a_k + b_k := T^{\rm per}_{N_k,R_k} v_k + \left(I - T^{\rm per}_{N_k,R_k}\right) v_k.$$

According to [EOS16b, Lemma 7.8] and [EOS16b, Proof of Theorem 7.7], one can find a subsequence of $(N_k)_{k\in\mathbb{N}}$ (not relabeled) and $R_k \uparrow \infty$ sufficiently slowly such that

$$\langle H_{N_k} a_k, b_k \rangle \to 0 \qquad \text{and} \qquad (D_\rho a_k, D_\sigma b_k)_{\ell^2(\Lambda_{N_k})} \to 0 \qquad \text{as } k \to \infty \tag{3.14}$$

for all $\rho, \sigma \in \mathcal{R}$. We split

$$\langle H_{N_k} v_k, v_k \rangle = \langle H_{N_k} a_k, a_k \rangle + 2\langle H_{N_k} a_k, b_k \rangle + \langle H_{N_k} b_k, b_k \rangle.$$

According to (3.14), the cross-term vanishes in the limit, $\langle H_{N_k} a_k, b_k \rangle \to 0$.

Since the support of Db_k does not intersect the defective region it is easy to see that

$$\langle H_{N_k} b_k, b_k \rangle = \left\langle \delta^2 \mathcal{E}^{\rm hom}_{N_k}(u^{\rm hom}_{N_k}) S^{\rm hom}_{N_k} b_k, S^{\rm hom}_{N_k} b_k \right\rangle,$$

where $u^{\rm hom}_{N_k} := S^{\rm hom}_{N_k} u_{N_k}$. Next, we observe that

$$\begin{aligned}
&\left|\left\langle \left[\delta^2 \mathcal{E}^{\rm hom}_{N_k}\left(u^{\rm hom}_{N_k}\right) - \delta^2 \mathcal{E}^{\rm hom}_{N_k}(0)\right] S^{\rm hom}_{N_k} b_k, S^{\rm hom}_{N_k} b_k \right\rangle\right| \\
&= \left| \sum_{\ell \in \Lambda^{\rm hom}_{N_k} \setminus \Lambda^{\rm hom}_{R_k/2}} \left(\nabla^2 V(Du^{\rm hom}_{N_k}(\ell)) - \nabla^2 V(0)\right) \left[DS^{\rm hom}_{N_k} b_k(\ell), DS^{\rm hom}_{N_k} b_k(\ell)\right] \right| \\
&\lesssim \epsilon_k \|DS^{\rm hom}_{N_k} b_k\|^2_{\ell^2\left(\Lambda^{\rm per,hom}_{N_k}\right)} \\
&\lesssim \epsilon_k \|b_k\|^2_{W^{\rm per}_{N_k}},
\end{aligned}$$

where, according to (3.5),

$$\begin{aligned}
\epsilon_k &:= \max_{\ell \in \Lambda^{\rm hom}_{N_k} \setminus \Lambda^{\rm hom}_{R_k/2}} \left| D^{\rm h} u^{\rm hom}_{N_k}(\ell) \right| \\
&= \max_{\ell \in \Lambda_{N_k} \setminus \Lambda_{R_k/2}} \left| DT_{N_k} u(\ell) \right| \\
&\leq \|DT_{N_k} u\|_{\ell^2(\Lambda_{N_k} \setminus \Lambda_{R_k/2})} \\
&\leq \|Du\|_{\ell^2(\Lambda_{N_k} \setminus \Lambda_{R_k/2})} + \|DT_{N_k} u - Du\|_{\ell^2(\Lambda_{N_k})} \\
&\lesssim \|Du\|_{\ell^2(\Lambda_{N_k} \setminus \Lambda_{R_k/2})} \\
&\to 0 \quad \text{ as } k \to \infty.
\end{aligned}$$

In particular, using Lemma 3.7, we obtain

$$\begin{aligned}
\langle H_{N_k} b_k, b_k \rangle &\geq \left\langle \delta^2 \mathcal{E}^{\rm hom}_{N_k}(0) S^{\rm hom}_{N_k} b_k, S^{\rm hom}_{N_k} b_k \right\rangle - C\epsilon_k \|b_k\|^2_{W^{\rm per}_{N_k}} \\
&\geq (c_0 - C\epsilon_k) \|b_k\|^2_{W^{\rm per}_{N_k}} \geq c_0/2 \|b_k\|^2_{W^{\rm per}_{N_k}}
\end{aligned} \tag{3.15}$$

for k sufficienty large.

Finally, since Da_k are supported in $\Lambda_{N_k/4}$ we have

$$\begin{aligned}(T_{N_k}a_k, \psi_j)_{\dot{W}^{1,2}} &= \Big(a_k, T^{\rm per}_{N_k,N_k/2}\psi_j\Big)_{W^{\rm per}_{N_k}} + \big(T_{N_k}a_k, (I - T_{N_k/2})\psi_j\big)_{\dot{W}^{1,2}} \\ &= \Big(v_k, T^{\rm per}_{N_k,N_k/2}\psi_j\Big)_{W^{\rm per}_{N_k}} - \Big(b_k, T^{\rm per}_{N_k,N_k/2}\psi_j\Big)_{W^{\rm per}_{N_k}} + 0 \\ &= -\Big(b_k, T^{\rm per}_{N_k,N_k/2}\psi_j\Big)_{W^{\rm per}_{N_k}}.\end{aligned}$$

Hence, for all $j = 1, \ldots, q$,

$$\begin{aligned}|(T_{N_k}a_k, \psi_j)_{\dot{W}^{1,2}}| &= \left|\Big(b_k, T^{\rm per}_{N_k,N_k/2}\psi_j\Big)_{W^{\rm per}_{N_k}}\right| \\ &\lesssim \max_j \|D\psi_j\|_{\ell^2(\Lambda_{N_k}\setminus\Lambda_{R_k/2})} =: \gamma_k \to 0.\end{aligned}$$

Writing $T_{N_k}a_k = a_k^+ + a_k^-$ with $a_k^\pm \in W_\pm$, Lemma 3.9(ii) implies

$$\langle H_{N_k}a_k, a_k\rangle = \langle HT_{N_k}a_k, T_{N_k}a_k\rangle \geq c_1\|a_k^+\|^2_{\dot{W}^{1,2}} - C\|a_k^-\|^2_{\dot{W}^{1,2}} \geq c_1\|a_k\|^2_{W^{\rm per}_{N_k}} - C\gamma_k. \tag{3.16}$$

In summary, combining (3.16) with (3.15) and recalling again (3.14) we conclude that, for k sufficiently large,

$$\begin{aligned}\inf_{\substack{v\in W_{N_k,+}\\ \|v\|_{W^{\rm per}_{N_k}}=1}} \langle H_{N_k}v, v\rangle &= \langle H_{N_k}v_k, v_k\rangle \\ &\geq \min(c_0/2, c_1)\Big(\|a_k\|^2_{W^{\rm per}_{N_k}} + \|b_k\|^2_{W^{\rm per}_{N_k}}\Big) - C\gamma_k \\ &= \min(c_0/2, c_1)\|v_k\|^2_{W^{\rm per}_{N_k}} - 2\min(c_0/2, c_1)\,(a_k, b_k)_{W^{\rm per}_{N_k}} - C\gamma_k \\ &\geq \min(c_0/4, c_1/2).\end{aligned}$$

Due to the choice of the N_k, this means that for all N large enough,

$$\inf_{\substack{v\in W_{N,+}\\ \|v\|_{W^{\rm per}_{N}}=1}} \langle H_N v, v\rangle \geq \min(c_0/8, c_1/4). \qquad \square$$

As an immediate corollary of the inf-sup stability of the supercell approximation we obtain a convergence result in the energy norm.

THEOREM 3.11. *Let $\bar{u} \in \dot{\mathcal{W}}^{1,2}$ be an inf-sup stable solution to* (2.4)*; then, for N sufficiently large, there are $\bar{u}_N \in \mathcal{W}^{\rm per}_N$ satisfying* (2.8) *as well as*

$$\big\|D\bar{u}_N - DT^{\rm per}_N\bar{u}\big\|_{\ell^2} \lesssim N^{-d/2}.$$

Proof. The proof of this result is identical to that of [EOS16a, Theorem 2.6], replacing positivity of $\delta^2\mathcal{E}_N(T^{\rm per}_N\bar{u})$ with the new inf-sup stability result provided by Lemma 3.10. $\square$

3.5. Uniform convergence. Let $\bar{u} \in \dot{\mathcal{W}}^{1,2}$ be an inf-sup stable solution to (2.4). According to Theorem 3.11, there exists $\bar{u}_N \in \mathcal{W}^{\rm per}_N$ solving (2.8) and satisfying

$$\|D\bar{u} - D\bar{u}_N\|_{\ell^2} \lesssim N^{-d/2},$$

where we combined the truncation estimate (3.5) with the decay estimate (2.7) to see

$$\|D\bar{u} - DT^{\rm per}_N\bar{u}\|_{\ell^2(\Lambda)} \lesssim \|D\bar{u}\|_{\ell^2(\Lambda\setminus\Lambda_{N/2})} \lesssim N^{-d/2}.$$

Throughout the remainder of this section, we fix $\bar{u}$ and the sequences $\bar{u}_N$, as well as $v_N := T_N^{\rm per}\bar{u}, \bar{u}_N^{\rm hom} := S_N^{\rm hom}\bar{u}_N, v_N^{\rm hom} := S_N^{\rm hom} v_N$,

$$e_N := \bar{u}_N - v_N, \qquad \text{and} \qquad e_N^{\rm hom} := \bar{u}_N^{\rm hom} - v_N^{\rm hom}.$$

In particular we will also assume implicitly that N is sufficiently large so that the existence of $\bar{u}_N$ is guaranteed. We will prove a uniform convergence rate for e_N, from which Theorem 2.1 will readily follow.

Recall from the definition of $T_N^{\rm per}$ and from Corollary 3.3 that

$$\begin{aligned} Dv_N &= D\bar{u} \quad \text{in } \Lambda_{N/2} \qquad \text{and} \\ |D^j v_N| &\lesssim N^{1-d-j} \quad \text{in } \Lambda_N \setminus \Lambda_{N/3}, \quad j = 1, 2. \end{aligned} \tag{3.17}$$

First, we use our Green's function estimates to obtain an implicit estimate for De_N.

LEMMA 3.12. *There exist $r_0, C_1 > 0$ such that for all $\ell \in \Lambda_N \setminus \Lambda_{r_0}$*

$$|De_N(\ell)| \le C_1 \left(N^{-d} + \sum_{m \in \Lambda_N} \left(\text{dist}\left(\ell - m, 2N\mathsf{B}\mathbb{Z}^d\right) + 1\right)^{-d} (1 + |m|)^{-d} |De_N(m)| \right).$$

Proof. Let

$$\begin{aligned} \sigma_N^{\rm hom}(\ell) &:= \left(\nabla V\left(D^{\rm h}\bar{u}_N^{\rm hom}(\ell)\right) - \nabla V\left(D^{\rm h} v_N^{\rm hom}(\ell)\right)\right) \chi_{B_{R_{\rm def}+r_{\rm cut}}}(\ell), \\ \sigma_N^{\rm def}(\ell) &:= \left(\nabla V_\ell(D\bar{u}_N(\ell)) - \nabla V_\ell(Dv_N(\ell))\right)\chi_{R_{\rm def}+r_{\rm cut}}(\ell), \\ f_N^{\rm bdry}(\ell) &:= -\mathrm{Div}\nabla V_\ell(Dv_N(\ell)) \\ &:= \sum_{\rho \in -\mathcal{R}_\ell} \nabla_{D_\rho} V_{\ell-\rho}(Dv_N(\ell - \rho)) - \sum_{\rho \in \mathcal{R}_\ell} \nabla_{D_\rho} V_\ell(Dv_N(\ell)), \end{aligned}$$

where $\nabla_{D_\rho} V_\ell(Du(\ell)) = \partial V_\ell(Du(\ell))/\partial D_\rho u(\ell)$.

A straightforward algebraic manipulation then shows that, for $w \in \mathcal{W}_N^{\rm per}(\Lambda_N^{\rm hom})$,

$$\begin{aligned} &\left\langle \delta\mathcal{E}_N^{\rm hom}\left(\bar{u}_N^{\rm hom}\right) - \delta\mathcal{E}_N^{\rm hom}\left(v_N^{\rm hom}\right), w\right\rangle \\ &\quad = \left(\sigma_N^{\rm hom}, Dw\right)_{\ell^2(\Lambda_N^{\rm hom})} - \left(\sigma_N^{\rm def}, DS_N^{\rm def} w\right)_{\ell^2(\Lambda_N)} - \left(f_N^{\rm bdry}, S_N^{\rm def} w\right)_{\ell^2(\Lambda_N)}. \end{aligned}$$

Furthermore, for $N \ge 6r_{\rm cut}$, it is straightforward to establish that

$$\left|\sigma_N^{\rm hom}(\ell)\right| \lesssim \left|D^{\rm h} e_N^{\rm hom}(\ell)\right| \qquad \forall \ell \in \Lambda_N^{\rm hom} \cap B_{R_{\rm def}+r_{\rm cut}}, \tag{3.18}$$

$$\left|\sigma_N^{\rm def}(\ell)\right| \lesssim |De_N(\ell)| \qquad \forall \ell \in \Lambda_N \cap B_{R_{\rm def}+r_{\rm cut}}, \qquad \text{and} \tag{3.19}$$

$$\left|f_N^{\rm bdry}(\ell)\right| \lesssim \begin{cases} 0, & \ell \in \Lambda_{N/3}, \\ N^{-d-1}, & \ell \in \Lambda_N \setminus \Lambda_{N/3}. \end{cases} \tag{3.20}$$

The first two estimates follow simply from the fact that $V, V_\ell \in C^4$, while (3.20) follows from the second-order difference structure of $f_N^{\rm bdry}(\ell)$ and (3.17).

Furthermore, Taylor expansions of $\delta\mathcal{E}_N^{\rm hom}(\bar{u}_N^{\rm hom})$ and $\delta\mathcal{E}_N^{\rm hom}(v_N^{\rm hom})$ about 0 and some elementary manipulations yield

$$
\begin{aligned}
&\left\langle \delta\mathcal{E}_N^{\mathrm{hom}}\left(\bar{u}_N^{\mathrm{hom}}\right) - \delta\mathcal{E}_N^{\mathrm{hom}}\left(v_N^{\mathrm{hom}}\right), w\right\rangle \\
&\quad = \left\langle \delta^2\mathcal{E}_N^{\mathrm{hom}}(0)e_N^{\mathrm{hom}}, w\right\rangle + \int_0^1 \left\langle \left[\delta^2\mathcal{E}_N^{\mathrm{hom}}\left(tv_N^{\mathrm{hom}}\right) - \delta^2\mathcal{E}_N^{\mathrm{hom}}(0)\right] e_N^{\mathrm{hom}}, w\right\rangle\, dt \\
&\qquad\qquad\qquad\qquad + \int_0^1 \left\langle \left[\delta^2\mathcal{E}_N^{\mathrm{hom}}\left(t\bar{u}_N^{\mathrm{hom}}\right) - \delta^2\mathcal{E}_N^{\mathrm{hom}}\left(tv_N^{\mathrm{hom}}\right)\right] u_N^{\mathrm{hom}}, w\right\rangle\, dt \\
&\quad = \left\langle \delta^2\mathcal{E}_N^{\mathrm{hom}}(0)e_N^{\mathrm{hom}}, w\right\rangle \\
&\qquad + \int_0^1\int_0^t \left\langle \left[\delta^3\mathcal{E}_N^{\mathrm{hom}}\left(sv_N^{\mathrm{hom}}\right) e_N^{\mathrm{hom}}, v_N^{\mathrm{hom}}, w\right\rangle\, dt\, ds \\
&\qquad + \int_0^1\int_0^t \left\langle \delta^3\mathcal{E}_N^{\mathrm{hom}}\left((t-s)v_N^{\mathrm{hom}} + s\bar{u}_N^{\mathrm{hom}}\right) e_N^{\mathrm{hom}}, e_N^{\mathrm{hom}} + v_N^{\mathrm{hom}}, w\right\rangle\, dt\, ds.
\end{aligned}
$$

We test with $w(n) = D^{\mathrm{h}} G_N(n-\ell)$, then

$$
\left|\left(D^{\mathrm{h}}\right)^j w(n)\right| \lesssim \left(\mathrm{dist}\left(\ell - m, 2N\mathsf{B}\mathbb{Z}^d\right) + 1\right)^{1-d-j}, \tag{3.21}
$$

hence, for $|\ell| > R_{\mathrm{def}} + r_{\mathrm{cut}}$, we obtain

$$
\begin{aligned}
|De_N(\ell)| &= \left|D^{\mathrm{h}} e_N^{\mathrm{hom}}(\ell)\right| = \left\langle \delta^2\mathcal{E}_N^{\mathrm{hom}}(0)(\bar{u}_N^{\mathrm{hom}} - v_N^{\mathrm{hom}}), w\right\rangle \\
&\lesssim \left|\left(\sigma_N^{\mathrm{hom}}, D^{\mathrm{h}} w\right)_{\ell^2(\Lambda_N^{\mathrm{hom}})}\right| + \left|\left(\sigma_N^{\mathrm{def}}, DS_N^{\mathrm{def}} w\right)_{\ell^2(\Lambda_N)}\right| + \left|\left(f_N^{\mathrm{bdry}}, S_N^{\mathrm{def}} w\right)_{\ell^2(\Lambda_N)}\right| \\
&\quad + \sum_{m\in\Lambda_N^{\mathrm{hom}}} \left|De_N^{\mathrm{hom}}(m)\right|^2 |Dw(n)| \\
&\quad + \sum_{m\in\Lambda_N^{\mathrm{hom}}} \left|De_N^{\mathrm{hom}}(m)\right| |Dw(m)|\, \left|Dv_N^{\mathrm{hom}}(m)\right| \\
&=: \mathrm{T}_1 + \mathrm{T}_2 + \mathrm{T}_3 + \mathrm{T}_4 + \mathrm{T}_5.
\end{aligned}
$$

The fifth term is already of the form we require: We can employ (3.21) to bound Dw and (3.17) to bound Dv_N^{hom}. Furthermore, we use Lemma 3.5 to bound De_N^{hom} by De_N to arrive at

$$
\mathrm{T}_5 \lesssim \sum_{m\in\Lambda_N^{\mathrm{hom}}} |De_N(m)| \left(\mathrm{dist}(\ell - m, 2N\mathsf{B}\mathbb{Z}^d) + 1\right)^{-d} (1+|m|)^{-d}
$$

for $|\ell| > 2R_{\mathrm{S}}$. Using (3.20) in combination with (3.21), as well as using $\|De_N^{\mathrm{hom}}\|_{\ell^2} \le N^{-d/2}$, we get $\mathrm{T}_3 + \mathrm{T}_4 \lesssim N^{-d}$. Finally, for T_1 and T_2 and again $|\ell| > 2R_{\mathrm{S}}$, we use (3.18) and (3.19) to estimate

$$
\begin{aligned}
\mathrm{T}_1 + \mathrm{T}_2 &\lesssim \sum_{m\in\Lambda_N^{\mathrm{hom}}\cap B_{R_{\mathrm{S}}}} |D^{\mathrm{h}} e_N^{\mathrm{hom}}(m)||D^2\mathcal{G}(\ell - m)| + \sum_{m\in\Lambda_N\cap B_{R_{\mathrm{S}}}} |De_N(m)||DS^{\mathrm{def}} D^{\mathrm{h}}\mathcal{G}(\ell - m)| \\
&\lesssim \sum_{k\in\Lambda_N^{\mathrm{hom}}\cap B_{R_{\mathrm{S}}}} \sum_{m\in\Lambda_N\cap B_{R_{\mathrm{S}}}} |De_N(m)||D^2\mathcal{G}(\ell - k)| \\
&\lesssim \sum_{m\in\Lambda_N^{\mathrm{hom}}\cap B_{R_{\mathrm{S}}}} |De_N(m)|\left(\mathrm{dist}(\ell - m, 2N\mathsf{B}\mathbb{Z}^d) + 1\right)^{-d}.
\end{aligned}
$$

∎

Next, we prove a discrete Caccioppoli estimate.

LEMMA 3.13. *There exist $r_1, C_2 > 0$ such that, for $r_1 \le r \le N/4$,*

$$\|De_N\|_{\ell^2(\Lambda_{r/2})} \le C_2 \|De_N\|_{\ell^2(\Lambda_{2r}\setminus\Lambda_{r/2})}.$$

Proof. Inf-sup stability of v_N established in Lemma 3.10 and the convergence $\|De_N\|_{\ell^2} \to 0$ (cf. Theorem 3.11) imply that there exists $c_1 > 0$ such that, for all N sufficiently large,

$$\sup_{\substack{w\in\mathcal{W}_N^{\rm per} \\ \|Dw\|_{\ell^2}=1}} \int_0^1 \big\langle \delta^2\mathcal{E}_N(v_N + te_N)z, w\big\rangle \, dt \ge c_1 \|Dz\|_{\ell^2} \qquad \forall z \in \mathcal{W}_N^{\rm per}.$$

In the rest of this proof we will write $\sup_w = \sup_{w\in\mathcal{W}_N^{\rm per}, \|Dw\|_{\ell^2}=1}$. Fix $r > 0$ and insert $z = T_{N,r}^{\rm per} e_N$ in the inf-sup condition; then we can use the fact that the supports of Dz and $D(I - T_{N,2r}^{\rm per})w$ do not overlap to write

$$\begin{aligned}
\|Dz\|_{\ell^2} &\lesssim \sup_w \int_0^1 \big\langle \delta^2\mathcal{E}_N(v_N + te_N)z, w\big\rangle \, dt \\
&= \sup_w \int_0^1 \Big\langle \delta^2\mathcal{E}_N(v_N + te_N)z, T_{N,2r}^{\rm per} w\Big\rangle \, dt \\
&= \sup_w \bigg(\int_0^1 \Big\langle \delta^2\mathcal{E}_N(v_N + te_N)(T_{N,r}^{\rm per} - I)e_N, T_{N,2r}^{\rm per} w\Big\rangle \, dt \\
&\qquad\qquad + \Big\langle \delta\mathcal{E}_N(\bar u_N) - \delta\mathcal{E}_N(v_N), T_{N,2r}^{\rm per} w\Big\rangle \bigg).
\end{aligned}$$

We clearly have $\langle \delta\mathcal{E}_N(\bar u_N), T_{N,2r}^{\rm per} w\rangle = 0$. Moreover,

$$\begin{aligned}
\big\langle \delta\mathcal{E}_N(v_N), T_{N,2r}^{\rm per} w\big\rangle &= \sum_{\ell\in\Lambda_{2r}} \nabla V_\ell(Dv_N(\ell)) \Big[DT_{N,2r}^{\rm per} w\Big] \\
&= \sum_{\ell\in\Lambda_{2r}} \nabla V_\ell(D\bar u(\ell)) \big[DT_{2r} w\big] \\
&= \big\langle \delta\mathcal{E}(\bar u), T_{2r} w\big\rangle = 0,
\end{aligned}$$

which leaves us with only the term

$$\|Dz\|_{\ell^2} \lesssim \sup_w \int_0^1 \Big\langle \delta^2\mathcal{E}_N(v_N + te_N)\left(T_{N,r}^{\rm per} - I\right) e_N, T_{N,2r}^{\rm per} w\Big\rangle \, dt.$$

Since $DT_{N,2r}^{\rm per} w = 0$ in $\Lambda \setminus \Lambda_{2r}$ we can estimate this further by

$$\begin{aligned}
\|Dz\|_{\ell^2} &\lesssim \sup_w \sum_{\ell\in\Lambda_{2r}} \Big| D\left(T_{N,r}^{\rm per} - I\right) e_N(\ell)\Big| \, \big|DT_{N,2r}^{\rm per} w(\ell)\big| \\
&\lesssim \sup_w \Big\| D\left(T_{N,r}^{\rm per} - I\right) e_N(\ell)\Big\|_{\ell^2(\Lambda_{2r})} \Big\|DT_{N,2r}^{\rm per} w\Big\|_{\ell^2} \\
&\lesssim \Big\| D\left(T_{N,r}^{\rm per} - I\right) e_N(\ell)\Big\|_{\ell^2(\Lambda_{2r})},
\end{aligned}$$

where, in the last estimate, we used Lemma 3.2 to bound $\|DT_{N,2r}^{\rm per} w\|_{\ell^2} \lesssim \|Dw\|_{\ell^2} \lesssim 1$.

Using Lemma 3.2 a second time we finally deduce that

$$\begin{aligned}
\|De_N\|_{\ell^2(\Lambda_{r/2})} \le \|Dz\|_{\ell^2(\Lambda_N)} &\lesssim \|D(T_r - I)e_N(\ell)\|_{\ell^2(\Lambda_{2r})} \\
&\lesssim \|D(T_r - I)e_N(\ell)\|_{\ell^2(\Lambda_r)} + \|De_N(\ell)\|_{\ell^2(\Lambda_{2r}\setminus\Lambda_r)} \\
&\lesssim \|De_N(\ell)\|_{\ell^2(\Lambda_{2r}\setminus\Lambda_{r/2})}.
\end{aligned}$$

∎

Our main result, Theorem 2.1, will follow from the next intermediate result, which is of independent interest.

THEOREM 3.14. *Under the conditions of Theorem* 2.1*,*

$$\|De_N\|_{\ell^\infty(\Lambda_N)} \lesssim N^{-d}.$$

Proof. Let $\omega(r) := \|De_N\|_{\ell^\infty(\Lambda_N\setminus\Lambda_r)}$; then according to Lemma 3.12, for $r \geq r_0$,

$$\begin{aligned}
\omega(r) &\lesssim N^{-d} + \sup_{\ell\in\Lambda_N\setminus\Lambda_r} \sum_{m\in\Lambda_N} \big(\mathrm{dist}(\ell - m, 2N\mathsf{B}\mathbb{Z}^d) + 1\big)^{-d} (1+|m|)^{-d} |De_N(m)| \\
&\lesssim N^{-d} + \omega(r) \sup_{\ell\in\Lambda_N\setminus\Lambda_r} \sum_{m\in\Lambda_N\setminus\Lambda_r} \big(\mathrm{dist}(\ell - m, 2N\mathsf{B}\mathbb{Z}^d) + 1\big)^{-d} (1+|m|)^{-d} \\
&\qquad + \sup_{\ell\in\Lambda_N\setminus\Lambda_r} \sum_{m\in\Lambda_r} (1+|\ell-m|)^{-d}(1+|m|)^{-d}|De_N(m)| \\
&\lesssim N^{-d} + \omega(r) \sup_{\ell\in\Lambda_N\setminus\Lambda_r} \sum_{z\in\{-1,0,1\}^d} \sum_{m\in\Lambda_N} (1+|\ell - m - 2N\mathsf{B}z|)^{-d}(1+|m|)^{-d} \\
&\qquad + \sup_{\ell\in\Lambda_N\setminus\Lambda_r} \Bigg(\sum_{m\in\Lambda_r} (1+|\ell-m|)^{-2d}(1+|m|)^{-2d}\Bigg)^{1/2} \|De_N\|_{\ell^2(\Lambda_r)} \\
&\lesssim N^{-d} + \omega(r) \sup_{\ell\in\Lambda_N\setminus\Lambda_r} \max_{z\in\{-1,0,1\}^d} |\ell - 2N\mathsf{B}z|^{-d} \log|\ell - 2N\mathsf{B}z| \\
&\qquad + \sup_{\ell\in\Lambda_N\setminus\Lambda_r} |\ell|^{-d} \|De_N\|_{\ell^2(\Lambda_r)} \\
&\lesssim N^{-d} + \omega(r) r^{-d}\log(r) + r^{-d}\|De_N\|_{\ell^2(\Lambda_r)}.
\end{aligned}$$

Here we used that, for $|\ell| \geq 2$,

$$\sum_{m\in\Lambda} (1+|\ell-m|)^{-d}(1+|m|)^{-d} \lesssim |\ell|^{-d}\log|\ell| \qquad \text{and}$$
$$\sum_{m\in\Lambda} (1+|\ell-m|)^{-2d}(1+|m|)^{-2d} \lesssim |\ell|^{-2d}.$$

We apply the Caccioppoli inequality, Lemma 3.13, further restricting to $r_1/2 \leq r \leq N/8$, to continue to estimate

$$\begin{aligned}
\omega(r) &\lesssim N^{-d} + \omega(r) r^{-d}\log(r) + \|De_N\|_{\ell^2(\Lambda_{4r}\setminus\Lambda_r)} r^{-d} \\
&\lesssim N^{-d} + \omega(r) r^{-d}\log(r) + r^{d/2}\|De_N\|_{\ell^\infty(\Lambda_{4r}\setminus\Lambda_r)} r^{-d} \\
&\leq C_3\big(N^{-d} + \omega(r) r^{-d/2}\big).
\end{aligned}$$

For $r_2 := (2C_3)^{2/d}$ and $r \geq r_3 := \max\{r_0, r_1, r_2\}$, we thus find $\omega(r) \leq 2C_3N^{-d}$. That is, we have proven that $|De_N(\ell)| \lesssim N^{-d}$ for all $\ell \in \Lambda_N \setminus \Lambda_{r_3}$, where r_3 is independent of N.

It thus remains only to consider $\ell \in \Lambda_{r_3}$, a finite subdomain. Using Lemma 3.13 a second time we obtain

$$|De_N(\ell)| \leq \|De_N\|_{\ell^2(\Lambda_{r_3})} \lesssim \|De_N\|_{\ell^2(\Lambda_{4r_3}\setminus\Lambda_{r_3})} \lesssim \omega(r_3) \lesssim N^{-d}. \qquad \square$$

Proof of Theorem 2.1. We split

$$\begin{aligned}\|D\bar{u}_N - D\bar{u}\|_{\ell^\infty(\Lambda_N)} &\le \|De_N\|_{\ell^\infty(\Lambda_N)} + \|Dv_N - D\bar{u}\|_{\ell^\infty(\Lambda_N)} \\ &\lesssim N^{-d} + \|Dv_N - D\bar{u}\|_{\ell^\infty(\Lambda_N)},\end{aligned}$$

where we used Theorem 3.14. For $\ell \in \Lambda_{N/2}$, $Dv_N(\ell) - D\bar{u}(\ell) = 0$. Conversely, for $\ell \in \Lambda_N \setminus \Lambda_{N/2}$, (3.17) and (2.7) imply that

$$|Dv_N(\ell) - D\bar{u}(\ell)| \le |Dv_N(\ell)| + |D\bar{u}(\ell)| \lesssim N^{-d}. \qquad \square$$

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