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MATHEMATICAL FRAMEWORK FOR LATTICE PROBLEMS

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Dedicated to Professor Max Gunzburger on the occasion of his 60th birthday

Abstract. We propose a mathematical framework to effectively study lattice materials with periodic and non-periodic structures over entire spaces in one, two, and three dimensions. The existence and uniqueness of solutions for periodic lattice problems with absolute terms are proved in discrete Sobolev spaces. By Fourier transform discrete lattice problems are converted to semi-discrete problems for which similar results are establish in semi-discrete Sobolev spaces. For lattice problems without absolute terms, additional conditions are imposed on data for the existence and uniqueness of solutions in discrete energy spaces in one,two and three dimensions. Two concrete examples are analyzed in the proposed mathematical framework. The mathematical framework, methodology and techniques in this paper can be utilized or generalized to non-periodic lattices on entire spaces and boundary value problems on lattices.

Key Words. lattice, cell, multi-scale, periodic structures, grids, absolute term, linear interpolation, Fourier transform.

1. Introduction

Lattice materials are porous materials consisting of periodic cells or non-periodic cells. The cells are composed of rods, or shells, or solid structures. The size of cell is usually small with respect to the size of the body filled with the lattice materials. The lattice materials with simple micro-structures are characterized by a single length scale, for instance, Lattice Block Materials which are developed by JAMCORP corporation. The hierarchic lattice materials have hierarchic multi-scale structures. In either case, we deal with a multi-scale problem. The lattice materials can offer significantly higher strength-to-weight and stiffness-to-weight ratio than their base materials. Hence they can be potentially advantageous in practical engineering applications.

Various micro mechanical models for the lattice materials with periodic and non-periodic structures have been studied for the analysis of the overall properties, crack propagation, etc. There are papers addressing these problems, especially in the mechanics, material science, and physics literatures [8, 12, 17, 19, 21]. For mathematical theory which is related to the problem of the lattice materials we refer to the book [5] and her various papers,e.g. [4, 6, 7]. Recently, asymptotic analysis for periodic lattice problem and multi-scale numerical method based on Fourier transform and homogenization appeared in [13, 14, 15, 20]. In these papers, the scale of cells is assumed so small that asymptotic arguments can be utilized and only problems in presence of absolute term are addressed so that the corresponding bilinear form satisfies the inf-sup condition on a pair of Sobolev spaces. In practical

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applications, these assumptions may not be valid, a substantial adjustment and generalization are needed.

In our paper we focus on periodic lattice materials composed of rods and balls in entire spaces. Such a structure results in a system of difference equations with infinite number of unknowns. We intend to establish a mathematical framework for systematical research on such lattice problems in entire spaces of one, two, and three dimensions. This framework can be used or generalized for lattice materials with complicated micro-structures such as plates and shells, or three dimensional solid structures. The analysis and method developed in this paper can be utilized for boundary value problems on lattices and non-periodic lattice problems, which will be illustrated in a coming paper [9, 10].

For lattice problems with absolute term, the existence and uniqueness of the solutions of variational equation and equilibrium equation are proved in these discrete Sobolev spaces over lattices. The Fourier transform is a powerful tool for studying periodic lattice problems, deriving homogenization results and designing effective computations. The Fourier transform converts discrete lattice problems to semi-discrete problems for which the theorem on existence and uniqueness of solutions is proved in proper semi-discrete Sobolev spaces.

For the lattice problems without absolute terms, we impose additional condition on the data, and substantially modify the discrete Sobolev spaces for the existence and uniqueness of solutions. For proving the results in two and three dimensional lattice problems, we need to utilize the properties of functions in $H^1(R^d), d = 2, 3$, which are attached in Appendix. To utilizing these properties we extend a grid function defined on a lattice to a continuous and piecewise linear function defined over whole space $R^d, d = 2, 3$ based on a proper triangular or tetrahedral partition of R^d, and establish the equivalence of discrete Sobolev norms of grid functions and Sobolev norms of its extension. The techniques of partition and extension can be generalized to non-periodic lattice problems.

The paper is organized as the follows. In Section 2, we first introduce various discrete Sobolev and energy spaces, and prove the existence and uniqueness of the solutions of variational equation for the lattice problems with absolute term. With help of Fourier transform, we convert a fully discrete problem over lattices to a semi-discrete problem over a combination of a bounded domain and the micro structure of the cells. The existence and uniqueness of the solutions for the semi-discrete problems are proved, which are parallel to those for fully discrete problems. In Section 3 we address the lattice problems without absolute terms in the energy spaces for data in the weighted discrete L^2 spaces, which lead to the existence and uniqueness of the solutions. We develop a representation formula for the solutions of the lattice problems in terms of Fourier transform and its inverse in Section 4. We present two examples of lattice problem in the last section, one is a one-dimensional model, another is two-dimensional model. Some concrete formulas for these examples will be derived, which are very helpful to understand lattice problems in general setting. In Appendix, we give some important properties of functions in $H^1(R^d), d = 2, 3$, which are essential to analysis of lattice problems without absolute terms.

2. General Setting in d-dimensions

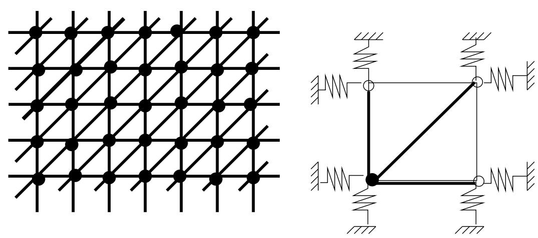
2.1. Lattice in entire spaces

Let Q be a master cell in $\mathbf{R}^d$ with unit size. A typical lattice and its master cell are shown in Fig. 2.1. We assume that the master cell is a d-dimensional cube without losing generality because a non-cubic cell can be mapped to cube by a linear transformation, e.g. as shown in Fig 2.2. The master cell is extended periodically in entire space by an integer translation:

$$Q_m = \{y \in \mathbf{R}^d \big| y = x + \sum_{i=1}^{d} m_i t^{(i)}, x \in Q\}, m \in \mathcal{Z}^d. \tag{2.1}$$

where $\mathcal{Z} = \{0, \pm1, \pm2, \dots\}$ denotes the set of all integers, and $t^{(i)}$ is a unit vector in the x_i axis. There is a set K_Q of nodes $\{x^{(\kappa)}\}_{\kappa=1}^q$ in the master cell Q, and a set K_m is the integer translation of K_Q by

$$K_m = \{x^{(m,\kappa)} = x^{(\kappa)} + \sum_{i=1}^{d} m_i t^{(i)}, x^{(\kappa)} \in K_Q\}, m \in \mathcal{Z}^d. \tag{2.2}$$



(a) A lattice (b) Master cell Q furnished with springs

Fig. 2.1 A periodic lattice in two dimension

Note that the indices κ of nodes in each cell Q_m are the same although the locations of these points in different cells are different. Hence we denote the set of indices $\{1, 2, \dots, q\}$ by $\mathcal{K}$. Without losing generality, we assume that the cells Q_m's and sets K_m's are mutually disjoint, namely,

$$Q_n \cap Q_m = \emptyset, K_n \cap K_m = \emptyset, n \neq m, n, m \in \mathcal{Z}^d.$$

For example, $Q = [0, 1)^2$ and nodes within such a cell, shown in Fig. 5.2, will satisfy the above assumption.

We now further specify the connectivity of lattices. By $\mathbf{b}^{(m,\kappa,n,\lambda)}$, we denote an elastic rod connecting the nodes $x^{(m,\kappa)}$ and $x^{(n,\lambda)}$ with intersect area A and length $b^{(m,\kappa,n,\lambda)}$. We assume that

(C.1) Each node is connected to others by the rods, at least one node and at most M nodes;

(C.2) Any two nodes $x^{(m,\kappa)}$ and $x^{(n,\lambda)}$ are linked by the shortest chain $L_{m,\kappa,n,\lambda}$: $x^{(m,\kappa)} = x^{(n_1,\lambda_1)} \to x^{(n_2,\lambda_2)} \to x^{(n_3,\lambda_3)} \to \cdots \to x^{(n_s,\lambda_s)} = x^{(n,\lambda)}$ such that $x^{(n_t,\lambda_t)}$ is connected to $x^{(n_{t+1},\lambda_{t+1})}, 1 \leq t \leq s-1$, and

$$|x^{(m,\kappa)} - x^{(n,\lambda)}| \leq \sum_{1 \leq t \leq s-1} |x^{(n_{t+1},\lambda_{t+1})} - x^{(n_t,\lambda_t)}| \leq \eta |x^{(m,\kappa)} - x^{(n,\lambda)}|,$$

where η is independent of m, n, κ and λ;

(C.3) The length of rods are uniformly bounded, i.e. for any $x^{(m,\kappa)}$ and $x^{(n,\lambda)}$ which are connected, there holds

$$b_1 \leq b^{(m,\kappa,n,\lambda)} = |x^{(m,\kappa)} - x^{(n,\lambda)}| \leq b_2.$$

To effectively describe the connectivity of the lattice, we introduce B_κ and $B_{\kappa,\lambda}$

$$B_\kappa = \{(n,\lambda) \in \mathcal{Z}^d \times \mathcal{K} \text{ such that } x^{(0,\kappa)} \text{ and } x^{(n,\lambda)} \text{ are connected } \} \qquad (2.3a)$$

and

$$B_{\kappa,\lambda} = \{n \in \mathcal{Z}^d \text{ such that } (n,\lambda) \in B_\kappa\}. \qquad (2.3b)$$

B_κ and $B_{\kappa,\lambda}$, based on the connectivity of the nodes $x^{(0,\kappa)}$ in the cell Q_0, can be periodically generalized to sets $B_\kappa^{(m)}$ and $B_{\kappa,\lambda}^{(m)}$ for all $m \in \mathcal{Z}^d$ by the integer translation. Due to the periodicity , it is easy to verify that

$$n \in B_{\kappa,\lambda} \text{ if and only if } -n \in B_{\lambda,\kappa}. \qquad (2.4)$$

For the sake of simplicity, we will omit cell index m whenever $m = 0$. For instance, we write $x^{(0,\kappa)} = x^{(\kappa)}$, $\mathbf{b}^{(0,\kappa,n,\lambda)} = \mathbf{b}^{(\kappa,n,\lambda)}$, etc. By $E^{(\kappa,n,\lambda)}$ we denote the Young's modules of the elastic rod $\mathbf{b}^{(\kappa,n,\lambda)}$. By (2.4) it holds that

$$E^{(\kappa,n,\lambda)} = E^{(\lambda,-n,\kappa)}. \qquad (2.5)$$

A lattice is characterize by the local structure $\mathcal{K}$, the global and periodical translation on $\mathcal{Z}^d$, and the connectivity B_κ. We now denote the lattice with the above structures by $\mathcal{G} = \mathcal{G}(\mathcal{K}, \mathcal{Z}^d, B_\kappa)$.

2.2. A truss problem on unscaled lattice

Let $u = (u_m)_{m\in Z^d}$ and $u_m = (u_{m,\kappa})_{\kappa\in\mathcal{K}}$ be a grid functions on $\mathcal{G}$ and $\mathcal{K}$, respectively, and each $u_{m,\kappa}$ is a vector $(u^1_{m,\kappa}, u^2_{m,\kappa}, \ldots, u^s_{m,\kappa})^\top$ with s-components. In one dimension, $s = d = 1$, and $u_{m,\kappa}$ denotes the displacement for elastic rods or the temperature of heat problems at the node $x^{(m,\kappa)}$. For two and three dimensional heat transform problems , $u_{m,\kappa}$ denotes the temperature if $s = 1$. For two and three dimensional elastic problem, $s \geq d$. If the connections of rods are non-rigid, then $s = d$, and $u_{m,\kappa}$ denotes the displacement at the node $x^{(m,\kappa)}$. If the connection of rods are rigid, then $s = d + 3^{d-2}$ for $d = 2, 3$, and $u_{m,\kappa}$ denotes the displacement and rotation at the node $x^{(m,\kappa)}$. We furnish the rods with springs in the axis directions at each node with Hook's coefficients denoted by diagonal matrices $\mathbf{C}^{(m,\kappa)} = \mathbf{C}^{(\kappa)}, m \in \mathcal{Z}^d, \kappa \in \mathcal{K}$. We assume that the ratio of the length of rods and the intersect area A of rods >> 1. For the convenience to characterize the nature of our methodology, we will focus on the case that s=d, namely, a trust problem without bending.

If external forces exert on the rods at the nodes, denoted by $f = (f_m, m \in Z^d)$ with $f_m = (f_{m,1}, f_{m,2}, \cdots, f_{m,q})$, we have the equilibrium equation

$$-\sum_{(n,\lambda)\in B_\kappa} \mathbf{E}^{(\kappa,n,\lambda)} \left(u_{m+n,\lambda} - u_{m,\kappa}\right) + \mathbf{C}^{(\kappa)} u_{m,\kappa} = f_{m,\kappa}, \forall m \in \mathcal{Z}^d, \forall \kappa \in \mathcal{K}. \quad (2.6)$$

with

$$\mathbf{E}^{(\kappa,n,\lambda)} = AE^{(\kappa,n,\lambda)} \frac{(x^{(n,\lambda)} - x^{(\kappa)})}{|x^{(n,\lambda)} - x^{(\kappa)}|^2} \frac{(x^{(n,\lambda)} - x^{(\kappa)})^\top}{|x^{(n,\lambda)} - x^{(\kappa)}|^2} \qquad (2.7a)$$

and

$$\mathbf{C}^{(\kappa)} = diag(C_1^{(\kappa)}, C_2^{(\kappa)}, \ldots, C_d^{(\kappa)}), \qquad C_\ell^{(\kappa)} \geq 0. \qquad (2.7b)$$

Let $H^1(\mathcal{G})$ and $L^2(\mathcal{G})$ be the Sobolev spaces over the lattice $\mathcal{G}$ with the norms

$$\|u\|^2_{L^2(\mathcal{G})} = \sum_{m\in\mathcal{Z}^d} \sum_{\kappa\in\mathcal{K}} |u_{m,\kappa}|^2 \qquad (2.8)$$

and

$$\|u\|^2_{H^1(\mathcal{G})} = |u|^2_{H^1(\mathcal{G})} + \|u\|^2_{L^2(\mathcal{G})} \qquad (2.9a)$$

where $|u|_{H^1(\mathcal{G})}$ is the semi-norm,

$$|u|^2_{H^1(\mathcal{G})} = \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}}\sum_{(n,\lambda)\in B_\kappa} \frac{|u_{m+n,\lambda}-u_{m,\kappa}|^2}{|x^{(m+n,\lambda)}-x^{(m,\kappa)}|^2}. \tag{2.9b}$$

The corresponding variational problem is defined as

$$B(u,v) = F(v) \tag{2.10}$$

with the bilinear form on $H^1(\mathcal{G})\times H^1(\mathcal{G})$

$$\begin{aligned} B(u,v) \;&= \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}}\Big\{\langle \mathbf{C}^{(\kappa)}u_{m,\kappa}, v_{m,\kappa}\rangle \\ &+\sum_{(n,\lambda)\in B_\kappa}\langle\frac{1}{2}\mathbf{E}^{(\kappa,n,\lambda)}(u_{m+n,\lambda}-u_{m,\kappa}),(v_{m+n,\lambda}-v_{m,\kappa})\rangle\Big\} \end{aligned} \tag{2.11}$$

and the linear functional on $H^1(\mathcal{G})$

$$F(v) = \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}}\langle f_{m,\kappa}, v_{m,\kappa}\rangle, \tag{2.12}$$

where $\langle x,y\rangle = \sum_{j=1}^d x_j y_j$ is the inner product of two vectors in $\mathbf{R}^d$, and $|x|^2 = \langle x,x\rangle$.

The strain energy of the trust is

$$\begin{aligned} G(u) \;&= B(u,u) = \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}}\Big\{\langle \mathbf{C}^{(\kappa)}u_{m,\kappa}, u_{m,\kappa}\rangle \\ &+\sum_{(n,\lambda)\in B_\kappa}\langle\frac{1}{2}\mathbf{E}^{(\kappa,n,\lambda)}(u_{m+n,\lambda}-u_{m,\kappa}),(u_{m+n,\lambda}-u_{m,\kappa})\rangle\Big\}. \end{aligned} \tag{2.13}$$

The energy space denoted by $E(\mathcal{G})$ is the family of all grid functions u on $\mathcal{G}$ with finite energy $G(u)$, and $\|u\|_{E(\mathcal{G})}= G(u)^{1/2}$ is referred as the energy norm.

Note that

$$\begin{aligned} &\langle\mathbf{E}^{(\kappa,n,\lambda)}\frac{(u_{m+n,\lambda}-u_{m,\kappa})}{|x^{(m+n,\lambda)}-x^{(m,\kappa)}|},\frac{(u_{m+n,\lambda}-u_{m,\kappa})}{|x^{(m+n,\lambda)}-x^{(m,\kappa)}|}\rangle \\ &= \frac{E}{|x^{(m+n,\lambda)}-x^{(m,\kappa)}|^4}|\langle x^{(m+n,\lambda)}-x^{(m,\kappa)}, u_{m+n,\lambda}-u_{m,\kappa}\rangle|^2 \\ &= \frac{E}{|x^{(m+n,\lambda)}-x^{(m,\kappa)}|^2}|u_{m+n,\lambda}-u_{m,\kappa}|^2 cos^2\phi_{\kappa,n,\lambda} \end{aligned}$$

where $\phi_{\kappa,n,\lambda}$ is the angle between the vectors $x^{(m+n,\lambda)}-x^{(m,\kappa)}$ and $u_{m+n,\lambda}-u_{m,\kappa}$. For $s=1$, u is scale, $cos\phi_{\kappa,n,\lambda}\equiv 1$. Hence

$$\langle\mathbf{E}^{(\kappa,n,\lambda)}\frac{(u_{m+n,\lambda}-u_{m,\kappa})}{|x^{(m+n,\lambda)}-x^{(m,\kappa)}|},\frac{(u_{m+n,\lambda}-u_{m,\kappa})}{|x^{(m+n,\lambda)}-x^{(m,\kappa)}|}\rangle = 0 \tag{2.14}$$

if and only if $u_{m+n,\lambda}-u_{m,\kappa}\equiv 0$ for all $m\in\mathcal{Z}^d, \kappa\in\mathcal{K}$, i.e. u is a constant function on $\mathcal{G}$. For $s=d=2, cos\phi_{\kappa,n,\lambda}\not\equiv 1$, then (2.15) holds if and only if $u_{m+n,\lambda}-u_{m,\kappa}\equiv 0$ or $(u_{m+n,\lambda}-u_{m,\kappa})\perp(x^{(m+n,\lambda)}-x^{(m,\kappa)})$, i.e. $u_{m,\kappa}=\sum_{1\le i\le 2}c_ie_i+c_3\tau_3$, where $e_i, 1\le i\le 2$ is a unit vector in the x_i-axis, which denotes the translation, $\tau_3 = (x_2^{(m,\kappa)}, -x_1^{(m,\kappa)})^\top$ for all $m\in\mathcal{Z}^d, \kappa\in\mathcal{K}$,which denotes the rotation. Similarly, (2.14) holds for $s=d=3$ if and only if $u_{m,\kappa}=\sum_{1\le i\le 3}c_ie_i+c_{i+3}\tau_{i+3}$ where $e_i, 1\le i\le 3$ is a unit vector in the x_i-axis, which denotes the translation, $\tau_4 = (x_2^{(m,\kappa)}, -x_1^{(m,\kappa)}, 0)^\top$, $\tau_5 = (0, x_3^{(m,\kappa)}, -x_2^{(m,\kappa)})^\top$, and $\tau_6 = (-x_3^{(m,\kappa)}, 0, x_1^{(m,\kappa)})^\top$ for all $m\in\mathcal{Z}^d, \kappa\in\mathcal{K}$,which denote the rotations around the axes.

Let

$$\mathcal{P}_r = P_c = \text{ all constant functions on } \mathcal{G} \text{ for } s = 1, 1 \le d \le 3 \tag{2.15a}$$

and

$$\mathcal{P}_r = span\{e_i, 1 \le i \le d, \tau_{d+j}, 1 \le j \le d(d-1)/2\} \text{ for } 1 < s = d \le 3. \tag{2.15b}$$

which denotes the rigid body motions for truss problems in two and three dimensions. Then we conclude with the following lemma based the analysis above.

Proposition 2.1 Let $\mathcal{P}_r$ be the set of grid functions on $\mathcal{G}$ as given in (2.15). Then

$$\langle \mathbf{E}^{(\kappa,n,\lambda)} \frac{(u_{m+n,\lambda} - u_{m,\kappa})}{|x^{(m+n,\lambda)} - x^{(m,\kappa)}|}, \frac{(u_{m+n,\lambda} - u_{m,\kappa})}{|x^{(m+n,\lambda)} - x^{(m,\kappa)}|} \rangle = 0$$

if and only if $u \in \mathcal{P}_r$.

A lattice is called mechanically rigid if the strain energy is zero if and only if the motion of lattices is rigid body motion. All lattices considered in this paper are assumed rigid.

Lemma 2.2 The variational form B on $H^1(\mathcal{G}) \times H^1(\mathcal{G})$ given in (2.10) is continuous, and it is coercive if $\mathbf{C}^{(\kappa)} \not\equiv 0$ for all $\kappa \in \mathcal{K}$.

Proof. Note that

$$\frac{(x^{(n,\lambda)} - x^{(\kappa)})^T}{|x^{(n,\lambda)} - x^{(\kappa)}|} \frac{(x^{(n,\lambda)} - x^{(\kappa)})}{|x^{(n,\lambda)} - x^{(\kappa)}|} = (cos\theta_1, \cdots, cos\theta_d)^T (cos\theta_1, \cdots, cos\theta_d)$$

where θ_ℓ is the angle between the rod $\mathbf{b}^{(\kappa,n,\lambda)}$ and the x_ℓ-axis. We have immediately

$$|B(u,v)| \le C \|u\|_{H^1(\mathcal{G})} \|v\|_{H^1(\mathcal{G})}$$

with

$$C = Max\{ \max_{n \in B_{\kappa,\lambda}, \kappa, \lambda \in \mathcal{K}} E^{(\kappa,n,\lambda)}, \max_{1 \le \ell \le d, \kappa \in \mathcal{K}} C_\ell^{(\kappa)} \}.$$

If $\mathbf{C}^{(\kappa)} > 0$ for all $\kappa \in \mathcal{K}$, then

$$B(u,u) \ge d_1 |u|^2_{H^1(\mathcal{G})} + d_2 \|u\|^2_{L^2(\mathcal{G})}$$

with

$$d_1 = \min_{n \in B_{\kappa,\lambda}, \kappa, \lambda \in \mathcal{K}} E^{(\kappa,n,\lambda)} > 0, \;\; d_2 = \min_{1 \le \ell \le d, \kappa \in \mathcal{K}} C_\ell^{(\kappa)} > 0.$$

Therefore

$$B(u,u) \ge d \|u\|^2_{H^1(\mathcal{G})}$$

with $d = min\{d_1, d_2\}$.

If $\mathbf{C}^{(\kappa)} = 0$ for some $\kappa \in \mathcal{K}$, but there is at least one $\mathbf{C}^{(\kappa)} > 0$, e.g. $C_\ell^{(\kappa_0)} > 0$ for some $\kappa_0 \in \mathcal{K}$ and $\ell = 1, 2, \ldots, d$, and $\mathbf{C}^{(\kappa)} = 0$ (null matrix) for all other $\kappa \in \mathcal{K}$, we have

$$B(u,u) \ge d_1 |u|^2_{H^1(\mathcal{G})} + \sum_{m \in \mathcal{Z}^d} \langle \mathbf{C}^{(\kappa_0)} u_{m,\kappa_0}, u_{m,\kappa_0} \rangle.$$

Note that

$$\|u\|^2_{L^2(\mathcal{G})} = \sum_{m \in \mathcal{Z}^d} \sum_{\kappa \in \mathcal{K}} |u_{m,\kappa}|^2 \le 2 \sum_{m \in \mathcal{Z}^d} \Big(\sum_{\kappa \in \mathcal{K}} |u_{m,\kappa} - u_{m,\kappa_0}|^2 + |u_{m,\kappa_0}|^2 \Big)$$

$x^{(m,\kappa)}$ and $x^{(m,\kappa_0)}$ may not be connected, but they are linked by a chain L_{m,κ,m,κ_0}: $x^{(m,\kappa)} = x^{(n_1,\lambda_1)} \to x^{(n_2,\lambda_2)} \to \cdots \to x^{(n_s,\lambda_s)} = x^{(m,\kappa_0)}$, and due to the assumptions (C.2) and (C.3), there holds

$$\begin{aligned} sb_1 &\le |x^{(m,\kappa)} - x^{(m,\kappa_0)}| \le \sum_{1\le t\le s-1} |x^{(n_{t+1},\lambda_{t+1})} - x^{(n_t,\lambda_t)}| \\ &\le \eta |x^{(m,\kappa)} - x^{(m,\kappa_0)}| \le \eta d_Q \end{aligned}$$

where d_Q is the diameter of the master cell Q, which implies that the number s of the nodes on the chain is uniformly bounded,

$$s \le \frac{\eta d_Q}{b_1}. \tag{2.16}$$

Therefore, we have

$$\sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}} |u_{m,\kappa} - u_{m,\kappa_0}|^2 \le C \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}}\sum_{(n,\lambda)\in B_\kappa} |u_{m,\kappa} - u_{n+m,\lambda}|^2.$$

This leads directly to

$$\begin{aligned} \|u\|^2_{L^2(\mathcal{G})} &\le C\Big(|u|^2_{H^1(\mathcal{G})} + \frac{1}{C^0}\sum_{m\in\mathcal{Z}^d} \langle \mathbf{C}^{(\kappa_0)} u_{m,\kappa_0}, u_{m,\kappa_0}\rangle\Big) \\ &\le C\Big(\frac{1}{d_1} B(u,u) + \frac{1}{C^0}\sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}} \langle \mathbf{C}^{(\kappa)} u_{m,\kappa}, u_{m,\kappa}\rangle\Big) \le \frac{1}{\hat{d}_2} B(u,u) \end{aligned}$$

with $\hat{d}_2 = (\frac{C}{d_1} + \frac{C}{C^0})^{-1}$, and $C^0 = \min_{1\le \ell\le d}\{C_\ell^{(\kappa_0)}\} > 0$, which implies

$$B(u,u) \ge \frac{d_1}{2}|u|^2_{H^1(\mathcal{G})} + \frac{\hat{d}_2}{2}\|u\ |^2_{L^2(\mathcal{G})} \ge d\|u\|^2_{H^1(\mathcal{G})}$$

with $d = \frac{1}{2}\min\{d_1, \hat{d}_2\}$. □

Theorem 2.3 Suppose that $\mathbf{C}^{(\kappa)} \not\equiv 0$ for all $\kappa \in \mathcal{K}$. Then, for any $f \in (H^1(\mathcal{G}))^{-1}$, the variational equation (2.7) has a unique solution $u \in H^1(\mathcal{G})$, and

$$\|u\|_{H^1(\mathcal{G})} \le C\|f\|_{(H^1(\mathcal{G}))^{-1}}.$$

In particular, if $f \in L^2(\mathcal{G})$, there holds

$$\|u\|_{H^1(\mathcal{G})} \le C\|f\|_{L^2(\mathcal{G})}. \tag{2.17}$$

Proof. The theorem follows from the previous lemma and Lax-Milgram Theorem. □

Remark 2.1 If $C_\ell^{(\kappa)} \not\equiv 0$ for all $\kappa \in \mathcal{K}$, the energy norm $\|u\|_{E(\mathcal{G})}$ is equivalent to the norm $\|u\|_{H^1(\mathcal{G})}$. If $C_\ell^{(\kappa)} \equiv 0$, $\|u\|_{E(\mathcal{G})}$ is equivalent to the semi-norm $|u|_{H^1(\mathcal{G})}$. The bilinear form B and linear functional F are defined on energy space $E(\mathcal{G})$, which is no longer a normed space. Therefore Theorem 2.3 can not stand because the energy space $E(\mathcal{G})$ is not imbeded in $L^2(\mathcal{G})$.

In next theorem we deal with the relation between the solution of the equilibrium equation (2.6) and the solution of the variational equation (2.10).

Theorem 2.4 If $u \in H^1(\mathcal{G})$ is the solution of the variational equation (2.10), then it satisfies the equilibrium equation (2.6). Vice versa, If $u \in H^1(\mathcal{G})$ solves the equilibrium equation (2.6), it satisfies the variational equation (2.10).

Proof. We first prove that the solution u of the equilibrium equation (2.6) satisfies the variation equation (2.10). For $v \in H^1(\mathcal{G})$, multiplying (2.6) with $v_{m,k}$ and summarizing with respect to m and κ, we have

$$- \sum_{m\in\mathcal{Z}^d}\sum_{\kappa,\lambda\in\mathcal{K}}\sum_{n\in B_{\kappa,\lambda}} \langle \mathbf{E}^{(\kappa,n,\lambda)}\left(u_{m+n,\lambda}-u_{m,\kappa}\right), v_{m,\kappa}\rangle$$
$$+ \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}}\langle \mathbf{C}^{(\kappa)}u_{m,\kappa}, v_{m,\kappa}\rangle = \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}}\langle f_{m,\kappa}, v_{m,\kappa}\rangle.$$

The above sums exist since $u, v \in H^1(\mathcal{G})$. Letting $m+n = m'$ and $n = -n'$, we get

$$\sum\nolimits_{m\in\mathcal{Z}^d} \sum_{\kappa,\lambda\in\mathcal{K}}\sum_{n\in B_{\kappa,\lambda}} \langle \mathbf{E}^{(\kappa,n,\lambda)}\left(u_{m+n,\lambda}-u_{m,\kappa}\right), v_{m,\kappa}\rangle$$
$$= \sum\nolimits_{m'\in\mathcal{Z}^d} \sum_{\kappa,\lambda\in\mathcal{K}}\sum_{-n'\in B_{\kappa,\lambda}} \langle \mathbf{E}^{(\kappa,-n,\lambda)}\left(u_{m',\lambda}-u_{m'+n',\kappa}\right), v_{m'+n',\kappa}\rangle$$

Due to the properties (2.4) and (2.5), there holds

$$\sum\nolimits_{m'\in\mathcal{Z}^d} \sum_{\kappa,\lambda\in\mathcal{K}}\sum_{-n'\in B_{\kappa,\lambda}} \langle \mathbf{E}^{(\kappa,-n',\lambda)}\left(u_{m',\lambda}-u_{m'+n',\kappa}\right), v_{m'+n',\kappa}\rangle$$
$$= - \sum\nolimits_{m'\in\mathcal{Z}^d} \sum_{\kappa,\lambda\in\mathcal{K}}\sum_{n'\in B_{\lambda,\kappa}} \langle \mathbf{E}^{(\lambda,n',\kappa)}\left(u_{m'+n',\kappa}-u_{m',\lambda}\right), v_{m'+n',\kappa}\rangle$$

Which leads to the (2.10) immediately.

We now show that the variational solution $u \in H^1(\mathcal{G})$ solves the equilibrium equation (2.10). Let $v \in H^1(\mathcal{G})$ be such that $v_{m,\kappa} = 0$ for all $\kappa \in \mathcal{K}$ except $\kappa = 1$. Then the variational equation leads to

$$\sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}}\sum_{n\in B_{\kappa,1}} \langle \frac{1}{2}\mathbf{E}^{(\kappa,n,1)}\left(u_{m+n,1}-u_{m,\kappa}\right), v_{m+n,1}\rangle + \sum_{m\in\mathcal{Z}^d}\langle \mathbf{C}^{(\kappa)}u_{m,1},, v_{m,1}\rangle$$
$$-\sum_{m\in\mathcal{Z}^d}\sum_{\lambda\in\mathcal{K}}\sum_{n\in B_{1,\lambda}} \langle \frac{1}{2}\mathbf{E}^{(1,n,1)}\left(u_{m+n,\lambda}-u_{m,1}\right), v_{m,1}\rangle = \sum_{m\in\mathcal{Z}^d}\langle f_{m,1}, v_{m,1}\rangle.$$

Selecting $v_{m,1}$ such that $v_{m,1} = 0$ for all $m \in \mathcal{Z}$ except $v_{1,1}$, we obtain

$$-\sum_{\lambda\in B_\kappa}\sum_{n\in B_{1,\lambda}} \langle \mathbf{E}^{(\kappa,n,\lambda)}\left(u_{1+n,\lambda}-u_{1,1}\right), v_{1.1}\rangle + \langle \mathbf{C}^{(1)}u_{1,1}, v_{1.1}\rangle = \langle f_{1,1}, v_{1.1}\rangle$$

which implies

$$-\sum_{\lambda\in B_\kappa}\sum_{n\in B_{1,\lambda}} \mathbf{E}^{(\kappa,n,\lambda)}\left(u_{1+n,\lambda}-u_{1,1}\right) + \mathbf{C}^{(1)}u_{1,1} = f_{1,1}$$

Similarly, there holds for any $m \in \mathcal{Z}^d$

$$-\sum_{\lambda\in B_\kappa}\sum_{n\in B_{1,\lambda}} \mathbf{E}^{(\kappa,n,\lambda)}\left(u_{m+n,\lambda}-u_{m,1}\right) + \mathbf{C}^{(1)}u_{m,1} = f_{m,1},$$

Actually, the above argument can be carried for any $\kappa \in \mathcal{K}$. Thus, we have the equation (2.6). □

2.3 Fourier transform for lattice problems

For grid functions u on the lattice $\mathcal{G}$ we introduce the Fourier transform

$$\mathcal{F}(u) = \sum_{m\in\mathcal{Z}^d} u_m e^{i\langle m,t\rangle} = \hat{u}(t) \tag{2.18a}$$

which is a linear functional over the space $C^{\infty}_{per}(I^d) = \{\hat{u} \in C^{\infty}(I^d) | \hat{u}(t)$ is a 2π-periodic function $\}$ with $I^d = (-\pi, \pi)^d$. $\hat{u}(t)$ is a complex-valued vector function $(\hat{u}_1(t), \hat{u}_1(t), \cdots, \hat{u}_q(t))$, and each $\hat{u}_\kappa(t)$ has s components $\hat{u}^\ell_\kappa(t), 1 \le \ell \le s$, and

$$\hat{u}_\kappa(t) = \sum_{m \in \mathcal{Z}^d} u_{m,\kappa} e^{i<m,t>}, \qquad \forall \kappa \in \mathcal{K}. \tag{2.18b}$$

The inverse Fourier transform is defined as

$$\mathcal{F}^{-1}(\hat{u}) = (u_m)_{m \in \mathcal{Z}^d} \tag{2.19a}$$

for any $\hat{u}(t) \in C^{\infty}_{per}(I^d)$, and

$$u_m = (2\pi)^{-d} \int_{I^d} \hat{u}(t) e^{-i<m,t>} dt \tag{2.19b}$$

For lattice problems we are interested in some of specific spaces over $\mathcal{G}$, e.g. $L^2(\mathcal{G})$, then $\mathcal{F}(u) \in L^2(I^d)$, which has a stronger topology than the linear functional on the space $C^{\infty}_{per}(I^d)$. In particular, we are interested in the Fourier transform on the spaces $L^2_\nu(\mathcal{G}), \nu \ge 0$ with the norm

$$\|u\|^2_{L^2_\nu(\mathcal{G})} = \sum_{m \in \mathcal{Z}^d} \sum_{\kappa \in \mathcal{K}} (1 + |m|^2)^\nu |u_{m,\kappa}|^2.$$

Lemma 2.5 The Fourier transform realizes isomorphism: $L^2(\mathcal{G}) \leftrightarrow L^2(I^d)$ and $L^2_\nu(\mathcal{G}) \leftrightarrow H^\nu_{per}(I^d)$, where $H^\nu_{per}(I^d)$ is the subspace of 2π- periodic functions in $H^\nu(I^d)$, and

$$\|u\|^2_{L^2(\mathcal{G})} = (2\pi)^{-d} \|\hat{u}\|^2_{L^2(I^d)}, \tag{2.20a}$$

$$\|u\|^2_{L^2_\nu(\mathcal{G})} \cong \|\hat{u}\|^2_{H^\nu(I^d)}. \tag{2.20b}$$

Hereafter "$\cong$" means equivalent with constants independent of major subjects, e.g. the functions u and $\hat{u}$.

Proof It is easy to verify that

$$\begin{aligned}\|\hat{u}\|^2_{L^2(I^d)} &= \int_{I^d} \sum_{m \in \mathcal{Z}^d} \sum_{\kappa \in \mathcal{K}} \sum_{0 \le \ell \le s} |\hat{u}^\ell_\kappa|^2 dt = \int_{I^d} \sum_{m \in \mathcal{Z}^d} \sum_{\kappa \in \mathcal{K}} \sum_{0 \le \ell \le s} |u^\ell_{m,\kappa} e^{i<m,t>}|^2 dt \\ &= (2\pi)^d \sum_{m \in \mathcal{Z}^d} \sum_{\kappa \in \mathcal{K}} \sum_{0 \le \ell \le s} |u^\ell_{m,\kappa}|^2 = (2\pi)^d \sum_{m \in \mathcal{Z}^d} |u_m|^2 = (2\pi)^d \|u\|^2_{L^2(\mathcal{G})}\end{aligned}$$

which implies an isomorphism : $L^2(\mathcal{G}) \leftrightarrow L^2(I^d)$ and (2.20a). For $\hat{u}(t) \in H^\nu_{per}(I^d)$ with integer $\nu \ge 0$, there holds

$$D^\alpha \hat{u}(t) = \prod_{\ell=1}^{d} (im_\ell)^{\alpha_\ell} \hat{u}(t)$$

for any $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d)$ with $|\alpha| = \sum_{1 \le i \le d} \alpha_i \le \nu$, which leads to

$$\|\hat{u}\|^2_{H^\nu(I^d)} \cong \sum_{m \in \mathcal{Z}^d} (1 + |m|^2)^\nu |u_m|^2 = \|u\|^2_{L^2_\nu(\mathcal{G})}.$$

For non-integer $\nu > 0, H^\nu_{per}(I^d)$ is defined as an interpolation space, and (2.19b) stands for non-integer ν as well. □

We now apply Fourier transform to the variational problem (2.10). We introduce a bilinear form $\hat{B}$ and a linear functional $\hat{F}$, namely,

$$\begin{aligned}\hat{B}(\hat{u},\hat{v}) &= \int_{I^d} \sum_{\kappa\in\mathcal{K}} \Big\{ \sum_{(n,\lambda)\in B_\kappa} \frac{1}{2} \langle \mathbf{E}^{(\kappa,n,\lambda)} (\hat{u}_\lambda e^{-i<n,t>} - \hat{u}_\kappa), \\ &\quad (\hat{v}_\lambda e^{-i<n,t>} - \hat{v}_\kappa)\rangle \langle \mathbf{C}^{(\kappa)} \hat{u}_\kappa, \hat{v}_\kappa\rangle \Big\} dt \end{aligned} \tag{2.21a}$$

and

$$\hat{F}(\hat{v}) = \sum_{\kappa\in\mathcal{K}} \int_{I^d} \langle \hat{f}, \hat{v}_\kappa\rangle dt. \tag{2.21b}$$

Lemma 2.6 Let $u, v \in H^1(\mathcal{G})$ and $f \in L^2(\mathcal{G})$, and let $\hat{u}, \hat{v}, \hat{f}$ be their Fourier transforms, respectively. Then there hold

$$B(u,v) = (2\pi)^{-d} B(\hat{u},\hat{v}) \tag{2.22}$$

and

$$F(v) = (2\pi)^{-d} \hat{F}(\hat{v}). \tag{2.23}$$

Proof. For $\hat{v} = \sum_{m\in\mathcal{Z}^d} v_m e^{i<m,t>}$ and $\hat{f} = \sum_{m\in\mathcal{Z}^d} f_m e^{i<m,t>}$, there holds

$$\begin{aligned}\hat{F}(\hat{v}) &= \sum_{\kappa\in\mathcal{K}} \int_{I^d} \langle \hat{f}_\kappa, \hat{v}_\kappa\rangle dt = \sum_{\kappa\in\mathcal{K}} \int_{I^d} \langle \sum_{n\in\mathcal{Z}^d} f_{n,\kappa} e^{i<n,t>}, \sum_{m\in\mathcal{Z}^d} v_{m,\kappa} e^{i<m,t>}\rangle dt \\ &= \sum_{\kappa\in\mathcal{K}} \int_{I^d} \sum_{n,m\in\mathcal{Z}^d} \langle f_{n,\kappa}, v_{m,\kappa}\rangle e^{i<(n-m),t>} dt \\ &= (2\pi)^d \sum_{\kappa\in\mathcal{K}} \sum_{m\in\mathcal{Z}^d} < f_{m,\kappa}, v_{m,\kappa} > . \end{aligned}$$

This leads to (2.23). Similarly we have

$$\sum_{\kappa\in\mathcal{K}} \int_{I^d} \langle \mathbf{C}^{(\kappa)} \hat{u}_\kappa, \hat{v}_\kappa\rangle dt = (2\pi)^d \sum_{\kappa\in\mathcal{K}} \sum_{m\in\mathcal{Z}^d} \langle \mathbf{C}^{(\kappa)} u_{m,\kappa}, v_{m,\kappa}\rangle. \tag{2.24}$$

It is easy to see that

$$\begin{aligned}&\int_{I^d} \sum_{\kappa\in\mathcal{K}} \sum_{(n,\lambda)\in B_\kappa} \frac{1}{2} \langle \mathbf{E}^{(\kappa,n,\lambda)} \left(\hat{u}_\lambda e^{-i<n,t>} - \hat{u}_\kappa\right), \left(\hat{v}_\lambda e^{-i<n,t>} - \hat{v}_\kappa\right)\rangle dt \\ = &\int_{I^d} \sum_{\kappa\in\mathcal{K}} \sum_{(n,\lambda)\in B_\kappa} \frac{1}{2} \langle \mathbf{E}^{(\kappa,n,\lambda)} (\sum_{m\in\mathcal{Z}^d} u_{m,\lambda} e^{i<(m-n),t>} - \sum_{m\in\mathcal{Z}^d} u_{m,\kappa} e^{i<m,t>}), \\ &(\sum_{m'\in\mathcal{Z}^d} v_{m',\lambda} e^{-i<m'-n,t>} - \sum_{m'\in\mathcal{Z}^d} v_{m',\kappa} e^{i<m',t>})\rangle dt \\ = &\int_{I^d} \sum_{\kappa\in\mathcal{K}} \sum_{(n,\lambda)\in B_\kappa} \sum_{m\in\mathcal{Z}^d} \frac{1}{2} \langle \mathbf{E}^{(\kappa,n,\lambda)} \left(u_{m+n,\lambda} - u_{m,\kappa}\right), \left(v_{m+n,\lambda} - v_{m,\kappa}\right)\rangle dt \\ = &(2\pi)^d \sum_{m\in Z^d} \sum_{\kappa\in\mathcal{K}} \sum_{(n,\lambda)\in B_\kappa} \frac{1}{2} \langle \mathbf{E}^{(\kappa,n,\lambda)} \left(u_{m+n,\lambda} - u_{m,\kappa}\right), \left(v_{m+n,\lambda} - v_{m,\kappa}\right)\rangle. \end{aligned}$$

which together with (2.24) yields (2.22). □

In order to properly define a variational problem over $I^d \times K_Q$,we need to introduce new function spaces. Let $L^2(K_Q)$ and $H^1(K_Q)$ be the spaces of grid functions on K_Q with the following norms

$$\|w\|^2_{L^2(K_Q)} = \sum_{\kappa\in\mathcal{K}} |w_\kappa|^2 = \sum_{\kappa\in\mathcal{K}} \sum_{1\le\ell\le s} |w^\ell_\kappa|^2$$

and

$$\|w\|^2_{H^1(K_Q)} = \sum_{\kappa\in\mathcal{K}} \sum_{(n,\lambda)\in B_\kappa} \frac{|w_{n,\lambda} - w_\kappa|^2}{|x^{(n,\lambda)} - x^{(\kappa)}|^2} + \|w\|^2_{L^2(K_Q)}.$$

$L^2\left(I^d, H^1(K_Q)\right)$ and $L^2\left(I^d, L^2(K_Q)\right)$ are spaces furnished with the norms :

$$\|\hat{w}\|^2_{L^2(I^d,H^1(K_Q))} = \int_{I^d} \|\hat{w}(t)\|^2_{H^1(K_Q)} dt$$

and

$$\|\hat{w}\|^2_{L^2(I^d,L^2(K_Q))} = \int_{I^d} \|\hat{w}(t)\|^2_{L^2(K_Q)} dt.$$

Lemma 2.7 If $f \in H^\ell(\mathcal{G})$, then $\hat{f}(t) \in L^2\left(I^d, H^\ell(K_Q)\right), \ell = 0, 1$, and

$$\|\hat{f}(t)\|_{L^2(I^d,H^\ell(K_Q))} = (2\pi)^d \|f\|_{H^\ell(\mathcal{G})}$$

Proof. The assertion follows easily from the definition of the spaces. □

Remark 2.2 The functions $\hat{u} = \hat{u}(t)$ in the space $H^l(I^d), l = 0, 1$ are vector functions with sq components, and the functions $\hat{u} = \hat{u}(t, x^{(\kappa)})$ in $L^2\left(I^d, L^2(K_Q)\right)$ are those defined on a semi-discrete domain $I^d \times K_Q$ with s components,. Obviously, the space $L^2\left(I^d\right)$ coincides with the space $L^2\left(I^d, L^2(K_Q)\right)$, and

$$\|\hat{f}\|_{L^2(I^d,L^2(K_Q))} = \|\hat{f}\|_{L^2(I^d)}.$$

But the space $H^1(I^d)$ is totally different from the space $L^2\left(I^d, H^1(K_Q)\right)$. The latter is related to the connectivity B_κ, and the former is not. Furthermore, the space $H^1(I^d)$ is an isomorphism of the space $L^2_1(\mathcal{G})$ according to Lemma 2.5, and the space $L^2\left(I^d, H^1(K_Q)\right)$ is an isomorphism of the space $H^1(\mathcal{G})$ according to Lemma 2.6.

The bilinear form $\hat{B}$ in (2.20) and linear functional $\hat{F}$ in (2.21) are defined on $L^2\left(I^d, H^1(K_Q)\right) \times L^2\left(I^d, H^1(K_Q)\right)$ and $L^2\left(I^d, H^1(K_Q)\right)$, respectively. The energy space $\hat{E} = \hat{E}\left(I^d \times K_Q\right)$ is defined as one equivalent to $L^2\left(I^d, H^1(K_Q)\right)$ if $\mathbf{C}^{(\kappa)} \not\equiv 0$, with an energy norm

$$\|\hat{w}\|^2_{\hat{E}(I^d\times K_Q)} = \hat{B}(\hat{w}, \hat{w})^{1/2}.$$

We are now able to precisely address the variational problem over the domain $I^d \times K_Q$.

Theorem 2.8 Let $\hat{B}$ be the bilinear form on $L^2\left(I^d, H^1(K_Q)\right) \times L^2\left(I^d, H^1(K_Q)\right)$ and $\hat{F}$ be linear functional on $L^2\left(I^d, H^1(K_Q)\right)$ as given in (2.20) and (2.21), respectively. If $\hat{f} \in L^2\left(I^d, L^2(K_Q)\right)$ and $\mathbf{C}^{(\kappa)} \not\equiv 0, \forall\kappa \in \mathcal{K}$, then the problem:

$$\hat{B}\left(\hat{u}, \hat{v}\right) = \hat{F}(\hat{v}),\ \forall \hat{v} \in L^2\left(I^d, H^1(K_Q)\right) \tag{2.25}$$

has a unique solution $\hat{u} \in L^2\left(I^d, H^1(K_Q)\right)$, and

$$\|\hat{u}\|_{L^2(I^d,H^1(K_Q))} \le C\|\hat{f}\|_{(L^2(I^d,L^2(K_Q)))}. \tag{2.26}$$

Remark 2.3 Combining Theorem 2.7 with Theorem 2.2 and Lemma 2.5, we have the equivalence between the problem (2.10) and the problem (2.27), i.e. the equation (2.25) has a unique solution $\hat{u} \in L^2\left(I^d, H^1(K_Q)\right)$ and the estimate (2.26) holds for $\hat{f} \in \left(I^d, L^2(K_Q)\right)$ if and only if the problem (2.10) has a unique solution $u \in H^1(\mathcal{G})$ and the estimate (2.17) holds for $f = \mathcal{F}^{-1}(\hat{f}) \in L^2(\mathcal{G})$, and $u = \mathcal{F}^{-1}(\hat{u})$.

Applying the Fourier transform to the variational equation (2.10) yields the variational equation (2.25). Applying Fourier transform to the equilibrium Equations (2.6) leads to a equilibrium Equations over $I^d \times K_Q$

$$-\sum_{(n,\lambda)\in B_\kappa} \mathbf{E}^{(\kappa,n,\lambda)} \left(\hat{u}_\lambda e^{-i<n,t>} - \hat{u}_\kappa\right) + \mathbf{C}^{(\kappa)}\hat{u}_\kappa = \hat{f}_\kappa, \forall \kappa \in \mathcal{K}. \tag{2.27}$$

Then we have a theorem indicating the relation between the solution of (2.25) and the solution of (2.27).

Theorem 2.9 If $\hat{u} \in L^2\left(I^d, H^1(K_Q)\right)$ is the solution of the variational equation (2.25) with $\hat{f} \in L^2\left(I^d, L^2(K_Q)\right)$, then it satisfies the equilibrium equation (2.27). Vice versa, if $\hat{u} \in L^2\left(I^d, H^1(K_Q)\right)$ solves the equilibrium equation (2.27) with $\hat{f} \in L^2\left(I^d, L^2(K_Q)\right)$, then it satisfies the variational equation (2.25).

Proof. The proof is analogous to that for Theorem 2.3. □

3. Lattice Problems Without Absolute Terms

In practical applications, many lattice problems are associated with no absolute terms, i.e. $\mathbf{C}^{(\kappa)} \equiv 0$ for all $\kappa \in \mathcal{K}$. We seek $u \in E(\mathcal{G})$ such that

$$B(u,v) = F(v), \ \forall v \in E(\mathcal{G}) \tag{3.1}$$

with

$$B(u,v) = \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}}\sum_{(n,\lambda)\in B_\kappa} \frac{1}{2}\langle \mathbf{E}^{(\kappa,n,\lambda)}\left(u_{m+n,\lambda}, -u_{m,\kappa}\right), \left(v_{m+n,\lambda} - v_{m,\kappa}\right)\rangle \quad (3.2a)$$

and

$$F(v) = \langle f, v\rangle_{\mathcal{G}} = \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}} \langle f_{m,\kappa}, v_{m,\kappa}\rangle. \quad (3.2b)$$

It is extremely important for us to address properly these problems. Without the absolute term the energy space $E(\mathcal{G})$ is not equivalent to the space $H^1(\mathcal{G})$, and $E(\mathcal{G})$ is not embedded in $L^2(\mathcal{G})$. Actually, the "energy norm" $\|u\|_{E(\mathcal{G})}$ is equivalent to the semi-norm $|u|_{H^1(\mathcal{G})}$. Consequently, the solution of the lattice problem is not unique in $E(\mathcal{G})$ and may not exist in $H^1(\mathcal{G})$. Hence we have to modify the space $H^1(\mathcal{G})$, such that the solution exists uniquely in modified space $\tilde{H}^1(\mathcal{G})$ with the norm equivalent to semi-norm of $H^1(\mathcal{G})$.

The modification of the spaces in one, two and three dimensions are quite different. We shall address them differently in this section. We need to introduce a weighted space $L^2_{\nu,\sigma}(\mathcal{G})$ for all dimensions with the norm

$$\|u\|_{L^2_{\nu,\sigma}(\mathcal{G})} = \left\{\sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}} \left(1+|m|^2\right)^\nu \log^{2\sigma}(1+|m|)\,|u_{m,\kappa}|^2\right\}^{\frac{1}{2}} \tag{3.3}$$

where ν and σ are real numbers. We shall write $L^2_{0,0}(\mathcal{G}) = L^2(\mathcal{G}), L^2_{\nu,0}(\mathcal{G}) = L^2_\nu(\mathcal{G})$. Obviously, $L^2_{\nu,\sigma}(\mathcal{G}) \supseteq L^2(\mathcal{G})$ if $\nu,\sigma \le 0$, and $L^2_{\nu,\sigma}(\mathcal{G}) \subseteq L^2(\mathcal{G})$ if $\nu,\sigma \ge 0$.

3.1 Lattice problems with $\mathbf{C}^{(\kappa)} \equiv 0$ in one dimension

Lemma 3.1 If $v \in E(\mathcal{G})$, and $v_{0,1} = 0$, then

$$\|v\|_{L^2_{-1}(\mathcal{G})} \le C|v|_{H^1(\mathcal{G})}. \tag{3.4}$$

Proof. First, suppose that $x^{(n,\kappa)}$ and $x^{(n,1)}$ are always connected for any $\kappa \in \mathcal{K}$ with $\kappa \neq 1$. Then

$$\begin{aligned}\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}}\frac{|v_{m,\kappa}|^2}{1+m^2} &\leq C\Big(\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}}(v_{m,\kappa}-v_{m,1})^2+\sum_{m\in\mathcal{Z}}\frac{|v_{m,1}|^2}{1+m^2}\Big)\\ &\leq C\Big(|v|^2_{H^1(\mathcal{G})}+\sum_{m\in\mathcal{Z}}\frac{|v_{m,1}|^2}{1+m^2}\Big).\end{aligned}\tag{3.5}$$

If there are some $\kappa \in \mathcal{K}$ such that $x^{(m,\kappa)}$ and $x^{(m,1)}$ are not connected, there always exists by (C.3) a chain $L_{m,1,m,\kappa} : x^{(m,1)} = x^{(n_1,\lambda_1)} \to x^{(n_2,\lambda_2)} \cdots \to x^{(n_s,\lambda_s)} = x^{(m,\kappa)}$, and due to (2.15)

$$\sum_{m\in\mathcal{Z}}|v_{m,\kappa}-v_{m,1}|^2 \leq C\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}}\sum_{(n,\lambda)\in B_{\mathcal{K}}}|x^{(m+n,\lambda)}-x^{(m,\kappa)}|^2 \leq C|v|^2_{H^1(\mathcal{G})}. \tag{3.6}$$

Hence, (3.5) holds for the cases that $x^{(m,\kappa)}$ and $x^{(m,1)}$ are connected or not connected.

Let $w_m = v_{m,1}$. It is sufficient to show that

$$\sum_{m=1}^{\infty}\frac{|w_m|^2}{1+m^2} \leq C\sum_{m=1}^{\infty}|w_m-w_{m-1}|^2 \tag{3.7}$$

Since $w_0 = 0$ and $w_m = \sum_{j=1}^{m}(w_j - w_{j-1})$, we have with $\varepsilon > 0$ by Cauchy inequality

$$\begin{aligned}\sum_{m=1}^{\infty}\frac{|w_m|^2}{1+m^2} &\leq \sum_{m=1}^{\infty}\frac{1}{1+m^2}\left(\sum_{j=1}^{m}(w_j-w_{j-1})^2 j^{\varepsilon}\right)\left(\sum_{j=1}^{m}j^{-\varepsilon}\right)\\ \leq\quad & C\sum_{m=1}^{\infty}\frac{m^{1-\varepsilon}}{1+m^2}\sum_{j=1}^{m}(w_j-w_{j-1})^2 j^{\varepsilon} \leq C\sum_{j=1}^{\infty}(w_j-w_{j-1})^2 j^{\varepsilon}\sum_{m=j}^{\infty}\frac{m^{-\varepsilon}}{1+m^2}.\end{aligned}$$

Note that

$$\sum_{m=j}^{\infty}\frac{m^{-\varepsilon}}{1+m^2} \leq C\sum_{m=j}^{\infty}m^{-1-\varepsilon} \leq C\int_j^{\infty}\xi^{-1-\varepsilon}d\xi \leq Cj^{-\varepsilon}$$

which leads to (3.7). Therefore

$$\sum_{m=1}^{\infty}\frac{|v_{m,1}|^2}{1+m^2} \leq C\sum_{m=1}^{\infty}|v_{m,1}-v_{m-1,1}|^2. \tag{3.8a}$$

Similarly, it can be prove that

$$\sum_{m=-\infty}^{0}\frac{|v_{m,1}|^2}{1+m^2} \leq C\sum_{m=0}^{-\infty}|v_{m,1}-v_{m-1,1}|^2. \tag{3.8b}$$

Combining (3.8a) and (3.8b), we have

$$\sum_{m\in\mathcal{Z}}\frac{|v_{m,1}|^2}{1+m^2} \leq C\sum_{m\in\mathcal{Z}}|v_{m,1}-v_{m-1,1}|^2. \tag{3.9}$$

Although $v_{m,1}$ and $v_{m-1,1}$ may be connected or not connected, we have due to (C.3)

$$\sum_{m\in\mathcal{Z}}|v_{m,1}-v_{m-1,1}|^2 \leq C\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}}\sum_{(n,\lambda)\in B_{\kappa}}|v_{m+n,\lambda}-v_{m,\kappa}|^2 \leq C\,|v|^2_{H^1(\mathcal{G})},$$

which together with (3.5) and (3.9) leads to (3.4). □

Theorem 3.2 If $f \in L^2_1(\mathcal{G})$ and $\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} = 0$, then for any $v \in E(\mathcal{G})$ it holds that

$$|\langle f, v\rangle_{\mathcal{G}}| = \left|\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} v_{m,\kappa}\right| \le C\|f\|_{L^2_1(\mathcal{G})}|v|_{H^1(\mathcal{G})} \tag{3.10}$$

Proof. Note that by Schwarz inequality

$$\left(\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} |f_{m,\kappa}|\right)^2 \le \sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} |f_{m,\kappa}|^2(1+m^2)\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} \frac{1}{1+m^2} \le C\|f|\|_{L^2_1(\mathcal{G})}.$$

Hence, $f \in L^1(\mathcal{G})$. Because $\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} = 0$, we have by Lemma 3.1

$$\begin{aligned} |\langle f, v\rangle_{\mathcal{G}}| &= \left|\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} v_{m,\kappa}\right| = \left|\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa}\left(v_{m,\kappa} - v_{0,1}\right)\right| \\ &\le \left(\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} \left(1+m^2\right)|f_{m,\kappa}|^2\right)^{1/2}\left(\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} \frac{\left(v_{m,\kappa}-v_{0,1}\right)^2}{1+m^2}\right)^{1/2} \\ &\le C\|f\|_{L^2_1(\mathcal{G})}|v|_{H^1(\mathcal{G})}. \end{aligned}$$

□

We introduce the space $\tilde{H}^1(\mathcal{G})$ with the norm

$$\|u\|_{\tilde{H}^1(\mathcal{G})} = \left\{\|u\|^2_{L^2_{-1}(\mathcal{G})} + |u|^2_{H^1(\mathcal{G})}\right\}^{1/2},$$

and a quotient space

$$\hat{H}^1(\mathcal{G}) = \tilde{H}^1(\mathcal{G})/P_0$$

with norm

$$\|u\|_{\hat{H}^1(\mathcal{G})} = \inf_{\alpha\in P_0}\|u-\alpha\|_{\tilde{H}^1(\mathcal{G})}$$

where P_0 is a subspace of $\tilde{H}^1(\mathcal{G})$, containing all constant grid functions on $\mathcal{G}$. Due to Lemma 3.1 it is easy to show that

$$\|u\|_{\hat{H}^1(\mathcal{G})} \cong |u|_{H^1(\mathcal{G})}.$$

In the framework of the space $\tilde{H}^1(\mathcal{G})$ and $\hat{H}^1(\mathcal{G})$ we are addressing the existence and uniqueness of the solution of the variational problem (3.1) with $d = 1$.

Theorem 3.3 If $f \in L^2_1(\mathcal{G})$ and $\sum_{m\in\mathcal{Z}}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} = 0$, then the problem (3.1) with $d = 1$ has a solution $u \in E(\mathcal{G})$, and

$$|u|_{H^1(\mathcal{G})} \le C\|f\|_{L^2_1(\mathcal{G})}. \tag{3.11}$$

The solution is unique up to a constant.

Proof. Due to the equivalence between $|u|_{H^1(\mathcal{G})}$ and $\|u\|_{\hat{H}^1(\mathcal{G})}$

$$|B(u,v)| \quad \le C|u|_{H^1(\mathcal{G})}|v|_{H^1(\mathcal{G})} \le C\|u\|_{\hat{H}^1(\mathcal{G})}\|v\|_{\hat{H}(\mathcal{G})}$$

and

$$|B(u,u)| \ge D|u|^2_{H^1(\mathcal{G})} \ge D\|u\|_{\hat{H}^1(\mathcal{G})}.$$

By Theorem 3.2, it holds that

$$|F(v)| \le C\|f\|_{L^2_1(\mathcal{G})}\|v\|_{\hat{H}^1(\mathcal{G})}.$$

By Lax-Milgram Theorem, the variational problem has a unique solution $u \in \hat{H}^1(\mathcal{G})$, and

$$\|u\|_{\hat{H}^1(\mathcal{G})} \leq C\|f\|_{L_1^2(\mathcal{G})},$$

which implies (3.11) and the uniqueness of the solution in $E(\mathcal{G})$ up to a constant.

3.2 Lattice problems with $C^{(\kappa)} \equiv 0$ in two dimensions

As in one dimensional $L^2(\mathcal{G})$ and $H^1(\mathcal{G})$ are not suitable spaces for the right hand side f of the equation (3.1) and the solution of the lattice problem, respectively. In the framework of $L^2_{\nu,\sigma}(\mathcal{G})$ and $\tilde{H}^1(\mathcal{G})$ we are able to establish the existence and uniqueness of the solution for Lattice problems.

Theorem 3.4 If $f \in L^2_{1,1}(\mathcal{G})$, and $\sum_{m\in\mathcal{Z}^2}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} = 0$, then for any $v \in E(\mathcal{G})$,

$$|\langle f, v\rangle_{\mathcal{G}}| = \left|\sum_{m\in\mathcal{Z}^2}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa}v_{m,\kappa}\right| \leq C\|f\|_{L^2_{1,1}(\mathcal{G})}|v|_{H^1(\mathcal{G})} \tag{3.12}$$

with constant C independent of f and v.

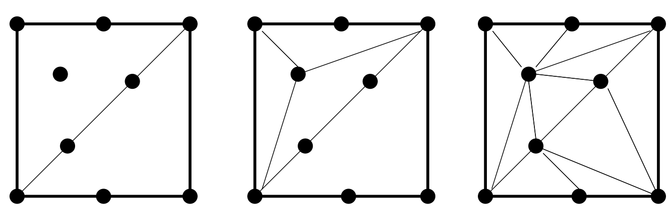
The theorem is parallel to Theorem 3.2 for one dimension, but the proof for two dimensions needs properties of functions in $H^1(R^2)$, which is contained in the appendix. In order to apply these properties, we have to extend by linear interpolation grid functions on $\mathcal{G}$ to whole space R^2.

Let $\bar{K}_m$ be a set of nodes which are located in $\bar{Q}_m$ where $\bar{Q}_m$ is the closure of the cell Q_m. Obviously, $x^{(m,\kappa)} \in \bar{K}_m$ for all $\kappa \in \mathcal{K}$, and some nodes $x^{(n,\kappa)}$ in neighboring cells are included as well. Let K_m^V, K_m^I and K_m^E be subsets of $\bar{K}_m$ for nodes at vertices, on edges (not including vertices) and in the interior of Q_m, respectively. Then $\bar{K}_m = K_m^E \cup K_m^V \cup K_m^I$.

By $\mathcal{T}_m = \{t_i, i = 1, 2, \ldots, T\}$, we denote a triangular partition of $\bar{Q}_m$ satisfying the following conditions:

(T.1) $V_{\mathcal{T}} = \bar{K}_m$, where $V_{\mathcal{T}}$ denote a set of all vertices of the partition $\mathcal{T}_m$;

(T.2) The partition is regular, i.e. $t_i \cap t_j$ for $i \neq j$ is a vertex, or a whole edge, or empty.



(a) Initial Partition T_m^0 (b) Partition T_m^1 (c) Partition $T_m^2 = T_m$

Fig. 3.1 Triangular partition of cell $\bar{Q}_m$

The construction of such a partition can be started with an initial partition $\mathcal{T}_m^0$ of $\bar{Q}_m$ for which (T.2) holds and $V_{\mathcal{T}_m^0} = K_m^V$ as shown in Fig. 3.1(a). If a node $x^{(n,\kappa)} \in K_m^I$ is in the interior of a triangle t_i, we divide t_i into three smaller triangles by connecting $x^{(n,\kappa)}$ to three vertices of t_i, as shown in Fig. 3.1(b). Repeating the process for each node in the interiors of all simplices, we have a partition $\mathcal{T}_m^1$ of $\bar{Q}_m$ for which (T.2) holds and no node $x^{(n,\kappa)} \in \bar{K}_m$ is located in the interiors of all triangles. If there are l nodes are on an (open)edge of a triangle t_i and $l \leq 1$, we divide the triangle t_i into $l+1$ smaller triangles by connecting these l nodes and the vertex opposite to the edge,as shown in Fig. 3.1(c). If this edge is shared by a pair of triangles t_i and t_j, we divide each of these two triangles into $l+1$ smaller triangles. Applying this process to each edge of the triangles will results in a triangular partition $\mathcal{T}_m$ satisfying (T.1) and (T.2).

For a periodic lattice $\mathcal{G}$, the triangular partition $\mathcal{T}_m$ of the cell $\bar{Q}_m$ can be periodically carried out, a combination of the triangular partitions $\mathcal{T}_m$ for all $m \in Z^2$ forms a partition $\mathcal{T}$ of R^2 for which (T.2) holds and $V_{\mathcal{T}} = \cup_{m\in Z^2} K_m$.

Based on such a partition $\mathcal{T}$, we can extend a grid function u on $\mathcal{G}$ to a function $\tilde{u}(x)$ for $x \in R^2$ by a linear interpolation. Let $\phi_i(x)$ be a linear function in t_i such that $\phi_i(x^{(n,\kappa)}) = u_{n,\kappa}$ at all vertices of t_i, and let $\psi_m(x)$ be a piecewise linear function in $\bar{Q}_m$ such that $\psi_m(x) = \phi_i(x)$ in $t_i, 1 \le i \le T$. Then, there holds

$$\begin{aligned} |\psi_m(x)|^2_{H^1(Q_m)} &= \sum_{1\le i\le T} |\phi_i(x)|^2_{H^1(t_i)} \\ &\le C \sum_{t_i\subseteq \bar{Q}_m} \sum_{x^{(n,\kappa)},x^{(l,\lambda)}\in t_i} \frac{|u_{n,\kappa}-u_{l,\lambda}|^2}{|x^{(n,\kappa)}-x^{(l,\lambda)}|^2} \\ &\le C \sum_{t_i\subseteq \bar{Q}_m} \sum_{x^{(n,\kappa)},x^{(l,\lambda)}\in t_i} |u_{n,\kappa}-u_{l,\lambda}|^2. \end{aligned} \tag{3.13}$$

Let $\tilde{u}(x) = \psi_m(x)$ in $\bar{Q}_m$ for all $m \in \mathcal{Z}^2$. Then, $\tilde{u}(x)$ is continuous and piecewise linear function in R^2, and

$$|\tilde{u}|^2_{H^1(R^2)} \le C \sum_{m\in\mathcal{Z}^2} \sum_{t_i\subseteq \bar{Q}_m} \sum_{x^{(n,\kappa)},x^{(l,\lambda)}\in t_i} |u_{n,\kappa}-u_{l,\lambda}|^2. \tag{3.14}$$

Note that if the vertices $x^{(n,\kappa)}$ and $x^{(l,\lambda)}$ of t_i in $\bar{Q}_m$ are not connected, (C.2) and (2.15) indicate that they are linked by the shortest chain $L_{n,\kappa,l,\lambda} : x^{(n_1,\lambda_1)} = x^{(n,\kappa)} \to x^{(n_2,\lambda_2)} \cdots \to x^{(n_s,\lambda_s)} = x^{(l,\lambda)}$ with s uniformly bounded, where the node $x^{(n_j,\lambda_j)}$ is connected to the node $x^{(n_{j+1},\lambda_{j+1})}$ for $1 \le j \le s-1$. Hence, there holds

$$|u_{n,\kappa} - u_{l,\lambda}| \le C \sum_{1\le j\le s-1} |u_{n_j,\lambda_j} - u_{n_{j+1},\lambda_{j+1}}|$$

which with (3.14) implies that

$$|\tilde{u}|^2_{H^1(R^2)} \le C \sum_{m\in\mathcal{Z}^2} \sum_{\kappa\in\mathcal{K}} \sum_{(n,\lambda)\in B_\kappa} |u_{m,\kappa} - u_{n+m,\lambda}|^2. \tag{3.15}$$

Theorem 3.5 Let u be a grid function on the lattice $\mathcal{G}$, and let $\tilde{u}$ be the extension of u by a linear interpolation, described as above. Then $|u|_{H^1(\mathcal{G})} \cong |\tilde{u}|_{H^1(R^2)}$, and $|u|_{L^2_{\nu,\sigma}(\mathcal{G})} \cong |\tilde{u}|_{L^2_{\nu,\sigma}(R^2)}$, i.e. there are two positive constants C_1 and C_2 independent of u and $\tilde{u}$ such that

$$C_1 |u|_{H^1(\mathcal{G})} \le |\tilde{u}|_{H^1(R^2)} < C_2 |u|_{H^1(\mathcal{G})} \tag{3.16}$$

and

$$C_1 |u|_{L^2_{\nu,\sigma}(\mathcal{G})} \le |\tilde{u}|_{L^2_{\nu,\sigma}(R^2)} < C_2 |u|_{L^2_{\nu,\sigma}(\mathcal{G})} \tag{3.17}$$

Proof. Since $\tilde{u}(x)$ is a piecewise linear function interpolating the grid function u at each node $x^{(m,\kappa)}$, and for $x \in \bar{Q}_m$,

$$(1+x^2)^\nu \log^{2\sigma}(1+|x|) \cong (1+|m|^2)^\nu \log^{2\sigma}(1+|m|),$$

it holds that

$$\|\tilde{u}(x)\|^2_{L^2_{\nu,\sigma}(\bar{Q}_m)} \cong \sum_{x^{(n,\kappa)}\in \bar{K}_m} (1+|m|^2)^\nu \log^{2\sigma}(1+|m|) |u_{n,\kappa}|^2$$

which implies (3.17).

The second inequality of (3.16) follows from (3.15). It suffices to show the first inequality of (3.16). Suppose that $x^{(m,\kappa)}$ and $x^{(n+m,\lambda)}$ are connected. If $x^{(m,\kappa)}$ and $x^{(n+m,\lambda)}$ are in the cell $\bar{Q}_m$, it is easy to see that

$$|u_{m,\kappa} - u_{n+m,\lambda}| \le C|\psi_m|_{H^1(Q_m)}. \tag{3.18}$$

We next consider two connected nodes $x^{(m,\kappa)}$ and $x^{(n+m,\lambda)}$ which are located in different cells $\bar{Q}_m$ and $\bar{Q}_n$. Let $Q_{n_j}, 1 \le j \le J$ be a sequence of cells with $Q_{n_1} = Q_m$ and $Q_{n_J} = Q_n$ such that Q_{n_j} is neighboring to $Q_{n_{j+1}}$. Due to the assumption (C.3), J is uniformly bounded. Select a common vertex $x^{(n_j,\lambda_j)}$ of the cell $\bar{Q}_{n_j}$ and $\bar{Q}_{n_{j+1}}, 1 \le j \le J-1$. Therefore, we have

$$\begin{aligned} |u_{m,\kappa} - u_{n+m,\lambda}| \quad &\le |u_{m,\kappa} - u_{n_1,\lambda_1}| + |u_{m+n,\lambda} - u_{n_J,\lambda_J}| \\ &+ \textstyle\sum_{1\le j\le J-1} |u_{n_j,\lambda_j} - u_{n_{j+1},\lambda_{j+1}}| \end{aligned} \tag{3.19}$$

Since $x^{(n_j,\lambda_j)}$ and $x^{(n_{j+1},\lambda_{j+1})}$ are in the same cell $\bar{Q}_{n_{j+1}}$, we have for $1 \le j \le J-2$

$$|u_{n_j,\lambda_j} - u_{n_{j+1},\lambda_{j+1}}| \le C|\psi_{n_{j+1}}|_{H^1(Q_{n_{j+1}})}, \tag{3.20a}$$

Similarly, there hold

$$|u_{m,\kappa} - u_{n_1,\lambda_1}| \le C|\psi_m|_{H^1(Q_m)}, \tag{3.20b}$$

and

$$|u_{m+n,\lambda} - u_{n_{J-1},\lambda_{J-1}}| \le C|\psi_n|_{H^1(Q_n)}. \tag{3.20c}$$

A combination of (3.19) and (3.20) leads to

$$|u_{m,\kappa} - u_{n+m,\lambda}| \le C \sum_{1\le j\le J} |\psi_{n_j}|_{H^1(Q_{n_j})}. \tag{3.21}$$

The first inequality of (3.16) follows easily from (3.18) and (3.21). □

Lemma 3.6 For $u \in \tilde{H}^1(\mathcal{G})$ there exists a constant α such that

$$\|u - \alpha\|_{L^2_{-1,-1}(\mathcal{G})} \le C|u|_{H^1(\mathcal{G})} \tag{3.22}$$

Proof. Let $\tilde{u}(x)$ be the extension described above and $\alpha = \int_\Gamma \tilde{u}(x)dx$ where $\Gamma = \{x \in R^2 \mid |x| = 2\}$. By Theorem A.1 there holds

$$\int_S |\tilde{u} - \alpha|^2\, dx + \int_{S^c} \frac{|\tilde{u} - \alpha|^2}{|x|^2 \log^2 |x|} dx \le C|\tilde{u}|^2_{H^1(R^2)}$$

where $S = \{x \in R^2 \mid |x| \le 2\}, S^c = R^2 \setminus S$. This estimation and Theorem 3.5 leads (3.22). □

We are now able to prove Theorem 3.4.

Proof of Theorem 3.4 Let $\tilde{v}(x)$ be the extension of v, and $\alpha = \int_\Gamma \tilde{v}(x)dx$. Suppose that circle centered at the origin with radius 2 is contained in a rectangle $D = \{x \in R^2 \mid |x_i| \le b, i = 1,2\}$, then

$$\alpha = \int_\Gamma \tilde{v}(x)dx = \sum_{\substack{n\in\mathcal{Z}^2\\ |n_i|\le b}} \sum_{\kappa\in\mathcal{K}} \beta_{n,\kappa} v_{n,\kappa}$$

with the coefficients $\beta_{n,\kappa}$. Since $\sum_{n\in\mathcal{Z}^2}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa}=0$, we have by Lemma 3.5 and Lemma 3.6

$$\begin{aligned}|\langle f,v\rangle_{\mathcal{G}}| &= |\langle f,v-\alpha\rangle_{\mathcal{G}}| \le C\|f\|_{L^2_{1,1}(\mathcal{G})}\|v-\alpha\|_{L^2_{-1,-1}(\mathcal{G})}\\ &\le C\|f\|_{L^2_{1,1}(\mathcal{G})}\|\tilde{v}-\alpha\|_{L^2_{-1,-1}(R^2)} \le C\|f\|_{L^2_{1,1}(\mathcal{G})}|\tilde{v}|_{H^1(R^2)}\\ &\le C\|f\|_{L^2_{1,1}(\mathcal{G})}|v|_{H^1(\mathcal{G})}.\end{aligned}$$

□

We now define $\tilde{H}^1(\mathcal{G})$ with the norm

$$\|u\|_{\tilde{H}^1(\mathcal{G})}=\left\{\|u\|^2_{L^2_{-1,-1}(\mathcal{G})}+|u|^2_{H^1(\mathcal{G})}\right\}^{\frac{1}{2}}$$

and define a quotient space $\hat{H}^1(\mathcal{G})$ by

$$\hat{H}^1(\mathcal{G})=\tilde{H}^1(\mathcal{G})/P_0$$

with P_0 denoting a set of constant grid functions on $\mathcal{G}$. Obviously, $P_0\subset\tilde{H}^1(\mathcal{G})$, and for any $u\in\hat{H}^1(\mathcal{G})$.

$$C_1\|u\|_{\hat{H}^1(\mathcal{G})}\le|u|_{H^1(\mathcal{G})}\le C_2\|u\|_{\hat{H}^1(\mathcal{G})}$$

with C_1 and C_2 independent of u. □

We are able to address the existence and uniqueness of the solution of the problem (3.1) with $d=2$ in the framework of the space $\hat{H}^1(\mathcal{G})$.

Theorem 3.7 If $f\in L^2_{1,1}(\mathcal{G})$ and $\sum_{n\in\mathcal{Z}^2}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa}=0$, then the problem (3.1) with $d=2$ has a solution $u\in E(\mathcal{G})$, and the

$$|u|_{H^1(\mathcal{G})}\le C\|f\|_{L^2_{1,1}(\mathcal{G})}. \tag{3.23}$$

The solution is unique in $E(\mathcal{G})$ up to a constant.

Proof By the property of the bilinear form

$$|B(u,v)|\le C|u|_{H^1(\mathcal{G})}|v|_{H^1(\mathcal{G})}\le C\|u\|_{\hat{H}^1(\mathcal{G})}\|v\|_{\hat{H}^1(\mathcal{G})}$$

and

$$B(u,u)\ge D|u|^2_{H^1(\mathcal{G})}\ge D\|u\|^2_{\hat{H}^1(\mathcal{G})}.$$

Due to Theorem 3.4

$$F(v)=|\langle f,v\rangle_{\mathcal{G}}|\le C\|f\|_{L^2_{-1,-1}(\mathcal{G})}\|v\|_{\hat{H}^1(\mathcal{G})}.$$

By Lax-Milgram Theorem, there exists a unique solution $u\in\hat{H}^1(\mathcal{G})$ such that

$$\|u\|_{\hat{H}^1(\mathcal{G})}\le C\|f\|_{L^2_{-1,-1}(\mathcal{G})}$$

which leads to the assertion of the theorem. □

Since $L^2_\nu(\mathcal{G})\subset L^2_{1,1}(\mathcal{G})$ for $\nu>1$, we have immediately the following corollary.

Corollary 3.8 If $f\in L^2_\nu(\mathcal{G})$ with $\nu>1$ and $\sum_{m\in\mathcal{Z}^2}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa}=0$, the result of Theorem 3.7 holds.

3.3 Lattice problems with $\mathbf{C}^{(\kappa)}\equiv 0$ in three dimensions

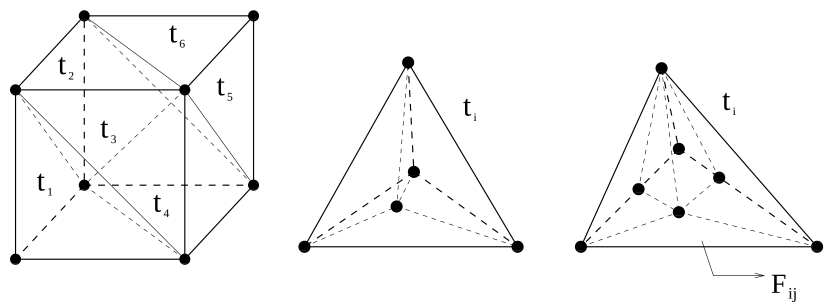
Since constant grid functions on $\mathcal{G}$ in three dimensions do not belong to the spaces $L^2_{-1}(\mathcal{G})$ and $L^2_{-1,-1}(\mathcal{G})$, we will not address lattice problems without absolute terms by introducing the quotient spaces, which are successfully used for problems in one and two dimensions. Instead, we shall develop a different approach for three-dimensional lattice problems. For the approach in three dimensions we shall utilize some properties of functions $H^1(R^3)$. To this end we have to establish the extension of grid functions on three dimensional lattice $\mathcal{G}$ to whole space R^3 by a linear interpolation.

Let $\bar{Q}_m$ be the closure of Q_m, and let $\bar{K}_m$ be a set of all nodes in $\bar{Q}_m$. By K_m^V, K_m^E, K_m^F and K_m^I, we denote the subsets of $\bar{K}_m$ for nodes at vertices, on the edges (not including the vertices), on faces (not including nodes on the edges and at vertices), and in the interior of $\bar{Q}_m$, respectively.

By $\mathcal{T} = \{t_i, 1 \le i \le T\}$ we denote a tetrahedral partition of $\bar{Q}_m$ satisfying the conditions :

(T.3) $V_{\mathcal{T}} = \bar{K}_m$, where $V_{\mathcal{T}}$ denotes a set of all vertices of the partition $\mathcal{T}$;

(T.4) for $i \neq j, t_i \cap t_j$ is a vertex, or an edge of t_i, or a face of t_i, or empty.



(a) Initial Partition T_m^0 of cell $\bar{Q}_m$ with 6 simplices (b) Partition of a simplex t_i with a node in the interior (c) Partition of simplex t_i with nodes on a face F_{ij}

Fig. 3.2 Tetrahedral partition $\mathcal{T}_m$ of cell $\bar{Q}_m$

Each t_i is a simplex with faces $F_{ij}, 1 \le j \le 4$. The construction of such a partition can be started with an initial partition $\mathcal{T}_m^0$ of $\bar{Q}_m$ such that (T.4) hold and $V_{\mathcal{T}_m^0} = K_m^V$, shown in Fig. 3.2(a). For the partition $\mathcal{T}_m^0$ there may be some nodes in the interior of simplices t_is. If a node $x^{(n,\kappa)} \in K_m^I$ is in the interior of t_i, we divide t_i into four smaller simplices by connecting $x^{(n,\kappa)}$ to four vertices of t_i, shown in Fig. 3.2(b). Repeating the process for each node in the interiors of all simplices, we have a partition $\mathcal{T}_m^1$ of $\bar{Q}_m$ for which (T.4) holds and no node $x^{(n,\kappa)} \in \bar{K}_m$ is located in the interiors of all simplices. Note that nodes $x^{(n,\kappa)} \in K_m^I \cup K_m^F \cup K_m^E$ may be located on the closure of faces of t_is in the partition $\mathcal{T}_m^1$. Suppose there are several nodes are on $\bar{F}_{ij}$ which is the closure of F_{ij}. According to the triangular partition of a cell in two dimensions, described in previous subsection, there is a triangular partition $\mathcal{T}_{\bar{F}_{ij}} = \{\tau_l, 1 \le l \le L\}$ of $\bar{F}_{ij}$ such that (T.1) and (T.2) are satisfied. Connecting the vertices of the partition $\mathcal{T}_{\bar{F}_{ij}}$ and the vertex opposite to the face F_{ij}, we divide this simplex t_i into several smaller simplices. If F_{ij} is shared by a pair of simplices, the division can be done in each of them. Carrying this division on each face of simplices t_i and each simplex in the partition $\mathcal{T}_m^1$, we will obtain a desired partition $\mathcal{T}_m$ satisfying (T.3) and (T.4). A combination of the partitions $\mathcal{T}_m$ for all $m \in \mathcal{Z}^3$ form a tetrahedral partition $\mathcal{T}$ of R^3 for which (T.4) holds and $V_{\mathcal{T}} = \cup_{m \in \mathcal{Z}^3} K_m$.

As in two dimension, based on such a tetrahedral partition $\mathcal{T}$ of R^3, we can extend a grid function u defined on three dimensional lattice $\mathcal{G}$ to a function $\tilde{u}(x)$ for $x \in R^3$ by a linear interpolation. Let $\phi_i(x)$ be a linear function in t_i which interpolates u at the vertices of t_i, and let $\psi_m(x) = \phi_i(x)$ for $x \in t_i, 1 \le i \le T$, which is a piecewise linear and continuous function in $\bar{Q}_m$, and

$$\begin{aligned}|\psi_m|^2_{H^1(Q_m)} &\leq C \sum_{t_i \subseteq \bar{Q}_m} \sum_{x^{(n,\kappa)}, x^{(l,\lambda)} \in t_i} \frac{|u_{n,\kappa} - u_{l,\lambda}|^2}{|x^{(n,\kappa)} - x^{(l,\lambda)}|^2} \\ &\leq C \sum_{t_i \subseteq \bar{Q}_m} \sum_{x^{(n,\kappa)}, x^{(l,\lambda)} \in t_i} |u_{n,\kappa} - u_{l,\lambda}|^2.\end{aligned}$$

Let $\tilde{u}(x) = \psi_m(x)$ for $x \in \bar{Q}_m, m \in \mathcal{Z}^3$. Then, $\tilde{u}(x)$ is a continuous and piecewise linear function in R^3, and

$$|\tilde{u}|^2_{H^1(R^3)} \leq C \sum_{m \in \mathcal{Z}^3} \sum_{t_i \subseteq \bar{Q}_m} \sum_{x^{(n,\kappa)}, x^{(l,\lambda)} \in t_i} |u_{n,\kappa} - u_{l,\lambda}|^2.$$

Note that vertices of a simplex t_i may not be connected. Arguing as in two dimensions for (3.15), we have

$$|\tilde{u}|^2_{H^1(R^3)} \leq C \sum_{m \in \mathcal{Z}^3} \sum_{\kappa \in \mathcal{K}} \sum_{(n,\lambda) \in B_\kappa} |u_{m,\kappa} - u_{m+n,\lambda}|^2 \leq C|u|^2_{H^1(\mathcal{G})}.$$

The arguments for the equivalence between norms of u and its extension $\tilde{u}(x)$ in two dimensions can be carried out in the three dimensions. Hence we have the following theorem which is parallel to Theorem 3.5.

Theorem 3.9 Let u be a grid function on a lattice $\mathcal{G}$, and let $\tilde{u}$ be the extension of u by a linear interpolation, described as above. Then, $|u|_{H^1(\mathcal{G})} \cong |\tilde{u}|_{H^1(R^3)}$ and $|u|_{L^2_{\nu,\sigma}(\mathcal{G})} \cong |\tilde{u}|_{L^2_{\nu,\sigma}(R^3)}$, i.e. there are two positive constants independent of u and $\tilde{u}$ such that

$$C_1|u|_{H^1(\mathcal{G})} \leq |\tilde{u}|_{H^1(R^3)} \leq C_2|u|_{H^1(\mathcal{G})} \tag{3.24}$$

and

$$C_1|u|_{L^2_{\nu,\sigma}(\mathcal{G})} \leq |\tilde{u}|_{L^2_{\nu,\sigma}(R^3)} \leq C_2|u|_{L^2_{\nu,\sigma}(\mathcal{G})}. \tag{3.25}$$

Lemma 3.10 For $v \in E(\mathcal{G})$ there exists a constant α such that

$$\|v - \alpha\|_{L^2_{-1}(\mathcal{G})} \leq C|v|_{H^1(\mathcal{G})} \tag{3.26}$$

Proof. Let $\tilde{v}$ be the extension of v described above, and let

$$\alpha = \lim_{r \to \infty} \frac{1}{|S|} \int_S \tilde{v}(r, \theta, \phi) dS.$$

where S is the unit sphere centered at the origin. By Lemma A.8 the above limit exists. Due to Theorem 3.9 and Lemma A.9, we have

$$\|v - \alpha\|_{L^2_{-1}(\mathcal{G})} \quad \leq \quad C \int_{R^3} \frac{|\tilde{v} - \alpha|^2}{r^2} dx \leq C \int_{R^3} |\nabla \tilde{v}|^2 dx \leq C|v|_{H^1(\mathcal{G})}.$$

□

Theorem 3.11 If $f \in L^2_1(\mathcal{G})$, and $\sum_{n \in \mathcal{Z}^3} \sum_{\kappa \in \mathcal{K}} f_{m,\kappa} = 0$, then for any $v \in E(\mathcal{G})$,

$$|\langle f, v \rangle_{\mathcal{G}}| = \left| \sum_{m \in \mathcal{Z}^3} \sum_{\kappa \in \mathcal{K}} f_{m,\kappa} v_{n,\kappa} \right| \leq C\|f\|_{L^2_1(\mathcal{G})} |v|_{H^1(\mathcal{G})} \tag{3.27}$$

Proof. Let $\tilde{v}$ be the extension of v, and let

$$\alpha = \lim_{r \to \infty} \frac{1}{|S|} \int_S \tilde{v}(r, \theta, \phi) dS.$$

as in previous lemma. Then by Cauchy inequality and Lemma 3.5 and Lemma 3.9

$$\begin{aligned} |\langle f, v\rangle_{\mathcal{G}}| &= |\langle f, v-\alpha\rangle_{\mathcal{G}}| \le C\|f\|_{L^2_1(\mathcal{G})}\|v-\alpha\|_{L^2_{-1}(\mathcal{G})} \\ &\le C\|f\|_{L^2_1(\mathcal{G})}\|\tilde{v}-\alpha\|_{L^2_{-1}(R^3)} \le C\|f\|_{L^2_1(\mathcal{G})}|\tilde{v}|_{H^1(R^3)} \\ &\le C\|f\|_{L^2_1(\mathcal{G})}|v|_{H^1(\mathcal{G})}. \end{aligned}$$

□

Theorem 3.12 If $f \in L^2_1(\mathcal{G})$ and $\sum_{m\in\mathcal{Z}^3}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} = 0$, then the problem (3.1) with $d=3$ has a solution $u \in E(\mathcal{G})$, and the

$$|u|_{H^1(\mathcal{G})} \le C\|f\|_{L^2_1(\mathcal{G})}. \tag{3.28}$$

The solution is unique in $E(\mathcal{G})$ up to a rigid body motion.

Proof. It is shown that

$$|B(u,v)| \le C|u|_{H^1(\mathcal{G})}|v|_{H^1(\mathcal{G})}$$

and

$$B(u,u) \ge d_1|u|^2_{H^1(\mathcal{G})}.$$

By Theorem 3.11, $F(v)$ defines a linear functional over $E(\mathcal{G})$, and

$$|F(v)| = |\langle f, v\rangle_{\mathcal{G}}| \le C\|f\|_{L^2_1(\mathcal{G})}|v|_{H^1(\mathcal{G})}.$$

If functions with zero energy are regarded as a "zero" element in the space $E(\mathcal{G})$, then $E(\mathcal{G})$ is a Hilbert space with the energy norm which is equivalent to the semi-norm of $H^1(\mathcal{G})$. By Lax-Milgram Theorem, there exists a solution $u \in E(\mathcal{G})$ such that

$$|u|_{H^1(\mathcal{G})} \approx \|u\|_{E(\mathcal{G})} \le C\|f\|_{L^2_{1,1}(\mathcal{G})}.$$

The solution is unique up to a grid function of rigid body motion on $\mathcal{G}$. □

If $\sum_{m\in\mathcal{Z}^3}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} = A$ exists but $A \ne 0$, we need to construct a special solution for the lattice problem (3.1) with f having a compact support. Let $f^0 \in L^2(\mathcal{G})$ such that $f^0_{m,\kappa} = 1$ for $m \in \mathcal{Z}^3_L = \{n \in \mathcal{Z}^3 \,|\, |n_i| < L, 1 \le i \le 3\}$ and $f^0_{m,\kappa} = 0$ for $m \notin \mathcal{Z}^3_L$. Consider the problem

$$-\sum_{(n,\lambda)\in B_\kappa} \mathbf{E}^{(\kappa,n,\lambda)}\left(u_{m+n,\lambda} - u_{m,\kappa}\right) + \mathbf{C}^{(\kappa)}u_{m,\kappa} = f^0_{m,\kappa}, m \in \mathcal{Z}^3, \kappa \in \mathcal{K}. \tag{3.29}$$

Using the arguments based on Fourier transform, e.g. see Theorem 2.15 of [13], it can be proved that the problem (3.29) has a unique solution u^0 in $E(\mathcal{G})$, and

$$|u^0|_{H^1(\mathcal{G})} \le C\|f^0\|_{L^1(\mathcal{G})} \le C\|f^0\|_{L^2(\mathcal{G})}.$$

Let $w = u - c_0u^0$ with $c_0 = \dfrac{\sum_{m\in\mathcal{Z}^3}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa}}{\sum_{m\in\mathcal{Z}^3}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa}}$. Then w satisfies the equation

$$-\sum_{(n,\lambda)\in B_\kappa} \mathbf{E}^{(\kappa,n,\lambda)}\left(w_{m+n,\lambda} - w_{m,\kappa}\right) + \mathbf{C}^{(\kappa)}w_{m,\kappa} = (f - c_0f^0)_{m,\kappa}, m \in \mathcal{Z}^3, \kappa \in \mathcal{K}.$$

Since $\sum_{m\in\mathcal{Z}^3}\sum_{\kappa\in\mathcal{K}}(f - f^0)_{m,\kappa} = 0$, by Theorem 3.12, the problem (3.30) has unique solution $w \in E(\mathcal{G})$, and

$$|w|_{H^1(\mathcal{G})} \le C\|f - f^0\|_{L^2_1(\mathcal{G})}$$

which implies that

$$|u|_{H^1(\mathcal{G})} \le C(\|f\|_{L^2_1(\mathcal{G})} + |A|).$$

Therefore, we have a theorem dealing with the case $\sum_{m\in\mathcal{Z}^3}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} \ne 0$.

Theorem 3.13 If $f \in L^2_1(\mathcal{G})$ and $\sum_{m\in\mathcal{Z}^3}\sum_{\kappa\in\mathcal{K}} f_{m,\kappa} = A$ exists, then the problem (3.1) with $d = 3$ has a solution $u \in E(\mathcal{G})$, and the

$$|u|_{H^1(\mathcal{G})} \leq C(\|f\|_{L^2_{1,1}(\mathcal{G})} + |A|). \tag{3.30}$$

The solution is unique in $E(\mathcal{G})$ up to a rigid body motion.

4. Solutions of lattice problems

In this section we shall derive a solution formula for lattice problems on a unscaled lattice $\mathcal{G}$.

4.1 Properties of Matrix $\boldsymbol{\sigma}$

The equation (2.23) gives us a system of linear equations

$$\boldsymbol{\sigma}(t)\hat{u}(t) = \hat{f}(t) \tag{4.1}$$

where $\hat{u} = \left(\hat{u}_1^T, \hat{u}_2^T \dots \hat{u}_q^T\right)^T$, and $\hat{u}_\kappa = \left(\hat{u}_1^1, \dots \hat{u}_\kappa^s\right)^T, \kappa \in \mathcal{K}$. $\hat{u}$ and $\hat{f}$ are vectors with sq components, and $\boldsymbol{\sigma}$ is a matrix called the symbol with entries denoted by $\sigma_{m,n}$. We can also write $\boldsymbol{\sigma}$ as a block matrix

$$\boldsymbol{\sigma} = (\boldsymbol{\sigma}_{\kappa,\lambda})_{1\leq\kappa,\lambda\leq q},$$

each of block $\boldsymbol{\sigma}_{\kappa\lambda}$ is a $s \times s$ matrix:

$$\left((\boldsymbol{\sigma}_{\kappa,\lambda})_{\ell,t}\right)_{1\leq\ell,t\leq s},$$

then

$$(\boldsymbol{\sigma}_{\kappa,\lambda})_{\ell,t} = \sigma_{m,n}$$

with $m = (\kappa-1)q + \ell$ and $n = (\lambda-1)q + t$. It follows from (2.23) that

$$\boldsymbol{\sigma}_{\kappa,\kappa} = \sum_{n\in B_{\kappa\kappa}} \left(1 - e^{-i<n,t>}\right)\mathbf{E}^{(\kappa,n,\kappa)} + \mathbf{C}^{(\kappa)}, \tag{4.2a}$$

$$\boldsymbol{\sigma}_{\kappa,\lambda} = -\sum_{n\in B_{\kappa\lambda}} e^{-i<n,t>}\mathbf{E}^{(\kappa,n,\lambda)}. \tag{4.2b}$$

Lemma 4.1 $\boldsymbol{\sigma}$ is a Hermitian matrix and Hermitian block matrix.

Proof. It follows from (4.2) and (2.4)- (2.5) that

$$\begin{aligned}
\boldsymbol{\sigma}_{\kappa,\lambda} &= -\sum_{n\in B_{\kappa\,\lambda}} e^{-i<n,t>}\mathbf{E}^{(\kappa,n,\lambda)} = -\sum_{n\in B_{\lambda,\kappa}} e^{-i<n,t>}\mathbf{E}^{(\kappa,n,\lambda)} \\
&= -\sum_{m\in B_{\lambda,\kappa}} e^{i<m,t>}\mathbf{E}^{(\kappa,-m,\lambda)} = -\sum_{m\in B_{\lambda,\kappa}} e^{i<m,t>}\mathbf{E}^{(\lambda,m,\kappa)} = \overline{\boldsymbol{\sigma}}_{\lambda,\kappa}.
\end{aligned}$$

For $\kappa = \lambda$, we shall write

$$B_{\kappa,\kappa} = B^-_{\kappa,\kappa} \cup B^+_{\kappa,\kappa}$$

where

$$B^+_{\kappa\kappa} = \{n = (n_1, n_2 \dots n_d) \in B_{\kappa\kappa} \mid n_\ell \geq 0, 1 \leq \ell \leq d\}$$
$$B^-_{\kappa\kappa} = \{n = (n_1, n_2 \dots n_d) \in B_{\kappa\kappa} \mid n_\ell \leq 0, 1 \leq \ell \leq d\}.$$

Due to the definition (2.3) of $B_{\kappa,\lambda}, 0 \notin B_{\kappa,\kappa}$, which implies $R^+_{\kappa,\kappa} \cap R^-_{\kappa,\kappa} = \emptyset$. By the property (2.4), $n \in B^+_{\kappa,\kappa}$ if and only if $-n \in B^-_{\kappa,\kappa}$. Therefore

$$\boldsymbol{\sigma}_{\kappa,\kappa} = \mathbf{C}^{(\kappa)} + 4\sum_{n\in B^+_{\kappa,\kappa}} \sin^2\frac{<n,t>}{2}\mathbf{E}^{(\kappa,n,\kappa)} \tag{4.3}$$

$\boldsymbol{\sigma}_{\kappa,\kappa}$ is a real matrix. Thus we have shown that $\boldsymbol{\sigma}$ is Hermitian block matrix. Note that $\mathbf{C}^{(\kappa)}$ and $\mathbf{E}^{(\kappa,n,\lambda)}$ are symmetric matrices, which implies the $\boldsymbol{\sigma}$ is a Hermitian matrix as well.

Lemma 2.2 $\boldsymbol{\sigma}_{\kappa\lambda}(-t) = \boldsymbol{\sigma}_{\lambda,\kappa}(t)^T$ for $\lambda, \kappa \in \mathcal{K}$, and $\boldsymbol{\sigma}(-t) = \boldsymbol{\sigma}(t)^T$.

Proof. For $\lambda \neq \kappa$, by the properties (2.4) and

$$\begin{aligned}\boldsymbol{\sigma}_{\kappa,\lambda}(-t) &= -\sum_{n\in B_{\kappa,\lambda}} e^{-i<n,-t>}\mathbf{E}^{(\kappa,n,\lambda)} = -\sum_{-n\in B_{\lambda,\kappa}} e^{-i<-n,t>}\mathbf{E}^{(\kappa,n,\lambda)} \\ &= -\sum_{m\in B_{\lambda,\kappa}} e^{-i<m,t>}\mathbf{E}^{(\kappa,-m,\lambda)} = -\sum_{m\in B_{\lambda,\kappa}} e^{-i<m,t>}\mathbf{E}^{(\lambda,m,\kappa)} \\ &= \boldsymbol{\sigma}_{\lambda,\kappa}(t).\end{aligned}$$

It is trivial that $\boldsymbol{\sigma}_{\kappa,\kappa}(t) = \boldsymbol{\sigma}_{\kappa,\kappa}(-t), \forall\kappa \in \mathcal{K}$. Since each block $\boldsymbol{\sigma}_{\lambda,\kappa}(t)$ is symmetric, we have $\boldsymbol{\sigma}(-t) = \boldsymbol{\sigma}(t)^\top$. □

Corollary 4.3 $\boldsymbol{\sigma}^{-1}(-t) = \left(\boldsymbol{\sigma}^{-1}(t)\right)^\top = \boldsymbol{\sigma}^{-\top}(t)$, and $\det(\boldsymbol{\sigma}(t))$ and the eigenvalues of $\boldsymbol{\sigma}(t)$ are even functions in t.

Lemma 4.4 Let $\hat{b}(t) = \left(\hat{b}_\kappa(t)\right)_{\kappa\in\mathcal{K}} \in L^2\left(I^d, H^1(K_Q)\right)$. If $C^{(\kappa)} \not\equiv 0$ for $\kappa \in \mathcal{K}$, there exist constants d_1 and d_2 independent of t and $\hat{b}(t)$ such that

$$\int_{I^d}\langle\boldsymbol{\sigma}(t)\hat{b}(t),\hat{b}(t)\rangle dt \geq d_1\int_{I^d}|\hat{b}(t)|^2_{H^1(K_Q)}dt + d_2\int_{I^d}\|\hat{b}(t)\|^2_{L^2(K_Q)}dt \tag{4.4}$$

Proof. Let $b \in \mathcal{F}^{-1}\left(\hat{b}(t)\right)$. Then, by Lemma 2.7, $b \in H^1(\mathcal{G})$, and

$$\begin{aligned}&\int_{I^d}\langle\boldsymbol{\sigma}(t)\hat{b}(t),\hat{b}(t)\rangle dt = B(b,b) \\ &= \sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in K_Q}\sum_{(n,\lambda)\in B_\kappa}\langle\mathbf{E}^{(\kappa,n,\lambda)}\left(u_{m+n,\lambda}-u_{m,\kappa}\right),\left(u_{m+n,\lambda}-u_{m,\kappa}\right)\rangle \\ &\quad+\sum_{\kappa\in\mathcal{K}}\langle\mathbf{C}^{(\kappa)}u_{m+\kappa},u_{m+\kappa}\rangle \geq d_1|b|^2_{H^1(\mathcal{G})} + d_2\|b\|^2_{L^2(\mathcal{G})}\end{aligned}$$

where d_1 and d_2 are given in (2.14). Note that

$$\|b\|^2_{H^1(\mathcal{G})} = \int_{I^d}|\hat{b}(t)|^2_{H^1(K_Q)}dt$$

and

$$\|b\|^2_{L^2(\mathcal{G})} = \int_{I^d}\|\hat{b}(t)\|^2_{L^2(K_Q)}dt.$$

(4.4) follows immediately.

Lemma 4.5 If $\mathbf{C}^{(\kappa)} \not\equiv 0$ for $\kappa \in \mathcal{K}$, then $\boldsymbol{\sigma}(t)$ is a positive definite matrix for all $t \in I^d$.

Proof. For any $\hat{b}(t) \in L^2\left(I^d, H^1(K_Q)\right)$, there holds by Lemma 4.4

$$\int_{I^d}\langle\boldsymbol{\sigma}(t)\hat{b}(t),\hat{b}(t)\rangle dt \geq d_1\int_{I^d}|\hat{b}(t)|^2_{H^1(K_Q)}dt + d_2\int_{I^d}\|\hat{b}(t)\|^2_{L^2(K_Q)}dt$$

Which implies that for almost every $t \in I^d$

$$\langle\sigma(t)\hat{b}(t),\hat{b}(t)\rangle \geq d_1|\hat{b}(t)|^2_{H^1(K_Q)} + d_2\|\hat{b}(t)\|^2_{L^2(K_Q)} \geq d_2\|\hat{b}(t)\|^2_{L^2(K_Q)}. \tag{4.5}$$

with $d_2 > 0$. Note that $\boldsymbol{\sigma}(t)$ is a Hermitian matrix and analytic in t. Hence $\boldsymbol{\sigma}(t)$ is positive definite for all $t \in I^d$. □

4.2 **Solution Representation Theorem**

Theorem 4.6 If $\mathbf{C}^{(\kappa)} \not\equiv 0$ for $\kappa \in \hat{\mathcal{K}}$ and $\hat{f} \in L^2\left(I^d\right)$, then

$$u = \mathcal{F}^{-1}\left(\boldsymbol{\sigma}(t)^{-1}\hat{f}(t)\right) \tag{4.6a}$$

is a solution of the equation (2.7) in $H^1(\mathcal{G})$, with

$$u_m = (2\pi)^{-d}\int_{I^d}\boldsymbol{\sigma}^{-1}\hat{f}(t)e^{-i<m,t>}dt \tag{4.6b}$$

and

$$\|\mathcal{F}^{-1}\left(\boldsymbol{\sigma}(t)^{-1}\hat{f}(t)\right)\|_{H^1(\mathcal{G})} \leq C\|\hat{f}\|_{L^2(I^d)} \tag{4.7}$$

where $\boldsymbol{\sigma}(t)$ is the matrix defined in (4.2).

Proof. Since $\boldsymbol{\sigma}(t)$ is positive definite for all $t \in I^d$ if $\mathbf{C}^{(\kappa)} \not\equiv 0$, by Theorem 2.4 the solution of the equation (4.1)

$$\hat{u} = \boldsymbol{\sigma}^{-1}(t)\hat{f}(t)$$

solves the variational equation (2.22), and

$$\|\hat{u}\|_{L^2(I^d,H^1(K_Q))} \leq C\|\hat{f}\|_{L^2(I^d,L^2(K_Q))}.$$

Let $u = \mathcal{F}^{-1}(\hat{u}(t))$. Due to Corollary 2.6 $u \in H^1(\mathcal{G})$ and solves the variational equation (2.8), and

$$\begin{aligned}\|\mathcal{F}^{-1}\left(\boldsymbol{\sigma}(t)^{-1}\hat{f}(t)\right)\|_{H^1(\mathcal{G})} &= \|u\|_{H^1(\mathcal{G})} \leq C\|\hat{u}\|_{L^2(I^d,H^1(K_Q))}\\ &\leq C\|\hat{f}\|_{L^2(I^d,L^2(K_Q))}.\end{aligned}$$

According to Remark 2.2, $L^2\left(I^d, L^2(K_Q)\right) = L^2(I^d)$, and the theorem is proved. □

If $\mathbf{C}^{(\kappa)} \equiv 0$ for all $\kappa \in \mathcal{K}$, there holds

$$\langle\boldsymbol{\sigma}(t)b(t), \hat{b}(t)\rangle \geq d_1|\hat{b}(t)|^2_{H^1(K_Q)} \geq 0.$$

Therefore, $\boldsymbol{\sigma}(t)$ is semi-positive definite for all $t \in I^d$. It was shown in [20] that $\det(\boldsymbol{\sigma}(t)) = 0$ if and only if $t = 0$, which implies that $\boldsymbol{\sigma}(t)$ is positive definite if $t \neq 0$. $\boldsymbol{\sigma}^{-1}(t)$ has a pole at the origin, and $\hat{u}(t)$ is singular at $t = 0$ if $\hat{f}(t) \in L^2(I^d)$. Hence, the integral (4.6b) may diverge due to the singularity at the origin.

On other hand, it was proved in previous section that lattice problems without absolute term have uniqueness solutions if $\sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}} f_{n,\kappa} = 0$ and $f \in H^\nu(\mathcal{G})$ with $\nu \geq 1$. This implies that the representation formula (4.6) can be valid for Lattice problems with $\mathbf{C}^{(\kappa)} \equiv 0$ for $\hat{f}$ belonging to some spaces stronger than $L^2(I^d)$.

Theorem 4.7 If $\hat{f} \in H^\nu_{per}\left(I^d\right)$ with $\nu > 1$ for $d = 2$ and $\nu = 1$ for $d = 1, 3$ and vanishes at $t = 0$, then the representation formula (4.6) for the lattice problems with $\mathbf{C}^{(\kappa)} \equiv 0$ holds, which realizes a mapping : $H^\nu_{pes}\left(I^d\right) \to E(\mathcal{G})$, and

$$\|\mathcal{F}^{-1}\left(\boldsymbol{\sigma}(t)^{-1}\hat{f}(t)\right)\|_{H^1(\mathcal{G})} \leq C\|\hat{f}\|_{H^\nu_{per}(I^d)}. \tag{4.8}$$

Proof. Let $f = \mathcal{F}^{-1}\left(\hat{f}\right)$. Then

$$\sum_{m\in\mathcal{Z}^d}\sum_{\kappa\in\mathcal{K}} f_{n,\kappa} = \hat{f}(0) = 0,$$

and $f \in L^2_\nu(\mathcal{G})$ by Lemma 3.5. By Theorem 3.3, Corollary 3.8 and Theorem 3.12, there exists a solution $u \in E(\mathcal{G})$ of the lattice problem (3.1) with $\mathbf{C}^{(\kappa)} \equiv 0, \forall \kappa \in \mathcal{K}$. Therefore $\hat{u}(t) = F(u) \in L^2\left(I^d, \hat{H}^1(K_Q)\right)$ and

$$\int_{I^d} |\hat{u}(t)|^2_{H^1(K_Q)}\, dt \cong |u|^2_{H^1(\mathcal{G})} \le C\|f\|_{L^2_\nu(\mathcal{G})}$$

which implies that the integral converges and that the representation formula (4.6) holds and realizes a mapping : $H^\nu_{per}\left(I^d\right) \to E(\mathcal{G})$, and

$$\|\mathcal{F}^{-1}\left(\boldsymbol{\sigma}^{-1}\hat{f}\right)\|_{H^1(\mathcal{G})} \le C\|\hat{f}\|_{H^\nu_{per}(I^d)}.$$

□

5. Two Lattice Problems

We will analyze two lattice problems. One is one-dimensional, and another is two-dimensional. Although the structures of these two problems are simple, the analysis we carry out here can be generalized to other lattice problems.

5.1. A lattice problem in one dimension

Suppose elastic rode of two different materials with half-unit length and intersection area A are connected by hinges at nodes, see Fig. 5.1. The master cell $Q = [0, 1)$, containing two nodes $x^{(\kappa)}, \kappa \in \mathcal{K} = \{1, 2\}$. The nodes in cells Q_m for $m \in \mathcal{Z}$ are denoted by $x^{(m,\kappa)}, \kappa = 1, 2$. Let $\mathcal{M} = \{x^{(m,\kappa)}, m \in \mathcal{Z}, \kappa = 1, 2\}$ denote the global mesh containing all nodes. Suppose that the rods are furnished with springs at each node. By E_1 and E_2 we denote the Young's modulus of the rode, and by $4C_1$ and $4C_2$, the Hook's constant of the springs, respectively. A lattice $\mathcal{G}$ denotes such a structure, connectivity and periodic translation.

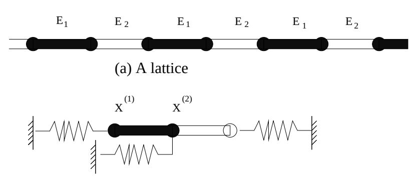


Fig. 5.1 Elastic rods of two materials in one dimension

Equilibrium Equation

Let u_j and f_j denotes the displacement of the rods and external force at the nodes x_j, we have the following equilibrium equations

$$\begin{aligned} -A\{E_1(u_{m,2} - u_{m,1}) + E_2(u_{m,1} - u_{m-1,2})\} + C_1 u_{m,1} &= f_{m,1} \\ -A\{E_2(u_{m+1,1} - u_{m,2}) + E_1(u_{m,2} - u_{m,1})\} + C_2 u_{m,2} &= f_{m,2} \end{aligned} \tag{5.1}$$

Variational Equation

The corresponding variational equation

$$B(u, v) = F(v).$$

where u, v and f are functions defined on $\mathcal{G}$, with the bilinear form

$$\begin{aligned} B(u,v) = & \sum_{m\in\mathcal{Z}} (u_{m,2}-u_{m,1})AE_1(v_{m,2}-u_{m,1}) + C_1 u_{m,1}v_{m,1} \\ + & \sum_{m\in\mathcal{Z}} (u_{m+1,1}-u_{m,2})AE_2(v_{m+1,1}-v_{m,2}) + C_2 u_{m,2}v_{m,2} \end{aligned} \qquad (5.2a)$$

and the linear functional

$$F(v) = \sum_{m\in\mathcal{Z}} \sum_{j=1,2} f_{m,j}v_{m,j} \qquad (5.2b)$$

The energy space $E(\mathcal{G})$ contains functions on $\mathcal{G}$ with finite energy $E(u)$,

$$\begin{aligned} E(u) = \tfrac{1}{2}B(u,u) = & \ \tfrac{1}{2}\sum_{m\in\mathcal{Z}} AE_1(u_{m,2}-u_{m,1})^2 + C_1 u_{m,1}^2 \\ + & \ \tfrac{1}{2}\sum_{m\in\mathcal{Z}} AE_2(u_{m+1,1}-u_{m,2})^2 + C_2 u_{m,2}^2. \end{aligned}$$

The spaces $H^1(\mathcal{G})$ and $L^2(\mathcal{G})$ are furnished with the norms

$$\|u\|^2_{H^1(\mathcal{G})} = |u|^2_{H^1(\mathcal{G})} + \|u\|^2_{L^2(\mathcal{G})} = \sum_{m\in\mathcal{Z}} (u_{m,2}-u_{m,1})^2 + (u_{m+1,1}-u_{m,2})^2 + \|u\|^2_{L^2(\mathcal{G})}$$

and

$$\|u\|^2_{L^2(\mathcal{G})} = \sum_{m\in\mathcal{Z}} |u_{m,1}|^2 + |u_{m,2}|^2.$$

Hence, the energy norm $\|u\|_{E(\mathcal{G})} = E(u)^{1/2}$ is equivalent to the norm of the space $H^1(\mathcal{G})$ if $C_1 + C_2 \neq 0$, and equivalent to the semi-norm of the space $H^1(\mathcal{G})$ if $C_1 + C_2 = 0$.

Fourier transform

For $f = f(m), m \in \mathcal{Z}$, we introduce the Fourier transform

$$\mathcal{F}(f) = \hat{f}(t) = \sum_n f(m)e^{imt}, t \in I = (-\pi,\pi)$$

which realizes an isomorphism between $L^2(\mathcal{G})$ and $L^2(I)$, and between $L^2_\nu(\mathcal{G})$ and $H^\nu_(I)$, where the space $L^2_\nu(\mathcal{G})$ is defined as a weighted space with a weighted L^2-norm

$$\|u\|^2_{L^2_\nu(\mathcal{G})} = \sum_{m\in\mathcal{Z}} (1+m^2)^\nu(|u_{m,1}|^2 + |u_{m,2}|^2).$$

The inverse Fourier transform gives $f = \mathcal{F}^{-1}(\hat{f})$ with

$$f(m) = \frac{1}{2\pi}\int_I \hat{f}(t)e^{-imt}dt.$$

Applying the Fourier transform to the equations (5.1), we obtain

$$\begin{aligned} A(E_1+E_2)\hat{u}_1 - A(E_1+E_2e^{it})\hat{u}_2 + C_1\hat{u}_1 &= \hat{f}_1 \\ -A(E_1+E_2e^{-it})\hat{u}_1 + A(E_1+E_2)\hat{u}_2 + C_2\hat{u}_2 &= \hat{f}_2 \end{aligned} \qquad (5.3)$$

The corresponding matrix

$$\boldsymbol{\sigma}(t) = \begin{pmatrix} E_{11} & -E_{12} \\ -E_{21} & E_{22} \end{pmatrix}$$

with $E_{11} = A(E_1+E_2)+C_1, E_{22} = A(E_1+E_2)+C_2, E_{12} = A(E_1+E_2e^{it})$ and $E_{21} = A(E_1+E_2e^{-it})$. $\boldsymbol{\sigma}(t)$ is a Hermit matrix, and

$$det(\boldsymbol{\sigma}) = 4A^2E_1E_2sin^2t/2 + A(C_1+C_2)(E_1+E_2) + C_1C_2.$$

Obviously, if $C_1 + C_2 > 0$, $\boldsymbol{\sigma}(t)$ is positive definite for $t \in I$, $\boldsymbol{\sigma}^{-1}(t)$ exists,

$$\boldsymbol{\sigma}^{-1}(t) = \frac{1}{det(\boldsymbol{\sigma})} \begin{pmatrix} E_{02} & E_{21} \\ E_{12} & E_{01} \end{pmatrix} \tag{5.4}$$

which leads to the solution of equation (5.3)

$$\begin{pmatrix} \hat{u}_1 \\ \hat{u}_2 \end{pmatrix} = \boldsymbol{\sigma}^{-1}(t) \begin{pmatrix} \hat{f}_1 \\ \hat{f}_2 \end{pmatrix}. \tag{5.5}$$

Therefore, the solution of the problem (5.1) can be represented as

$$u_\kappa = \mathcal{F}^{-1}(\hat{u}_\kappa(t)) = \mathcal{F}^{-1}(\sum_{1\le\ell\le2} \phi_{\kappa,\ell}(t)\hat{f}_\ell(t)),\ \kappa = 1, 2 \tag{5.6a}$$

with

$$\begin{aligned} \phi_{1,1}(t) &= \tfrac{1}{det(\boldsymbol{\sigma}(t))}E_{02},\ \phi_{2,2}(t) = \tfrac{1}{det(\boldsymbol{\sigma}(t))}E_{01}, \\ \phi_{1,2}(t) &= \tfrac{1}{det(\boldsymbol{\sigma}(t))}E_{21},\ \phi_{2,1}(t) = \tfrac{1}{det(\boldsymbol{\sigma}(t))}E_{11}. \end{aligned} \tag{5.6b}$$

If $C_1 = C_2 = 0, \boldsymbol{\sigma}(t)$ is positive definite for $t \in I$ and $t \neq 0$, and (5.4)-(5.6) hold. According to Theorem 4.6, if $\hat{f} \in H^1(I)$ and $\hat{f}(0) = 0$, then $\hat{u} \in L^2(I, H^1(K_Q))$ and $u \in E(\mathcal{G})$.

5.2 A lattice problem in two dimensions

Suppose elastic rods with intersection area A and unit length are connected by hinges at nodes $x_{k,j} = (k, j) \in \mathcal{Z}^2$, periodically, as shown Fig. 2.1. The master cell $Q = [0, 1)^2$, in which there is only one node $x^{(1)}$, and the index set $\mathcal{K} = \{1\}$. The mash $\mathcal{M} = \cup_{m=(k,j)\in\mathcal{Z}^2} x^{(m,1)} = \cup_{(k,j)\in\mathcal{Z}^2} x_{k,j} = \cup_{(k,j)\in\mathcal{Z}^2}(k, j)$. We will use $x_{k,j}$ to denote the nodes in stead of $x^{(m,1)}$. Suppose that the rods are furnished with springs at each node. By E and $\mathbf{C} = diag(C, C)$, we denote the Young's modulus of the rods, and the Hook's constant of the springs, respectively. A lattice $\mathcal{G}$ in two dimensions denotes such a structure, connectivity and periodicity.

Equilibrium Equation

Let $u_{k,j} = (u^{(1)}_{k,j}, u^{(2)}_{k,j})$ and $f_{k,j} = (f^{(1)}_{k,j}, f^{(2)}_{k,j})$ be the displacement vector and external force vector at the node $x_{k,j} = (k, j)$. We have the following equilibrium equation

$$\begin{aligned} AE(-\Delta_1 u^{(1)}_{k,j} + \Delta_1 u^{(1)}_{k-1,j}) &+ \tfrac{1}{2}AE\sum_{\ell=1,2}(-\Delta_{12}u^{(\ell)}_{k,j} + \Delta_{12}u^{(\ell)}_{k-1,j-1}) \\ &+ C\,u^{(1)}_{k,j} = f^{(1)}_{k,j}, \\ AE(-\Delta_2 u^{(2)}_{k,j} + \Delta_2 u^{(2)}_{k,j-1}) &+ \tfrac{1}{2}AE\sum_{\ell=1,2}(-\Delta_{12}u^{(\ell)}_{k,j} + \Delta_{12}u^{(\ell)}_{k-1,j-1}) \\ &+ C\,u^{(2)}_{k,j} = f^{(2)}_{k,j} \end{aligned} \tag{5.7}$$

where

$$\Delta_1 u^{(\ell)}_{k,j} = u^{(\ell)}_{k+1,j} - u^{(\ell)}_{k,j},\ \Delta_2 u^{(\ell)}_{k,j} = u^{(\ell)}_{k,j+1} - u^{(\ell)}_{k,j},\ \Delta_{12}u^{(\ell)}_{k,j} = (u^{(\ell)}_{k+1,j+1} - u^{(\ell)}_{k,j})/\sqrt{2}.$$

Variational Equation

The corresponding variational equation is

$$B(u, v) = F(v) \tag{5.8}$$

where the linear functional F and the bilinear form B are defined as

$$F(v) = \sum_{(k,j)\in\mathcal{Z}^2} f^T_{k,j} v_{k,j}$$

and

$$B(u,v) = \sum_{(k,j)\in\mathcal{Z}^2} (\Delta_1 u_{k,j})^T \mathbf{E} \Delta_1 v_{k,j} + (\Delta_2 u_{k,j})^T \mathbf{E} \Delta_2 v_{k,j}$$

$$+\tfrac{1}{2}(\Delta_{12} u_{k,j})^T \mathbf{E}^* \Delta_{12} u_{k,j} + C u_{k,j}^T v_{k,j}$$

where $\mathbf{E} = AE\mathcal{I}$ and $\mathbf{E}^* = AE\mathbf{b}\mathbf{b}^T$, $\mathcal{I}$ is an identity 2×2 matrix, and $\mathbf{b}$ is a vector $= (cos\frac{\pi}{4}, sin\frac{\pi}{4})^T$.

Fourier Transform

We introduce the Fourier transform for functions $f = \{f_{k,j}, (k,j) \in \mathcal{Z}^2\}$

$$\mathcal{F}(f) = \hat{f}(t) = \sum_{(k,j)\in\mathcal{Z}^2} f_{k,j} e^{i(kt_1+jt_2)},\ t = (t_1,t_2) \in (-\pi,\pi)^2$$

which leads to an equation in matrix form

$$\boldsymbol{\sigma}(t)\hat{u}(t) = \hat{f}(t) \tag{5.9}$$

where

$$\boldsymbol{\sigma}(t) = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}$$

with

$$\begin{aligned} \sigma_{11} &= AE(4sin^2\tfrac{t_1}{2} + \sqrt{2}sin^2\tfrac{(t_1+t_2)}{2}) + C \\ \sigma_{12} &= \sigma_{21} = -\sqrt{2}AEsin^2\tfrac{(t_1+t_2)}{2} \\ \sigma_{22} &= AE(4sin^2\tfrac{t_2}{2} + \sqrt{2}sin^2\tfrac{(t_1+t_2)}{2}) + C \end{aligned}$$

$\boldsymbol{\sigma}(t)$ is a real and symmetric matrix, and

$$\begin{aligned} det(\boldsymbol{\sigma}) = \ & A^2E^2(16sin^2\tfrac{t_1}{2}sin^2\tfrac{t_2}{2} + 4\sqrt{2}sin^2\tfrac{(t_1+t_2)}{2}(sin^2\tfrac{t_1}{2} + sin^2\tfrac{t_2}{2})) \\ & +2AEC(2sin^2\tfrac{t_1}{2} + 2sin^2\tfrac{t_2}{2} + \sqrt{2}sin^2\tfrac{(t_1+t_2)}{2}) + C^2. \end{aligned}$$

If $C > 0$, the matrix $\boldsymbol{\sigma}^{-1}(z)$ is analytic in a strip $\Sigma_\delta = \{z : |Imz| \le \delta\}$ with $\delta > 0$, and $\boldsymbol{\sigma}(t)$ is positive definite for $t \in (-\pi,\pi)^2$, and

$$\boldsymbol{\sigma}^{-1}(t) = \frac{1}{det(\boldsymbol{\sigma})}\begin{pmatrix} \sigma_{22} & -\sigma_{21} \\ -\sigma_{12} & \sigma_{11} \end{pmatrix}. \tag{5.10}$$

Representation Formula

If $C > 0$, then $\boldsymbol{\sigma}(t)$ is positive definite, then we a solution of the equation (5.9)

$$(\hat{u}^{(1)}(t), \hat{u}^{(2)}(t))^T = \boldsymbol{\sigma}^{-1}(t)(\hat{f}^{(1)}(t), \hat{f}^{(2)}(t))^T. \tag{5.11}$$

Then solution of the equation (5.7) can be represented as

$$\begin{aligned} (u^{(1)}, u^{(2)})^T &= \mathcal{F}^{-1}(\boldsymbol{\sigma}^{-1}(t)(\hat{f}^{(1)}(t), \hat{f}^{(2)}(t))^T) \\ &= \mathcal{F}^{-1}\Big(\sum_{1\le\ell\le 2}\phi_{1,\ell}(t)\hat{f}^{(\ell)}(t), \sum_{1\le\ell\le 2}\phi_{2,\ell}(t)\hat{f}^{(\ell)}(t)\Big)^T. \end{aligned} \tag{5.12a}$$

with

$$\begin{aligned} \phi_{1,1}(t) &= \tfrac{1}{det(\boldsymbol{\sigma})}(AE(4sin^2\tfrac{t_2}{2} + \sqrt{2}sin^2\tfrac{(t_1+t_2)}{2}) + C), \\ \phi_{1,2}(t) &= \phi_{2,1}(t) = \tfrac{1}{det(\boldsymbol{\sigma})}\sqrt{2}AEsin^2\tfrac{(t_1+t_2)}{2}, \\ \phi_{2,2}(t) &= \tfrac{1}{det(\boldsymbol{\sigma})}(AE(4sin^2\tfrac{t_1}{2} + \sqrt{2}sin^2\tfrac{(t_1+t_2)}{2}) + C). \end{aligned} \tag{5.12b}$$

If $C = 0, \boldsymbol{\sigma}(t)$ is positive definite for $t \in I^2$ and $t \neq 0$, and (5.10)-(5.12) hold. $\boldsymbol{\sigma}(t)^{-1}$ has a pole of order of 2 at $t = 0$. If $\hat{f}(t)$ has a zero of order 1 at $t = 0$, the solution presented in (5.12) is valid, which confirms Theorem 4.7, i.e. $\hat{u} \in L^2(I, H^1(K_Q))$ and $u \in E(\mathcal{G})$ if $\hat{f} \in H^\nu(I^2)$ with $\nu > 1$ and $\hat{f}(0) = 0$.

Appendix

In this appendix we investigate the properties of functions with finite semi-norm of $H^1(R^d), d = 2, 3$, which are essential to prove the existence and uniqueness of solutions for lattice problems without absolute terms. Let

$$H(R^d) = \left\{u \mid u \in H^1_{local}(R^d), |u|_{H^1(R^d)} < \infty\right\}$$

and let

$$H_0(R^d) = \left\{u \in H(R^d) \mid \int_\Gamma u ds = 0\right\}$$

where $\Gamma = \{x \in R^d \mid |x| = 2\}$ is the surface of the ball $S = \{x \in R^d \mid |x| \le 2\}$.

A.1 Two dimensional case

Let $\tilde{H}^1\left(R^2\right)$ be a closure of C^∞ functions with the norm

$$\|u\|^2_{\tilde{H}^1(R^2)} = \int_S |u|^2 dx + \int_{S^c} \frac{|u|^2}{r^2 \log^2 r} dx + \int_{R^2} |\nabla u|^2 dx \tag{A.2}$$

where (r, θ) are the polar coordinates, the disc $S = \{x \in R^2 | r = |x| \le 2\}$ and $S^c = R^2 \setminus S$. By $L^2_{\nu,\sigma}\left(R^2\right)$ we denote a weighted space with the norm

$$\|u\|^2_{L^2_{\nu,o}(R^2)} = \int_S |u|^2 dx + \int_{S^c} |u|^2 r^{2\nu} \log^{2\sigma} r dx. \tag{A.3}$$

Then we have

$$\|u\|^2_{\tilde{H}^1(R^2)} = \|u\|^2_{L^2_{-1,-1}(R^2)} + |u|^2_{H^1(R^d)}.$$

We introduce the spaces

$$H_\Gamma(S^c) = \left\{u \mid \int_{S^c} |\nabla u|^2 dx < \alpha, u \mid_\Gamma = 0\right\}$$

with $\Gamma = \partial S$, and we define a quotient space

$$\hat{H}^1(R^2) = \tilde{H}^1(R^2)/P_0 \tag{A.4a}$$

with the norm

$$\|u\|_{\hat{H}^1(R^2)} = \inf_{\alpha \in P_0} \|u - \alpha\|_{H^1(R^2)} \tag{A.4b}$$

where P_0 is the set of all real numbers. Since $P_0 \subset \tilde{H}^1(R^2)$, the quotient space is well defined.

Theorem A.1 If $u \in H_0\left(R^2\right)$, then

$$\int_S |u|^2 dx + \int_{S^c} \frac{|u|^2}{r^2 \log^2 r} dx \le C \int_{R^2} |\nabla u|^2 dx \tag{A.5}$$

with constant C independent of u.

To prove this theorem we need several lemmas.

Lemma A.2 Let $u(t)$ be a function on $(0, \infty)$ satisfying $u(2) = 0$ and

$$\int_2^\infty \left|\frac{du}{dt}\right|^2 t dt < \infty.$$

Then

$$\int_2^\infty \frac{|u|^2}{t\log^2 t}dt \le C\int_2^\infty \left|\frac{du}{dt}\right|^2 vdt \tag{A.6}$$

Proof. Due to Theorem 1.14 of [18]

$$\int_2^\infty |u|^2 wdt \le C_L\int_2^\infty \left|\frac{du}{dt}\right|^2 vdt$$

where $w = \dfrac{1}{t\log^2 t}, v = t$ and $C_L = \sup_{2\le t\le\infty} F_L(t)$, with

$$\begin{aligned} F_L(t) &= \left(\int_t^\infty wdt\right)^{\frac{1}{2}}\left(\int_2^t v^{-1}dt\right)^{\frac{1}{2}} \\ &= \sqrt{\frac{\log t - \log 2}{\log t}} \le 1 \text{ for } 2\le t\le\infty. \end{aligned}$$

Then (A.6) follows immediately. □

Lemma A.3 If $u \in H_\Gamma(S^c)$, then

$$\int_{S^c} \frac{|u|^2}{r^2\log^2 r}dx \le C\int_{S^c} |\nabla u|^2 dx \tag{A.7}$$

Proof. Note that $u(r,\theta)\,|_{r=2}= 0$, which implies by Lemma A.2 that

$$\int_2^\infty |u|^2\frac{1}{r\log^2 r}dr \le C\int_2^\infty \left|\frac{\partial u}{\partial r}\right|^2 rdr$$

with constant C independent of θ. Integrating with respect to θ from 0 to 2π we have (A.6). □

Lemma A.4 Let $u \in H^1(S)$. Then the following norm

$$|||u|||_{H^1(S)} = \left\{|u|^2_{H^1(S)} + |\int_\Gamma uds|^2\right\}^{\frac{1}{2}} \tag{A.8}$$

is equivalent to the norm, $\|u\|_{H^1(S)}$.

Proof. Obviously $|||u|||_{H^1(S)}$ is a norm to $H^1(S)$. Note that

$$\Big|\int_\Gamma uds\Big|^2 \le C\int_\Gamma |u|^2ds \le C\|u\|_{H^{\frac{1}{2}}(\Gamma)} \le C\|u\|_{H^1(S)}$$

which implies

$$|||u|||_{H^1(S)} \le C_1\|u\|_{H^1(S)}.$$

We need to show that

$$\|u\|_{H^1(S)} \le C_2|||u|||_{H^1(S)}.$$

If it is false, there exists a sequence $u_j \in H^1(S), j = 1,2,\ldots$ such that $\|u_j\|_{H^1(S)} = 1$, and

$$|||u_j|||^2_{H^1(S)} = |u_j|^2_{H^2(S)} + \Big|\int_\Gamma uds\Big|^2 \to 0 \text{ as } j\to\infty$$

Since $H^1(S) \subset\subset L^2(S)$, there exists a subsequence denoted by u_j again, which is a Cauchy sequence in $L^2(S)$. Since $|u_j|_{H^2(S)} \to 0$ as $j\to\infty$, $\{u_j\}_{j=1}^\infty$ is a Cauchy sequence in $H^1(S)$ as well. Hence $\lim_{j\to\infty} u_j = u_0$ in $H^1(S)$. This implies that $D^\alpha u_0 = \lim_{j\to\infty} D^\alpha u_j = 0$ for $|\alpha| = 1$. Therefore u_0 is a constant in S. Note that

$$\Big|\int_\Gamma (u_j - u_0)\,ds\Big|^2 \le C\int_\Gamma (u_j-u_0)^2\,ds \le C\|u_j - u_0\|^2_{H^1(S)} \to 0 \text{ as } j\to\infty,$$

which leads to

$$\int_\Gamma u_0 ds = \lim_{j\to\infty} \int u_j ds = 0.$$

Hence $u_0 \equiv 0$ in S. It contradicts the fact that $\|u_0\|_{H^1(S)} = \lim_{j\to\infty} \|u_j\|_{H^1(S)} = 1$. Thus the lemma is proved. $\square$

Lemma A.5 If $u \in H_0\left(R^2\right), u$ has the Fourier series on Γ:

$$u(2,\theta) = \sum_{k=1}^{\infty} a_k \cos k\theta + b_k \sin k\theta$$

and

$$\sum_{k=1}^{\infty} \left(a_k^2 + b_k^2\right) k \le C|u|^2_{H^1(S)} \le C|u|^2_{H^1(R^2)}$$

Proof. Since $\int_\Gamma u ds = 0$, $u(2,\theta)$ has the Fourier expansion

$$u(2,\theta) = \sum_{k=1}^{\infty} \left(a_k \cos k\theta + b_k \sin k\theta\right).$$

Then by the trace theorem and by Lemma A.4 we have

$$\sum_{k=1}^{\infty} \left(a_k^2 + b_k^2\right) k \le C\|u\|^2_{H^{1/2}(\Gamma)} \le C\|u\|^2_{H^1(S)} \le C|||u|||^2_{H^1(S)} = C|u|^2_{H^1(S)}.$$

$\square$

We are now able to prove Theorem A.1.

Proof of Theorem A.1. For $u \in H_0\left(R^2\right)$ we can find a harmonic function u_1 such that $(u-u_1)|_\Gamma = 0$ and $\int_{S^c} |\nabla u_1|^2 dx < \infty$. Let $u_2 = u - u_1$. Then $u_2 \in H_0\left(S^c\right)$, and by Lemma A.3

$$\int_{S^c} |u_2|^2 \frac{1}{r^2 \log^2 r} dx \le C \int_{S^c} |\nabla u_2|^2 dx \qquad (A.9)$$

Since $u_1(2,\theta) = u(2,\theta), u_1$ has a Fourier series on Γ

$$u_1(2,\theta) = \sum_{k=1}^{\infty} \left(a_k \cos k\theta + b_k \sin k\theta\right)$$

with $a_0 = 0$. Because u_1 is harmonic in S^c,

$$u_1(r,\theta) = \sum_{k=1}^{\infty} \left(a_k \cos k\theta + b_k \sin k\theta\right) \left(\frac{2}{r}\right)^k$$

and by Lemma A.5

$$\begin{aligned} \int_{S^c} |u_1|^2 \frac{1}{r^2 \log^2 r} r dr d\theta &\le C \textstyle\sum_{k=1}^{\infty} \left(a_k^2 + b_k^2\right) 4^k \displaystyle\int_2^\infty \frac{r dr}{r^{2k+2} \log^2 r} \\ &\le C \textstyle\sum_{k=1}^{\infty} \left(a_k^2 + b_k^2\right) k \le C|u|^2_{H^1(S)} \end{aligned} \qquad (A.10)$$

Note that $u_2 |_\Gamma = 0$ and $\Delta u_1 = 0$ in S^c, which implies that

$$\int_{S^c} \nabla u_1 \nabla u_2 dx = \int_\Gamma u_2 \frac{\partial u_1}{\partial n} ds - \int_{S^c} u_2 \Delta u_1 dx = 0.$$

Hence

$$|u|^2_{H^1(S^c)} = |u_1|^2_{H^1(S^c)} + |u_2|^2_{H^1(S^c)},$$

which together with (A.9)-(A.10) leads to

$$\begin{aligned} \|u\|^2_{L^2_{-1,-1}(S^c)} &\leq C\left(\|u_1\|^2_{L^2_{-1,1}(S^c)} + \|u_2\|^2_{L^2_{-1,1}(S^c)}\right) \\ &\leq C\left(|u_1|^2_{H^1(S)} + |u_2|^2_{H^1(S^c)}\right) \\ &\leq C|u|^2_{H^1(R^2)}. \end{aligned} \tag{A.11}$$

We next shall show that

$$\|u\|_{L^2(S)} \leq C|u|_{H^1(S)} \tag{A.12}$$

Let v_1 be harmonic in S and $v_1|_\Gamma = u|_\Gamma$, and let $v_2 = u - v_1$. Since $v_2|_\Gamma = 0$, by Lemma A.4

$$\|v_2\|_{L^2(S)} \leq \|v_2\|_{H^1(S)} \leq C\,|v_2|_{H^1(S)}\,. \tag{A.13}$$

Since v_1 is harmonic and $\int_\Gamma v_1 ds = \int_\Gamma u ds = 0$

$$v_1(r,\theta) = \sum_{k=1}^{\infty} (a_k \cos k\theta + b_k \sin k\theta)\left(\frac{r}{2}\right)^k$$

where $\sum_{k=1}^{\infty} a_k \cos k\theta + b_k \sin k\theta$ is the Fourier series of $v_1(2,\theta) = u(2,\theta)$. By Lemma A.5

$$\|v_1\|^2_{L^2(S)} \leq C\sum_{k=1}^{\infty}\left(a_k^2 + b_k^2\right)k \leq C|u|^2_{H^1(S)}. \tag{A.14}$$

Since v_1 is harmonic and v_2 vanishes on Γ, we have, by the argument above for u_1 and u_2, that

$$|v|^2_{H^1(S)} = |v_1|^2_{H^1(S)} + |v_2|^2_{H^1(S)}$$

which together with (A.13)-(A.14) leads to (A.12) immediately. A combination of (A.11) and (A.12) yields (A.5). □

Corollary A.6 The norm $\|u\|_{\hat{H}^1(R^2)}$ is equivalent to $|u|_{H^1(R^2)}$, and the spaces $\hat{H}^1(R^2)$ and $H(R^2)$ are equivalent.

Remark A.1. The weight function $w(x) = 1$ in S, and $w(x) = r^{-2}\log^{-2} r$ in S^c. S^c excludes the origin and unit circle. We may select others weight, e.g., $w(x) = \left(1 + r^2\right)^{-1}\log^{-2}(2+r)$ for all $x \in R^2$. It is essential for the selection of the weight that

$$|w| = O\left(|x|^{-2}\log^{-2}|x|\right) \text{ for large } |x|.$$

Also S can be selected to any bounded domain with Lipschitz boundary, and it is not necessary to be the disk centered at the origin and with radius 2.

A.2 Three dimensional case

We introduce

$$\tilde{u}(r) = \frac{1}{|S|}\int_S u(r,\theta,\phi)dS = \frac{1}{|S|}\int_0^{2\pi}\int_0^{\pi} u(r,\theta,\phi) sin\theta\, d\theta\, d\phi \tag{A.15}$$

where S denotes the unit sphere, and (r,θ,ϕ) are the spherical coordinates.

Lemma A.7 If $u \in H(R^3)$, then $\lim\limits_{r\to\infty} \tilde{u}(r) = A$ exists.

Proof. For $r \geq 1$,

$$\tilde{u}(r) = \frac{1}{|S|}\int_S \int_1^r \frac{\partial u(t,\theta,\phi)}{\partial t} dt dS + v(1)$$

Let $r_j, j = 1, 2, \ldots$ be an arbitrary sequence with $\lim_{j\to\infty} r_j = \infty$. For $r_j > r_i$ we have

$$\begin{aligned} |\tilde{u}(r_j) - \tilde{u}(r_i)| &= \frac{1}{|S|}\int_S \int_{r_i}^{r_j} \frac{\partial u(t,\theta,\phi)}{\partial t} dt dS \\ &\le C\left(\int_S \int_{r_i}^{r_j} |\frac{\partial u(t,\theta,\phi)}{\partial t}|^2 t^2 dt dS\right)^{1/2} \left(\int_{r_i}^{r_j} t^{-2} dt\right)^{1/2} \\ &\le C\left(\frac{1}{r_i} - \frac{1}{r_j}\right)^{1/2} |u|_{H^1(R^3)} \end{aligned}$$

This implies that $\{\tilde{u}(r_j)\}_{j=1}^{\infty}$ is a Cauchy sequence and that $\tilde{u}(r_j)$ converges to the same limit A for all sequence $\{r_j\}_{j=1}^{\infty}$ with $\lim_{j\to\infty} r_j = \infty$. Therefore, $\lim_{r\to\infty} \tilde{u}(r)$ exists, and $\lim_{r\to\infty} \tilde{u}(r) = A$. □

Lemma A.8 Let $\tilde{u}(r)$ be given in (A.17) and $A = \lim_{r\to\infty} \tilde{u}(r)$. Then

$$\int_0^{\infty} |\tilde{u}(r) - A|^2 dr \le C \int_0^{\infty} |\tilde{u}'(r)|^2 r^2 dr \le C|u|_{H^1(R^3)}. \tag{A.16}$$

Proof Let $w(r) = \tilde{u}(r) - A$. Then $\lim_{r\to\infty} w(r) = 0$. By Hardy inequality 330 [11], we have

$$\int_0^{\infty} |w(r)|^2 dr \le C \int_0^{\infty} |w'(r)|^2 r^2 dr$$

which is the first inequality of (A.18). The second one follows from

$$\int_0^{\infty} |\tilde{u}'(r)|^2 r^2 dr \le \int_0^{\infty} \int_S |\frac{\partial u(r,\theta,\phi)}{\partial r}| r^2 dr dS.$$

□

Theorem A.9 If $|u|_{H^1(R^3)} < \infty$, then there exist a constant α such that

$$\int_{R^3} \frac{|u-\alpha|^2}{r^2} dx \le C \int_{R^3} |\nabla u|^2 dx.$$

Proof. Let $\alpha = A = \lim_{r\to\infty} \tilde{u}(r)$. Then

$$\int_{R^3} \frac{|u-\alpha|^2}{r^2} dx \le C\left(\int_{R^3} \frac{|\tilde{u}(r)-\alpha|^2}{r^2}|dx + \int_{R^3} \frac{|u-\tilde{u}(r)|^2}{r^2}|dx\right) \tag{A.17}$$

For the first term on the right hand side of (A.17), we have by Lemma A.11

$$\int_{R^3} \frac{|\tilde{u}(r)-\alpha|^2}{r^2} dx \le \int_S \int_0^{\infty} |\tilde{u}(r) - \alpha|^2 dr dS \le C|u|^2_{H^1(R^3)}. \tag{A.18}$$

For the second term we write

$$u(r,\theta,\phi) - \tilde{u}(r) = \frac{1}{|S|}\int_S (u(r,\theta,\phi) - u(r,\theta',\phi'))\, sin\theta'\, d\theta'\, d\phi'$$

and

$$u(r,\theta,\phi) - u(r,\theta',\phi') = u(r,\theta,\phi) - u(r,\theta',\phi) + u(r,\theta',\phi) - u(r,\theta',\phi').$$

Note that

$$|u(r,\theta,\phi) - u(r,\theta',\phi)|^2 \quad = \quad |\int_{\theta'}^{\theta} \frac{\partial u(r,\tau,\phi)}{\partial \tau} d\tau|^2 \le C\int_0^{\pi} |\frac{\partial u(r,\theta,\phi)}{\partial \theta}|^2 d\theta$$

which implies

$$\int_S |u(r,\theta,\phi) - u(r,\theta',\phi)|^2 dS \le \int_S |\frac{\partial u(r,\theta,\phi)}{\partial\theta}|^2 dS$$

and

$$\int_{R^3} \frac{|u(r,\theta,\phi) - u(r,\theta',\phi)|^2}{r^2} dx \le C \int_{R^3} |\nabla u|^2 dx. \qquad (A.19)$$

Similarly, it can be shown that

$$\int_{R^3} \frac{|u(r,\theta',\phi) - u(r,\theta',\phi')|^2}{r^2} dx \le C \int_{R^3} |\nabla u|^2 dx. \qquad (A.22)$$

A combination of (A.17)-(A.20) leads to (A.16). □

Theorem A.10 If $f \in L^2_1(R^3)$, and $\int_{R^3} f dx = \lim_{R\to\infty} \int_{D_R} f dx = 0$, then for any $v \in H^(R^3)$,

$$|\int_{R^3} fvdx| \le C\|f\|_{L^2_1(R^3)} |v|^2_{H^1(R^3)}. \qquad (A.21)$$

Hereafter D_R denote a ball centered at the origin with radius R, and

$$\|f\|^2_{L^2_1(R^3)} = \int_{R^3} (1+r^2)|f|^2 dx.$$

Proof. Since $\int_{R^3} f dx = 0$, we have

$$\int_{R^3} fvdx = \int_{R^3} f(v-A)dx$$

with $A = \lim_{r\to\infty} \frac{1}{|S|} \int_S v(r,\theta,\phi)dS$. By Lemma A.8,

$$\begin{aligned} \Big|\int_{R^3} fvdx\Big| &\le C\Big\{\int_{R^3} |f|^2(1+r^2)dx\Big\}^{1/2}\Big\{\int_{R^3} \frac{|v|^2}{(1+r^2)}dx\Big\}^{1/2} \\ &\le C\|f\|_{L^2_1(R^3)}|v|_{H^1(R^3)}. \end{aligned}$$

□

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