

HOMOGENIZATION OF MATERIALS WITH PERIODIC TRUSS OR FRAME MICRO-STRUCTURES

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The equations that govern elastostatic equilibrium between a prescribed force field and an unknown displacement field for materials with periodic skeletal micro-structures are studied. It is shown that as the size of the micro-structure tends to zero, the displacement field will converge to the solution of a constant coefficient partial differential equation. This equation is shown to be either a classical or a micro-polar continuum elasticity equation, depending on the micro-structural geometry and the nature of the external load field. Convergence is proved for representative model problems in Sobolev energy norms and in the maximum norm. In addition, it is shown that by considering pseudo-differential homogenized equations, any order of convergence can be achieved.

Keywords: Homogenization; lattice; mechanical truss.

1. Introduction

We study the mechanics of materials with periodic skeletal micro-structures called “lattice materials.” Specifically, we study the problem of determining the displacement field in an infinite piece of lattice material subjected to a prescribed load. Modeling the micro-structure as an assembly of discrete struts, we formulate an equilibrium equation that is defined on the integer lattice \mathbb{Z}^d . We will demonstrate that when the size of the unit cell in the lattice is much smaller than the length-scale over which the load changes, an approximate solution to the equilibrium equation can be determined by solving a partial differential equation with constant coefficients, known as the *homogenized* equation.

Depending on the geometry of its skeletal micro-structure, a lattice material derives its main strength from either the axial or the bending stiffness of the struts.⁹

Materials of the first kind are usually modeled as mechanical trusses, whereas materials of the second kind are modeled as frames. As an illustration, among the materials illustrated in Fig. 1, (b) and (c) are treated as trusses, and (a) and (d) as frames. Frame materials are generally less stiff than truss materials since the axial stiffness of a slender bar is significantly higher than the bending stiffness. We will consider both of these models, as well as a model for heat conduction. The lowest order homogenized equation will be Poisson's equation for conduction problem and the classical equations of elasticity for truss materials. For frame materials, the corresponding equation will be an equation of micro-polar (Cosserat) elasticity. We will also consider higher order approximations that do not correspond to classical continuum theories.

The homogenized equations are useful in that they provide valuable heuristic information about the macro-scopic behavior of the material in terms of, e.g., the effective stiffness tensor. Moreover, knowledge about the asymptotic behavior of solutions to the lattice equations is essential to the construction of fast numerical solution techniques. We wish to emphasize that we do not advocate the common technique of dealing with heterogeneous media by solving a homogenized equation using a standard PDE solver. Such methods tend to perform poorly in any situation where non-smooth boundaries, inclusions, or non-smooth loads are present. Techniques that do not have this shortcoming include multigrid solvers for the lattice equations developed by Xu and co-workers,²³ finite element techniques that embed the subscale modeling in the construction of the approximation functions,²² techniques based on lattice Green's functions,¹¹ and discrete boundary equation techniques coupled with fast matrix-vector multiplication algorithms.^{12,21} In order to optimize the performance of such techniques, it is very useful to know the asymptotic behavior of solutions to the lattice equation on infinite domains; describing this behavior is the subject of the present paper.

The technical analysis will rely heavily on a Korn-type inequality in the Fourier domain that was proved by Martinsson and Babuška¹³ (which in turn was inspired by Morgan and Babuška^{16,17}). Since they are obtained using Fourier techniques, the results of this paper rely on both the periodicity of the geometry and the linearity of the equilibrium equations. For techniques applicable to non-linear problems, see, e.g., Blanc *et al.*⁵ and the references therein. For the case of non-periodic network

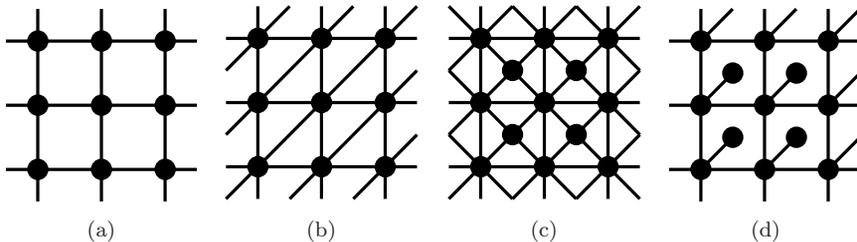


Fig. 1. Examples of lattice geometries.

problems, see, e.g., Babuška and Sauter² and Berlyand and Kolpakov.⁴ While we consider static problems only, Fourier techniques similar to the ones used here can also be used to study dynamical problems, see e.g., Mielke¹⁵ and Martinsson and Movchan.¹⁴ For a review of the engineering literature on lattice problems, see Ostoja-Starzewski.¹⁹

Remark 1.1. The analysis in this paper takes as its starting point a discrete lattice model obtained using classical techniques from structural mechanics. An alternative approach would be to start by modeling the lattice material as a perforated continuum. The equilibrium equations would then be defined on a geometry that is governed by two small parameters: ε , which denotes the size of the periodic cell, and δ , which denotes the diameter of a strut relative to the cell size (so that its absolute diameter is $\delta\varepsilon$). Using homogenization techniques such as the “multiple-scale method” and the variational technique of Tartar it is then possible to study the asymptotic behavior of solutions to the continuum equilibrium equations as ε and δ tend to zero, see for instance Bakhvalov and Panasenko³ Panasenko,²⁰ and in particular Cioranescu and Saint Jean Paulin.⁶ Such an analysis has an advantage over our approach in that it allows a detailed study of the relationship between the small parameter δ and the homogenized equations. On the other hand, the approach given here seems to be much simpler; it is a trivial matter to calculate the homogenized equations even for complicated geometries (using symbolic algebra software, homogenized equations for geometries involving dozens of struts and nodes in each unit cell have been computed¹²). Moreover, high-order homogenized equations can be obtained with ease. In a sense, the method presented here can be viewed as short-cut for obtaining the homogenized equation in the limit $\delta \rightarrow 0$ (at least at first glance, the end result appears to be the same).

This paper is structured as follows. In Sec. 2 we describe our notation and introduce a scaled Fourier transform. In Sec. 3.1 we describe how to determine the asymptotic behavior of the solution to the equilibrium equation by computing a power series in Fourier space; this technique is then applied to the problem of thermostatics in Sec. 3.2 and elastostatics on truss and frame lattices in Secs. 3.3 and 3.4, respectively. For each model, we first present two examples that illustrate the homogenization process and then give general results. In Section 4, we rigorously prove that the solution of the lattice equation converges to the solution of the homogenized equation as the lattice cell size tends to zero. The full proofs will be given for the conduction problem only; the extension to mechanical problems is straightforward.

2. Preliminaries

In this section we introduce notation for describing lattice geometries and lattice functions, and describe the general form of the equations under consideration. We also introduce a discrete Fourier transform.

For periodic media, the term *reference cell* refers to a minimal cell that reproduces the entire structure when repeated periodically. We restrict our attention to infinite periodic lattice geometries in \mathbb{R}^d whose reference cell is the cube $[0, \varepsilon]^d$. The restriction to cubic symmetry simplifies the notation but is strictly aesthetic (see Ref. 12 for the general case). The cells in the lattice are labeled using an integer index $m \in \mathbb{Z}^d$. Letting q denote the number of nodes in a unit cell, we label the nodes inside cell m with the composite indices $(m, 1), \dots, (m, q)$. Thus, $(m, \kappa) \in \mathbb{Z}^d \times \{1, \dots, q\}$ uniquely labels a node, (see Fig. 2). With each node we associate a potential (a temperature, or a displacement) $\mathbf{u}^{(\varepsilon)}(m, \kappa) \in \mathbb{C}^r$ and a load (a heat source, or an external force) $\mathbf{f}^{(\varepsilon)}(m, \kappa) \in \mathbb{C}^r$. Collecting the q vectors $\mathbf{u}^{(\varepsilon)}(m, 1), \dots, \mathbf{u}^{(\varepsilon)}(m, q)$ into a single vector $\mathbf{u}^{(\varepsilon)}(m) \in \mathbb{C}^{qr}$, we consider equilibrium equations of the form

$$[\mathbf{A}^{(\varepsilon)}\mathbf{u}^{(\varepsilon)}](m) = \mathbf{f}^{(\varepsilon)}(m), \quad \forall m \in \mathbb{Z}^d, \tag{2.1}$$

where the equilibrium operator $\mathbf{A}^{(\varepsilon)}$ is a convolution operator of the form

$$[\mathbf{A}^{(\varepsilon)}\mathbf{u}^{(\varepsilon)}](m) = \sum_{n \in \mathbb{B}} A^{(n, \varepsilon)}\mathbf{u}^{(\varepsilon)}(m - n),$$

for some $qr \times qr$ matrices $A^{(n, \varepsilon)}$ and a *finite* set $\mathbb{B} \subset \mathbb{Z}^d$. Equations of the form (2.1) describe a wide range of equilibrium equations, including elastostatic equilibrium on truss and frame lattices. Several examples are given in Sec. 3.

The asymptotic analysis in this paper is based on Fourier techniques. We define a discrete Fourier transform as follows:

$$\tilde{\mathbf{u}}^{(\varepsilon)}(\xi) = [\mathbf{F}^{(\varepsilon)}\mathbf{u}^{(\varepsilon)}](\xi) = \varepsilon^d \sum_{m \in \mathbb{Z}^d} e^{i\mathbf{e}m \cdot \xi} \mathbf{u}^{(\varepsilon)}(m), \quad \forall \xi \in I_\varepsilon^d = (-\pi/\varepsilon, \pi/\varepsilon)^d, \tag{2.2}$$

where $\mathbf{i} = \sqrt{-1}$. The scaling in ε is set in such a way that when $\mathbf{u}^{(\varepsilon)}$ is defined by $\mathbf{u}^{(\varepsilon)}(m) := \mathbf{u}(\varepsilon m)$ for some function \mathbf{u} of a continuous variable, then $\tilde{\mathbf{u}}^{(\varepsilon)}(\xi)$ is a

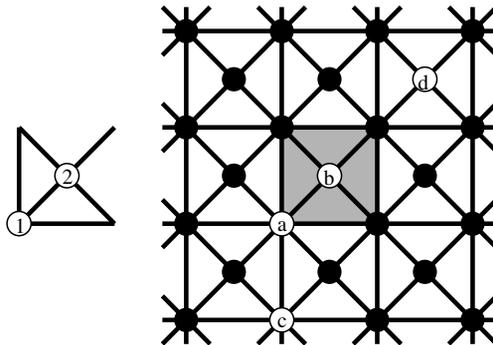


Fig. 2. Lattice notation. To the left, an irreducible unit cell is depicted. Each node is marked with its type, κ . To the right, the cell $m = [0, 0]$ is marked in grey. The node marked “a” is a node of type $\kappa = 1$ in cell $m = [0, 0]$. Thus node “a” is labeled $(1, [0, 0])$. Node “b” is of type $\kappa = 2$ and has the label $(2, [0, 0])$. Node “c” is labeled $(1, [0, -1])$, and node “d” is labeled $(2, [1, 1])$.

Riemann sum of the continuous Fourier transform

$$\hat{u}(\xi) = [\mathcal{F}u](\xi) := \int_{\mathbb{R}^d} e^{ix \cdot \xi} u(x) dx.$$

The inverse of $\mathbf{F}^{(\varepsilon)}$ is given by

$$\mathbf{u}^{(\varepsilon)}(m) = [(\mathbf{F}^{(\varepsilon)})^{-1} \tilde{\mathbf{u}}^{(\varepsilon)}](m) = \frac{1}{(2\pi)^2} \int_{I_\varepsilon^d} e^{-im \cdot \xi} \tilde{\mathbf{u}}^{(\varepsilon)}(\xi) d\xi. \tag{2.3}$$

Taking the Fourier transform of both sides of (2.1) we obtain the algebraic equation

$$\sigma^{(\varepsilon)}(\xi) \tilde{\mathbf{u}}^{(\varepsilon)}(\xi) = \tilde{\mathbf{f}}^{(\varepsilon)}(\xi), \quad \forall \xi \in I_\varepsilon^d, \tag{2.4}$$

where the symbol $\sigma^{(\varepsilon)}$ of $\mathbf{A}^{(\varepsilon)}$ is defined by

$$\sigma^{(\varepsilon)}(\xi) := \mathbf{F}^{(\varepsilon)} \mathbf{A}^{(\varepsilon)} \left(\mathbf{F}^{(\varepsilon)} \right)^{-1} = \sum_{n \in \mathbb{B}} e^{i(\varepsilon n) \cdot \xi} A^{(n, \varepsilon)}.$$

3. Derivation of the Homogenized Equations

In this section, we determine the asymptotic behavior of the solution to the equilibrium equation, as the cell size ε tends to zero, by computing a power series in ε in the Fourier domain. The general procedure is described in Sec. 3.1. In Sec. 3.2 we apply the technique to derive the homogenized equations for the equations of thermostatic equilibrium on a lattice and then in Secs. 3.3 and 3.4, we study the equations that govern the elastostatic equilibrium on truss and frame lattices, respectively. The presentation is largely example-driven and convergence proofs are postponed until Sec. 4.

3.1. The general case

In this section, we briefly describe how to formally derive an asymptotic expansion of the solution $\mathbf{u}^{(\varepsilon)}$ of the generic equation (2.1) (specific examples are given in Secs. 3.2, 3.3 and 3.4). First we note that from Eq. (2.4), we obtain $\tilde{\mathbf{u}}^{(\varepsilon)}(\xi) = [\sigma^{(\varepsilon)}(\xi)]^{-1} \tilde{\mathbf{f}}^{(\varepsilon)}(\xi)$, whence the Fourier inversion formula (2.3) yields

$$\mathbf{u}^{(\varepsilon)}(m) = \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} e^{-i(\varepsilon m) \cdot \xi} \left[\sigma^{(\varepsilon)}(\xi) \right]^{-1} \tilde{\mathbf{f}}^{(\varepsilon)}(\xi) d\xi. \tag{3.1}$$

For all equations under consideration in this paper, the inverse symbol $\sigma^{(\varepsilon)}(\xi)^{-1}$ has an $O(|\xi|^{-2})$ singularity at the origin and the integral (3.1) is absolutely integrable when $d \geq 3$ (the case $d = 2$ is discussed in Refs. 12 and 13). In order to derive the limiting behavior of $\mathbf{u}^{(\varepsilon)}$, as $\varepsilon \rightarrow 0$, we assume that there exists a fixed function f of a continuous variable such that

$$\tilde{\mathbf{f}}^{(\varepsilon)}(\xi) = \hat{f}(\xi) + O(\varepsilon^k) \tag{3.2}$$

for some integer k . This assumption is easily justified by observing that for any k , it is possible to find a weight function μ such that the sequence of lattice function

$\{\mathbf{f}^{(\varepsilon)}\}_{\varepsilon \rightarrow 0}$ defined by

$$\mathbf{f}^{(\varepsilon)}(m) := \frac{1}{\varepsilon^d} \int_{\mathbb{R}^d} f(x) \mu\left(\frac{x - \varepsilon m}{\varepsilon}\right) dx,$$

satisfies (3.2) provided that f is sufficiently smooth (see Sec. 4.1). Now, letting $\varepsilon \rightarrow 0$ and $|m| \rightarrow \infty$ in such a fashion that $x = \varepsilon m$ stays constant, we find that

$$\mathbf{u}^{(\varepsilon)}(m) \rightarrow u^{(0)}(x) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-ix \cdot \xi} S^{(0)}(\xi) \hat{f}(\xi) d\xi = \mathcal{F}^{-1} \left[S^{(0)}(\xi) \hat{f}(\xi) \right], \quad (3.3)$$

where $S^{(0)}(\xi)$ is the limit of the inverse symbol,

$$S^{(0)}(\xi) := \lim_{\varepsilon \rightarrow 0} [\sigma^{(\varepsilon)}(\xi)]^{-1}. \quad (3.4)$$

We observe that $u^{(0)}$ is a vector of q functions, $u^{(0)}(x) = [u^{(0)}(x, 1), \dots, u^{(0)}(x, q)]^t$, where each $u^{(0)}(x, \kappa)$ is a scalar or a vector valued function, depending on whether we consider thermostatics or elastostatics. For either case, we will prove that $S^{(0)}(\xi)$ is the inverse of a matrix whose entries are polynomials in ξ , and thus the function $u^{(0)}$ will be the solution of a constant coefficient partial differential equation with f at the right-hand side. At this point we have not specified the mathematical meaning of the limit (3.3), but in Sec. 4 we demonstrate that if f is sufficiently smooth, convergence occurs both in pointwise and in Sobolev norms.

More generally, we let $S^{(\varepsilon,p)}(\xi)$ denote the p -term MacLaurin expansion of $\sigma^{(\varepsilon)}(\xi)^{-1}$ and set

$$u^{(\varepsilon,p)} := \mathcal{F}^{-1} [S^{(\varepsilon,p)}(\xi) \hat{f}(\xi)].$$

Then, assuming that f is sufficiently smooth (this requirement gets more severe as p increases),

$$\mathbf{u}^{(\varepsilon)}(m) = u^{(\varepsilon,p)}(\varepsilon m) + O(\varepsilon^{p+1}).$$

Each entry of the matrix $S^{(\varepsilon,p)}(\xi)$ is a rational function in ξ , and thus the function $u^{(\varepsilon,p)}$ is the solution of a constant coefficient pseudo-differential equation in physical space.

Remark 3.1. As a practical matter, we mention that even for quite simple structures, it would be prohibitively toilsome to compute $\sigma^{(\varepsilon)}$ and evaluate the inverse and the limit in (3.4) by hand. Fortunately, these tasks can very easily be performed by symbolic algebra software (the examples given in this paper were calculated using the program “Maple”).

3.2. The thermostatic equilibrium equation

Consider a lattice subjected to an applied field of nodal heat sources $\mathbf{f}^{(\varepsilon)}$. When the lattice is in thermostatic equilibrium, the nodal temperatures $\mathbf{u}^{(\varepsilon)}$ satisfy an equation of the form (2.1) which represents the condition that at each node, the

sum of fluxes through the links that connect to the node equals the prescribed heat source.

In order to determine how this model scales with the cell size ε , we first consider a lattice with cell size 1, which we refer to as the “unscaled” lattice. Let $\mathbf{A}^{(\text{us})}$ denote the stiffness operator associated with this lattice and let $\sigma^{(\text{us})}(\xi)$ denote the corresponding symbol. If this lattice is shrunk by a factor of ε , the cross section of a strut will decrease by a factor ε^{d-1} and its length by ε . The scaled load $\mathbf{f}^{(\varepsilon)}$ is defined so that the actual external heat flux is $\varepsilon^d \mathbf{f}^{(\varepsilon)}(m)$. The equilibrium equation at scale ε therefore reads

$$\frac{\varepsilon^{d-1}}{\varepsilon} [\mathbf{A}^{(\text{us})} \mathbf{u}^{(\varepsilon)}](m) = \varepsilon^d \mathbf{f}^{(\varepsilon)}(m), \quad \forall m \in \mathbb{Z}^d, \tag{3.5}$$

which we convert into (2.1) by defining

$$\mathbf{A}^{(\varepsilon)} := \varepsilon^{-2} \mathbf{A}^{(\text{us})}.$$

Likewise, we define

$$\sigma^{(\varepsilon)}(\xi) := \varepsilon^{-2} \sigma^{(\text{us})}(\varepsilon \xi).$$

Before giving the general results, we illustrate the limit process with two examples.

A mono-atomic lattice We consider the lattice in Fig. 1(a). Setting the conductivity of each link to 1, the condition for thermostatic equilibrium at node $m = (m_1, m_2)$ reads

$$\begin{aligned} & \frac{1}{\varepsilon^2} (\mathbf{u}^{(\varepsilon)}(m_1, m_2) - \mathbf{u}^{(\varepsilon)}(m_1 + 1, m_2)) + \frac{1}{\varepsilon^2} (\mathbf{u}^{(\varepsilon)}(m_1, m_2) - \mathbf{u}^{(\varepsilon)}(m_1 - 1, m_2)) \\ & + \frac{1}{\varepsilon^2} (\mathbf{u}^{(\varepsilon)}(m_1, m_2) - \mathbf{u}^{(\varepsilon)}(m_1, m_2 + 1)) \\ & + \frac{1}{\varepsilon^2} (\mathbf{u}^{(\varepsilon)}(m_1, m_2) - \mathbf{u}^{(\varepsilon)}(m_1, m_2 - 1)) = \mathbf{f}^{(\varepsilon)}(m_1, m_2). \end{aligned}$$

The lattice equilibrium operator is thus given by

$$[\mathbf{A}^{(\varepsilon)} \mathbf{u}^{(\varepsilon)}](m) = \frac{1}{\varepsilon^2} \left[4\mathbf{u}^{(\varepsilon)}(m) - \mathbf{u}^{(\varepsilon)}(m + e_1) - \mathbf{u}^{(\varepsilon)}(m - e_1) - \mathbf{u}^{(\varepsilon)}(m + e_2) - \mathbf{u}^{(\varepsilon)}(m - e_2) \right],$$

where $e_1 = [1, 0]$ and $e_2 = [0, 1]$. The Fourier representation of $\mathbf{A}^{(\varepsilon)}$ is then

$$\sigma^{(\varepsilon)}(\xi) = \frac{1}{\varepsilon^2} (4 - e^{-i\varepsilon\xi_1} - e^{i\varepsilon\xi_1} - e^{-i\varepsilon\xi_2} - e^{i\varepsilon\xi_2}) = \frac{1}{\varepsilon^2} \left(4 \sin^2 \frac{\varepsilon\xi_1}{2} + 4 \sin^2 \frac{\varepsilon\xi_2}{2} \right).$$

In order to determine $S^{(\varepsilon,p)}$ we series expand $\sigma^{(\varepsilon)}(\xi)^{-1}$ in ε and find that

$$[\sigma^{(\varepsilon)}(\xi)]^{-1} = \varepsilon^2 \left(4 \sin^2 \frac{\varepsilon\xi}{2} + 4 \sin^2 \frac{\varepsilon\xi}{2} \right)^{-1} = \frac{1}{|\xi|^2} + O(\varepsilon^2), \quad \text{as } \varepsilon \rightarrow 0.$$

Letting $\varepsilon \rightarrow 0$, we see that $S^{(0)}(\xi) = |\xi|^{-2}$, and so the limit function $u^{(0)}$ satisfies $|\xi|^2 \hat{u}^{(0)} = \hat{f}$. The homogenized equation is then

$$-\Delta u^{(0)} = f. \tag{3.6}$$

For this case, $S^{(\varepsilon,1)}(\xi) = S^{(0)}(\xi)$; so Eq. (3.6) is $O(\varepsilon^2)$ -accurate. □

A multi-atomic lattice Consider the X-braced square lattice in Fig. 1(c), again setting the conductivity of all links in the unscaled lattice to 1. Here

$$\sigma^{(\varepsilon)}(\xi) = \frac{1}{\varepsilon^2} \begin{pmatrix} 4 + 4 \sin^2 \frac{\varepsilon \xi_1}{2} + 4 \sin^2 \frac{\varepsilon \xi_2}{2} & -1 - e^{i\varepsilon \xi_1} - e^{i\varepsilon \xi_2} - e^{i(\varepsilon \xi_1 + \varepsilon \xi_2)} \\ -1 - e^{-i\varepsilon \xi_1} - e^{-i\varepsilon \xi_2} - e^{-i(\varepsilon \xi_1 + \varepsilon \xi_2)} & 4 \end{pmatrix}.$$

We find that

$$\det \sigma^{(\varepsilon)}(\xi) = \varepsilon^{-2} (8|\xi|^2 + O(\varepsilon^2)),$$

and so

$$[\sigma^{(\varepsilon)}(\xi)]^{-1} = \frac{1}{8|\xi|^2 + O(\varepsilon^2)} \times \begin{pmatrix} 4 & 1 + e^{-i\varepsilon \xi_1} + e^{-i\varepsilon \xi_2} + e^{-i(\varepsilon \xi_1 + \varepsilon \xi_2)} \\ 1 + e^{i\varepsilon \xi_1} + e^{i\varepsilon \xi_2} + e^{i(\varepsilon \xi_1 + \varepsilon \xi_2)} & 4 + 4 \sin^2 \frac{\varepsilon \xi_1}{2} + 4 \sin^2 \frac{\varepsilon \xi_2}{2} \end{pmatrix}. \tag{3.7}$$

Taylor expanding the right-hand side of (3.7) in ε , we find that

$$[\sigma^{(\varepsilon)}(\xi)]^{-1} = \frac{1}{2|\xi|^2} \left(\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \begin{bmatrix} 0 & -i\varepsilon(\xi_1 + \xi_2)/2 \\ i\varepsilon(\xi_1 + \xi_2)/2 & 0 \end{bmatrix} + O(|\varepsilon \xi|^2) \right). \tag{3.8}$$

The lowest order homogenized equations read

$$\begin{cases} -2\Delta u^{(0)}(x, 1) = f(x, 1) + f(x, 2), \\ -2\Delta u^{(0)}(x, 2) = f(x, 1) + f(x, 2). \end{cases} \tag{3.9}$$

Since $u^{(0)}(x, 1)$ and $u^{(0)}(x, 2)$ represent the limiting temperatures of the two nodal temperature fields $\mathbf{u}^{(\varepsilon)}(m, 1)$ and $\mathbf{u}^{(\varepsilon)}(m, 2)$, respectively, the fact that the two equations in (3.9) are identical implies that $\mathbf{u}^{(\varepsilon)}(m, 1) = \mathbf{u}^{(\varepsilon)}(m, 2) + O(\varepsilon)$. The difference between the two temperature fields, surfaces in the $O(\varepsilon^2)$ -accurate homogenized equations:

$$\begin{cases} -2\Delta u^{(\varepsilon,1)}(x, 1) = (f(x, 1) + f(x, 2)) + \varepsilon \frac{1}{2}(\partial_1 + \partial_2)f(x, 2), \\ -2\Delta u^{(\varepsilon,1)}(x, 2) = (f(x, 1) + f(x, 2)) - \varepsilon \frac{1}{2}(\partial_1 + \partial_2)f(x, 1), \end{cases} \tag{3.10}$$

where ∂_j denotes the partial differentiation operator with respect to x_j . We note that Eqs. (3.10) require higher regularity in f to be well-posed than do (3.9). □

In order to make a statement about general lattice geometries, we need the following result about the nature of the unscaled lattice (Theorem 4.9 of Ref. 13): For any connected lattice, there exists a positive definite matrix M (which can be calculated from $\sigma^{(\text{us})}(\xi)$ through a simple formula), such that, setting $\sigma^{(0)}(\xi) := \xi \cdot M\xi$, we have, as $|\xi| \rightarrow 0$,

$$\sigma^{(\text{us})}(\xi)^{-1} = \begin{pmatrix} \sigma^{(0)}(\xi)^{-1} & \sigma^{(0)}(\xi)^{-1} & \dots & \sigma^{(0)}(\xi)^{-1} \\ \sigma^{(0)}(\xi)^{-1} & & & \vdots \\ \vdots & & & \\ \sigma^{(0)}(\xi)^{-1} & \dots & & \sigma^{(0)}(\xi)^{-1} \end{pmatrix} + O(|\xi|^{-1}). \quad (3.11)$$

Inserting the scaling $\sigma^{(\varepsilon)}(\xi) = \varepsilon^{-2}\sigma^{(\text{us})}(\varepsilon\xi)$ into (3.11) and letting $\varepsilon \rightarrow 0$, we obtain

$$S^{(0)}(\xi) = \begin{pmatrix} \sigma^{(0)}(\xi)^{-1} & \sigma^{(0)}(\xi)^{-1} & \dots & \sigma^{(0)}(\xi)^{-1} \\ \sigma^{(0)}(\xi)^{-1} & & & \vdots \\ \vdots & & & \\ \sigma^{(0)}(\xi)^{-1} & \dots & & \sigma^{(0)}(\xi)^{-1} \end{pmatrix}.$$

This shows that to lowest order, the homogenized equations are the same for all the fields $\mathbf{u}^{(\varepsilon)}(\cdot, \kappa)$. To be precise, $\mathbf{u}^{(\varepsilon)}(m, \kappa) = u^{(0)}(\varepsilon m) + O(\varepsilon)$, where $u^{(0)}$ is specified by the equation

$$-\nabla \cdot M\nabla u^{(0)}(x) = \sum_{\lambda=1}^q f(x, \lambda).$$

We leave the discussion of higher order homogenizations to Sec. 4.

3.3. Elastostatic equilibrium of mechanical trusses

Lattice geometries such as in Figs. 1(b) and 1(c) can accurately be modeled as systems of axial springs that are pin-jointed at the nodes, i.e. as trusses. This simplistic model can be justified by noting that the bending stiffness of the struts is so much smaller than the axial stiffness that it can safely be neglected, (see Refs. 9 and 13).

Since the axial stiffness of a strut scales in exactly the same way as its conductivity, the analysis of the mechanical truss problem follows the conduction case closely. In particular, it is still the case that $\sigma^{(\varepsilon)}(\xi) = \varepsilon^{-2}\sigma^{(\text{us})}(\varepsilon\xi)$. However, the algebra gets considerably more cumbersome since the potential is vector-valued, so we will consider only the lowest order homogenized equations. If needed, higher order models can be derived using the techniques demonstrated for the conduction problem.

A mono-atomic example Consider the square lattice with a single diagonal brace (Fig. 1(b)). Letting the axial stiffness of all bars be unity, we find that

$$\sigma^{(\varepsilon)}(\xi) = \frac{1}{\varepsilon^2} \begin{pmatrix} 4 \sin^2 \frac{\varepsilon \xi_1}{2} + 2 \sin^2 \frac{\varepsilon \xi_1 + \varepsilon \xi_2}{2} & 2 \sin^2 \frac{\varepsilon \xi_1 + \varepsilon \xi_2}{2} \\ 2 \sin^2 \frac{\varepsilon \xi_1 + \varepsilon \xi_2}{2} & 4 \sin^2 \frac{\varepsilon \xi_2}{2} + 2 \sin^2 \frac{\varepsilon \xi_1 + \varepsilon \xi_2}{2} \end{pmatrix}.$$

Since each term has a finite non-zero limit as $\varepsilon \rightarrow 0$, it is possible to interchange the order of the limit and the matrix inversion in (3.4); in other words

$$\begin{aligned} S^{(0)}(\xi) &= \lim_{\varepsilon \rightarrow 0} [\sigma^{(\varepsilon)}(\xi)]^{-1} = \left[\lim_{\varepsilon \rightarrow 0} \sigma^{(\varepsilon)}(\xi) \right]^{-1} \\ &= \begin{pmatrix} \xi_1^2 + \frac{1}{2}(\xi_1 + \xi_2)^2 & \frac{1}{2}(\xi_1 + \xi_2)^2 \\ \frac{1}{2}(\xi_1 + \xi_2)^2 & \xi_2^2 + \frac{1}{2}(\xi_1 + \xi_2)^2 \end{pmatrix}^{-1}. \end{aligned}$$

The system of equations for the homogenized displacement field $u^{(0)} = [u_1^{(0)}, u_2^{(0)}]^t$ is then

$$\begin{aligned} - \left(\partial_1^2 + \frac{1}{2}(\partial_1 + \partial_2)^2 \right) u_1^{(0)} - \frac{1}{2}(\partial_1 + \partial_2)^2 u_2^{(0)} &= f_1, \\ - \frac{1}{2}(\partial_1 + \partial_2)^2 u_1^{(0)} - \left(\partial_2^2 + \frac{1}{2}(\partial_1 + \partial_2)^2 \right) u_2^{(0)} &= f_2. \end{aligned} \tag{3.12}$$

By setting $\sigma^{(0)}(\xi) := S^{(0)}(\xi)^{-1}$ we can write (3.12) compactly as $\sigma^{(0)}(\mathbf{i}\partial)u^{(0)} = f^{(0)}$, where we used the vector of differential operators $\partial = [\partial_1, \partial_2]^t$. Not unexpectedly, (3.12) are the equations of (plane strain) elasticity with a non-isotropic stiffness tensor. □

A multi-atomic lattice We consider the X-braced square lattice in Fig. 1(c), again letting all struts have axial stiffness 1. The symbol is given by

$$\sigma^{(\varepsilon)}(\xi) = \frac{1}{\varepsilon^2} \left[\begin{array}{cc|cc} 4 \sin^2 \frac{\varepsilon \xi_1}{2} + 2 & 0 & 1 + e^{i\varepsilon \xi_1} + e^{i\varepsilon \xi_2} + e^{i(\varepsilon \xi_1 + \varepsilon \xi_2)} & 1 - e^{i\varepsilon \xi_1} - e^{i\varepsilon \xi_2} + e^{i(\varepsilon \xi_1 + \varepsilon \xi_2)} \\ * & 4 \sin^2 \frac{\varepsilon \xi_2}{2} + 2 & 1 - e^{i\varepsilon \xi_1} - e^{i\varepsilon \xi_2} + e^{i(\varepsilon \xi_1 + \varepsilon \xi_2)} & 1 + e^{i\varepsilon \xi_1} + e^{i\varepsilon \xi_2} + e^{i(\varepsilon \xi_1 + \varepsilon \xi_2)} \\ \hline * & * & 2 & 0 \\ * & * & * & 2 \end{array} \right].$$

Computing the matrix inverse and sending ε to zero we find that

$$S^{(0)}(\xi) = \begin{bmatrix} \sigma^{(0)}(\xi)^{-1} & \sigma^{(0)}(\xi)^{-1} \\ \sigma^{(0)}(\xi)^{-1} & \sigma^{(0)}(\xi)^{-1} \end{bmatrix}, \quad \text{where } \sigma^{(0)}(\xi) = \begin{bmatrix} \frac{3}{2}\xi_1^2 + \frac{1}{2}\xi_2^2 & \xi_1 \xi_2 \\ \xi_1 \xi_2 & \frac{1}{2}\xi_1^2 + \frac{3}{2}\xi_2^2 \end{bmatrix}.$$

This means that the lowest order homogenized equations are the same for the two potential fields. To be precise, for $\kappa = 1, 2$, we have

$$\begin{cases} - \left(\frac{3}{2}\partial_1^2 + \frac{1}{2}\partial_2^2 \right) u_1^{(0)}(x, \kappa) - \partial_1 \partial_2 u_2^{(0)}(x, \kappa) = f_1(x, 1) + f_1(x, 2), \\ - \partial_1 \partial_2 u_1^{(0)}(x, \kappa) - \left(\frac{1}{2}\partial_1^2 + \frac{3}{2}\partial_2^2 \right) u_2^{(0)}(x, \kappa) = f_2(x, 1) + f_2(x, 2). \end{cases} \tag{3.13}$$

Using the compact vector notation introduced in the mono-atomic example, we could write (3.13) as $\sigma^{(0)}(\mathbf{i}\partial)u^{(0)}(x, \kappa) = f(x, 1) + f(x, 2)$. □

The extension to arbitrary lattice geometries is completely analogous to the conduction problem. For lattices that can be modeled as trusses there exists a $d \times d$ matrix $\sigma^{(0)}(\xi)$ such that an identity analogous to (3.11) holds (Theorem 6.5 of Ref. 13). The matrix $\sigma^{(0)}(\xi)$ can be computed from $\sigma^{(\text{us})}(\xi)$ through a simple formula. All its entries are second-order polynomials in ξ and moreover, all its eigenvalues satisfy $c|\xi|^2 \leq \lambda_i \leq C|\xi|^2$ for some $c > 0$ and $C < \infty$ (Lemma 4.1 of Ref. 13). Since $\sigma^{(\varepsilon)}(\xi) = \varepsilon^{-2}\sigma^{(\text{us})}(\varepsilon\xi)$ we find that each one of the q^2 blocks of $S^{(0)}(\xi)$ equals $\sigma^{(0)}(\xi)^{-1}$. As a result, all the lattice functions $\{\mathbf{u}^{(\varepsilon)}(m, \kappa)\}_{\kappa=1}^q$, representing the displacements of the q different species of nodes, satisfy the relation $\mathbf{u}^{(\varepsilon)}(m, \kappa) = u^{(0)}(\varepsilon m) + O(\varepsilon)$, where the homogenized displacement field $u^{(0)}$ satisfies the equation

$$\sigma^{(0)}(\mathbf{i}\partial)u^{(0)}(x) = \sum_{\lambda=1}^q f(x, \lambda).$$

3.4. Elastostatics of mechanical frames

When modeling lattices such as in Figs. 1(a) and 1(d), we must include the bending stiffnesses of the struts. Each node now locks the relative angles of the struts that connect to it, and the nodal displacement must therefore include rotational as well as translational degrees of freedom. Thus $\mathbf{u}^{(\varepsilon)}(m, \kappa) = [\mathbf{u}_t^{(\varepsilon)}(m, \kappa), \mathbf{u}_r^{(\varepsilon)}(m, \kappa)] \in \mathbb{R}^r$, where $r = 3$ in two dimensions and $r = 6$ in three. In this model, different components of $\sigma^{(\varepsilon)}(\xi)$ scale differently with ε as will be illustrated in the next two examples.

A mono-atomic lattice. Consider again the simple square lattice in Fig. 1(a). The nodal potential for the unscaled lattice is $\mathbf{u}(m) = [\mathbf{u}_1(m), \mathbf{u}_2(m), \mathbf{u}_3(m)]$, where $[\mathbf{u}_1(m), \mathbf{u}_2(m)]$ denotes the translational displacement and $\mathbf{u}_3(m)$ the rotational (counted anti-clockwise). Likewise, $\mathbf{f}(m) = [\mathbf{f}_1(m), \mathbf{f}_2(m), \mathbf{f}_3(m)]$, where $[\mathbf{f}_1(m), \mathbf{f}_2(m)]$ denotes an external force and $\mathbf{f}_3(m)$ an external torque. Modeling each strut as an Euler beam with length L , cross-sectional area A , moment of inertia I and Young’s modulus E , the equilibrium equation for the unscaled lattice reads

$$\begin{pmatrix} \frac{EA}{L} 4 \sin^2 \frac{\xi_1}{2} + \frac{12EI}{L^3} 4 \sin^2 \frac{\xi_2}{2} & 0 & \frac{12EI}{L^2} \mathbf{i} \sin \xi_2 \\ 0 & \frac{EA}{L} 4 \sin^2 \frac{\xi_2}{2} + \frac{12EI}{L^3} 4 \sin^2 \frac{\xi_1}{2} & -\frac{12EI}{L^2} \mathbf{i} \sin \xi_1 \\ -\frac{12EI}{L^2} \mathbf{i} \sin \xi_2 & \frac{12EI}{L^2} \mathbf{i} \sin \xi_1 & \frac{4EI}{L} (4 + \cos \xi_1 + \cos \xi_2) \end{pmatrix} \times \begin{pmatrix} \tilde{\mathbf{u}}_1(\xi) \\ \tilde{\mathbf{u}}_2(\xi) \\ \tilde{\mathbf{u}}_3(\xi) \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{f}}_1(\xi) \\ \tilde{\mathbf{f}}_2(\xi) \\ \tilde{\mathbf{f}}_3(\xi) \end{pmatrix}.$$

Now, as the lattice is shrunk by a factor of ε we have $L = \varepsilon L_0$, $A = \varepsilon^{d-1} A_0$ and $I = \varepsilon^{d+1} I_0$ (provided that the width-to-length ratio of all bars are kept constant). In these formulas we kept the dimension d explicit in order to simplify generalization to higher dimensions (although for now, $d = 2$). Recalling that $\mathbf{f}^{(\varepsilon)}$ is defined so

load ($f_3 = 0$). In either case, the rotational degree of freedom u_3 decays faster than the translational, $[u_1, u_2]$. We also see that in the case of a pure force load, we can eliminate the rotational variable u_3 , thus recovering a system of equations representing classical elasto-static equilibrium:

$$\begin{aligned} (\partial_1^2 + \gamma \frac{1}{2} \partial_2^2) u_1^{(0)} + \gamma \frac{1}{2} \partial_1 \partial_2 u_2^{(0)} &= f_1, \\ \gamma \frac{1}{2} \partial_1 \partial_2 u_1^{(0)} + (\partial_2^2 + \gamma \frac{1}{2} \partial_1^2) u_2^{(0)} &= f_2. \end{aligned} \tag{3.14}$$

□

Remark 3.2. The quantity $\gamma = 12I_0/L_0^2A_0$ that we introduced represents the quotient between the bending stiffness and the axial stiffness of a bar with the properties I_0 , L_0 and A_0 . Letting R_0 denote the width of the bar, we know that $I_0 \sim R_0^4$ and that $A_0 \sim R_0^2$. Thus $\gamma \sim (R_0/L_0)^2$ which means that $\gamma \ll 1$ for a slender bar. This in turn means that the homogenized equations typically show highly non-isotropic behavior. For instance, Eqs. (3.14) represent a material that is compliant to shear loads but stiff with respect to hydrostatic pressure.

A multi-atomic lattice We consider the square lattice augmented with a strut that leads to an isolated node (Fig. 1(b)). Due to the algebraic complexity of this case, we will skip the intermediate steps and directly give the result of the limit process. We find that

$$S^{(0)}(\xi) = \begin{pmatrix} \sigma_{[11]}^{(0)}(\xi)^{-1} & \sigma_{[12]}^{(0)}(\xi)^{-1} \\ \sigma_{[21]}^{(0)}(\xi)^{-1} & \sigma_{[22]}^{(0)}(\xi)^{-1} \end{pmatrix},$$

where

$$\sigma_{[11]}^{(0)}(\xi) = \sigma_{[12]}^{(0)}(\xi) = \sigma_{[21]}^{(0)}(\xi) = \begin{pmatrix} \xi_1^2 + \gamma \xi_2^2 & 0 & \mathbf{i} \gamma \xi_2 \\ 0 & \xi_2^2 + \gamma \xi_1^2 & -\mathbf{i} \gamma \xi_1 \\ -\mathbf{i} \gamma \xi_2 & \mathbf{i} \gamma \xi_1 & 2\gamma \end{pmatrix},$$

$$\begin{aligned} \sigma_{[22]}^{(0)}(\xi) &= \frac{1}{1 + 12\sqrt{2}} \\ &\times \begin{pmatrix} (1 + 12\sqrt{2})\xi_1^2 + \gamma(1 + 6\sqrt{2})\xi_2^2 & 6\sqrt{2}\gamma\xi_1\xi_2 & \mathbf{i}\gamma\xi_2 \\ 6\sqrt{2}\gamma\xi_1\xi_2 & \gamma(1 + 6\sqrt{2})\xi_1^2 + (1 + 12\sqrt{2})\xi_2^2 & -\mathbf{i}\gamma\xi_1 \\ -\mathbf{i}\gamma\xi_2 & \mathbf{i}\gamma\xi_1 & 2\gamma \end{pmatrix}. \end{aligned}$$

We note that in the frame model, the blocks of $S^{(0)}(\xi)$ may be different. However, some vestiges of the invariance we saw for the other models can be recovered by eliminating the rotational degrees of freedom. To do this, split each of the matrices

$\sigma_{[\kappa\lambda]}^{(0)}$ into rotational and translational components,

$$\sigma_{[\kappa\lambda]}^{(0)}(\xi) = \begin{bmatrix} \sigma_{[\kappa\lambda],tt}^{(0)}(\xi) & \sigma_{[\kappa\lambda],tr}^{(0)}(\xi) \\ \sigma_{[\kappa\lambda],rt}^{(0)}(\xi) & \sigma_{[\kappa\lambda],rr}^{(0)}(\xi) \end{bmatrix}.$$

If we then eliminate the rotational component by forming the Schur complements, we find that, for $\kappa, \lambda = 1, 2$,

$$\begin{aligned} \sigma_{[\kappa\lambda],\text{reduced}}^{(0)}(\xi) &= \sigma_{[\kappa\lambda],tt}^{(0)}(\xi) - \sigma_{[\kappa\lambda],tr}^{(0)}(\xi) [\sigma_{[\kappa\lambda],rr}^{(0)}(\xi)]^{-1} \sigma_{[\kappa\lambda],rt}^{(0)}(\xi) \\ &= \begin{bmatrix} \xi_1^2 + \frac{1}{2}\gamma\xi_2^2 & \frac{1}{2}\gamma\xi_1\xi_2 \\ \frac{1}{2}\gamma\xi_1\xi_2 & \xi_2^2 + \frac{1}{2}\gamma\xi_1^2 \end{bmatrix}. \end{aligned}$$

In words: the four blocks $\sigma_{[\kappa\lambda]}^{(0)}(\xi)$ have identical Schur complements. □

When discussing the general case, we start by noting that the analysis of the scaling in the first example remains valid in any dimension $d \geq 2$. Thus, if we split the $\kappa\lambda$ -block of the unscaled symbol, $\sigma_{[\kappa\lambda]}^{(\text{us})}(\xi)$, into rotational and translational components,

$$\sigma_{[\kappa\lambda]}^{(\text{us})}(\xi) = \begin{pmatrix} \sigma_{[\kappa\lambda],tt}^{(\text{us})}(\xi) & \sigma_{[\kappa\lambda],tr}^{(\text{us})}(\xi) \\ \sigma_{[\kappa\lambda],rt}^{(\text{us})}(\xi) & \sigma_{[\kappa\lambda],rr}^{(\text{us})}(\xi) \end{pmatrix},$$

then

$$\sigma_{[\kappa\lambda]}^{(\varepsilon)}(\xi) = \begin{bmatrix} \varepsilon^{-2}\sigma_{[\kappa\lambda],tt}^{(\text{us})}(\varepsilon\xi) & \varepsilon^{-1}\sigma_{[\kappa\lambda],tr}^{(\text{us})}(\varepsilon\xi) \\ \varepsilon^{-1}\sigma_{[\kappa\lambda],rt}^{(\text{us})}(\varepsilon\xi) & \sigma_{[\kappa\lambda],rr}^{(\text{us})}(\varepsilon\xi) \end{bmatrix}.$$

We made two observations in the second example: (i) the blocks of $S^{(0)}(\xi)$ need not be identical and (ii) if each such block is inverted and the rotational degrees of freedom are then eliminated, the result is the same for every block. That the second observation is generally true follows from Theorem 7.5 of Ref. 13 which states the following: given a connected frame lattice, there exists a $d \times d$ matrix $\sigma^{(0)}(\xi)$ with the same properties as the corresponding matrix for the truss lattices, such that the $\kappa\lambda$ -block of $\sigma^{(\text{us})}(\xi)^{-1}$ satisfies, as $|\xi| \rightarrow 0$,

$$\begin{aligned} [\sigma^{(\text{us})}(\xi)^{-1}]_{[\kappa\lambda]} &= \begin{pmatrix} [\sigma^{(\text{us})}(\xi)^{-1}]_{[\kappa\lambda],tt} & [\sigma^{(\text{us})}(\xi)^{-1}]_{[\kappa\lambda],tr} \\ [\sigma^{(\text{us})}(\xi)^{-1}]_{[\kappa\lambda],rt} & [\sigma^{(\text{us})}(\xi)^{-1}]_{[\kappa\lambda],rr} \end{pmatrix} \\ &= \begin{pmatrix} \sigma^{(0)}(\xi)^{-1} + O(|\xi|^{-1}) & O(|\xi|^{-1}) \\ O(|\xi|^{-1}) & O(1) \end{pmatrix}. \end{aligned}$$

The implication of this statement is that we find ourselves in radically different situations depending on whether torque loads are prescribed: if they are, then we will necessarily have to solve a potentially very large mixed order elliptic system that involves all the $qd(d+1)/2$ variables. If on the other hand there are no torque loads, then upon elimination of the rotational degrees of freedom the large system

decouples into q unrelated equations with d variables each. Thus, $\mathbf{u}_t^{(\varepsilon)}(m, \kappa) = u_t^{(0)}(\varepsilon m) + O(\varepsilon)$, where

$$\sigma^{(0)}(\mathbf{i}\partial)u_t^{(0)}(x) = \sum_{\lambda=1}^q f_t(x, \lambda).$$

Furthermore, $\sigma^{(0)}(\xi)$ is the Schur complement of any of the matrices $\sigma_{[\kappa\lambda]}^{(0)}(\xi)$.

Remark 3.3. If we were to consider finite structures, then the presence of boundaries would have much the same effect as the presence of external torque loads in a boundary layer. This explains why several researchers, (see Lakes¹⁰ and Noor¹⁸), have found that the use of Cosserat continuum models gives higher accuracy than classical models for skeletal structures consisting of large cells (compared to their macroscopic dimension).

4. Convergence Analysis

In this section, we provide rigorous mathematics proofs for the statements that were heuristically derived in Sec. 3. We start in Sec. 4.1 by demonstrating how to create a sequence of lattice load functions $\{\mathbf{f}^{(\varepsilon)}\}_{\varepsilon \rightarrow 0}$ out of a function f in such a fashion that for a given integer k , $\hat{\mathbf{f}}^{(\varepsilon)}(\xi) = \hat{f}(\xi) + O(\varepsilon^k)$. In Secs. 4.2 and 4.3 we will then present the asymptotic analysis relevant to mono- and multi-atomic conduction problems, respectively. Throughout, we will only consider the problems in three dimensions and higher since the one- and two-dimensional cases require certain renormalizations of the integrals involved (see Ref. 12). Moreover, we consider only the conduction model, since the proofs for the elastostatic cases are analogous.

4.1. Preliminaries

Given a function of a continuous variable v , we create a lattice function $P_\varepsilon v$ by taking local averages

$$[P_\varepsilon v](m) = \frac{1}{\varepsilon^d} \int_{\mathbb{R}^d} v(x)\mu(\varepsilon^{-1}x - m) dx, \tag{4.1}$$

where μ is a compactly supported function such that $\int \mu = 1$. We use the same function μ to map a lattice function $\mathbf{v}^{(\varepsilon)}$ to a function of a continuous variable $P_\varepsilon^* \mathbf{v}^{(\varepsilon)}$ as follows:

$$[P_\varepsilon^* \mathbf{v}^{(\varepsilon)}](x) = \sum_{m \in \mathbb{Z}^d} \mathbf{v}^{(\varepsilon)}(m)\mu(\varepsilon^{-1}x - m).$$

The compact support of μ is important because it guarantees the continuity of the map $P_\varepsilon : L^p \rightarrow l_\varepsilon^p$, where l_ε^p is defined as the closure of the compactly supported functions on \mathbb{Z}^d under the norms

$$\|\mathbf{v}^{(\varepsilon)}\|_{l_\varepsilon^p} := \left[\varepsilon^d \sum_{m \in \mathbb{Z}^d} |\mathbf{v}^{(\varepsilon)}(m)|^p \right]^{1/p}, \quad \text{and} \quad \|\mathbf{v}^{(\varepsilon)}\|_{l_\varepsilon^\infty} := \sup_{m \in \mathbb{Z}^d} |\mathbf{v}^{(\varepsilon)}(m)|.$$

Lemma 4.1. *If μ is bounded and compactly supported, then for any $p \in [1, \infty]$, there exists a finite C_p (that does not depend on ε) such that $\|P_\varepsilon v\|_{l_\varepsilon^p} \leq C_p \|v\|_{L^p}$.*

Proof. Consider first the case $p < \infty$ and let ω denote the support of μ ; then

$$\begin{aligned} \|P_\varepsilon v\|_{l_\varepsilon^p}^p &= \varepsilon^d \sum_{m \in \mathbb{Z}^d} \left| \frac{1}{\varepsilon^d} \int_{\mathbb{R}^d} \mu\left(\frac{x - \varepsilon m}{\varepsilon}\right) v(x) dx \right|^p \\ &= \varepsilon^d \sum_{m \in \mathbb{Z}^d} \left| \int_{\omega + m} \mu(y - m) v(\varepsilon y) dy \right|^p. \end{aligned}$$

Apply Hölder’s inequality, with $q = p/(p - 1)$,

$$\begin{aligned} \|P_\varepsilon v\|_{l_\varepsilon^p}^p &\leq \varepsilon^d \sum_{m \in \mathbb{Z}^d} \left[\int_{\omega + m} |\mu(y - m)|^q dy \right]^{p/q} \left[\int_{\omega + m} |v(\varepsilon y)|^p dy \right] \\ &\leq \|\mu\|_{L^q}^p \sum_{m \in \mathbb{Z}^d} \int_{\omega + m} |v(x)|^p dx \leq C \|\mu\|_{L^q}^p \|f\|_{L^p}^p, \end{aligned}$$

where in the last step, we used that ω is finite. The case $p = \infty$ is trivial. □

The next result describes how the Fourier transform of $P_\varepsilon v$ relates to \hat{v} , and conversely, how the Fourier transform of $P_\varepsilon^* \mathbf{v}^{(\varepsilon)}$ relates to $\tilde{\mathbf{v}}^{(\varepsilon)}$.

Lemma 4.2. (a) *If v is a function such that the right-hand side below is well-defined, then*

$$[\mathbf{F}^{(\varepsilon)} P_\varepsilon v](\xi) = \hat{v}(\xi) \hat{\mu}(\varepsilon \xi) + \sum_{m \in \mathbb{Z}^d, m \neq 0} \hat{v}\left(\xi + \frac{2\pi}{\varepsilon} m\right) \hat{\mu}(\varepsilon \xi + 2\pi m).$$

(b) *If $\mathbf{v}^{(\varepsilon)} \in l_\varepsilon^1$, then*

$$[\mathcal{F} P_\varepsilon^* \mathbf{v}^{(\varepsilon)}](\xi) = \tilde{\mathbf{v}}^{(\varepsilon)}(\xi) \hat{\mu}(\varepsilon \xi).$$

Proof. For part (a), set $\mu_{\varepsilon, m}(x) = \mu(\varepsilon^{-1} x - m)$ and apply Plancherel’s theorem to (4.1),

$$[P_\varepsilon v](m) = \frac{1}{\varepsilon^d (2\pi)^d} \int_{\mathbb{R}^d} \hat{v}(\zeta) \hat{\mu}_{\varepsilon, m}(-\zeta) d\zeta = \frac{1}{\varepsilon^d (2\pi)^d} \int_{\mathbb{R}^d} \hat{v}(\zeta) \varepsilon^d e^{-i\varepsilon m \cdot \zeta} \hat{\mu}(\varepsilon \zeta) d\zeta. \tag{4.2}$$

Inserting (4.2) into the definition of $\mathbf{F}^{(\varepsilon)}$, (2.2), we obtain the expression

$$[\mathbf{F}^{(\varepsilon)} P_\varepsilon v](\xi) = \int_{\mathbb{R}^d} \hat{v}(\zeta) \hat{\mu}(\varepsilon \zeta) \left(\frac{\varepsilon^d}{(2\pi)^d} \sum_{m \in \mathbb{Z}^d} e^{i\varepsilon(\xi - \zeta) \cdot m} \right) d\zeta. \tag{4.3}$$

Applying Poisson’s summation formula to the function $m \mapsto e^{i\varepsilon(\xi - \zeta) \cdot m}$ we find that

$$\frac{\varepsilon^d}{(2\pi)^d} \sum_{m \in \mathbb{Z}^d} e^{i\varepsilon(\xi - \zeta) \cdot m} = \sum_{m \in \mathbb{Z}^d} \delta\left(\xi - \zeta + \frac{2\pi}{\varepsilon} m\right).$$

This identity in combination with (4.3) proves the claim.

Part (b) is straightforward;

$$\begin{aligned} [\mathcal{F}P_\varepsilon^* \mathbf{v}^{(\varepsilon)}](\xi) &= \sum_{n \in \mathbb{Z}^d} \mathbf{v}^{(\varepsilon)}(n) \int_{\mathbb{R}^d} e^{ix \cdot \xi} \mu\left(\frac{x}{\varepsilon} - n\right) dx \\ &= \sum_{n \in \mathbb{Z}^d} \mathbf{v}^{(\varepsilon)}(n) \int_{\mathbb{R}^d} e^{i\varepsilon(y+n) \cdot \xi} \mu(y) \varepsilon^d dy = \hat{\mathbf{v}}^{(\varepsilon)}(\xi) \hat{\mu}(\varepsilon\xi). \end{aligned} \quad \square$$

For our purposes, it is desirable that $[\mathbf{F}^{(\varepsilon)} P_\varepsilon f](\xi) = \hat{f}(\xi) + O(\varepsilon^k)$ for some large integer k . In view of Lemma 4.2, this question appears to be related to whether $\hat{\mu}(\xi) - 1$ has a higher order zero at the origin. In fact, for $O(\varepsilon^{2p+2})$ approximation we need to ask that

$$|\hat{\mu}(\xi) - 1| \leq C|\xi|^{2+l}, \quad \text{for } -2 \leq l \leq 2p. \quad (4.4)$$

It is also required that $\hat{\mu}(\xi)$ decays fast for large ξ (which corresponds to a regularity requirement in physical space) and that $\hat{\mu}(\xi)$ has a high order zero around all points $2\pi n$, for $n \in \mathbb{Z}^d \setminus \{0\}$, i.e.

$$|\hat{\mu}(\xi - 2\pi n)| \leq C|\xi|^{2+l} \prod_{j=1}^d \frac{1}{1 + n_j^{2(p+1)}}, \quad \text{for } -2 \leq l \leq 2p \text{ and } n \in \mathbb{Z}^d \setminus \{0\}. \quad (4.5)$$

These conditions were first formulated by Babuška¹ and later by Fix and Strang.^{7,8} They correspond to a requirement that μ and its translates should be able to reproduce polynomials of degree $2p+2$. The following result is a direct consequence of Lemma 4.2.

Lemma 4.3. *Suppose that μ satisfies (4.4) and (4.5), that P_ε is the corresponding map and that $\mathbf{f}^{(\varepsilon)} = P_\varepsilon f$. Then $|\hat{\mathbf{f}}^{(\varepsilon)}(\xi) - \hat{f}(\xi)| \leq C|\varepsilon\xi|^{2p+2} \|f\|_{L^1}$.*

We will next demonstrate that it is possible to construct a compactly supported function μ that satisfies (4.4) and (4.5) from basic spline functions. Start by defining the lowest order spline, $\psi^{(1)}$, as the characteristic function for the cube $[-1/2, 1/2]^d$, in other words, $\psi^{(1)}(x) = \prod_{j=1}^d \chi_{[-1/2, 1/2]}(x_j)$. Then define the higher splines through successive convolutions $\psi^{(k)} = \psi^{(1)} * \psi^{(k-1)}$ so that

$$\hat{\psi}^{(k)}(\xi) = \prod_{j=1}^d \left(\frac{\sin(\xi_j/2)}{\xi_j/2} \right)^k.$$

Now, $\psi^{(2)}$ satisfies both (4.4) and (4.5) for $p = 0$, so picking $\mu = \psi^{(2)}$ is sufficient for $O(\varepsilon^2)$ approximation. As k increases, the functions $\hat{\psi}^{(k)}$ attain higher order zeros at the points $2\pi n$ but the zero of $\hat{\psi}^{(k)}(\xi) - 1$ remains of order 2. We can increase

this order by forming linear combinations of high order splines. For instance,

$$\mu(x) := 3\psi^{(4)}(x) - 2\psi^{(6)}(x)$$

gives $O(\varepsilon^4)$ approximation order and

$$\mu(x) := 10\psi^{(6)}(x) - 15\psi^{(8)}(x) + 6\psi^{(10)}(x)$$

gives $O(\varepsilon^6)$. We have verified that such constructions exist at least up to $O(\varepsilon^{10})$. Henceforth, we will suppose that the maps P_ε and P_ε^* are defined using these spline-based weight-functions but in principle, any compactly supported and bounded μ that satisfies (4.4) and (4.5) could be used.

Before proceeding to the main results of this section we define Sobolev semi-norms by

$$|u|_{H^k} := \left[\int_{\mathbb{R}^d} |\xi|^{2k} |\hat{u}(\xi)|^2 d\xi \right]^{1/2}.$$

4.2. Homogenization of mono-atomic lattices

Studying heat conduction on connected mono-atomic lattices in dimension $d \geq 3$, in this section we will: (i) state an equation for the scaled lattice potential $\mathbf{u}^{(\varepsilon)}$ and prove that it is well posed, (ii) give a rigorous definition of the homogenized solution $u^{(\varepsilon, 2p)}$, and (iii) prove that in a certain sense $\mathbf{u}^{(\varepsilon)}(m) = u^{(\varepsilon, 2p)}(\varepsilon m) + O(\varepsilon^{2p+2})$. Before we do any of this, we need to describe how $\sigma^{(\varepsilon)}(\xi)^{-1}$ behaves for small ξ .

The symbol of the unscaled lattice $\sigma^{(\text{us})}(\xi)$ is a trigonometric polynomial and as such has an absolutely convergent power series. It follows from Lemma 4.1 in Ref. 13 that for any connected mono-atomic lattice there exists a positive definite matrix M such that this series takes the form

$$\sigma^{(\text{us})}(\xi) = \xi \cdot M\xi + \sum_{j=2}^{\infty} b_j(\xi),$$

where the $b_j(\xi)$'s are homogeneous polynomials of order $2j$. Letting Π^{2j} denote the set of all such polynomials, we write $b_j \in \Pi^{2j}$. Using induction, it is not difficult to prove that (see Ref. 12) there exist $a_{2j} \in \Pi^{4j}$ such that

$$\frac{1}{\sigma^{(\text{us})}(\xi)} = \frac{1}{\xi \cdot M\xi} + \sum_{j=1}^p \frac{a_{2j}(\xi)}{(\xi \cdot M\xi)^{j+1}} + \hat{R}_p(\xi), \quad \text{where } |\partial^\alpha \hat{R}_p(\xi)| \leq C|\xi|^{2p-|\alpha|}.$$

The relation $\sigma^{(\varepsilon)}(\xi) = \varepsilon^{-2}\sigma^{(\text{us})}(\varepsilon\xi)$ then implies that

$$\frac{1}{\sigma^{(\varepsilon)}(\xi)} = \frac{1}{\xi \cdot M\xi} + \sum_{j=1}^p \varepsilon^{2j} \frac{a_{2j}(\xi)}{(\xi \cdot M\xi)^{j+1}} + \hat{R}_p^{(\varepsilon)}(\xi), \tag{4.6}$$

where $|\partial^\alpha \hat{R}_p^{(\varepsilon)}(\xi)| \leq C\varepsilon^{2p+2}|\xi|^{2p-|\alpha|}$. The series expansion of $\sigma^{(\varepsilon)}(\xi)^{-1}$ is thus

$$S^{(\varepsilon, 2p)}(\xi) := \frac{1}{\xi \cdot M\xi} + \sum_{j=1}^p \varepsilon^{2j} \frac{a_{2j}(\xi)}{(\xi \cdot M\xi)^{j+1}}. \tag{4.7}$$

The only other information we need about $\sigma^{(us)}(\xi)$ is that it is strictly positive in $I^d \setminus \{0\}$. This fact follows from Lemma 4.1 of Ref. 13.

In order to strictly define the lattice equilibrium equation, we suppose that $f \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ is a fixed load function. Then given ε , set $\mathbf{f}^{(\varepsilon)} := P_\varepsilon f$ and consider the lattice equation

$$\begin{cases} \mathbf{A}^{(\varepsilon)} \mathbf{u}^{(\varepsilon)} = \mathbf{f}^{(\varepsilon)}, \\ \|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}} < \infty, \end{cases} \tag{4.8}$$

where the energy norm $\|\cdot\|_{\mathbf{A}^{(\varepsilon)}}$ is defined by

$$\|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}}^2 := \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} \overline{\tilde{\mathbf{u}}^{(\varepsilon)}(\xi)} \sigma^{(\varepsilon)}(\xi) \tilde{\mathbf{u}}^{(\varepsilon)}(\xi) d\xi. \tag{4.9}$$

For $\mathbf{u}^{(\varepsilon)}$ such that $\|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}} < \infty$ the familiar definition $\|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}}^2 = \langle \mathbf{u}^{(\varepsilon)}, \mathbf{A}^{(\varepsilon)} \mathbf{u}^{(\varepsilon)} \rangle_{I_\varepsilon^d}$ holds but note that there exist functions $\mathbf{u}^{(\varepsilon)}$ such that $\|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}} = \infty$ even though $\mathbf{A} \mathbf{u} = 0$. We will prove that an explicit solution of (4.8) is given by

$$\mathbf{u}^{(\varepsilon)}(m) := \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} e^{-i(\varepsilon m) \cdot \xi} \sigma^{(\varepsilon)}(\xi)^{-1} \tilde{\mathbf{f}}^{(\varepsilon)}(\xi) d\xi. \tag{4.10}$$

Proposition 4.1. *If $f \in L^1 \cap L^2$ and $\mathbf{f}^{(\varepsilon)} = P_\varepsilon f$, then the integral in (4.10) is absolutely convergent and defines a solution of Eq. (4.8). This solution is unique up to a constant and satisfies $\|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}} \leq C (\|f\|_{L^1} + \|f\|_{L^2})$.*

Proof. To see that the integral is absolutely convergent, note that $f \in L^1$ which implies that $\mathbf{f}^{(\varepsilon)} \in l_\varepsilon^1$ which in turn implies that $\tilde{\mathbf{f}}^{(\varepsilon)}$ is continuous. As a result of (4.6), the integrand thus has an $O(|\xi|^{-2})$ singularity at the origin which is integrable in three dimensions and higher. To see that the proposed solution indeed solves the equation, simply apply $\mathbf{A}^{(\varepsilon)}$ to the integral, use the absolute convergence to move it inside the integral and note that when it hits $e^{-i(\varepsilon m) \cdot \xi}$ it produces a factor $\sigma^{(\varepsilon)}(\xi)$ that cancels the factor $\sigma^{(\varepsilon)}(\xi)^{-1}$.

Next we prove the bound on the energy. Letting B denote the unit ball in \mathbb{R}^d we obtain

$$\begin{aligned} \|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}}^2 &= \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} \sigma^{(\varepsilon)}(\xi) |\tilde{\mathbf{u}}^{(\varepsilon)}(\xi)|^2 d\xi = \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} \sigma^{(\varepsilon)}(\xi)^{-1} |\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)|^2 d\xi \\ &= \frac{1}{(2\pi)^d} \int_B \sigma^{(\varepsilon)}(\xi)^{-1} |\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)|^2 d\xi + \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d \setminus B} \sigma^{(\varepsilon)}(\xi)^{-1} |\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)|^2 d\xi \\ &\leq \int_B \frac{C}{|\xi|^2} \|\tilde{\mathbf{f}}^{(\varepsilon)}\|_{l_\varepsilon^\infty}^2 d\xi + \int_{I_\varepsilon^d \setminus B} C |\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)|^2 d\xi \leq C \left(\|\mathbf{f}^{(\varepsilon)}\|_{l_\varepsilon^1}^2 + \|\mathbf{f}^{(\varepsilon)}\|_{l_\varepsilon^2}^2 \right) \\ &\leq C (\|f\|_{L^1}^2 + \|f\|_{L^2}^2). \end{aligned}$$

To prove uniqueness suppose that $\mathbf{v}^{(\varepsilon)}$ is another solution and set $\mathbf{w}^{(\varepsilon)} := \mathbf{u}^{(\varepsilon)} - \mathbf{v}^{(\varepsilon)}$. Then $\mathbf{A}^{(\varepsilon)} \mathbf{w}^{(\varepsilon)} = 0$ and $\|\mathbf{w}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}} < \infty$. This implies that $\|\mathbf{w}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}}^2 = \langle \mathbf{w}^{(\varepsilon)}, \mathbf{A}^{(\varepsilon)} \mathbf{w}^{(\varepsilon)} \rangle = 0$, so $\mathbf{w}^{(\varepsilon)}$ must be constant. \square

We next define the homogenized solution. With $S^{(\varepsilon, 2p)}(\xi)$ defined by (4.7) we set

$$u^{(\varepsilon, 2p)} := \mathcal{F}^{-1} \left[S^{(\varepsilon, 2p)} \hat{f} \right], \tag{4.11}$$

where the inverse Fourier transform is to be understood in the sense of tempered distributions. Since $f \in L^1$ and $S^{(\varepsilon, 2p)}$ is a locally integrable rational function, the function $u^{(\varepsilon, 2p)}$ is well-defined. In many cases, Eq. (4.11) can be rewritten as a (quasi-) partial differential equation but for such an equation to have a unique solution, it must be coupled with finite energy conditions that depend on the order of the equation, we do not give details.

Even though the abstract definition of $u^{(\varepsilon, 2p)}$ as a tempered distribution is occasionally necessary, the Fourier integral in (4.11) is typically absolutely integrable and $u^{(\varepsilon, 2p)}$ is a continuous function.

Proposition 4.2. *The function $u^{(\varepsilon, 2p)}$ defined by (4.11) is continuous if $f \in L^1 \cap H^{2p+k}$ for some $k > d/2 - 2$.*

Proof. We prove the claim by proving that $\hat{u}^{(\varepsilon, 2p)} \in L^1$. With B the unit ball, we find that

$$\begin{aligned} \|\hat{u}^{(\varepsilon, 2p)}\|_{L^1} &= \int_{\mathbb{R}^d} |S^{(\varepsilon, 2p)}(\xi) \hat{f}(\xi)| \, d\xi \leq C \int_B \frac{|\hat{f}(\xi)|}{|\xi|^2} \, d\xi + C \int_{B^c} |\xi|^{2p-2} |\hat{f}(\xi)| \, d\xi \\ &\leq C \int_B \frac{\|f\|_{L^1}^2}{|\xi|^2} \, d\xi + C \left[\int_B |\xi|^{-2k-4} \, d\xi \int_{B^c} |\xi|^{4p+2k} |\hat{f}(\xi)|^2 \, d\xi \right]^{1/2}, \end{aligned}$$

which is finite precisely when $f \in L^1 \cap H^{2p+k}$ and $2k + 4 > d$. □

The next two theorems assert that $\mathbf{P}_\varepsilon^* \mathbf{u}^{(\varepsilon)} - u^{(\varepsilon, 2p)} \rightarrow 0$ in some Sobolev H^k norm and that $\mathbf{u}^{(\varepsilon)}(m) - u^{(\varepsilon, 2p)}(\varepsilon m) \rightarrow 0$ pointwise.

Theorem 4.1. Suppose that $d \geq 3$, let $\mathbf{u}^{(\varepsilon)}$ be the solution of the lattice equation (4.8), where $\mathbf{f}^{(\varepsilon)} = \mathbf{P}_\varepsilon f$, and let $u^{(\varepsilon, 2p)}$ be the approximation defined by (4.11). For ε small and k and l positive integers such that $2p - 2 \leq l \leq 2p$ and $k \leq 2 + l - 2p$ we have, for $f \in H^l$,

$$|\mathbf{P}_\varepsilon^* \mathbf{u}^{(\varepsilon)} - u^{(\varepsilon, 2p)}|_{H^k} \leq C \varepsilon^{2+l-k} \|f\|_{H^l}. \tag{4.12}$$

Proof. For notational convenience, we set $\sigma^{(\varepsilon, 2p)}(\xi) := S^{(\varepsilon, 2p)}(\xi)^{-1}$. Then, since $|\varepsilon \xi|$ is bounded when $\xi \in I_\varepsilon^d$, Eq. (4.6) implies that:

$$\left| \frac{1}{\sigma^{(\varepsilon)}(\xi)} - \frac{1}{\sigma^{(\varepsilon, 2p)}(\xi)} \right| \leq C \varepsilon^2 |\varepsilon \xi|^l, \quad \text{for } \xi \in I_\varepsilon^d \text{ and } 0 \leq l \leq 2p. \tag{4.13}$$

By invoking Plancherel’s equality, the inequality (4.12) can be proved on the Fourier side;

$$\begin{aligned}
 |P_\varepsilon^* \mathbf{u}^{(\varepsilon)} - u^{(\varepsilon,2p)}|_{H^k}^2 &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |\xi|^{2k} |\tilde{\mathbf{u}}^{(\varepsilon)}(\xi) \hat{\mu}(\varepsilon\xi) - \hat{u}^{(\varepsilon,2p)}(\xi)|^2 d\xi \\
 &= \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} |\xi|^{2k} |\tilde{\mathbf{u}}^{(\varepsilon)}(\xi) \hat{\mu}(\varepsilon\xi) - \hat{u}^{(\varepsilon,2p)}(\xi)|^2 d\xi \\
 &\quad + \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d \setminus I_\varepsilon^d} |\xi|^{2k} |\tilde{\mathbf{u}}^{(\varepsilon)}(\xi) \hat{\mu}(\varepsilon\xi)|^2 d\xi \\
 &\quad + \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d \setminus I_\varepsilon^d} |\xi|^{2k} |\hat{u}^{(\varepsilon,2p)}(\xi)|^2 d\xi =: K_1 + K_2 + K_3.
 \end{aligned}$$

Applying Lemma 4.2 we find that

$$\begin{aligned}
 K_1 &= \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} |\xi|^{2k} \left| \frac{\tilde{\mathbf{f}}^{(\varepsilon)}(\xi) \hat{\mu}(\varepsilon\xi)}{\sigma^{(\varepsilon)}(\xi)} - \frac{\hat{f}(\xi)}{\sigma^{(\varepsilon,2p)}(\xi)} \right|^2 d\xi \\
 &\leq C\varepsilon^{-2k} \underbrace{\int_{I_\varepsilon^d} \left| \frac{\hat{f}(\xi) \hat{\mu}(\varepsilon\xi)^2}{\sigma^{(\varepsilon)}(\xi)} - \frac{\hat{f}(\xi)}{\sigma^{(\varepsilon,2p)}(\xi)} \right|^2 d\xi}_{=:K_{11}} \\
 &\quad + C\varepsilon^{-2k} \underbrace{\int_{I_\varepsilon^d} \left| \frac{\hat{\mu}(\varepsilon\xi)}{\sigma^{(\varepsilon)}(\xi)} \sum_{n \neq 0} \hat{f}\left(\xi + \frac{2\pi}{\varepsilon}n\right) \hat{\mu}(\varepsilon\xi + 2\pi n) \right|^2 d\xi}_{=:K_{12}}.
 \end{aligned}$$

When bounding K_{11} we use that, by (4.13) and (4.4),

$$\left| \frac{\hat{\mu}^2(\varepsilon\xi)}{\sigma^{(\varepsilon)}(\xi)} - \frac{1}{\sigma^{(\varepsilon,2p)}(\xi)} \right|^2 \leq \left| \frac{\hat{\mu}^2(\varepsilon\xi) - 1}{\sigma^{(\varepsilon)}(\xi)} \right|^2 + \left| \frac{1}{\sigma^{(\varepsilon)}(\xi)} - \frac{1}{\sigma^{(\varepsilon,2p)}(\xi)} \right|^2 \leq C\varepsilon^4 |\varepsilon\xi|^{2l}.$$

Then, since $|\xi| \leq C\varepsilon^{-1}$ for $\xi \in I_\varepsilon^d$,

$$\begin{aligned}
 K_{11} &\leq C\varepsilon^{-2k} \int_{I_\varepsilon^d} \left| \frac{\hat{\mu}^2(\varepsilon\xi)}{\sigma^{(\varepsilon)}(\xi)} - \frac{1}{\sigma^{(\varepsilon,2p)}(\xi)} \right|^2 |\hat{f}(\xi)|^2, \\
 d\xi &\leq C\varepsilon^{4+2l-2k} \int_{I_\varepsilon^d} |\xi|^{2l} |\hat{f}(\xi)|^2 d\xi \leq C\varepsilon^{4+2l-2k} \|f\|_{H^l}^2.
 \end{aligned}$$

When bounding K_{12} use first that $|\hat{\mu}(\varepsilon\xi)|$ is bounded,

$$\begin{aligned}
 K_{12} &\leq \sum_{n \neq 0} \sum_{m \neq 0} C\varepsilon^{-2k} \int_{I_\varepsilon^d} \frac{1}{\sigma^{(\varepsilon)}(\xi)^2} \hat{f} \\
 &\quad \times \left(\xi + \frac{2\pi}{\varepsilon}n \right) \hat{\mu}(\varepsilon\xi + 2\pi n) \overline{\hat{f}\left(\xi + \frac{2\pi}{\varepsilon}m\right) \hat{\mu}(\varepsilon\xi + 2\pi m)} d\xi \\
 &\leq \sum_{n \neq 0} \sum_{m \neq 0} C\varepsilon^{-2k} \int_{I_\varepsilon^d} \left(\left| \hat{f}\left(\xi + \frac{2\pi}{\varepsilon}n\right) \right|^2 + \left| \hat{f}\left(\xi + \frac{2\pi}{\varepsilon}m\right) \right|^2 \right) \\
 &\quad \times \frac{\hat{\mu}(\varepsilon\xi + 2\pi n)}{\sigma^{(\varepsilon)}(\xi)} \frac{\hat{\mu}(\varepsilon\xi + 2\pi m)}{\sigma^{(\varepsilon)}(\xi)} d\xi.
 \end{aligned}$$

Noting that the two terms have the same sum we find that

$$K_{12} \leq \sum_{n \neq 0} \sum_{m \neq 0} C \varepsilon^{-2k} \int_{I_\varepsilon^d} \left| \hat{f} \left(\xi + \frac{2\pi}{\varepsilon} n \right) \right|^2 \frac{\hat{\mu}(\varepsilon \xi + 2\pi n)}{\sigma^{(\varepsilon)}(\xi)} \frac{\hat{\mu}(\varepsilon \xi + 2\pi m)}{\sigma^{(\varepsilon)}(\xi)} d\xi.$$

Then we use (4.5),

$$\begin{aligned} K_{12} &\leq \sum_{n \neq 0} \sum_{m \neq 0} C \varepsilon^{-2k} \int_{I_\varepsilon^d} \left| \hat{f} \left(\xi + \frac{2\pi}{\varepsilon} n \right) \right|^2 \frac{|\varepsilon \xi|^{2+l}}{|\xi|^2} \frac{|\varepsilon \xi|^{2+l}}{|\xi|^2 \prod_{j=1}^d (1 + m_j^{2(p+1)})} d\xi \\ &\leq \sum_{n \neq 0} C \varepsilon^{4+2l-2k} \int_{I_\varepsilon^d} |\xi|^{2l} \left| \hat{f} \left(\xi + \frac{2\pi}{\varepsilon} n \right) \right|^2 d\xi \leq C \varepsilon^{4+2l-2k} \|f\|_{H^l}^2. \end{aligned}$$

We next turn to bounding K_2 . By definition

$$\begin{aligned} K_2 &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d \setminus I_\varepsilon^d} |\xi|^{2k} \left| \frac{\tilde{\mathbf{f}}^{(\varepsilon)}(\xi) \hat{\mu}(\varepsilon \xi)}{\sigma^{(\varepsilon)}(\xi)} \right|^2 d\xi \\ &= \frac{1}{(2\pi)^d} \sum_{n \neq 0} \int_{I_\varepsilon^d} \left| \xi + \frac{2\pi}{\varepsilon} n \right|^{2k} \left| \frac{\tilde{\mathbf{f}}^{(\varepsilon)}(\xi) \hat{\mu}(\varepsilon \xi + 2\pi n)}{\sigma^{(\varepsilon)}(\xi)} \right|^2 d\xi. \end{aligned}$$

Now we invoke the inequality (4.5),

$$\begin{aligned} K_2 &\leq \sum_{n \neq 0} \int_{I_\varepsilon^d} \left| \frac{n}{\varepsilon} \right|^{2k} |\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)|^2 \frac{|\varepsilon \xi|^{4+2l}}{|\xi|^4 \prod_{j=1}^d (1 + n_j^{2(p+1)})} d\xi \\ &\leq C \varepsilon^{4+2l-2k} \int_{I_\varepsilon^d} |\xi|^{2l} |\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)|^2 d\xi. \end{aligned}$$

We need to prove that the integral in the last expression is bounded by $\|f\|_{H^l}^2$; by Lemma 4.2,

$$\begin{aligned} \int_{I_\varepsilon^d} |\xi|^{2l} |\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)|^2 d\xi &\leq \int_{I_\varepsilon^d} |\xi|^{2l} |\hat{f}(\xi) \hat{\mu}(\varepsilon \xi)|^2 d\xi \\ &\quad + \int_{I_\varepsilon^d} |\xi|^{2l} \left| \sum_{n \neq 0} \hat{f} \left(\xi + \frac{2\pi}{\varepsilon} n \right) \hat{\mu}(\varepsilon \xi + 2\pi n) \right|^2 d\xi. \end{aligned}$$

Expanding the sum as in the bound for K_{12} we find that

$$\begin{aligned} &\int_{I_\varepsilon^d} |\xi|^{2l} |\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)|^2 d\xi \\ &\leq C \|f\|_{H^l}^2 + C \sum_{n \neq 0} \sum_{m \neq 0} \int_{I_\varepsilon^d} |\xi|^{2l} \left| \hat{f} \left(\xi + \frac{2\pi}{\varepsilon} n \right) \right|^2 \hat{\mu}(\varepsilon \xi + 2\pi n) \hat{\mu}(\varepsilon \xi + 2\pi m) d\xi. \end{aligned}$$

By (4.5) the sum over m produces nothing more than a constant. Then use that $\hat{u}(\varepsilon\xi + 2\pi n)$ is bounded to obtain

$$\begin{aligned} \int_{I_\varepsilon^d} |\xi|^{2l} |\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)|^2 d\xi &\leq C \|f\|_{H^l}^2 + C \sum_{n \neq 0} \int_{I_\varepsilon^d} |\xi|^{2l} \left| \hat{f}\left(\xi + \frac{2\pi}{\varepsilon}n\right) \right|^2 d\xi \\ &\leq C \|f\|_{H^l}^2 + C \sum_{n \neq 0} \int_{I_\varepsilon^d} \left| \xi + \frac{2\pi}{\varepsilon}n \right|^{2l} \left| \hat{f}\left(\xi + \frac{2\pi}{\varepsilon}n\right) \right|^2 d\xi \\ &\leq C \|f\|_{H^l}^2, \end{aligned}$$

which shows that K_2 is bounded as required.

Finally we bound K_3 . By definition

$$K_3 = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d \setminus I_\varepsilon^d} |\xi|^{2k} \left| \frac{\hat{f}(\xi)}{\sigma^{(\varepsilon, 2p)}(\xi)} \right|^2 d\xi \leq C \int_{\mathbb{R}^d \setminus I_\varepsilon^d} \left(\frac{|\xi|^k}{\sigma^{(\varepsilon, 2p)}(\xi)} \right)^2 |\hat{f}(\xi)|^2 d\xi.$$

Now using that for $\xi \in \mathbb{R}^d \setminus I_\varepsilon^d$,

$$\frac{|\xi|^k}{\sigma^{(\varepsilon, 2p)}(\xi)} \leq |\xi|^k C \varepsilon^{2p} |\xi|^{2p-2} = C \varepsilon^{2p} \frac{|\xi|^l}{|\xi|^{2+l-k-2p}} \leq C \varepsilon^{2+l-k} |\xi|^l,$$

since $2 + l - k - 2p \geq 0$. This immediately yields $K_3 \leq C \varepsilon^{4+2l-2k} \|f\|_{H^l}^2$ and completes the proof. \square

Theorem 4.2. *With the same assumptions as in Theorem 4.1 we have, for small ε , and $k > d/2 - 2$,*

$$\sup_{m \in \mathbb{Z}^d} |\mathbf{u}^{(\varepsilon)}(m) - u^{(\varepsilon, 2p)}(\varepsilon m)| \leq C \|f\|_{H^{2p+k}} \begin{cases} \varepsilon^{2p+2} & \text{if } k > d/2, \\ \varepsilon^{2p+2} |\log \varepsilon| & \text{if } k = d/2, \\ \varepsilon^{2p+2+k-d/2} & \text{if } k < d/2. \end{cases}$$

Proof. Due to translation invariance it is sufficient to prove that $|\mathbf{u}^{(\varepsilon)}(0) - u^{(\varepsilon, 2p)}(0)|$ is bounded as claimed. Defining $\sigma^{(\varepsilon, 2p)}$ as in the proof of Theorem 4.1, we have

$$\begin{aligned} \mathbf{u}^{(\varepsilon)}(0) - u^{(\varepsilon, 2p)}(0) &= \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} \frac{\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)}{\sigma^{(\varepsilon)}(\xi)} d\xi - \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\hat{f}(\xi)}{\sigma^{(\varepsilon, 2p)}(\xi)} d\xi \\ &= \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} \left(\frac{\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)}{\sigma^{(\varepsilon)}(\xi)} - \frac{\hat{f}(\xi)}{\sigma^{(\varepsilon, 2p)}(\xi)} \right) d\xi \\ &\quad + \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d \setminus I_\varepsilon^d} \frac{\hat{f}(\xi)}{\sigma^{(\varepsilon, 2p)}(\xi)} d\xi =: J_1 + J_2. \end{aligned}$$

By Lemma 4.2 we find that

$$J_1 = \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} \left(\frac{\hat{f}(\xi)\hat{\mu}(\varepsilon\xi)}{\sigma^{(\varepsilon)}(\xi)} - \frac{\hat{f}(\xi)}{\sigma^{(\varepsilon,2p)}(\xi)} \right) d\xi + \sum_{n \neq 0} \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} \frac{\hat{f}(\xi + \frac{2\pi}{\varepsilon}n)\hat{\mu}(\varepsilon\xi + 2\pi n)}{\sigma^{(\varepsilon)}(\xi)} d\xi =: J_{11} + J_{12}.$$

When bounding J_{11} use that (4.13) and (4.4) combined provide the inequality

$$\left| \frac{\hat{\mu}(\varepsilon\xi)}{\sigma^{(\varepsilon)}(\xi)} - \frac{1}{\sigma^{(\varepsilon,2p)}(\xi)} \right| \leq C\varepsilon^2 |\varepsilon\xi|^{2p},$$

and hence

$$|J_{11}| \leq C\varepsilon^{2+2p} \int_{I_\varepsilon^d} |\xi|^{2p} |\hat{f}(\xi)| d\xi.$$

Applying Cauchy’s inequality we obtain that

$$|J_{11}| \leq C\varepsilon^{2+2p} \left[\int_{I_\varepsilon^d} \frac{1}{(1 + |\xi|^2)^k} d\xi \int_{I_\varepsilon^d} (1 + |\xi|^2)^k |\xi|^{4p} |\hat{f}(\xi)|^2 d\xi \right]^{1/2} \leq C(\varepsilon, k, d)\varepsilon^{2+2p} \|f\|_{H^{2p+k}},$$

where

$$C(\varepsilon, k, d) = \begin{cases} C & \text{for } k > d/2, \\ C|\log \varepsilon| & \text{for } k = d/2, \\ C\varepsilon^{k-d/2} & \text{for } k < d/2. \end{cases}$$

When bounding J_{12} we need that

$$\frac{\hat{\mu}(\varepsilon\xi + 2\pi n)}{\sigma^{(\varepsilon)}(\xi)} \leq C\varepsilon^{2p} |\xi + \frac{2\pi}{\varepsilon}n|^{2p-2}, \quad \text{for } \xi \in I_\varepsilon^d. \tag{4.14}$$

When $p \geq 1$ the inequality (4.14) is proved from (4.4) as follows:

$$\frac{\hat{\mu}(\varepsilon\xi + 2\pi n)}{\sigma^{(\varepsilon)}(\xi)} \leq C \frac{|\varepsilon\xi|^{2p}}{|\xi|^2} \leq C\varepsilon^{2p} |\xi|^{2p-2} \leq C\varepsilon^{2p} \left| \xi + \frac{2\pi}{\varepsilon}n \right|^{2p-2},$$

since $2p - 2 \geq 0$ and $|\xi| \leq |\xi + \frac{2\pi}{\varepsilon}n|$. When $p = 0$ we use instead

$$\frac{\hat{\mu}(\varepsilon\xi + 2\pi n)}{\sigma^{(\varepsilon)}(\xi)} \leq C \frac{|\varepsilon\xi|^2}{|\xi|^2 \prod_{j=1}^d (1 + n_j^2)} \leq C \frac{1}{\prod_{j=1}^d (1 + (n_j/\varepsilon)^2)} \leq C \left| \xi + \frac{2\pi}{\varepsilon}n \right|^{-2}.$$

Now that we have proved (4.14) we use it to bound J_{12} as follows:

$$|J_{12}| \leq C \sum_{n \neq 0} \int_{I_\varepsilon^d} \left| \hat{f} \left(\xi + \frac{2\pi}{\varepsilon}n \right) \right| \varepsilon^{2p} \left| \xi + \frac{2\pi}{\varepsilon}n \right|^{2p-2} d\xi = C\varepsilon^{2p} \int_{\mathbb{R}^d \setminus I_\varepsilon^d} |\xi|^{2p-2} |\hat{f}(\xi)| d\xi \leq C\varepsilon^{2p} \left[\int_{\mathbb{R}^d \setminus I_\varepsilon^d} \frac{1}{|\xi|^4 (1 + |\xi|^2)^k} d\xi \right]^{1/2} \left[\int_{\mathbb{R}^d \setminus I_\varepsilon^d} |\xi|^{4p} (1 + |\xi|^2)^k |\hat{f}(\xi)|^2 d\xi \right]^{1/2}.$$

Since $2k > d - 4$ the first factor is bounded by $\varepsilon^{2+k-d/2}$, thus

$$J_{12} \leq C\varepsilon^{2p+2+k-d/2} \|f\|_{H^{2p+k}}.$$

Finally we note that J_2 satisfies

$$|J_2| \leq C \int_{\mathbb{R} \setminus I_\varepsilon^d} |\hat{f}(\xi)| \varepsilon^2 |\varepsilon \xi|^{2p-2} d\xi \leq C\varepsilon^{2p} \int_{\mathbb{R} \setminus I_\varepsilon^d} |\xi|^{2p-2} |\hat{f}(\xi)| d\xi,$$

and thus can be bounded like J_{12} . □

4.3. Homogenization of multi-atomic lattices

The analysis of multi-atomic lattices will closely follow the pattern of the previous section. We first investigate the nature of the inverse symbol, then we formulate the discrete lattice problem and define an approximate solution. Finally, we present a convergence proof. For brevity, we consider only $O(\varepsilon^2)$ -accurate approximations.

Since the symbol $\sigma^{(us)}(\xi)$ is a $q \times q$ matrix, its inverse is given by the formula

$$\sigma^{(us)}(\xi) = (\det \sigma^{(us)}(\xi))^{-1} L(\xi), \tag{4.15}$$

where $L(\xi)$ is the matrix of co-determinants of $\sigma^{(us)}(\xi)$. Corollary 4.4 of Ref. 13 asserts that

$$\det \sigma^{(us)}(\xi) = \xi \cdot M\xi + \sum_{j=2}^{\infty} a_j(\xi), \tag{4.16}$$

where M is a positive definite matrix and the sum consists of high order polynomials, $a_j \in \Pi^{2j}$. Moreover, Theorem 4.9 of Ref. 13 asserts that the lowest order terms of all the co-determinants of $\sigma^{(us)}(\xi)$ are identical; this means that the Taylor expansion of the $\kappa\lambda$ entry of $L(\xi)$ has the form

$$[L(\xi)]_{\kappa\lambda} = c_0 + \mathbf{i}v^{(\kappa\lambda)} \cdot \xi + O(|\xi|^2), \tag{4.17}$$

where $c_0 > 0$ is a constant, and $v^{(\kappa\lambda)} \in \mathbb{R}^d$ are vectors. Combining (4.15)–(4.17) with the relation $\sigma^{(\varepsilon)}(\xi) = \varepsilon^{-2}\sigma^{(us)}(\varepsilon\xi)$, we find that

$$\left[\sigma^{(\varepsilon)}(\xi)^{-1} \right]_{\kappa\lambda} = \varepsilon^2 \left(\varepsilon^2 \xi \cdot M\xi + \sum_{j=2}^{\infty} \varepsilon^{2j} a_j(\xi) \right)^{-1} (c_0 + \mathbf{i}v^{(\kappa\lambda)} \cdot \varepsilon\xi + O(|\varepsilon\xi|^2)). \tag{4.18}$$

The $O(\varepsilon^2)$ -accurate Taylor expansion of $[\sigma^{(\varepsilon)}(\xi)^{-1}]_{\kappa\lambda}$ is then

$$[S^{(\varepsilon,1)}(\xi)]_{\kappa\lambda} = (\xi \cdot M\xi)^{-1} (c_0 + \varepsilon \mathbf{i}v^{(\kappa\lambda)} \cdot \xi).$$

We will next state conditions on the load function $f(x) = [f(x, 1), \dots, f(x, q)]$ under which the lattice equilibrium equation is well posed. To this end, we split f

into a cell wise average f_a and a vector of differences f_d by setting

$$f_a(x) := \frac{1}{q} \sum_{\kappa=1}^q f(x, \kappa), \quad f_d(x, \kappa) := f(x, \kappa) - f_a(x).$$

We require that $f_a \in L^1 \cap L^2$ and that $f_d \in L^2$. Then we form the projection of f onto a lattice function, $\mathbf{f}^{(\varepsilon)} = P_\varepsilon f$, and formulate the lattice equilibrium equation by

$$\begin{cases} \mathbf{A}^{(\varepsilon)} \mathbf{u}^{(\varepsilon)} = \mathbf{f}^{(\varepsilon)}, \\ \|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}} < \infty. \end{cases} \tag{4.19}$$

An explicit solution is again given by

$$\mathbf{u}^{(\varepsilon)}(m) := \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} e^{-i(\varepsilon m) \cdot \xi} \sigma^{(\varepsilon)}(\xi)^{-1} \tilde{\mathbf{f}}^{(\varepsilon)}(\xi) d\xi. \tag{4.20}$$

Proposition 4.3. *The function $\mathbf{u}^{(\varepsilon)}$ defined by (4.20) is a solution of (4.19). This solution is unique up to a constant and satisfies $\|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}} \leq C(\|f_a\|_{L^1} + \|f_a\|_{L^2} + \varepsilon\|f_d\|_{L^2})$.*

Proof. Combining (4.9) with the relation $\mathbf{u}^{(\varepsilon)} = [\sigma^{(\varepsilon)}]^{-1} \mathbf{f}^{(\varepsilon)}$, we find that

$$\|\mathbf{u}^{(\varepsilon)}\|_{\mathbf{A}^{(\varepsilon)}}^2 = \frac{1}{(2\pi)^d} \int_{I_\varepsilon^d} \overline{\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)} \cdot [\sigma^{(\varepsilon)}(\xi)]^{-1} \tilde{\mathbf{f}}^{(\varepsilon)}(\xi) d\xi.$$

From (4.18), it follows that

$$\overline{\tilde{\mathbf{f}}^{(\varepsilon)}(\xi)} \cdot [\sigma^{(\varepsilon)}(\xi)]^{-1} \tilde{\mathbf{f}}^{(\varepsilon)}(\xi) \leq C \left(\max\{|\xi|^{-2}, 1\} |\tilde{\mathbf{f}}_a^{(\varepsilon)}(\xi)|^2 + \varepsilon^2 |\tilde{\mathbf{f}}_d^{(\varepsilon)}(\xi)|^2 \right).$$

The remainder of the proof is analogous to the proof of Proposition 4.1. □

Next we define the homogenized solution by

$$u^{(1,\varepsilon)} := \mathcal{F}^{-1}[S^{(1,\varepsilon)} \hat{f}]. \tag{4.21}$$

As long as $f \in L^2$ and $f_a \in L^1$, this is well defined as a tempered distribution. In order for this function to be continuous, somewhat sharper conditions on f are required than what was the case for mono-atomic lattices. The reason is that for large ξ , $S^{(1,\varepsilon)}(\xi)$ decays as $\varepsilon|\xi|^{-1}$ rather than $|\xi|^{-2}$.

Proposition 4.4. *The function $u^{(\varepsilon,1)}$ defined by (4.21) is continuous if $f \in L^1 \cap H^{2+k}$ for some $k > d/2 - 1$.*

We can now state and prove the core convergence result for multi-atomic lattices.

Theorem 4.3. *Suppose that $d \geq 3$, let $\mathbf{u}^{(\varepsilon)}$ be the solution of (4.20) with $\mathbf{f}^{(\varepsilon)} = \mathbf{P}_\varepsilon f$, and let $u^{(\varepsilon,1)}$ be the solution of (4.21). Then if ε is small and $k > d/2 - 1$,*

$$\sup_{m \in \mathbb{Z}^d} |\mathbf{u}^{(\varepsilon)}(m) - u^{(\varepsilon,1)}(\varepsilon m)| \leq C \|f\|_{H^{2p+k}} \begin{cases} \varepsilon^2 & \text{if } k > d/2, \\ \varepsilon^2 |\log \varepsilon| & \text{if } k = d/2, \\ \varepsilon^{2+k-d/2} & \text{if } k < d/2. \end{cases}$$

Proof. The proof follows the proof of Theorem 4.2 closely. Simply replace $[\sigma^{(\varepsilon,2p)}(\xi)]^{-1}$ by the matrix $S^{(\varepsilon,1)}(\xi)$ and then split the error into J_{11} , J_{12} and J_2 as before. Bound J_{11} using

$$|\hat{\mu}(\varepsilon\xi)[\sigma^{(\varepsilon)}(\xi)^{-1}]_{\kappa\lambda} - [S^{(\varepsilon,1)}(\xi)]_{\kappa\lambda}| \leq C\varepsilon^2, \quad \forall \xi \in I_\varepsilon^d.$$

The bound for J_{12} is also entirely analogous since $|\sigma^{(\varepsilon)}(\xi)^{-1}|_{\kappa\lambda} \leq C|\xi|^{-2}$ in I_ε^d .

The only real difference occurs in the bound for J_2 . Since $[S^{(\varepsilon,1)}(\xi)]_{\kappa\lambda}$ decays somewhat more slowly than $|\xi|^{-2}$ we get

$$\begin{aligned} |J_2| &\leq \max_{\kappa} \sum_{\lambda=1}^q \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d \setminus I_\varepsilon^d} |[S^{(\varepsilon,1)}(\xi)]_{\kappa\lambda}| |\hat{f}_\lambda(\xi)| d\xi \\ &\leq C \sum_{\lambda=1}^q \int_{\mathbb{R}^d \setminus I_\varepsilon^d} \left(\frac{1}{|\xi|^2} + \frac{\varepsilon}{|\xi|} \right) |\hat{f}_\lambda(\xi)| d\xi \\ &\leq C\varepsilon \sum_{\lambda=1}^q \int_{\mathbb{R}^d \setminus I_\varepsilon^d} \frac{1}{|\xi|} |\hat{f}_\lambda(\xi)| d\xi \\ &\leq C\varepsilon \sum_{\lambda=1}^q \left[\int_{\mathbb{R}^d \setminus I_\varepsilon^d} \frac{1}{|\xi|^2(1+|\xi|^2)^k} d\xi \int_{\mathbb{R}^d \setminus I_\varepsilon^d} (1+|\xi|^2)^k |\hat{f}(\xi)|^2 d\xi \right]^{1/2}. \end{aligned}$$

We see that the bound evaluates to the same quantity, $C\varepsilon^{2+k-d/2} \|f\|_{H^k}$, as in the mono-atomic case, but that a necessary condition for convergence of the first integral is that $k > d/2 - 1$. □

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