ARMA manuscript No.
(will be inserted by the editor)

Cauchy–Born Rule and the Stability of Crystalline Solids: Static Problems

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Abstract

We study the connection between atomistic and continuum models for the elastic deformation of crystalline solids at zero temperature. We prove, under certain sharp stability conditions, that the correct nonlinear elasticity model is given by the classical Cauchy–Born rule in the sense that elastically deformed states of the atomistic model are closely approximated by solutions of the continuum model with stored energy functionals obtained from the Cauchy–Born rule. The analysis is carried out for both simple and complex lattices, and for this purpose, we develop the necessary tools for performing asymptotic analysis on such lattices. Our results are sharp and they also suggest criteria for the onset of instabilities of crystalline solids.

1. Introduction

This series of papers [11, 17, 28, 29] and [30] is devoted to a mathematical study of the connection between atomistic and continuum models of crystalline solids at zero temperature. In the present paper, we study the simplest situation when classical potentials are used in the atomistic models, and when there are no defects in the crystal. In this case the bridge between the atomistic and continuum models is served by the classical Cauchy–Born rule [6, 13, 4]. Our main objective is to establish the validity of the Cauchy–Born rule, for static problems in the present paper and for dynamic problems in the next paper [11]. In doing so, we also establish a sharp criterion for the stability of crystalline solids under stress and this allows us to study instabilities and defect formation in crystals [29].

The characteristics of crystalline solids can be summarized as follows:

1. Atoms in solids stick together due to the cohesive forces. Consequently the atoms in a crystal are arranged on a lattice. The origin of the cohesive force and the choice of the lattice are determined by the electronic structure of the atoms. However, once the lattice is selected, its geometry has a profound influence on the mechanical properties of the solid.
2. If the applied force is not too large, the solid deforms elastically to respond to the applied force. In this regime, the mechanical properties of the solid are characterized mainly by its elastic parameters such as the elastic moduli.
3. Above a certain threshold, defects, such as dislocations, form in the crystal. The structure of the defects are influenced largely by the geometry of the lattice. However, as we will see in subsequent papers [28] and [30], this is not always the case, and more refined considerations about the nature of the bonding between atoms are sometimes necessary. In this regime, the mechanical properties of the solid are characterized by various barriers such as the Peierls stress for dislocation motion.

This paper is concerned with the second point. In particular, we are interested in how the atomistic and continuum models are related to each other in the elastic regime. Naturally there has been a long history of work on this topic, going back at least to Cauchy who derived expressions for the linear elastic moduli from atomistic pair potentials and the well-known Cauchy relations [20]. Modern treatment began with the treatise of B and H [6]. The basic result is the Cauchy–Born rule (see Section 2 for details) which establishes a relation between atomistic and continuum models for elastically deformed crystals. In the mathematics literature, B , D M and G studied atomistic models using the concept of Γ-convergence [7], and proved that certain discrete functionals with pairwise interaction converge to a continuum model. One interesting aspect of their work is that their results allow for fractures to occur in the material (see also the work of T [24]). B , L B and L assumed that the microscopic displacement of the atoms follows a smooth macroscopic displacement field, and derived, in the continuum limit, both bulk and surface energy expressions from atomistic models [5]. Their leading order bulk energy term is given by the Cauchy–Born rule. F and T [14] examined a special lattice and spring model. By extending the work on convexity of continuous functionals to discrete models, they succeeded quite remarkably in proving that in certain parameter regimes, the Cauchy–Born rule does give the energy of the global minimizer in the thermodynamic limit. They also identified parameter regimes for which this statement fails and they interpreted this as being the failure of the Cauchy–Born rule.

This paper is devoted to a proof that shows that the Cauchy–Born rule is always valid for elastically deformed crystals, as long as the right unit cell is used in formulating the Cauchy–Born rule. This statement is intuitively quite obvious. Indeed much of the work in this paper is devoted to the existence and characterization of

elastically deformed states for the atomistic model, and this is where the stability conditions, which are the key conditions for our theorems, come in. However, to formulate the right theorem, it is crucial to understand that elastically deformed states are in general only local minimizers of the energy, not global minimizers. This observation is not new (see for example [24, 10]) and can be seen from the following simple example.

Consider a chain of N atoms on a line with positions $x_1, \cdots, x_N$ (see Fig. 1). Their total potential energy is given by

$$E\{x_1, \cdots, x_N\} = \sum_{i=1}^{N-1} V_0\Big(\frac{x_{i+1} - x_i}{\varepsilon}\Big),$$

where

$$V_0 = 4(r^{-12} - r^{-6})$$

is the Lennard-Jones potential [16] and ε is the equilibrium bond length. In the absence of external loading, neglect boundary effects and consider only the nearest neighbor interaction, the equilibrium positions of the atoms are given approximately by $x_j = 2^{1/6} j\varepsilon$. We will consider the case when the following condition of external loading is applied: the position of the left-most atom is kept fixed, the right-most atom is displaced by an amount that we denote as D_0. To have a finite elastic strain, D_0 should scale as $D_0 \sim L = 2^{1/6}(N-1)\varepsilon$.

There are two obvious approximate solutions to this problem: the first is a uniformly deformed elastic state: $x_j = j(2^{1/6}\varepsilon + d)$ where $d = D_0/N$. The energy of this state is approximately

$$E_1 \sim (N-1)V_0(2^{1/6} + 2^{1/6} D_0/L),$$

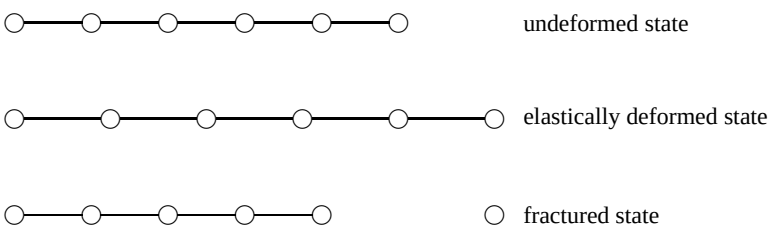

Fig. 1. A schematic figure for the one-dimensional chain example

The second approximate solution is a fractured state: $x_j \simeq 2^{1/6} j\varepsilon$ for $j \leqq N-1$ and $x_N = 2^{1/6} N\varepsilon + D_0$. The energy of this state is approximately:

$$E_2 \sim V_0(2^{1/6} + D_0/\varepsilon).$$

Obviously for large N, the fractured state has less energy than the elastically deformed state. This example indicates that elastically deformed states are sometimes only local minimizers at zero temperature. Fractured states may have less energy. The reason that crystals do not fracture spontaneously under loading is that the energy barrier for fracture is too high for real systems.

The fact that we have to deal with local minimizers simplifies the analysis at zero temperature, but complicates the situation at finite temperature. In the latter case, the right approach is to prove that elastically deformed states are metastable states. At the present time, this is still a difficult problem.

With these remarks, we can put previous results as well as the results obtained in this paper into perspective. First of all, we understand that the counterexamples constructed by Friesecke and Theil are due to the instabilities of the lattice which have caused either the onset of plastic deformation, phase transformation, or melting of the lattice. If the system undergoes phase transformation, then the Cauchy–Born rule has to be modified using the unit cell of the new phase. In other cases, we do not expect elasticity models to apply. The work of Braides *et al.* also analyzes global minimizers. The novelty of their work lies in that they have realized the analytical consequence of the example discussed above and allowed fracture states in their set-up by choosing the approximate function space over which $\Gamma-$convergence is discussed. Their results in high dimensions require that the atomistic potential satisfies the super-linear growth condition, a condition which is rarely met in real solids. The approach that is closest to ours is perhaps that of Blanc, Le Bris and Lions. The difference is that they *assumed* that the atomic displacement follows that of a macroscopically smooth vector field, whereas we *prove* that this is indeed the case under certain stability conditions. This difference is best seen from a simple example. Consider the Lennard-Jones potential with next nearest neighbor interaction on square and triangular lattices. As we show below, the stability conditions are satisfied by the triangular lattice but violated by the square lattice. Therefore, from Theorem 2.2, we are able to conclude that the Cauchy–Born rule is valid on the triangular lattice but not on the square lattice. In [17], we show that the square lattice is indeed unstable and spontaneous phase transformation occurs. In contrast, the results of [5] are equally valid for the triangular lattice and the square lattice. From a technical viewpoint, we can view the passage from the atomistic models to the continuum models as the convergence of some nonlinear finite difference schemes. The work of Blanc *et al.* is concerned with consistency. Our work proves convergence. The basic strategy is the same as that of S [22] for proving convergence of finite difference methods for nonlinear problems. Besides stability of the linearized problem, the other key component is asymptotic analysis of the atomistic model. Since we have at hand a highly unusual finite difference scheme, we have to develop the necessary tools for carrying out asymptotic and stability analysis in this setting. Indeed, much of the present paper is devoted exactly to that.

Since this is the first in this series of papers, we will discuss briefly the contents of subsequent papers. In the next paper, we will extend the results of the present paper to dynamic problems. This will allow us to formulate the sharp stability criteria for crystalline solids under stress. [29] is a natural growth of the present paper and [11], in which we carry out a systematic study of the onset of instability and plastic deformation of crystals, includes a classification of linear instabilities and the subsequent nonlinear and atomistic evolution of the crystal. [28] is devoted to the generalization of the classical Peierls–Nabarro model, which is a model of dislocations that combines an atomistic description on the slip surface and a continuum description of the linear elastic deformation away from the slip surface. The generalized Peierls–Nabarro model allows us to study the core structure and dynamics of dislocations and the influence of the underlying lattice. Finally [30] considers the generalization of the classical Cauchy–Born rule to low dimensional and curved structures such as plates, sheets and rods, with applications to the mechanical properties of carbon nanotubes.

One theme that we will emphasize throughout this series of papers is the interplay between the geometric and physical aspects of crystalline solids. As we said earlier, the geometry of the lattice has a profound influence on the physical properties of the crystal, such as the onset of plastic deformation, the core structure and the slip systems of dislocations, and the nature of the cracks. However, this is not the whole story. There are also examples of properties of solids which are not reflected at the level of geometry and have to be understood at the level of physics, e.g. the nature of the bonding between atoms. Some of these issues are discussed in [28].

2. The Generalities

We will begin with a brief discussion on atomic lattices and the atomistic potentials of solids.

2.1. Simple and complex lattices

Atoms in crystals are normally arranged on lattices. Common lattice structures are body-centered cubic (BCC), face-centered cubic (FCC), diamond lattice, hexagonal closed packing (HCP), etc [3]. Under normal experimental conditions, i.e. room temperature and pressure, iron (Fe) exists in BCC lattice, aluminum (Al) exists in FCC lattice, and silicon (Si) exists in diamond lattice.

Lattices are divided into two types: simple lattices and complex lattices.

Simple lattices. Simple lattices are also called Bravais lattices. They take the form:

$$L(\boldsymbol{e}_i, \boldsymbol{o}) = \Big\{\boldsymbol{x} \mid \boldsymbol{x} = \sum_{i=1}^{d} \nu^i \boldsymbol{e}_i + \boldsymbol{o} \qquad \nu^i \text{ are integers}\Big\}, \tag{2.1}$$

where $\{\boldsymbol{e}_i\}_{i=1}^d$ are the basis vectors, d is the dimension, and $\boldsymbol{o}$ is a particular lattice site, which can be taken as the origin, due to the translation invariance of lattices. The basis vectors are not unique.

Out of the examples listed above, BCC and FCC are simple lattices. For FCC, one set of basis vectors are

$$e_1 = \frac{\varepsilon}{2}(0,1,1), \quad e_2 = \frac{\varepsilon}{2}(1,0,1), \quad e_3 = \frac{\varepsilon}{2}(1,1,0).$$

For BCC, we may choose

$$e_1 = \frac{\varepsilon}{2}(-1,1,1), \quad e_2 = \frac{\varepsilon}{2}(1,-1,1), \quad e_3 = \frac{\varepsilon}{2}(1,1,-1).$$

as the basis vectors. Here and in what follows, we use ε to denote the equilibrium lattice constant.

Another example of a simple lattice is the two-dimensional triangular lattice. Its basis vectors can be chosen as:

$$e_1 = \varepsilon(1,0), \quad e_2 = \varepsilon(1/2, \sqrt{3}/2).$$

Complex lattices. In principle, any lattices can be regarded as a union of congruent simple lattices [12], i.e. they can be expressed in the form:

$$L = L(\boldsymbol{e}_i, \boldsymbol{o}) \cup L(\boldsymbol{e}_i, \boldsymbol{o} + \boldsymbol{p}_1) \cup \cdots L(\boldsymbol{e}_i, \boldsymbol{o} + \boldsymbol{p}_k)$$

for certain integer k, $\boldsymbol{p}_1, \cdots, \boldsymbol{p}_k$ are the shift vectors. For example, the two dimensional hexagonal lattice with lattice constant ε can be regarded as the union of two triangular lattices with shift vector $\boldsymbol{p}_1 = \varepsilon(-1/2, -\sqrt{3}/6)$. The diamond lattice is made up of two interpenetrating FCC lattices with shift vector $\boldsymbol{p}_1 = \varepsilon/4(1,1,1)$. The HCP lattice is obtained by stacking two simple hexagonal lattices with the shift vector $\boldsymbol{p}_1 = \varepsilon(1/2, \sqrt{3}/6, \sqrt{6}/3)$. Some solids consist of more than one species of atoms. Sodium chloride (NaCl), for example, has equal number of sodium ions and chloride ions placed at alternating sites of a simple cubic lattice. This can be viewed as the union of two FCC lattices: one for the sodium ions and one for the chloride ions.

In this paper, we focus on the case when $k = 1$. Generalization to high values of k is in principle straightforward but the technicalities can be quite tedious.

2.2. Potentials

We will restrict our attention to classical potentials of the form:

$$E\{\boldsymbol{y}_1, \cdots, \boldsymbol{y}_N\} = V(\boldsymbol{y}_1, \cdots, \boldsymbol{y}_N) - \sum_{j=1}^{N} f(\boldsymbol{x}_j)\boldsymbol{y}_j, \tag{2.2}$$

where V is the interaction potential between the atoms, $\boldsymbol{y}_j$ and $\boldsymbol{x}_j$ are the deformed and undeformed positions of the j-th atom respectively. V often takes the form:

$$V(\boldsymbol{y}_1, \cdots, \boldsymbol{y}_N) = \sum_{i,j} V_2(\boldsymbol{y}_i/\varepsilon, \boldsymbol{y}_j/\varepsilon) + \sum_{i,j,k} V_3(\boldsymbol{y}_i/\varepsilon, \boldsymbol{y}_j/\varepsilon, \boldsymbol{y}_k/\varepsilon) + \cdots,$$

where ε is the lattice constant as before.

Examples of the potentials include:

1. Lennard-Jones potential:

$$V_2(\boldsymbol{x}, \boldsymbol{y}) = V_0(r) \qquad \text{and} \quad V_3 = V_4 = \cdots = 0,$$

where $r = |\boldsymbol{x} - \boldsymbol{y}|$, and

$$V_0(r) = 4(r^{-12} - r^{-6}).$$

2. Embeded-atom methods: embeded-atom methods introduced by D B [8, 9] to model realistic metallic systems. The total energy consists of two parts: a function of the electron density and a term that accounts for the repulsive interaction when atoms get close to each other:

$$V = \sum_i F(\rho_i) + \frac{1}{2} \sum_{i \neq j} V_2(r_{ij}/\varepsilon),$$

where ρ_i is the electron density around the i-th atom, and V_2 is a pair potential, $r_{ij} = \left|\boldsymbol{x}_j - \boldsymbol{x}_i\right|$. The density ρ_i is usually defined as

$$\rho_i = \sum_{j \neq i} f(r_{ij}).$$

The functions f, V_2 and F are obtained empirically and calibrated by quantum mechanical calculations.

3. Stillinger–Weber potential [21]

$$V = \frac{1}{2} \sum_{i,j} V_2(r_{ij}/\varepsilon) + \frac{1}{3!} \sum_{i,j,k} V_3(\boldsymbol{x}_i/\varepsilon, \boldsymbol{x}_j/\varepsilon, \boldsymbol{x}_k/\varepsilon),$$

where V_2 is a pair potential and V_3 is an angular term which usually takes the form:

$$V_3(\boldsymbol{x}_i, \boldsymbol{x}_j, \boldsymbol{x}_k) = h(r_{ij}, r_{ik}, \theta_{jik}),$$

where

$$h(r_{ij}, r_{ik}, \theta_{jik}) = \lambda e^{[\gamma(r_{ij}-a)^{-1} + \gamma(r_{ik}-a)^{-1}]}(\cos\theta_{jik} + 1/3)^2$$

for some parameters λ and γ, θ_{jik} is angle between $\boldsymbol{x}_j - \boldsymbol{x}_i$ and $\boldsymbol{x}_k - \boldsymbol{x}_i$.

4. Tersoff potential: Tersoff potential [23] is introduced to describe the open structure of covalently bonded solids such as carbon and silicon. It takes the form:

$$V = \frac{1}{2}\sum_{i\neq j} f_C(r_{ij}/\varepsilon)(f_R(r_{ij}/\varepsilon) + b_{ij} f_A(r_{ij}/\varepsilon)).$$

Here f_C is a cut-off function and

$$f_R(r) = A\exp(-\lambda_1 r), \quad f_A(r) = -B\exp(-\lambda_2 r).$$

The term b_{ij} is a measure of local bond order,

$$b_{ij} = (1+\beta^n \xi_{ij}^n)^{(-1/2n)},$$

where the function ξ_{ij} is given by

$$\xi_{ij} = \sum_{k\neq i,j} f_C(r_{ik}/\varepsilon) g(\theta_{ijk}) \exp(\lambda_3^3 (r_{ij} - r_{ik})^3)$$

with

$$g(\theta) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos\theta)^2}.$$

The parameters $A, B, \lambda_1, \lambda_2, \lambda_3, \beta, n, c, d$ and h vary for different materials.

Clearly different potentials are required to model different materials. In this paper, we will work with general atomistic models, and we will make the following assumptions on the potential functions V.

1. V is translation invariant.
2. V is invariant with respect to rigid body motion.
3. V is smooth in a neighborhood of the equilibrium state.
4. V has finite range and consequently we will consider only interactions that involve a fixed number of atoms.

In fact, our presentation will be limited to potentials that contain only two-body or three-body potentials. However, it is straightforward to extend our results to more general potentials that satisfy these conditions. To avoid complication in notation, we will sometimes only write out the three-body terms in the expressions for the potential. Extensions to general multi-body terms should be quite straightforward from the three-body terms. The first two assumptions are general [6], while the latter two are specific technical assumptions. Note that a direct consequence of the invariance of V with respect to rigid body motion is that V is an even function, i.e.

$$V(\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N) = V(-\boldsymbol{x}_1, \cdots, -\boldsymbol{x}_N). \tag{2.3}$$

This is easily understood since V is a function of atom distances and angles by invariance with respect to rigid body motion [15].

At zero temperature, the atomistic model becomes a minimization problem:

$$\min_{\substack{\boldsymbol{y}_1,\cdots,\boldsymbol{y}_N \\ \text{subject to certain boundary condition}}} E\{\boldsymbol{y}_1,\cdots,\boldsymbol{y}_N\},$$

from which we determine the position of every atom. We define

$$\boldsymbol{u}_j = \boldsymbol{y}_j - \boldsymbol{x}_j$$

as the displacement of the j-th atom under the applied force.

In continuum model of solids, we describe the displacement by a vector field $\boldsymbol{u}$. Denote by Ω the domain occupied by the material in the undeformed state. The displacement field is determined by a variational problem:

$$\int_{\Omega} \Big\{ W(\nabla \boldsymbol{u}(\boldsymbol{x})) - f(\boldsymbol{x}) \cdot \boldsymbol{u}(\boldsymbol{x}) \Big\} \mathrm{d}\boldsymbol{x}, \tag{2.4}$$

subject to certain boundary conditions. Here W is the stored energy density, which in general is a function of the displacement gradient $\nabla \boldsymbol{u}$. A very important question is how to obtain W. In the continuum mechanics literature, W is often obtained empirically through fitting a few experimental parameters such as the elastic moduli. Here we will study how W can be obtained from the atomistic models.

For simplicity, we will concentrate on the case when the periodic boundary condition is imposed over the material: the displacement is assumed to be the sum of a linear function and a periodic function, the linear part is assumed to be fixed. Extending the analysis to nonperiodic boundary conditions requires substantial changes of the analysis, since new classes of instabilities may occur at the boundary.

There are two important length scales in this problem. One is the lattice constant. The other is the size of the material. Their ratio is a small parameter that we will use in our estimates below.

2.3. Cauchy–Born rule

2.3.1. Cauchy–Born rule for simple lattice First of all, let us fix the notations. We will fix one atom in a perfect lattice as the origin. All other atoms are viewed as translation of the origin, and we denote the translation vector generically as $\boldsymbol{s}$. In this way, we may write $V_2(\boldsymbol{s}) = V_2(\boldsymbol{0}, \boldsymbol{s})$ and $V_3(\boldsymbol{s}_1, \boldsymbol{s}_2) = V_3(\boldsymbol{0}, \boldsymbol{s}_1, \boldsymbol{s}_2)$. We assume that V is zero if one of the $\boldsymbol{s}_i$ is zero. Denote

$$\nabla V_3(\boldsymbol{s}_1, \boldsymbol{s}_2) = (\partial_{\alpha_1} V_3(\boldsymbol{s}_1, \boldsymbol{s}_2), \partial_{\alpha_2} V_3(\boldsymbol{s}_1, \boldsymbol{s}_2)).$$

We let

$$D^+_\ell \boldsymbol{x}_i = \boldsymbol{x}_{i+s_\ell} - \boldsymbol{x}_i, \qquad D^-_\ell \boldsymbol{x}_i = \boldsymbol{x}_i - \boldsymbol{x}_{i-s_\ell} \qquad \text{for} \quad \ell = 1, 2, \cdots, d,$$

where d is the dimension of the system, and $(\boldsymbol{s}_1, \cdots, \boldsymbol{s}_d)$ is a fixed basis for the lattice. Clearly, D_ℓ^+ and D_ℓ^- depend on $\boldsymbol{s}_\ell$. However, using this simplified notation will not cause confusion.

For complex lattices, we need an additional notation. Assuming that the lattice is made up of two simple lattices, one with atoms labeled by A and another with atoms labeled by B, we let:

$$D_{\boldsymbol{p}}^+ \boldsymbol{x}_i^A = \boldsymbol{x}_i^B - \boldsymbol{x}_i^A.$$

Here $\boldsymbol{x}_i^A$ and $\boldsymbol{x}_i^B$ belong to the same unit cell. The stored energy density W_{CB} is a function of $d \times d$ matrices. Given a $d \times d$ matrix A, $W_{\mathrm{CB}}(\mathsf{A})$ is computed by first deforming an infinite crystal uniformly with displacement gradient A, and then setting $W_{\mathrm{CB}}(\mathsf{A})$ to be the energy of the deformed unit cell

$$W_{\mathrm{CB}}(\mathsf{A}) = \lim_{m\to\infty} \frac{\sum_{\boldsymbol{y}_i,\boldsymbol{y}_j,\boldsymbol{y}_k \in (\mathsf{I}+\mathsf{A})L \cap mD} V(\boldsymbol{y}_i, \boldsymbol{y}_j, \boldsymbol{y}_k)}{|mD|}. \tag{2.5}$$

Here D is an arbitrary open domain in $\mathbb{R}^d$, L denotes the lattice $L(\boldsymbol{e}_i, \boldsymbol{o})$ defined in (2.1) and $|mD|$ denote the volume of mD.

The key point in (2.5) is that the lattice is uniformly deformed, i.e. no internal relaxation is allowed for the atoms in mD. This is contrary to the definition of energy densities in Γ-limits (see [7] and [14]). It is easy to check that this definition is independent of the choice of D.

The limit in (2.5) can be computed explicitly. For two-body potentials, we have

$$W_{\mathrm{CB}}(\mathsf{A}) = \frac{1}{2\vartheta_0} \sum_{\boldsymbol{s}} V_2((\mathsf{I}+\mathsf{A})\boldsymbol{s}), \tag{2.6}$$

where $\boldsymbol{s}$ runs over the ranges of the potential V_2, ϑ_0 is the volume of the unit cell. For simplicity of notation, we will omit the volume factor in subsequent presentation.

In particular, if the atomistic model is a Lennard-Jones potential on a one-dimensional simple lattice, we have

$$W_{\mathrm{CB}}(A) = \frac{\zeta^2(6)}{\zeta(12)}\Big(\frac{1}{4}|1+A|^{-12} - \frac{1}{2}|1+A|^{-6}\Big), \tag{2.7}$$

where $\zeta(\cdot)$ is the Riemann zeta function. See Fig. 2.

For three-body potentials, we have

$$W_{\mathrm{CB}}(\mathsf{A}) = \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \frac{1}{3!} V_3((\mathsf{I}+\mathsf{A})\boldsymbol{s}_1, (\mathsf{I}+\mathsf{A})\boldsymbol{s}_2). \tag{2.8}$$

For general many-body potentials,

$$W_{\mathrm{CB}}(\mathsf{A}) = \sum_{m=2} \frac{1}{m!} \sum_{\langle \boldsymbol{s}_1, \cdots, \boldsymbol{s}_{m-1} \rangle} V_m((\mathsf{I}+\mathsf{A})\boldsymbol{s}_1, \cdots, (\mathsf{I}+\mathsf{A})\boldsymbol{s}_{m-1}). \tag{2.9}$$

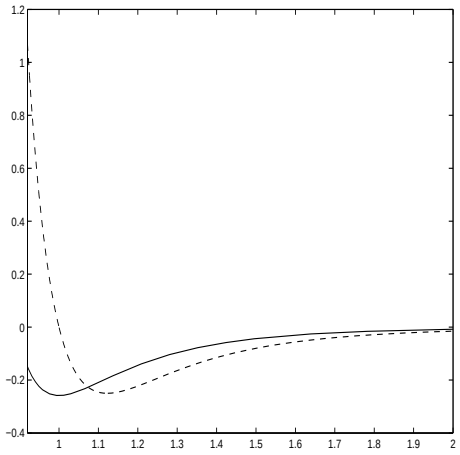

Fig. 2. Solid line: stored energy density obtained from the Lennard-Jones potential via CB rule in terms of $1 + A$. Dotted line: the original Lennard-Jones potential

For three-body potentials, the variational operator for W_{CB} is:

$$\operatorname{div}(D_{\mathsf{A}} W_{\mathrm{CB}}(\nabla \boldsymbol{u})) = \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \Big\{ (\partial^2_{\alpha_1} V_3)(\boldsymbol{s}_1 \cdot \nabla)^2 \boldsymbol{u} + (\partial^2_{\alpha_2} V_3)(\boldsymbol{s}_2 \cdot \nabla)^2 \boldsymbol{u} + 2(\partial_{\alpha_1 \alpha_2} V_3)(\boldsymbol{s}_1 \cdot \nabla)(\boldsymbol{s}_2 \cdot \nabla)\boldsymbol{u} \Big\}, \tag{2.10}$$

where $\partial^2_{\alpha_1} V_3, \partial_{\alpha_1 \alpha_2} V_3$ and $\partial^2_{\alpha_2} V_3$ are all evaluated at $(\boldsymbol{s}_1 + (\boldsymbol{s}_1 \cdot \nabla)\boldsymbol{u}, \boldsymbol{s}_2 + (\boldsymbol{s}_2 \cdot \nabla)\boldsymbol{u})$.

2.3.2. Cauchy–Born rule for complex lattice For a complex lattice, we first associate with it a Bravais sublattice denoted by L_0 so that the unit cell generated by the basis vectors coincides with the unit cell of the complex lattice. The remaining lattice points are treated as internal degrees of freedom, denoted by $\boldsymbol{p}$. These are the shift vectors. To simplify the notation, we will assume that the complex lattice is the union of two simple lattices ($k = 1$). To compute $W_{\mathrm{CB}}(\mathsf{A})$, we deform the Bravais sublattice uniformly with deformation gradient A. We then relax the internal degrees of freedom keeping the position of the deformed Bravais lattice fixed. This gives

$$W_{\mathrm{CB}}(\mathsf{A}) = \min_{\boldsymbol{p}} W(\mathsf{A}, \boldsymbol{p}), \tag{2.11}$$

where

$$W(\mathsf{A}, \boldsymbol{p}) = \lim_{m \to \infty} \frac{1}{|mD|} \sum V(\boldsymbol{y}_i + z_i \boldsymbol{p}, \boldsymbol{y}_j + z_j \boldsymbol{p}, \boldsymbol{y}_k + z_k \boldsymbol{p}). \tag{2.12}$$

Here the summation is carried out for $\boldsymbol{y}_i, \boldsymbol{y}_j, \boldsymbol{y}_k \in (\mathsf{I} + \mathsf{A})L \cap mD$ and $z_i, z_j, z_k = 0, 1$.

We will give two specific examples of W_{CB} for complex lattices. First we consider a one-dimensional chain with two alternating species of atoms A and B, with pairwise interactions. We denote the interaction potential between A atoms by V_{AA},

the interaction potential between B atoms by V_{BB}, and the interaction potential between A and B atoms by V_{AB}. Denote the shift of a B atom from its left neighboring A atom by p. Then $W_{\mathrm{CB}}(A) = \min_p W(A, p)$ with

$$W(A,p) = \sum_{j\in\mathbb{Z}}\Big(V_{AB}((1+A)(j+1)\varepsilon - p) + V_{AB}((1+A)j\varepsilon + p)\Big) + \sum_{j\in\mathbb{Z}}\Big(V_{AA}((1+A)j\varepsilon) + V_{BB}((1+A)j\varepsilon)\Big),$$

where ε is the lattice constant. Observe that for any A, $W(A, p)$ is symmetric with respect to $p^* = (1+A)\varepsilon/2$, and therefore $p^* = (1+A)\varepsilon/2$ is either a local maximum or a local minimum of $W(A, p)$. In the latter case, we have

$$W_{\mathrm{CB}}(A) = \sum_{j\in\mathbb{Z}}\Big(V_{AA}((1+A)j\varepsilon) + V_{BB}((1+A)j\varepsilon) + 2V_{AB}((1+A)(j+1/2)\varepsilon)\Big) \tag{2.13}$$

at that local minimum.

Next we consider the hexagonal lattice. We again assume that there are two species of atoms, A and B, located at the open and filled circles in Fig. 3, respectively. As in the one-dimensional case, there are three terms in $W(\mathsf{A}, \boldsymbol{p})$:

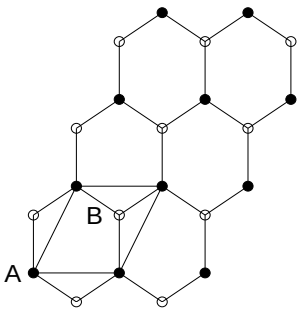

Fig. 3. Hexagonal Lattice. Two species of atoms: Atom A and atom B.

$$W(\mathsf{A}, \boldsymbol{p}) = W_{AA}(\mathsf{A}) + W_{AB}(\mathsf{A}, \boldsymbol{p}) + W_{BB}(\mathsf{A})$$

with

$$W_{\kappa\kappa}(\mathsf{A}) = \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2\rangle} V_{\kappa\kappa}((\mathsf{I}+\mathsf{A})\boldsymbol{s}_1, (\mathsf{I}+\mathsf{A})\boldsymbol{s}_2) \quad \kappa = \mathrm{A} \text{ or } \mathrm{B},$$

and

$$W_{AB}(\mathsf{A}, \boldsymbol{p}) = \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} [V_{AB}((\mathsf{I}+\mathsf{A})\boldsymbol{s}_1 + \boldsymbol{p}, (\mathsf{I}+\mathsf{A})\boldsymbol{s}_2 + \boldsymbol{p}) + V_{AB}((\mathsf{I}+\mathsf{A})\boldsymbol{s}_1 + \boldsymbol{p}, (\mathsf{I}+\mathsf{A})\boldsymbol{s}_2) + V_{AB}((\mathsf{I}+\mathsf{A})\boldsymbol{s}_1, (\mathsf{I}+\mathsf{A})\boldsymbol{s}_2 + \boldsymbol{p})].$$

A special case of this lattice is the graphite sheet for carbon. In that case, there is only one species of atoms. Hence V_{AA}, V_{BB} and V_{AB} are all equal.

We next derive the Euler–Lagrange equations in this case. There are two sets of Euler–Lagrange equations. The first comes from the local minimization with respect to the internal degree of freedom $\boldsymbol{p}$, i.e. (2.11), which reads:

$$\partial_{\boldsymbol{p}} W_{AB}(\mathsf{A}, \boldsymbol{p}) = \boldsymbol{0}, \tag{2.14}$$

namely,

$$\sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} [(\partial_{\alpha_1} + \partial_{\alpha_2}) V_{AB}((\mathsf{I}+\mathsf{A})\boldsymbol{s}_1 + \boldsymbol{p}, (\mathsf{I}+\mathsf{A})\boldsymbol{s}_2 + \boldsymbol{p}) + \partial_{\alpha_1} V_{AB}((\mathsf{I}+\mathsf{A})\boldsymbol{s}_1 + \boldsymbol{p}, (\mathsf{I}+\mathsf{A})\boldsymbol{s}_2) + \partial_{\alpha_2} V_{AB}((\mathsf{I}+\mathsf{A})\boldsymbol{s}_1, (\mathsf{I}+\mathsf{A})\boldsymbol{s}_2 + \boldsymbol{p})] = \boldsymbol{0}. \tag{2.15}$$

The second Euler–Lagrange equation comes from the minimization problem (2.4),

$$\operatorname{div}(D_{\mathsf{A}} W_{\mathrm{CB}}(\nabla \boldsymbol{u})) = \boldsymbol{f}, \tag{2.16}$$

where $D_{\mathsf{A}} W_{\mathrm{CB}}(\mathsf{A}) = D_{\mathsf{A}}(W_{AA}(\mathsf{A}) + W_{AB}(\mathsf{A}, \boldsymbol{p}) + W_{BB}(\mathsf{A}))$, and for $\kappa, \kappa' = A$ or B,

$$\operatorname{div}(D_{\mathsf{A}} W_{\kappa\kappa'}(\nabla \boldsymbol{u})) = \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{i,j=1}^{2} (\partial^2_{\alpha_i \alpha_j} V_{\kappa\kappa'})(\boldsymbol{s}_i \cdot \nabla)(\boldsymbol{s}_j \cdot \nabla)\boldsymbol{u},$$

where $\partial^2_{\alpha_i \alpha_j} V_{\kappa\kappa'}(\kappa, \kappa' = A \text{ or } B)$ is evaluated at $(\boldsymbol{s}_1 + (\boldsymbol{s}_1 \cdot \nabla)\boldsymbol{u}, \boldsymbol{s}_2 + (\boldsymbol{s}_2 \cdot \nabla)\boldsymbol{u})$.

It follows from the Hellmann–Feynman theorem [27] that

$$\begin{aligned} &\operatorname{div}(D_{\mathsf{A}} W_{AB}(\nabla \boldsymbol{u})) \\ &= \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{i,j=1}^{2} \partial^2_{\alpha_i \alpha_j} \widetilde{V}_{AB}(\boldsymbol{s}_i \cdot \nabla)(\boldsymbol{s}_j \cdot \nabla)\boldsymbol{u} \\ &\quad + \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} [(\partial^2_{\alpha_1}(V^1_{AB} + V^2_{AB}) + \partial_{\alpha_1 \alpha_2}(V^1_{AB} + V^3_{AB}))(\boldsymbol{s}_1 \cdot \nabla)(D_{\mathsf{A}} \boldsymbol{p} \cdot \nabla)\boldsymbol{u} \\ &\qquad + (\partial_{\alpha_1 \alpha_2}(V^1_{AB} + V^2_{AB}) + \partial^2_{\alpha_2}(V^1_{AB} + V^3_{AB}))(\boldsymbol{s}_1 \cdot \nabla)(D_{\mathsf{A}} \boldsymbol{p} \cdot \nabla)\boldsymbol{u}], \end{aligned}$$

where $\widetilde{V}_{AB} = V^1_{AB} + V^2_{AB} + V^3_{AB}$ with

$$V^1_{AB} = V_{AB}(\boldsymbol{s}_1 + (\boldsymbol{s}_1 \cdot \nabla)\boldsymbol{u} + \boldsymbol{p}(\nabla \boldsymbol{u}), \boldsymbol{s}_2 + (\boldsymbol{s}_2 \cdot \nabla)\boldsymbol{u} + \boldsymbol{p}(\nabla \boldsymbol{u})),$$
$$V^2_{AB} = V_{AB}(\boldsymbol{s}_1 + (\boldsymbol{s}_1 \cdot \nabla)\boldsymbol{u} + \boldsymbol{p}(\nabla \boldsymbol{u}), \boldsymbol{s}_2 + (\boldsymbol{s}_2 \cdot \nabla)\boldsymbol{u}),$$
$$V^3_{AB} = V_{AB}(\boldsymbol{s}_1 + (\boldsymbol{s}_1 \cdot \nabla)\boldsymbol{u}, \boldsymbol{s}_2 + (\boldsymbol{s}_2 \cdot \nabla)\boldsymbol{u} + \boldsymbol{p}(\nabla \boldsymbol{u})),$$

where $\boldsymbol{p}$ is obtained from the algebraic equations (2.14).

2.3.3. The elastic stiffness tensor For a given stored energy function W_{CB}, the elastic stiffness tensor can be expressed as

$$\mathsf{C}_{\alpha\beta\gamma\delta} = \frac{\partial^2 W_{\mathrm{CB}}}{\partial A_{\alpha\beta} \partial A_{\gamma\delta}}(\mathbf{0}) \qquad 1 \leqq \alpha, \beta, \gamma, \delta \leqq d.$$

If W_{CB} is obtained from a pairwise potential, we have

$$\mathsf{C}_{\alpha\beta\gamma\delta} = \sum_{\boldsymbol{s}} (V_2''(|\boldsymbol{s}|)\,|\boldsymbol{s}|^{-2} - V_2'(|\boldsymbol{s}|)\,|\boldsymbol{s}|^{-3}) s_\alpha s_\beta s_\gamma s_\delta, \tag{2.17}$$

where the summation is carried out for all $\boldsymbol{s} = (s_1, \cdots, s_d)$. The above formula is proven in Lemma 3.2. Discussions for the more general cases are found in Appendix B.

2.4. Spectral analysis of the dynamical matrix

A lot can be learned about the lattice statics and lattice dynamics from phonon analysis, which is the discrete Fourier analysis of lattice waves at the equilibrium or uniformly deformed states. This is standard material in textbooks on solid state physics (see for example [3] and [26]). As we need some of the terminology, we will briefly discuss a simple example of a *one-dimensional* chain.

Consider the following example:

$$M \frac{d^2 y_j}{dt^2} = -\frac{\partial V}{\partial y_j} = V'(y_{j+1} - y_j) - V'(y_j - y_{j-1}),$$

where M is the mass of the atom. Let $y_j = j\varepsilon + \widetilde{y}_j$, and linearizing the above equation, we get

$$M \frac{d^2 \widetilde{y}_j}{dt^2} = V''(\varepsilon)(\widetilde{y}_{j+1} - 2\widetilde{y}_j + \widetilde{y}_{j-1}). \tag{2.18}$$

Let $\widetilde{y}_j(k) = e^{i(k x_j - \omega t)}$, we obtain

$$\omega^2(k) = \frac{4}{M} V''(\varepsilon) \sin^2 \frac{k\varepsilon}{2},$$

where $k = \frac{2\pi\ell}{N\varepsilon}$ with $\ell = -[N/2], \cdots, [N/2]$.

For the more general case, it is useful to define the reciprocal lattice, which is the lattice of points in the k-space that satisfy $e^{i\boldsymbol{k}\cdot\boldsymbol{x}} = 1$ for all $\boldsymbol{x} \in L$. The first

Brillouin zone in the k-space is defined to be the subset of points that are closer to the origin than to any other point on the reciprocal lattice.

For complex lattices, the phonon spectrum contains both acoustic and optical branches [3], which will be denoted by ω_a and ω_o respectively.

What we really need in the present work is the spectral analysis of the dynamical matrix, which is the matrix defined by the right-hand side of (2.18). For the simple example discussed above, we consider the eigenvalue problem:

$$\widetilde{\omega}^2 y_j = -\frac{\partial V}{\partial y_j} = V'(y_{j+1} - y_j) - V'(y_j - y_{j-1}).$$

Then

$$\widetilde{\omega}^2(k) = 4V''(\varepsilon)\sin^2\frac{k\varepsilon}{2}.$$

The difference between the phonon spectrum and the spectrum of the dynamical matrix lies in the mass matrix. If there is only one specie of atoms, the mass matrix is a scalar matrix. In this case, the two spectra are the same up to a scaling factor. If there are more than one species of atoms, then the two spectra can be quite different. However, they are still closely related [18,26]. In particular, the spectrum of the dynamical matrix will have acoustic and optical branches, which will be denoted by $\widetilde{\omega}_a$ and $\widetilde{\omega}_c$ respectively.

In the general case, the dynamical matrix is defined by the discrete Fourier transform of the Hessian matrix of the potential function V, which is given by

$$\mathsf{H}(\boldsymbol{y}) = \{\mathsf{H}_{\alpha\beta}(i,j)\}(\boldsymbol{y}) := \frac{\partial^2 V}{\partial \boldsymbol{y}_i(\alpha)\partial \boldsymbol{y}_j(\beta)}(\boldsymbol{y}),$$

where $\boldsymbol{y}_i(\alpha)$ denotes the $\alpha-$th component of $\boldsymbol{y}_i$. Let $\mathsf{H}_0 = \mathsf{H}(\boldsymbol{x})$ be the Hessian matrix at the undeformed state. For a complex lattice with two species of atoms, for example, the Hessian matrix H_0 takes a block form

$$\mathsf{H}_0 = \begin{pmatrix} \mathsf{H}_{AA} & \mathsf{H}_{AB} \\ \mathsf{H}_{BA} & \mathsf{H}_{BB} \end{pmatrix},$$

where

$$\{\mathsf{H}_{\kappa\kappa'}\}_{\alpha\beta}(i,j) = \frac{\partial^2 V}{\partial \boldsymbol{y}_i^{\kappa}(\alpha)\partial \boldsymbol{y}_j^{\kappa'}(\beta)}(\boldsymbol{x})$$

for $\kappa, \kappa' = A$ or B. The dynamical matrix associated with each block is defined by

$$\{\mathsf{D}_{\kappa\kappa'}[n]\}_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{N}\{\mathsf{H}_{\kappa\kappa'}\}_{\alpha\beta}(i,j)e^{i(\boldsymbol{x}_j^{\kappa'} - \boldsymbol{x}_i^{\kappa})\cdot \boldsymbol{k}_n}$$

for $\kappa, \kappa' = A$ or B, $\boldsymbol{x}_i^{\kappa} = \boldsymbol{x}_i + \boldsymbol{x}(\kappa)$ with $\boldsymbol{x}(\kappa)$ being the shift vector, and $\{\boldsymbol{k}_n\}$ belongs to the reciprocal space. Obviously, D is a $2d \times 2d$ block matrix.

Using [18, equation (2.22)], we have that D is Hermitian. Therefore, all eigenvalues are real. Denote by $\{[\widetilde{\omega}(\boldsymbol{k})]^2\}$ the set of eigenvalues of D. We call $\widetilde{\omega}(\boldsymbol{k})$ the spectrum of the dynamical matrix D.

2.5. Main results

Let Ω be a bounded cube. For any nonnegative integer m and positive integer k, we denote by $W^{k,p}(\Omega;\mathbb{R}^m)$ the Sobolev space of mappings $\boldsymbol{y}\colon \Omega \to \mathbb{R}^m$ such that $\|\boldsymbol{y}\|_{W^{k,p}} < \infty$ (see [1] for the definition). In particular, $W^{k,p}_{\#}(\Omega;\mathbb{R}^m)$ denotes the Sobolev space of periodic functions whose distributional derivatives of order less than k are in the space $L^p(\Omega)$. We write $W^{1,p}(\Omega)$ for $W^{1,p}(\Omega;\mathbb{R}^1)$ and $H^1(\Omega)$ for $W^{1,2}(\Omega)$.

Summation convention will be used. We will use $|\cdot|$ to denote the absolute value of a scalar quantity, the Euclidean norm of a vector and the volume of a set. In several places we denote by $\|\cdot\|_{\ell_2}$ the ℓ_2 norm of a vector to avoid confusion. For a vector $\boldsymbol{v}$, $\nabla\boldsymbol{v}$ is the tensor with components $(\nabla\boldsymbol{v})_{ij} = \partial_j v_i$; for a tensor field S, $\operatorname{div}\mathsf{S}$ is the vector with components $\partial_j S_{ij}$. Given any function $y\colon \mathbb{R}^{d\times d} \to \mathbb{R}$, we define

$$D_{\mathsf{A}}\, y(\mathsf{A}) = \Big(\frac{\partial y}{\partial A_{ij}}\Big) \quad \text{and} \quad D^2_{\mathsf{A}}\, y(\mathsf{A}) = \Big(\frac{\partial^2 y}{\partial A_{ij}\partial A_{kl}}\Big),$$

where $\mathbb{R}^{d\times d}$ denotes the set of real $d\times d$ matrices. We also define $\mathbb{R}^{d\times d}_+$ as the set of real $d\times d$ matrices with positive determinant. For a matrix $\mathsf{A} = \{a_{ij}\} \in \mathbb{R}^{d\times d}$, we define the norm $\|\mathsf{A}\| := (\sum_{i=1}^d \sum_{j=1}^d a_{ij}^2)^{1/2}$.

For any $p > d$ and $m \geqq 0$ define

$$X := \left\{ \boldsymbol{v} \in W^{m+2,p}(\Omega;\mathbb{R}^d) \cap\ W^{1,p}_{\#}(\Omega;\mathbb{R}^d)\ \Big|\ \int_\Omega \boldsymbol{v} = \boldsymbol{0} \right\},$$

and $Y := W^{m,p}(\Omega;\mathbb{R}^d)$.

Let $\mathsf{B} \in \mathbb{R}^{d\times d}_+$. Given the total energy functional

$$I(\boldsymbol{v}) := \int_\Omega \Big\{ W_{\mathrm{CB}}(\nabla\boldsymbol{v}(\boldsymbol{x})) - \boldsymbol{f}(\boldsymbol{x})\cdot\boldsymbol{v}(\boldsymbol{x}) \Big\} \mathrm{d}\boldsymbol{x}, \tag{2.19}$$

where $W_{\mathrm{CB}}(\nabla\boldsymbol{v})$ is given by (2.5) or (2.11) with $\mathsf{A} = \nabla\boldsymbol{v}$, we seek a solution $\boldsymbol{u}$, such that $\boldsymbol{u} - \mathsf{B}\cdot\boldsymbol{x} \in X$ and

$$I(\boldsymbol{u}) = \min_{\boldsymbol{v}-\mathsf{B}\cdot\boldsymbol{x}\in X} I(\boldsymbol{v}).$$

The Euler–Lagrange equation of the above minimization problem is:

$$\begin{cases} \mathcal{L}(\boldsymbol{v}) := -\operatorname{div}(D_{\mathsf{A}} W_{\mathrm{CB}}(\nabla\boldsymbol{v})) = \boldsymbol{f} & \text{in} \quad \Omega, \\ \boldsymbol{v} - \mathsf{B}\cdot\boldsymbol{x} \ \text{ is periodic} & \text{on} \quad \partial\Omega. \end{cases} \tag{2.20}$$

As to the atomistic model, we assume that $\boldsymbol{y} - \boldsymbol{x} - \widetilde{\mathsf{B}}\cdot\boldsymbol{x}$ is periodic for $\boldsymbol{x}$ belongs to $L \cap \partial\Omega$, where $\widetilde{\mathsf{B}} = \mathsf{B} \otimes \mathsf{I}_{2N\times 2N}$. To guarantee the uniqueness of solutions, we require, for example, for the case there are two species of atoms,

$$\sum_{i=1}^{2N} \boldsymbol{y}_i = \boldsymbol{0}.$$

We write the minimization problem for the atomistic model as

$$\min_{\boldsymbol{y}\in\mathcal{A}} E\{\boldsymbol{y}_1, \cdots, \boldsymbol{y}_{2N}\} \tag{2.21}$$

where the admissible set $\mathcal{A}$ is defined as

$$\mathcal{A} = \left\{ \boldsymbol{y} \in \mathbb{R}^{2N\times d} \mid \boldsymbol{y} - \boldsymbol{x} - \widetilde{\mathsf{B}}\cdot\boldsymbol{x} \text{ is periodic for } \boldsymbol{x} \in L \cap \partial\Omega \text{ and } \sum_{i=1}^{2N} \boldsymbol{y}_i = \boldsymbol{0} \right\}.$$

The Euler–Lagrange equation associated with the above minimization problem is

$$\begin{cases} T(\boldsymbol{y}) = \boldsymbol{0}, \\ \quad \boldsymbol{y} - \boldsymbol{x} - \widetilde{\mathsf{B}}\cdot\boldsymbol{x} \text{ is periodic and for } \boldsymbol{x} \in L \cap \partial\Omega \text{ and } \sum_{i=1}^{2N} \boldsymbol{y}_i = \boldsymbol{0}, \end{cases} \tag{2.22}$$

where $T = (T_1, \cdots, T_{2N})$ with $T_i : \mathbb{R}^{2N\times d} \to \mathbb{R}^d$ defined by

$$T_i(\boldsymbol{y}) := -\frac{\partial V}{\partial \boldsymbol{y}_i} - \boldsymbol{f}(\boldsymbol{x}_i) \qquad 1 \leqq i \leqq 2N. \tag{2.23}$$

Definition 2.1. The function $\boldsymbol{v}_0 - \mathsf{B}\cdot\boldsymbol{x} \in X$ is a $W^{1,\infty}$ local minimizer of I if and only if there exists $\delta > 0$ such that

$$I(\boldsymbol{v}_0) \leqq I(\boldsymbol{v})$$

for all $\boldsymbol{v} - \mathsf{B}\cdot\boldsymbol{x} \in X$ satisfying

$$\|\boldsymbol{v} - \boldsymbol{v}_0\|_{W^{1,\infty}} < \delta.$$

Definition 2.2. $\boldsymbol{z}_0 \in \mathcal{A}$ is a discrete $W^{1,\infty}$ local minimizer of E if and only if there exists $\delta > 0$ such that

$$E(\boldsymbol{z}_0) \leqq E(\boldsymbol{z})$$

for all $\boldsymbol{z} \in \mathcal{A}$ satisfying

$$|\boldsymbol{z} - \boldsymbol{z}_0|_{1,\infty} < \delta,$$

where the discrete $W^{1,\infty}$–norm is defined for any $\boldsymbol{z} \in \mathbb{R}^{2N\times d}$ excluding the constant vector by

$$|\boldsymbol{z}|_{1,\infty} = \varepsilon^{-1} \max_{1\leqq i\leqq 2N} \max_{|\boldsymbol{x}_{ij}|=\varepsilon} \left|\boldsymbol{z}_i - \boldsymbol{z}_j\right|, \tag{2.24}$$

where $\boldsymbol{x}_{ij} = \boldsymbol{x}_i - \boldsymbol{x}_j$.

Our main assumption is the following:

Assumption A: There exist two constants Λ_1 and Λ_2, independent of ε, such that the acoustic and optical branches of the spectrum of the dynamical matrix satisfy

$$\widetilde{\omega}_a(\boldsymbol{k}) \geqq \Lambda_1 |\boldsymbol{k}|, \tag{2.25}$$

and

$$\widetilde{\omega}_o(\boldsymbol{k}) \geqq \Lambda_2/\varepsilon, \tag{2.26}$$

respectively, where $\boldsymbol{k}$ is any vector in the first Brillouin zone.

In the next section, we will discuss where the scaling factor ε in (2.26) comes from. In subsequent papers [17] and [29], we will show that if **Assumption A** is violated, then results of the type (2.27) cease to be valid. Therefore, **Assumption A** is not only sufficient for Theorems 2.1, 2.2 and 2.3, but also essentially necessary.

Our main results are:

Theorem 2.1. *If* **Assumption A** *holds and* $p > d, m \geqq 0$, *then there exist three constants* κ_1, κ_2 *and* δ *such that for any* $\mathsf{B} \in \mathbb{R}^{d\times d}_+$ *with* $\|\mathsf{B}\| \leqq \kappa_1$ *and for any* $\boldsymbol{f} \in Y$ *with* $\|\boldsymbol{f}\|_{W^{m,p}} \leqq \kappa_2$, *the problem* (2.20) *has one and only one solution* $\boldsymbol{u}_{CB}$ *that satisfies* $\|\boldsymbol{u}_{CB} - \mathsf{B}\cdot\boldsymbol{x}\|_{W^{m+2,p}} \leqq \delta$, *and* $\boldsymbol{u}_{CB}$ *is a* $W^{1,\infty}$ *local minimizer of the total energy functional* (2.19).

Theorem 2.2. *If* **Assumption A** *holds and* $p > d, m \geqq 6$, *then there exist two constants* M_1 *and* M_2 *such that for any* $\mathsf{B} \in \mathbb{R}^{d\times d}_+$ *with* $\|\mathsf{B}\| \leqq M_1$ *and for any* $\boldsymbol{f} \in Y$ *with* $\|\boldsymbol{f}\|_{W^{m,p}} \leqq M_2$, *the problem* (2.22) *has one and only one solution* $\boldsymbol{y}^\varepsilon$, *and* $\boldsymbol{y}^\varepsilon$ *is a discrete* $W^{1,\infty}$ *local minimizer of the energy functional* (2.2). *Moreover,* $\boldsymbol{y}^\varepsilon$ *satisfies*

$$\|\boldsymbol{y}^\varepsilon - \boldsymbol{y}_{CB}\|_d \leqq C\varepsilon, \tag{2.27}$$

where $\boldsymbol{y}_{CB} = \boldsymbol{x} + \boldsymbol{u}_{CB}(\boldsymbol{x})$. *The norm* $\|\cdot\|_d$ *is defined as*

$$\|\boldsymbol{z}\|_d := \varepsilon^{d/2}(\boldsymbol{z}^T \mathsf{H}_0 \boldsymbol{z})^{1/2} \tag{2.28}$$

for any $\boldsymbol{z} \in \mathbb{R}^{2N\times d}$ *excluding the constant vector, where* H_0 *is the Hessian matrix of the atomistic potential at the undeformed state.*

We will see later that $\|\cdot\|_d$ is a discrete analogue of the H^1 norm (cf. Lemma 6.4 and Lemma 6.5).

Theorem 2.3. *Under the same condition as in Theorem 2.2, if the crystal lattice is a simple lattice, then* (2.27) *can be improved to*

$$\|\boldsymbol{y}^\varepsilon - \boldsymbol{y}_{CB}\|_d \leqq C\varepsilon^2. \tag{2.29}$$

3. The Stability Condition

In this section, we will show that our **Assumption A** implies that $W(\mathsf{A}, \boldsymbol{p})$ satisfies a generalized *Legendre–Hadamard condition*. We will also discuss explicit examples of the stability conditions. This allows us to appreciate the difference between the results of Blanc *et al.* and the results of the present paper.

Lemma 3.1. *If* **Assumption A** *is valid, then* $W(\mathsf{A}, \boldsymbol{p})$ *satisfies the* generalized Legendre–Hadamard condition *at the undeformed configuration: there exist two constants* Λ_1 *and* Λ_2*, independent of* ε*, such that for all* $\boldsymbol{\xi}, \boldsymbol{\eta}, \boldsymbol{\zeta} \in \mathbb{R}^d$*,*

$$(\boldsymbol{\xi}\otimes\boldsymbol{\eta}, \boldsymbol{\zeta}) \begin{pmatrix} D^2_{\mathsf{A}} W(\mathbf{0}, \boldsymbol{p}_0) & D_{\mathsf{A}\boldsymbol{p}} W(\mathbf{0}, \boldsymbol{p}_0) \\ D_{\boldsymbol{p}\mathsf{A}} W(\mathbf{0}, \boldsymbol{p}_0) & D^2_{\boldsymbol{p}} W(\mathbf{0}, \boldsymbol{p}_0) \end{pmatrix} \begin{pmatrix} \boldsymbol{\xi}\otimes\boldsymbol{\eta} \\ \boldsymbol{\zeta} \end{pmatrix} \geqq \Lambda_1 |\boldsymbol{\xi}|^2 \left|\boldsymbol{\eta}\right|^2 + \Lambda_2 |\boldsymbol{\zeta}|^2 , \qquad (3.1)$$

where $\boldsymbol{p}_0$ *is the shift vector at the undeformed configuration.*

Proof. We first note the following equivalent form of (3.1), we call it **Assumption B**.

- $D^2_{\boldsymbol{p}} W(\mathbf{0}, \boldsymbol{p}_0)$ is positive definite.
- W_{CB} satisfies the Legendre–Hadamard condition at the undeformed configuration:

$$D^2_{\mathsf{A}} W_{\mathrm{CB}}(\mathbf{0})(\boldsymbol{\xi}\otimes\boldsymbol{\eta}, \boldsymbol{\xi}\otimes\boldsymbol{\eta}) \geqq \Lambda |\boldsymbol{\xi}|^2 \left|\boldsymbol{\eta}\right|^2 \qquad \text{for all } \boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^d.$$

The equivalence between (3.1) and **Assumption B** is a consequence of the following simple calculation: at $\mathsf{A} = \mathbf{0}$ and $\boldsymbol{p} = \boldsymbol{p}_0$, we have

$$\begin{pmatrix} \mathsf{I} & -D_{\mathsf{A}\boldsymbol{p}} W [D^2_{\boldsymbol{p}} W]^{-1} \\ \mathbf{0} & \mathsf{I} \end{pmatrix} \begin{pmatrix} D^2_{\mathsf{A}} W & D_{\mathsf{A}\boldsymbol{p}} W \\ D_{\boldsymbol{p}\mathsf{A}} W & D^2_{\boldsymbol{p}} W \end{pmatrix} \begin{pmatrix} \mathsf{I} & \mathbf{0} \\ -[D^2_{\boldsymbol{p}} W]^{-1} D_{\boldsymbol{p}\mathsf{A}} W & \mathsf{I} \end{pmatrix}$$
$$= \begin{pmatrix} D^2_{\mathsf{A}} W - D_{\mathsf{A}\boldsymbol{p}} W [D^2_{\boldsymbol{p}} W]^{-1} D_{\boldsymbol{p}\mathsf{A}} W & \mathbf{0} \\ \mathbf{0} & D^2_{\boldsymbol{p}} W \end{pmatrix} = \begin{pmatrix} D^2_{\mathsf{A}} W_{\mathrm{CB}} & \mathbf{0} \\ \mathbf{0} & D^2_{\boldsymbol{p}} W \end{pmatrix}.$$

In terms of the elastic stiffness tensor, the second condition of **Assumption B** can also be rewritten as:

$$\mathsf{C}(\boldsymbol{\xi}\otimes\boldsymbol{\eta}, \boldsymbol{\xi}\otimes\boldsymbol{\eta}) \geqq \Lambda |\boldsymbol{\xi}|^2 \left|\boldsymbol{\eta}\right|^2 \qquad \text{for all } \boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^d. \qquad (3.2)$$

Next we prove that **Assumption A** implies **Assumption B**. We only give the proof for the simple lattice here, while that for the complex lattice is postponed to Appendix C since it is much more involved.

Using the translation invariance of L, we write $\mathsf{D}[\boldsymbol{k}]$ as

$$\mathsf{D}_{\alpha\gamma}[\boldsymbol{k}] = \sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0, j) e^{i\boldsymbol{k}\cdot\boldsymbol{x}_j}.$$

For the simple lattice, each atom site is a center of inversion symmetry. Therefore, we rewrite $\mathsf{D}[\boldsymbol{k}]$ as

$$\mathsf{D}_{\alpha\gamma}[\boldsymbol{k}] = \frac{1}{2}\sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0,j)(e^{i\boldsymbol{k}\cdot\boldsymbol{x}_j} + e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_j}) = \sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0,j)\cos(\boldsymbol{k}\cdot\boldsymbol{x}_j).$$

By translation invariance, we have $\sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0,j) = \mathbf{0}$. Therefore,

$$\begin{aligned}\mathsf{D}_{\alpha\gamma}[\boldsymbol{k}] &= \sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0,j)(\cos(\boldsymbol{k}\cdot\boldsymbol{x}_j) - 1) = -2\sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0,j)\sin^2\frac{\boldsymbol{k}\cdot\boldsymbol{x}_j}{2} \\ &= -\frac{1}{2}\sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0,j)\left|\boldsymbol{k}\cdot\boldsymbol{x}_j\right|^2 \\ &\quad + 2\sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0,j)\Big[\Big(\frac{\boldsymbol{k}\cdot\boldsymbol{x}_j}{2}\Big)^2 - \sin^2\frac{\boldsymbol{k}\cdot\boldsymbol{x}_j}{2}\Big].\end{aligned}$$

Using the expression of C [26], we have

$$\mathsf{D}_{\alpha\gamma}[\boldsymbol{k}] = \mathsf{C}_{\alpha\beta\gamma\delta}k_\beta k_\delta + 2\sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0,j)\Big[\Big(\frac{\boldsymbol{k}\cdot\boldsymbol{x}_j}{2}\Big)^2 - \sin^2\frac{\boldsymbol{k}\cdot\boldsymbol{x}_j}{2}\Big]. \tag{3.3}$$

Using the basic inequality: $\cos x \leqq 1 - x^2/2 + x^4/(4!)$ for all $x \in \mathbb{R}$, we have

$$0 \leqq \Big(\frac{\kappa\cdot\boldsymbol{x}_j}{2}\Big)^2 - \sin^2\frac{\boldsymbol{k}\cdot\boldsymbol{x}_j}{2} \leqq \frac{|\boldsymbol{k}|^4\left|\boldsymbol{x}_j\right|^4}{12}. \tag{3.4}$$

Using the assumption that V has finite range and the fact that $\mathsf{H}_{\alpha\gamma} = O(\varepsilon^{-2})$, we get that there exists C independent of ε and $\boldsymbol{k}$ such that

$$2\left|\sum_{j=1}^{N} \mathsf{H}_{\alpha\gamma}(0,j)\Big[\Big(\frac{\boldsymbol{k}\cdot\boldsymbol{x}_j}{2}\Big)^2 - \sin^2\frac{\boldsymbol{k}\cdot\boldsymbol{x}_j}{2}\Big]\right| \leqq C\varepsilon^2|\boldsymbol{k}|^4.$$

Substituting the above two equations into (3.3), and using **Assumption A**, we obtain, for any $\boldsymbol{\eta} \in \mathbb{R}^d$ and $\boldsymbol{k} \in \mathbb{R}^d$ in the first Brillouin zone,

$$\begin{aligned}\mathsf{C}(\boldsymbol{k}\otimes\boldsymbol{\eta}, \boldsymbol{k}\otimes\boldsymbol{\eta}) &\geqq \boldsymbol{\eta}^T\mathsf{D}[\boldsymbol{k}]\boldsymbol{\eta} - C\varepsilon^2|\boldsymbol{k}|^4\left|\boldsymbol{\eta}\right|^2 \\ &\geqq (\Lambda_1 - C\varepsilon^2|\boldsymbol{k}|^2)|\boldsymbol{k}|^2\left|\boldsymbol{\eta}\right|^2 \\ &\geqq (\Lambda_1/2)|\boldsymbol{k}|^2\left|\boldsymbol{\eta}\right|^2,\end{aligned}$$

where we have used the fact that $\boldsymbol{k}$ is of $O(1)$ since they are in the first Brillouin zone. The above inequality is homogeneous with respect to $\boldsymbol{k}$, therefore, it is also valid for any $\boldsymbol{k} \in \mathbb{R}^d$. This gives **Assumption B**.

3.1. Stability condition for the continuum model

We shall prove that (3.2) is valid for the triangular lattice and fails for the square lattice with the Lennard-Jones potential. We write the Lennard-Jones potential as

$$V(r) = 4(r^{-12} - r^{-6}). \tag{3.5}$$

The following lemma simplifies the expression of the elastic stiffness tensor by exploiting the symmetry property of the underlying lattices.

Lemma 3.2. *The elastic stiffness tensor* C *is of the form:*

$$\mathsf{C}_{\alpha\beta\gamma\delta} = \sum_{\boldsymbol{s}} (V''(|\boldsymbol{s}|)\,|\boldsymbol{s}|^2 - V'(|\boldsymbol{s}|)\,|\boldsymbol{s}|)\,|\boldsymbol{s}|^{-4}\,\boldsymbol{s}_\alpha \boldsymbol{s}_\beta \boldsymbol{s}_\gamma \boldsymbol{s}_\delta. \tag{3.6}$$

Proof. A direct calculation gives

$$\begin{aligned}\mathsf{C}_{\alpha\beta\gamma\delta} = &\sum_{\boldsymbol{s}} (V''(|\boldsymbol{s}|)\,|\boldsymbol{s}|^2 - V'(|\boldsymbol{s}|)\,|\boldsymbol{s}|))\,|\boldsymbol{s}|^{-4}\,\boldsymbol{s}_\alpha \boldsymbol{s}_\beta \boldsymbol{s}_\gamma \boldsymbol{s}_\delta \\ &+ \sum_{\boldsymbol{s}} V'(|\boldsymbol{s}|)\,|\boldsymbol{s}|^{-1}\,\delta_{\alpha\gamma}\boldsymbol{s}_\beta \boldsymbol{s}_\delta.\end{aligned}$$

Using

$$D_{\mathsf{A}} W_{\mathrm{CB}}(\mathbf{0}) = \mathbf{0}, \tag{3.7}$$

we have

$$\sum_{\boldsymbol{s}} V'(|\boldsymbol{s}|)\,|\boldsymbol{s}|^{-1}\,\delta_{\alpha\gamma}\boldsymbol{s}_\beta \boldsymbol{s}_\delta = \delta_{\alpha\gamma} D_{\mathsf{A}} W_{\mathrm{CB}}(\mathbf{0}) = \mathbf{0}.$$

Thus (3.6) holds.

Using (3.6), we have

$$\begin{aligned}\mathsf{C}_{1111} = \mathsf{C}_{2222} &= \sum_{\boldsymbol{s}} (V''(|\boldsymbol{s}|)\,|\boldsymbol{s}|^2 - V'(|\boldsymbol{s}|)\,|\boldsymbol{s}|)\,|\boldsymbol{s}|^{-4}\,|\boldsymbol{s}_1|^4\,, \\ \mathsf{C}_{1122} = \mathsf{C}_{1212} &= \sum_{\boldsymbol{s}} (V''(|\boldsymbol{s}|)\,|\boldsymbol{s}|^2 - V'(|\boldsymbol{s}|)\,|\boldsymbol{s}|)\,|\boldsymbol{s}|^{-4}\,|\boldsymbol{s}_1|^2\,|\boldsymbol{s}_2|^2\,.\end{aligned} \tag{3.8}$$

For the triangular lattice, using the above lemma, we obtain

$$\begin{aligned}\mathsf{C}(\boldsymbol{\xi}\otimes\boldsymbol{\eta}, \boldsymbol{\xi}\otimes\boldsymbol{\eta}) &= \mathsf{C}_{1111}(\xi_1^2\eta_1^2 + \xi_2^2\eta_2^2) + 2\mathsf{C}_{1122}\xi_1\xi_2\eta_1\eta_2 \\ &\quad + \mathsf{C}_{1122}(\xi_1\eta_2 + \xi_2\eta_1)^2 \\ &= (\mathsf{C}_{1111} - \mathsf{C}_{1122})(\xi_1^2\eta_1^2 + \xi_2^2\eta_2^2) \\ &\quad + \mathsf{C}_{1122}[(\xi_1\eta_1 + \xi_2\eta_2)^2 + (\xi_1\eta_2 + \xi_2\eta_1)^2].\end{aligned}$$

Using the explicit form of V (3.5), a straightforward calculation gives

$$\mathsf{C}_{1111} - \mathsf{C}_{1122} > 0 \quad \text{and} \quad \mathsf{C}_{1122} > 0.$$

$$\mathsf{C}(\boldsymbol{\xi}\otimes\boldsymbol{\eta},\boldsymbol{\xi}\otimes\boldsymbol{\eta}) \geqq \min(\mathsf{C}_{1111}-\mathsf{C}_{1122},\mathsf{C}_{1122})[\xi_1^2\eta_1^2+\xi_2^2\eta_2^2+(\xi_1\eta_1+\xi_2\eta_2)^2 + (\xi_1\eta_2+\xi_2\eta_1)^2].$$

Using the elementary identity:

$$\begin{aligned}&\xi_1^2\eta_1^2+\xi_2^2\eta_2^2+(\xi_1\eta_1+\xi_2\eta_2)^2+(\xi_1\eta_2+\xi_2\eta_1)^2\\ &=\frac{1}{2}|\boldsymbol{\xi}|^2|\boldsymbol{\eta}|^2+\frac{3}{2}(\xi_1\eta_1+\xi_2\eta_2)^2+\frac{1}{2}(\xi_1\eta_2+\xi_2\eta_1)^2,\end{aligned}$$

we have

$$\mathsf{C}(\boldsymbol{\xi}\otimes\boldsymbol{\eta},\boldsymbol{\xi}\otimes\boldsymbol{\eta}) \geqq \Lambda|\boldsymbol{\xi}|^2|\boldsymbol{\eta}|^2$$

with $\Lambda=\frac{1}{2}\min(\mathsf{C}_{1111}-\mathsf{C}_{1122},\mathsf{C}_{1122})>0$.

For the square lattice, let $\xi_1=\eta_2=0$, we have

$$\mathsf{C}(\boldsymbol{\xi}\otimes\boldsymbol{\eta},\boldsymbol{\xi}\otimes\boldsymbol{\eta})=\mathsf{C}_{1122}\xi_2^2\eta_1^2<0$$

for any $\xi_2,\eta_1\neq 0$ since $\mathsf{C}_{1122}<0$ by $(3.8)_2$ and a direct calculation.

If we only consider the nearest neighborhood interaction, we have $\mathsf{C}_{1122}=\mathsf{C}_{1212}=0$, i.e., the shear modulus of the macroscopic model is zero. We refer to [17] for discussions on the manifestation of this instability.

3.2. Stability condition for the atomistic model

We will check **Assumption A** for $N\times N$ triangular and square lattices. Write

$$\widetilde{\omega}^2(\boldsymbol{k})=2\lambda(\boldsymbol{k}). \tag{3.9}$$

A straightforward calculation gives, in the case of triangular lattice with nearest neighbor interaction

$$\lambda(\boldsymbol{k})=a[\alpha+\beta+\gamma-((\alpha-\beta)^2+(\beta-\gamma)^2+(\gamma-\alpha)^2)^{1/2}/\sqrt{2}\,],$$

where $a=V''(\varepsilon)$, and

$$\alpha=\sin^2\frac{\pi}{N}k_1,\quad \beta=\sin^2\frac{\pi}{N}k_2,\quad \gamma=\sin^2\frac{\pi}{N}(k_1-k_2) \tag{3.10}$$

with $\boldsymbol{k}=(k_1,k_2)$.

If the next-nearest neighbor interaction is taken into account, then

$$\begin{aligned}\lambda(\boldsymbol{k})&=(a+b)(\alpha+\beta+\gamma)+(c+d)(\widetilde{\alpha}+\widetilde{\beta}+\widetilde{\gamma})\\ &\quad-\frac{1}{2}([(a-b)(2\alpha-\beta-\gamma)+(d-c)(2\widetilde{\beta}-\widetilde{\alpha}-\widetilde{\gamma})]^2\\ &\qquad+3[(a-b)(\beta-\gamma)+(c-d)(\widetilde{\alpha}-\widetilde{\gamma})]^2)^{1/2},\end{aligned}$$

where α,β and γ are the same as (3.10) while

$$\widetilde{\alpha}=\sin^2\frac{\pi}{N}(k_1+k_2),\ \widetilde{\beta}=\sin^2\frac{\pi}{N}(-k_1+2k_2),\ \widetilde{\gamma}=\sin^2\frac{\pi}{N}(-2k_1+k_2),$$

and

$$b = V'(\varepsilon)\varepsilon^{-1}, \quad c = V'(\sqrt{3}\varepsilon), \quad d = V'(\sqrt{3}\varepsilon)(\sqrt{3}\varepsilon)^{-1},$$

where

$$\varepsilon = \left(2\frac{1+3^{-6}}{1+3^{-3}}\right)^{1/6}.$$

For the square lattice, if we only consider the nearest neighbor interaction, then we have

$$\lambda_1(\boldsymbol{k}) = 2a\alpha, \qquad \lambda_2(\boldsymbol{k}) = 2a\beta,$$

where α, β are defined earlier. Obviously, there does not exist a constant Λ such that

$$\widetilde{\omega}(\boldsymbol{k}) \geqq \Lambda\,|\boldsymbol{k}|\,.$$

If we take into account the next-nearest neighbor interaction, then we have

$$\begin{aligned}\lambda(\boldsymbol{k}) = {} & (a+b)(\alpha+\beta) + (e+f)(\widetilde{\alpha}+\gamma) \\ & - ([(a-b)^2(\alpha-\beta)^2 + (e-f)^2(\widetilde{\alpha}-\gamma)^2)^{1/2},\end{aligned}$$

where

$$e = V''(\sqrt{2}\varepsilon), \quad f = V'(\sqrt{2}\varepsilon)(\sqrt{2}\varepsilon)^{-1},$$

and

$$\varepsilon = \left(2\frac{1+2^{-6}}{1+2^{-3}}\right)^{1/6}.$$

From Fig. 4 we see **Assumption A** is satisfied by the triangular lattice but fails for the square lattice. Therefore, our results imply that the Cauchy–Born rule is valid for the triangular lattice but not for the square lattice. Numerical results show that this is indeed the case [17]. Note that the work of Blanc *et al.* does not distinguish between the two cases.

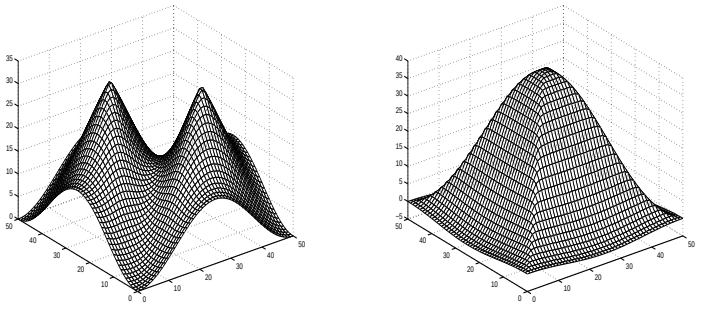

Fig. 4. Spectrum of the dynamical matrix corresponding to the larger wave speed for triangular (left) and square (right) lattices with next-nearest neighbor Lennard-Jones interaction.

Next we turn to complex lattices. Again we will consider a one-dimensional chain with two species of atoms A and B. We do not assume nearest neighbor interaction. The equilibrium equations for A and B are:

$$\begin{aligned} m_A \frac{d^2 y_i^A}{dt^2} &= V'_{AB}(y_i^B - y_i^A) + V'_{AA}(y_{i+1}^A - y_i^A) \\ &\quad - V'_{AB}(y_i^A - y_{i-1}^B) - V'_{AA}(y_i^A - y_{i-1}^A), \\ m_B \frac{d^2 y_i^B}{dt^2} &= V'_{AB}(y_{i+1}^A - y_i^B) + V'_{BB}(y_{i+1}^B - y_i^B) \\ &\quad - V'_{AB}(y_i^B - y_i^A) - V'_{BB}(y_i^B - y_{i-1}^B). \end{aligned}$$

We may assume $m_A = m_B = 1$ since we concern the spectrum of the dynamical matrix. Let $y_i^A = i\varepsilon + \widetilde{y}_i^A$ and $y_i^B = i\varepsilon + p + \widetilde{y}_i^B$, linearizing the above equation, and using the Euler–Lagrange equation for optimizing with respect to the shift p, we obtain

$$\begin{aligned} \frac{d^2 \widetilde{y}_i^A}{dt^2} &= V''_{AB}(p)(\widetilde{y}_i^B - \widetilde{y}_i^A) - V''_{AB}(\varepsilon - p)(\widetilde{y}_i^A - \widetilde{y}_{i-1}^B) \\ &\quad + V''_{AA}(\varepsilon)(\widetilde{y}_{i+1}^A - 2\widetilde{y}_i^A + \widetilde{y}_{i-1}^A), \\ \frac{d^2 \widetilde{y}_i^B}{dt^2} &= V''_{AB}(\varepsilon - p)(\widetilde{y}_{i+1}^A - \widetilde{y}_i^B) - V''_{AB}(p)(\widetilde{y}_i^B - \widetilde{y}_i^A) \\ &\quad + V''_{BB}(\varepsilon)(\widetilde{y}_{i+1}^B - 2\widetilde{y}_i^B + \widetilde{y}_{i-1}^B). \end{aligned}$$

Let $\widetilde{y}_i^A = \varepsilon_A e^{i(ki\varepsilon - \omega t)}$ and $\widetilde{y}_i^B = \varepsilon_B e^{i(ki\varepsilon - \omega t)}$, we get

$$\mathsf{D}[k](\varepsilon_A, \varepsilon_B)^T = (0,0)^T$$

with

$$\begin{aligned} D_{11} &= \omega^2 - 4V''_{AA}(\varepsilon)\sin^2 \tfrac{k\varepsilon}{2} - V''_{AB}(p) - V''_{AB}(\varepsilon - p), \\ D_{12} &= V''_{AB}(\varepsilon - p)e^{ik\varepsilon} + V''_{AB}(p)e^{ikp}, \\ D_{21} &= V''_{AB}(\varepsilon - p)e^{-ik\varepsilon} + V''_{AB}(p)e^{-ikp}, \\ D_{22} &= \omega^2 - 4V''_{BB}(\varepsilon)\sin^2 \tfrac{k\varepsilon}{2} - V''_{AB}(p) - V''_{AB}(\varepsilon - p). \end{aligned}$$

Solving the equation $\det \mathsf{D}[k] = 0$ we get

$$\begin{aligned} \omega_\pm^2 &= 2(V''_{AA}(\varepsilon) + V''_{BB}(\varepsilon))\sin^2 \frac{k\varepsilon}{2} + \frac{1}{4}(V''_{AB}(p) + V''_{AB}(\varepsilon - p)) \\ &\quad \pm \Big[4(V''_{BB}(\varepsilon) - V''_{AA}(\varepsilon))^2 \sin^4 \frac{k\varepsilon}{2} \\ &\quad + (V''_{AB}(p) + V''_{AB}(\varepsilon - p))^2 - 4V''_{AB}(p)V''_{AB}(\varepsilon - p)\sin^2 \frac{k\varepsilon}{2} \Big]^{1/2}. \end{aligned}$$

We have, for any $k \in \mathbb{R}$,

$$\varepsilon\omega_o(k) = \varepsilon\omega_+(k) \geqq \Lambda_2 \tag{3.11}$$

with

$$\Lambda_2 := \frac{1}{2}(V''_{AB}(p) + V''_{AB}(\varepsilon - p))^{1/2}\varepsilon.$$

Next we write the acoustic branch as

$$\omega_a^2(k) = \omega_-^2(k) = [\omega_+(k)\omega_-(k)]^2/\omega_+^2(k).$$

A direct calculation gives

$$[\omega_+\omega_-]^2 \geqq 4\Big(V''_{AA}(\varepsilon) + V''_{BB}(\varepsilon) + \frac{V''_{AB}(p)V''_{AB}(\varepsilon-p)}{V''_{AB}(p)+V''_{AB}(\varepsilon-p)}\Big) \times (V''_{AB}(p)+V''_{AB}(\varepsilon-p))\sin^2\frac{k\varepsilon}{2}.$$

We bound ω_+^2 as

$$\omega_+^2 \leqq 2(V''_{AB}(p)+V''_{AB}(\varepsilon-p)) + g(\sin k\varepsilon/2)$$

with

$$g(t) := \Big((V''_{BB}(\varepsilon)-V''_{AA}(\varepsilon))^2t^2 + \frac{1}{2}V''_{AB}(p)V''_{AB}(\varepsilon-p)\Big)^{1/2}|t| + (V''_{AA}(\varepsilon)+V''_{BB}(\varepsilon))t^2 \qquad \text{for all} \quad 0 \leqq t \leqq 1.$$

Therefore, we estimate ω_a^2 as

$$\omega_a^2(k) \geqq K_2\Big(V''_{AA}(\varepsilon)+V''_{BB}(\varepsilon)+\frac{V''_{AB}(p)V''_{AB}(\varepsilon-p)}{V''_{AB}(p)+V''_{AB}(\varepsilon-p)}\Big)\sin^2\frac{k\varepsilon}{2},$$

where

$$K_2 = \frac{2[V''_{AB}(p)+V''_{AB}(\varepsilon-p)]}{[V''_{AB}(p)+V''_{AB}(\varepsilon-p)]+g(\sin\frac{k\varepsilon}{2})}.$$

Obviously,

$$K_2 \geqq \frac{2[V''_{AB}(p)+V''_{AB}(\varepsilon-p)]}{[V''_{AB}(p)+V''_{AB}(\varepsilon-p)]+g(1)} =: K.$$

It is seen that K is independent of ε.

Using the basic inequality

$$\frac{\sin x}{x} \geqq \frac{2}{\pi} \quad \text{for all } |x| \leqq \frac{\pi}{2},$$

we obtain, for k in the first Brillouin zone, i.e. $|k\varepsilon| \leqq \pi/2$,

$$\omega_a(k) \geqq \sqrt{K}\Big(V''_{AA}(\varepsilon)+V''_{BB}(\varepsilon)+\frac{V''_{AB}(p)V''_{AB}(\varepsilon-p)}{V''_{AB}(p)+V''_{AB}(\varepsilon-p)}\Big)^{1/2}\Big|\sin\frac{k\varepsilon}{2}\Big| \geqq \Lambda_1|k|, \tag{3.12}$$

where

$$\Lambda_1 = \frac{\sqrt{K}}{\pi}\Big(V''_{AA}(\varepsilon)+V''_{BB}(\varepsilon)+\frac{V''_{AB}(p)V''_{AB}(\varepsilon-p)}{V''_{AB}(p)+V''_{AB}(\varepsilon-p)}\Big)^{1/2}\varepsilon.$$

It is obvious that Λ_1 is independent of ε.

In view of (3.12) and (3.11), we verify **Assumption A**.

In the general case, the factor $1/\varepsilon$ in $\widetilde{\omega}_o$ is a consequence of scaling: if we take the lattice constant to be $O(1)$, then $\widetilde{\omega}_o = O(1)$. If we take the lattice constant to be $O(\varepsilon)$ as we do, then $V''(\varepsilon) = O(\varepsilon^{-2})$, which gives $\widetilde{\omega}_o = O(\varepsilon^{-1})$.

In our analysis, it is sufficient to impose stability conditions on rank-one deformations only. This is due to the fact that we have fixed the linear part of the deformation gradient tensor through boundary conditions. If we allow the linear part to vary, we have to impose additional stability conditions with respect to deformations of higher rank. In this case, we need to require that the elastic moduli tensor be positive definite. We refer to [19] for a discussion.

4. Local Minimizers for the Continuum Model

In this section, we prove Theorem 2.1. The proof is quite standard. The main tool is the implicit function theorem.

The linearized operator of $\mathcal{L}$ at $\boldsymbol{u}$ is defined by:

$$\mathcal{L}_{\text{lin}}(\boldsymbol{u})\boldsymbol{v} = -\operatorname{div}(D^2_{\mathsf{A}} W_{\text{CB}}(\nabla \boldsymbol{u})\nabla \boldsymbol{v})$$

for any $\boldsymbol{v} \in W^{1,p}_{\#}(\Omega;\mathbb{R}^d)$

Proof of Theorem 2.1. For any $p > d$, define the map

$$T : Y \times X \to \mathbb{R}^d \quad \text{with} \quad T(\boldsymbol{f},\boldsymbol{v}) := \mathcal{L}(\boldsymbol{v} + \mathsf{B}\cdot\boldsymbol{x}) - \boldsymbol{f}.$$

Without loss of generality, we assume that Ω is a unit cube and write

$$\boldsymbol{v}(\boldsymbol{x}) = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} a_{\boldsymbol{n}} e^{i2\pi \boldsymbol{n}\cdot\boldsymbol{x}} \qquad \text{with} \qquad a_{\boldsymbol{n}} = \int_{\Omega} \boldsymbol{v}(\boldsymbol{x}) e^{-i2\pi\boldsymbol{n}\cdot\boldsymbol{x}} \mathrm{d}\boldsymbol{x}.$$

Therefore,

$$\begin{aligned}
&\int_{\Omega} \nabla \boldsymbol{v} \cdot D^2_{\mathsf{A}} W_{\text{CB}}(\boldsymbol{0}) \cdot \nabla \boldsymbol{v} \mathrm{d}\boldsymbol{x} \\
&= 4\pi^2 \sum_{\alpha,\beta,\gamma,\delta=1}^{d} \sum_{\boldsymbol{n},\boldsymbol{m}\in\mathbb{Z}^d} \mathsf{C}_{\alpha\beta\gamma\delta} n_\alpha m_\gamma a_{n_\beta} a_{m_\delta} \int_{\Omega} e^{i2\pi(\boldsymbol{n}-\boldsymbol{m})\cdot\boldsymbol{x}} \mathrm{d}\boldsymbol{x} \\
&= 4\pi^2 \sum_{\alpha,\beta,\gamma,\delta=1}^{d} \sum_{\boldsymbol{n}\in\mathbb{Z}^d} \mathsf{C}_{\alpha\beta\gamma\delta} n_\alpha n_\gamma a_{n_\beta} a_{n_\delta}.
\end{aligned}$$

By Lemma 3.1, we have **Assumption B**. Using the above expression, we obtain

$$\begin{aligned}
\int_{\Omega} \nabla \boldsymbol{v} \cdot D^2_{\mathsf{A}} W_{\text{CB}}(\boldsymbol{0}) \cdot \nabla \boldsymbol{v} \mathrm{d}\boldsymbol{x} &\geqq 4\pi^2 \Lambda \sum_{\boldsymbol{n}\in\mathbb{Z}^d} |\boldsymbol{n}|^2 |a_{\boldsymbol{n}}|^2 \\
&= \Lambda \int_{\Omega} |\nabla \boldsymbol{v}|^2 \, \mathrm{d}\boldsymbol{x}. \qquad (4.1)
\end{aligned}$$

Since $\int_\Omega \boldsymbol{v} = \mathbf{0}$, using Poincaré's inequality, we get

$$\int_\Omega \nabla \boldsymbol{v} \cdot D_{\mathsf{A}}^2 W_{\mathrm{CB}}(\mathbf{0}) \cdot \nabla \boldsymbol{v} \mathrm{d}\boldsymbol{x} \geqq C_1 \|\boldsymbol{v}\|_1^2, \tag{4.2}$$

where C_1 depends on Λ, e.g. $C_1 = \Lambda\pi^2/(1+\pi^2)$. Define $\kappa = \min(C_1/(2M), 1)$ with $M = \max_{\mathsf{A}\in\mathbb{R}^{d\times d}} \left|D_{\mathsf{A}}^3 W_{\mathrm{CB}}(\mathsf{A})\right|$. If $\|\mathsf{B}\| \leqq \kappa$, then

$$\left|D_{\mathsf{A}}^2 W_{\mathrm{CB}}(\mathsf{B}) - D_{\mathsf{A}}^2 W_{\mathrm{CB}}(\mathbf{0})\right| \leqq M\|\mathsf{B}\| \leqq C_1/2.$$

Therefore,

$$\int_\Omega \nabla \boldsymbol{v} \cdot D_{\mathsf{A}}^2 W_{\mathrm{CB}}(\mathsf{B}) \cdot \nabla \boldsymbol{v} \mathrm{d}\boldsymbol{x} \geqq (C_1/2)\|\boldsymbol{v}\|_1^2. \tag{4.3}$$

Notice that $T(\mathbf{0}, \mathbf{0}) = 0$. Standard regularity theory for elliptic systems (see [2]) allows us to conclude that $D_{\boldsymbol{v}} T(\mathbf{0}, \mathbf{0})$ is a bijection from X onto Y. Since $p > d$, we know that $W^{k,p}(\Omega; \mathbb{R}^d)$ is a Banach algebra [1] for any $k \geqq 1$. Therefore, it is easy to verify that $D_{\mathsf{A}} W_{\mathrm{CB}}$ is a C^2 function from $\mathbb{R}_+^{d\times d}$ to $\mathbb{R}^{d\times d}$. It follows from the implicit function theorem [25, Appendix I] that there exist two constants R and r such that for all $\boldsymbol{f}$ satisfying $\|\boldsymbol{f}\|_{W^{m,p}} \leqq r$, there exists one and only one solution $\boldsymbol{v}(\boldsymbol{f}) \in X$ that satisfies

$$T(\boldsymbol{f}, \boldsymbol{v}(\boldsymbol{f})) = \mathbf{0}, \qquad \|\boldsymbol{v}(\boldsymbol{f})\|_{m+2,p} \leqq R, \tag{4.4}$$

and $\boldsymbol{v}(\mathbf{0}) = \mathbf{0}$. Finally we let $\boldsymbol{u}_{\mathrm{CB}} = \boldsymbol{v}(\boldsymbol{f}) + \mathsf{B} \cdot \boldsymbol{x}$. It is clear that $\boldsymbol{u}_{\mathrm{CB}}$ satisfies equation (2.20), $\boldsymbol{u}_{\mathrm{CB}} - \mathsf{B} \cdot \boldsymbol{x}$ is periodic over $\partial\Omega$ and

$$\|\boldsymbol{u}_{\mathrm{CB}} - \mathsf{B} \cdot \boldsymbol{x}\|_{W^{m+2,p}} \leqq R. \tag{4.5}$$

Next we show that $\boldsymbol{u}_{\mathrm{CB}}$ is actually a $W^{1,\infty}$ local minimizer. Using a Taylor expansion around $\boldsymbol{u}_{\mathrm{CB}}$ and using (2.20) gives

$$\begin{aligned} & I(\boldsymbol{v}) - I(\boldsymbol{u}_{\mathrm{CB}}) \\ = & \int_\Omega \nabla(\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}) \cdot \Big(\int_0^1 (1-t) D_{\mathsf{A}}^2 W(\nabla \boldsymbol{u}^t) \mathrm{d}t \Big) \cdot \nabla(\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}) \mathrm{d}\boldsymbol{x}, \end{aligned} \tag{4.6}$$

where $\boldsymbol{u}^t = t\boldsymbol{v} + (1-t)\boldsymbol{u}_{\mathrm{CB}}$. It is clear that

$$\nabla \boldsymbol{u}^t - \mathsf{B} = t\nabla(\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}) + \nabla \boldsymbol{v}(\boldsymbol{f}).$$

Therefore, there exist κ and δ such that if $\|\boldsymbol{f}\|_{L^p} \leqq \kappa$ and $\|\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}\|_{1,\infty} \leqq \delta$, then

$$\int_\Omega \nabla(\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}) \cdot D_{\mathsf{A}}^2 W(\nabla \boldsymbol{u}^t) \cdot \nabla(\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}) \mathrm{d}\boldsymbol{x} \geqq (C_1/4)\|\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}\|_1^2 \tag{4.7}$$

for any $0 \leqq t \leqq 1$. It follows from the above inequality and (4.6) that

$$I(\boldsymbol{v}) - I(\boldsymbol{u}_{\mathrm{CB}}) \geqq (C_1/4)\|\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}\|_1^2.$$

This proves that $\boldsymbol{u}_{\mathrm{CB}}$ is a $W^{1,\infty}$ local minimizer of I. □

The next two sections are devoted to the proof of Theorem 2.2. We first construct an approximation solution that satisfies the equilibrium equations of the atomistic problem in § 5 with higher-order accuracy. To construct exact solutions, we analyze the stability of the atomistic model. This is done in § 6, by first constructing and characterizing the norm $\|\cdot\|_d$, and then proving a perturbation lemma for this norm. The existence of the solution of the atomistic model then follows from the fixed-point theorem.

5. Asymptotic Analysis on Lattices

In this section, we carry out asymptotic analysis on lattices. The results in this section not only serve as a preliminary step for proving Theorem 2.2, but also have interests of their own.

5.1. Asymptotic analysis on simple lattices

We first discuss asymptotic analysis on simple lattices. As we said earlier, without loss of generality, we will restrict our attention to the case where the potential V is a three-body potential. The equilibrium equation at the site i is of the form:

$$\mathcal{L}_\varepsilon(\boldsymbol{y}_i) = -\frac{\partial V}{\partial \boldsymbol{y}_i} = \boldsymbol{f}(\boldsymbol{x}_i), \tag{5.1}$$

where

$$\begin{aligned}\mathcal{L}_\varepsilon(\boldsymbol{y}_i) = \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} & [\partial_{\alpha_1} V(D_1^+ \boldsymbol{y}_i, D_2^+ \boldsymbol{y}_i) - \partial_{\alpha_1} V(D_1^- \boldsymbol{y}_i, D_2^+ \boldsymbol{y}_{i-\boldsymbol{s}_1}) \\ & + \partial_{\alpha_2} V(D_1^+ \boldsymbol{y}_i, D_2^+ \boldsymbol{y}_i) - \partial_{\alpha_2} V(D_1^+ \boldsymbol{y}_{i-\boldsymbol{s}_2}, D_2^- \boldsymbol{y}_i)].\end{aligned}$$

Here the summation runs over all $\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle \in L \times L$. In writing this expression, we have paired the interaction at $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ directions (see Fig. 5).

The plan is to carry out the analysis in two steps: the first is to approximate (5.1) by differential equations. The second is to carry out asymptotic analysis on these differential equations.

Assuming that $\boldsymbol{y}_i = \boldsymbol{x}_i + \boldsymbol{u}(\boldsymbol{x}_i)$ and substituting it into the above equilibrium equations, collecting terms of the same order, we may write

$$\mathcal{L}_\varepsilon(\boldsymbol{y}_i) = \mathcal{L}_0(\boldsymbol{u}(\boldsymbol{x}_i)) + \varepsilon \mathcal{L}_1(\boldsymbol{u}(\boldsymbol{x}_i)) + \varepsilon^2 \mathcal{L}_2(\boldsymbol{u}(\boldsymbol{x}_i)) + O(\varepsilon^3). \tag{5.2}$$

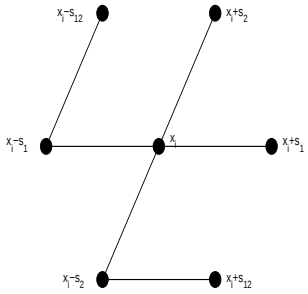

Fig. 5. A schematic example for the atomic interactions on simple lattices

Lemma 5.1. *The leading order operator $\mathcal{L}_0$ is the same as the variational operator for W_{CB}.*

Moreover, $\mathcal{L}_1 = 0$ and $\mathcal{L}_2$ is an operator in divergence form.

Proof. We may rewrite the operator $\mathcal{L}_\varepsilon(\boldsymbol{y}_i)$ as

$$\begin{aligned}\mathcal{L}_\varepsilon(\boldsymbol{y}_i) = &\sum_{\langle \boldsymbol{s}_1,\boldsymbol{s}_2\rangle} [\partial_{\boldsymbol{\alpha}_1} V(D_1^+\boldsymbol{y}_i, D_2^+\boldsymbol{y}_i) - \partial_{\boldsymbol{\alpha}_1} V(D_1^+\boldsymbol{y}_{i-\boldsymbol{s}_1}, D_2^+\boldsymbol{y}_{i-\boldsymbol{s}_1})\\ &\qquad + \partial_{\boldsymbol{\alpha}_2} V(D_1^+\boldsymbol{y}_i, D_2^+\boldsymbol{y}_i) - \partial_{\boldsymbol{\alpha}_2} V(D_1^+\boldsymbol{y}_{i-\boldsymbol{s}_2}, D_2^+\boldsymbol{y}_{i-\boldsymbol{s}_2})]\\ = &\sum_{\langle \boldsymbol{s}_1,\boldsymbol{s}_2\rangle} (D_1^-\partial_{\boldsymbol{\alpha}_1} V + D_2^-\partial_{\boldsymbol{\alpha}_2} V)(D_1^+\boldsymbol{y}_i, D_2^+\boldsymbol{y}_i).\end{aligned}$$

Denote by $\partial_{\boldsymbol{\alpha}_j} V(D_1^+\boldsymbol{y}_i, D_2^+\boldsymbol{y}_i) = \partial_{\boldsymbol{\alpha}_j} V_i$ for $j = 1, 2$. For any smooth function $\boldsymbol{\varphi}(\boldsymbol{x})$ satisfying the periodic boundary condition, after summation by parts, we have

$$\sum_{i=1}^N \mathcal{L}_\varepsilon(\boldsymbol{y}_i)\boldsymbol{\varphi}(\boldsymbol{x}_i) = -\sum_{i=1}^N \sum_{\langle \boldsymbol{s}_1,\boldsymbol{s}_2\rangle} \partial_{\boldsymbol{\alpha}_1} V_i D_1^+\boldsymbol{\varphi}(\boldsymbol{x}_i) + \partial_{\boldsymbol{\alpha}_2} V_i D_2^+\boldsymbol{\varphi}(\boldsymbol{x}_i). \tag{5.3}$$

Fix i, for $j = 1, 2$, Taylor expansion at $\boldsymbol{x}_i$ gives

$$\begin{aligned} D_j^+\boldsymbol{\varphi}(\boldsymbol{x}_i) &= (\boldsymbol{s}_j\cdot\nabla)\boldsymbol{\varphi}(\boldsymbol{x}_i) + \frac{1}{2}(\boldsymbol{s}_j\cdot\nabla)^2\boldsymbol{\varphi}(\boldsymbol{x}_i) + O(\varepsilon^3),\\ D_j^+\boldsymbol{y}_i &= \boldsymbol{s}_j + (\boldsymbol{s}_j\cdot\nabla)\boldsymbol{u}(\boldsymbol{x}_i) + \boldsymbol{a}_j + \boldsymbol{b}_j + O(\varepsilon^4),\end{aligned}$$

where

$$\boldsymbol{a}_j = \frac{1}{2}(\boldsymbol{s}_j\cdot\nabla)^2\boldsymbol{u}(\boldsymbol{x}_i) \qquad \text{and} \qquad \boldsymbol{b}_j = \frac{1}{6}(\boldsymbol{s}_j\cdot\nabla)^3\boldsymbol{u}(\boldsymbol{x}_i).$$

In what follows, we omit the argument of $\boldsymbol{u}$ and V since $\boldsymbol{u}$ is always evaluated at $\boldsymbol{x}_i$ and V is always evaluated at $((\boldsymbol{s}_1 + (\boldsymbol{s}_1\cdot\nabla)\boldsymbol{u}(\boldsymbol{x}_i), \boldsymbol{s}_2 + (\boldsymbol{s}_2\cdot\nabla)\boldsymbol{u}(\boldsymbol{x}_i))$.

$$\begin{aligned}\partial_{\boldsymbol{\alpha}_j} V_i = &\partial_{\boldsymbol{\alpha}_j} V + ((\boldsymbol{a}_1 + \boldsymbol{b}_1)\partial_{\boldsymbol{\alpha}_1} + (\boldsymbol{a}_2 + \boldsymbol{b}_2)\partial_{\boldsymbol{\alpha}_2})\partial_{\boldsymbol{\alpha}_j} V\\ &+ \frac{1}{2}((\boldsymbol{a}_1 + \boldsymbol{b}_1)\partial_{\boldsymbol{\alpha}_1} + (\boldsymbol{a}_2 + \boldsymbol{b}_2)\partial_{\boldsymbol{\alpha}_2})^2\partial_{\boldsymbol{\alpha}_j} V + O(\varepsilon^2).\end{aligned}$$

Substituting the above four equations into (5.3) and gathering terms of the same order, we obtain the expressions for the operators $\mathcal{L}_0$, $\mathcal{L}_1$ and $\mathcal{L}_2$:

$$\sum_{i=1}^{N} \mathcal{L}_0(\boldsymbol{u}(\boldsymbol{x}_i))\boldsymbol{\varphi}(\boldsymbol{x}_i) = -\sum_{i=1}^{N} \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{j=1}^{2} \partial_{\boldsymbol{\alpha}_j} V(\boldsymbol{s}_j \cdot \nabla)\boldsymbol{\varphi}(\boldsymbol{x}_i),$$

$$\begin{aligned}\sum_{i=1}^{N} \mathcal{L}_1(\boldsymbol{u}(\boldsymbol{x}_i))\boldsymbol{\varphi}(\boldsymbol{x}_i) = -\sum_{i=1}^{N} \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{j=1}^{2} [&(\boldsymbol{a}_1 \partial_{\alpha_1} + \boldsymbol{a}_2 \partial_{\alpha_2}) \partial_{\boldsymbol{\alpha}_j} V(\boldsymbol{s}_j \cdot \nabla)\boldsymbol{\varphi}(\boldsymbol{x}_i) \\ &+ \frac{1}{2} \partial_{\boldsymbol{\alpha}_j} V(\boldsymbol{s}_j \cdot \nabla)^2 \boldsymbol{\varphi}(\boldsymbol{x}_i)],\end{aligned}$$

and

$$\begin{aligned}&\sum_{i=1}^{N} \mathcal{L}_2(\boldsymbol{u}(\boldsymbol{x}_i))\boldsymbol{\varphi}(\boldsymbol{x}_i) \\ &= -\sum_{i=1}^{N} \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{j=1}^{2} [(\boldsymbol{b}_1 \partial_{\alpha_1} + \boldsymbol{b}_2 \partial_{\alpha_2}) \partial_{\boldsymbol{\alpha}_j} V(\boldsymbol{s}_j \cdot \nabla)\boldsymbol{\varphi}(\boldsymbol{x}_i) \\ &\qquad + \frac{1}{2} (\boldsymbol{a}_1 \partial_{\alpha_1} + \boldsymbol{a}_2 \partial_{\alpha_2}) \partial_{\boldsymbol{\alpha}_j} V(\boldsymbol{s}_j \cdot \nabla)^2 \boldsymbol{\varphi}(\boldsymbol{x}_i) \\ &\qquad + \frac{1}{6} \partial_{\boldsymbol{\alpha}_j} V(\boldsymbol{s}_j \cdot \nabla)^3 \boldsymbol{\varphi}(\boldsymbol{x}_i)].\end{aligned}$$

Passing to the limit, and integrating by parts, we have

$$\begin{aligned}\int_{\Omega} \mathcal{L}_0(\boldsymbol{u}(\boldsymbol{x}))\boldsymbol{\varphi}(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} &= -\int_{\Omega} \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{j=1}^{2} \partial_{\boldsymbol{\alpha}_j} V(\boldsymbol{s}_j \cdot \nabla)\boldsymbol{\varphi} \mathrm{d}\boldsymbol{x} \\ &= \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{j=1}^{2} \int_{\Omega} \operatorname{div}(\partial_{\boldsymbol{\alpha}_j} V \boldsymbol{s}_j)\boldsymbol{\varphi}(\boldsymbol{x}) \mathrm{d}\boldsymbol{x},\end{aligned}$$

which gives

$$\begin{aligned}\mathcal{L}_0(\boldsymbol{u}) = \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} (&\partial^2_{\boldsymbol{\alpha}_1} V(\boldsymbol{s}_1 \cdot \nabla)^2 \boldsymbol{u} + 2\partial_{\alpha_1 \alpha_2} V(\boldsymbol{s}_1 \cdot \nabla)(\boldsymbol{s}_2 \cdot \nabla)\boldsymbol{u} \\ &+ \partial^2_{\boldsymbol{\alpha}_2} V(\boldsymbol{s}_2 \cdot \nabla)^2 \boldsymbol{u}).\end{aligned}$$

We see that $\mathcal{L}_0$ is the same as the operator that appears in (2.10).

The proof for the fact that the operator $\mathcal{L}_2$ is of divergence form is similar.

Since each atom site in the simple lattice L is a center of inversion symmetric i.e. if $\boldsymbol{s} \in L$, then $-\boldsymbol{s} \in L$, and thus $\mathcal{L}_1 = \boldsymbol{0}$. This can also be proved by a straightforward but tedious calculation.

Next we expand the solution

$$\boldsymbol{u} = \boldsymbol{u}_0 + \varepsilon \boldsymbol{u}_1 + \varepsilon^2 \boldsymbol{u}_2 + \cdots .$$

Substituting it into (5.2), we obtain the equations for $\boldsymbol{u}_0$, $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$. The equation for $\boldsymbol{u}_0$ is simply the Euler–Lagrange equation (2.10), and $\boldsymbol{u}_0$ satisfies the same boundary condition as for $\boldsymbol{u}_{\mathrm{CB}}$. Therefore,

$$\boldsymbol{u}_0 = \boldsymbol{u}_{\mathrm{CB}}.$$

For $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$, we have

Lemma 5.2. *$\boldsymbol{u}_1$ satisfies*

$$\mathcal{L}_{lin}(\boldsymbol{u}_0)\boldsymbol{u}_1 = \boldsymbol{0}, \tag{5.4}$$

and $\boldsymbol{u}_2$ satisfies

$$\mathcal{L}_{lin}(\boldsymbol{u}_0)\boldsymbol{u}_2 = -\mathcal{L}_2(\boldsymbol{u}_0). \tag{5.5}$$

Moreover, if **Assumption A** *holds, then $\boldsymbol{u}_1 = \boldsymbol{0}$ and there exists a function $\boldsymbol{u}_2 \in X$ that satisfies* (5.5)*.*

Proof. A straightforward calculation gives

$$\mathcal{L}_{\mathrm{lin}}(\boldsymbol{u}_0)\boldsymbol{u}_1 = -\mathcal{L}_1(\boldsymbol{u}_0) = \boldsymbol{0}.$$

Using Lemma 5.1, we get (5.4). Using (4.7) with $t = 0$, there exists a constant κ such that if $\|\boldsymbol{f}\|_{L^p} \leqq \kappa$, then $\mathcal{L}_{\mathrm{lin}}$ is elliptic at $\boldsymbol{u}_{\mathrm{CB}} = \boldsymbol{u}_0$. Therefore, $\boldsymbol{u}_1 = \boldsymbol{0}$.

A simple calculation gives

$$\mathcal{L}_{\mathrm{lin}}(\boldsymbol{u}_0)\boldsymbol{u}_2 = -\frac{1}{2}\Big(\frac{\delta^2 \mathcal{L}_0}{\delta \boldsymbol{u}^2}(\boldsymbol{u}_0)\boldsymbol{u}_1\Big)\boldsymbol{u}_1 - \frac{\delta \mathcal{L}_1}{\delta \boldsymbol{u}}(\boldsymbol{u}_0)\boldsymbol{u}_1 - \mathcal{L}_2(\boldsymbol{u}_0) = -\mathcal{L}_2(\boldsymbol{u}_0),$$

which gives (5.5). It remains to prove that the right-hand side of (5.5) is orthogonal to a constant function, namely,

$$\int_{\Omega} \mathcal{L}_2(\boldsymbol{u}_0(\boldsymbol{x}))\mathrm{d}\boldsymbol{x} = 0. \tag{5.6}$$

This is true since $\mathcal{L}_2$ is of divergence form, see Lemma 5.1.

As a direct consequence of Lemma 5.1 and Lemma 5.2, we have

Corollary 5.1. *Define*

$$\widetilde{\boldsymbol{y}} = \boldsymbol{x} + \boldsymbol{u}_0(\boldsymbol{x}) + \varepsilon^2 \boldsymbol{u}_2(\boldsymbol{x}). \tag{5.7}$$

If $\boldsymbol{f} \in W^{6,p}(\Omega; \mathbb{R}^d)$, then there exists a constant C such that

$$\big|\mathcal{L}_\varepsilon(\widetilde{\boldsymbol{y}}) - \boldsymbol{f}\big| \leqq C\varepsilon^3. \tag{5.8}$$

Proof. Since $\boldsymbol{f} \in W^{6,p}(\Omega;\mathbb{R}^d)$, using Theorem 2.1, we conclude that $\boldsymbol{u}_0 \in W^{8,p}(\Omega;\mathbb{R}^d)$. Therefore, $\boldsymbol{u}_0 \in C^7(\overline{\Omega})$ by Sobolev embedding theorem. This gives that $\boldsymbol{u}_0 + \varepsilon^2\boldsymbol{u}_2 \in C^5(\overline{\Omega})$. Therefore,

$$\left|\mathcal{L}_\varepsilon(\widetilde{\boldsymbol{y}}) - \mathcal{L}_0(\boldsymbol{u}_0 + \varepsilon^2\boldsymbol{u}_2) - \varepsilon^2\mathcal{L}_2(\boldsymbol{u}_0 + \varepsilon^2\boldsymbol{u}_2)\right| \leqq C\varepsilon^3,$$

where the constant C depends on $\|\boldsymbol{u}_0\|_{C^7(\overline{\Omega})}$. Using $\mathcal{L}_0(\boldsymbol{u}_0) = \boldsymbol{f}$ and (5.5), we obtain

$$\left|\mathcal{L}_0(\boldsymbol{u}_0 + \varepsilon^2\boldsymbol{u}_2) + \varepsilon^2\mathcal{L}_2(\boldsymbol{u}_0 + \varepsilon^2\boldsymbol{u}_2) - \boldsymbol{f}\right| \leqq C\varepsilon^4,$$

where the constant C depends on $\|\boldsymbol{u}_0\|_{C^4(\overline{\Omega})}$. A combination of the above two inequalities leads to (5.8).

5.2. Asymptotic analysis on complex lattices

Assume that in equilibrium, the crystal consists of two types of atoms, *A* and *B*, each of which occupy a simple lattice. Let us express the equilibrium equations for atoms *A* and *B* in the form:

$$\mathcal{L}_\varepsilon^A(\boldsymbol{y}_i^A, \boldsymbol{y}_i^B) = \boldsymbol{f}(\boldsymbol{x}_i^A) \qquad \text{and} \qquad \mathcal{L}_\varepsilon^B(\boldsymbol{y}_i^A, \boldsymbol{y}_i^B) = \boldsymbol{f}(\boldsymbol{x}_i^B). \tag{5.9}$$

We will make the following ansatz:

$$\begin{aligned}
\boldsymbol{y}_i^A &= \boldsymbol{x}_i^A + \boldsymbol{u}(\boldsymbol{x}_i^A),\\
\boldsymbol{y}_i^B &= \boldsymbol{y}_i^A + \varepsilon\boldsymbol{v}_1(\boldsymbol{x}_i^A) + \varepsilon^2\boldsymbol{v}_2(\boldsymbol{x}_i^A) + \varepsilon^3\boldsymbol{v}_3(\boldsymbol{x}_i^A) + \varepsilon^4\boldsymbol{v}_4(\boldsymbol{x}_i^A) + \cdots.
\end{aligned}$$

Substituting this ansatz into (5.9), we obtain

$$\begin{aligned}
\mathcal{L}_\varepsilon^A &= \frac{1}{\varepsilon}\widetilde{\mathcal{L}}_{-1}^A(\boldsymbol{u},\boldsymbol{v}_1) + \widetilde{\mathcal{L}}_0^A(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2) + \varepsilon\widetilde{\mathcal{L}}_1^A(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3)\\
&\quad + \varepsilon^2\widetilde{\mathcal{L}}_2^A(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3,\boldsymbol{v}_4) + O(\varepsilon^3), \qquad (5.10)\\
\mathcal{L}_\varepsilon^B &= \frac{1}{\varepsilon}\widetilde{\mathcal{L}}_{-1}^B(\boldsymbol{u},\boldsymbol{v}_1) + \widetilde{\mathcal{L}}_0^B(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2) + \varepsilon\widetilde{\mathcal{L}}_1^B(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3)\\
&\quad + \varepsilon^2\widetilde{\mathcal{L}}_2^B(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3,\boldsymbol{v}_4) + O(\varepsilon^3). \qquad (5.11)
\end{aligned}$$

Therefore,

$$\begin{aligned}
\mathcal{L}_\varepsilon^A + \mathcal{L}_\varepsilon^B &= \frac{1}{\varepsilon}(\widetilde{\mathcal{L}}_{-1}^A(\boldsymbol{u},\boldsymbol{v}_1) + \widetilde{\mathcal{L}}_{-1}^B(\boldsymbol{u},\boldsymbol{v}_1)) + \widetilde{\mathcal{L}}_0^A(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2) + \widetilde{\mathcal{L}}_0^B(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2)\\
&\quad + \varepsilon[\widetilde{\mathcal{L}}_1^A(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3) + \widetilde{\mathcal{L}}_1^B(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3)]\\
&\quad + \varepsilon^2[\widetilde{\mathcal{L}}_2^A(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3,\boldsymbol{v}_4) + \widetilde{\mathcal{L}}_2^B(\boldsymbol{u},\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3,\boldsymbol{v}_4)] + O(\varepsilon^3).
\end{aligned}$$

We will show later that

1. $\widetilde{\mathcal{L}}_{-1}^B + \widetilde{\mathcal{L}}_{-1}^A = \boldsymbol{0}$.
2. $\boldsymbol{v}_{i+2}$ cancels out in the $O(\varepsilon^i)$ term for $i \geqq 0$.

Therefore we may write

$$\frac{1}{2}(\mathcal{L}_\varepsilon^A + \mathcal{L}_\varepsilon^B) = \mathcal{L}_0(\boldsymbol{u}, \boldsymbol{v}_1) + \varepsilon \mathcal{L}_1(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2) + \varepsilon^2 \mathcal{L}_2(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3) + O(\varepsilon^3) \tag{5.12}$$

with

$$\begin{aligned}
\mathcal{L}_0(\boldsymbol{u}, \boldsymbol{v}_1) &= [\widetilde{\mathcal{L}}_0^A(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{0}) + \widetilde{\mathcal{L}}_0^B(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{0})]/2, \\
\mathcal{L}_1(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2) &= [\widetilde{\mathcal{L}}_1^A(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{0}) + \widetilde{\mathcal{L}}_1^B(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{0})]/2, \\
\mathcal{L}_2(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3) &= [\widetilde{\mathcal{L}}_2^A(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3, \boldsymbol{0}) + \widetilde{\mathcal{L}}_2^B(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3, \boldsymbol{0})]/2.
\end{aligned}$$

Next consider $\mathcal{L}_\varepsilon^A - \mathcal{L}_\varepsilon^B$, we obtain

$$\begin{aligned}
\widetilde{\mathcal{L}}_{-1}^A(\boldsymbol{u}, \boldsymbol{v}_1) - \widetilde{\mathcal{L}}_{-1}^B(\boldsymbol{u}, \boldsymbol{v}_1) &= \boldsymbol{0}, \\
\widetilde{\mathcal{L}}_0^A(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2) - \widetilde{\mathcal{L}}_0^B(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2) &= -(\boldsymbol{p}_0 \cdot \nabla)\boldsymbol{f}, \\
\widetilde{\mathcal{L}}_1^A(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3) - \widetilde{\mathcal{L}}_1^B(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3) &= -\frac{1}{2}(\boldsymbol{p}_0 \cdot \nabla)^2 \boldsymbol{f}, \\
\widetilde{\mathcal{L}}_2^A(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3, \boldsymbol{v}_4) - \widetilde{\mathcal{L}}_2^B(\boldsymbol{u}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3, \boldsymbol{v}_4) &= -\frac{1}{6}(\boldsymbol{p}_0 \cdot \nabla)^3 \boldsymbol{f}.
\end{aligned}$$

Observe that these are algebraic equations for $\boldsymbol{v}_1$, $\boldsymbol{v}_2$, $\boldsymbol{v}_3$ and $\boldsymbol{v}_4$ respectively. Their solvability will be proved in Lemma 5.3.

In the second step, we assume

$$\boldsymbol{u} = \boldsymbol{u}_0 + \varepsilon \boldsymbol{u}_1 + \varepsilon^2 \boldsymbol{u}_2 + \cdots .$$

Substituting the above ansatz into (5.12), we obtain the equations satisfied by $\boldsymbol{u}_0, \boldsymbol{u}_1$ and $\boldsymbol{u}_2$:

$$\mathcal{L}_0(\boldsymbol{u}_0, \boldsymbol{v}_1) = \boldsymbol{0}, \tag{5.13}$$

$$\mathcal{L}_{\mathrm{lin}}(\boldsymbol{u}_0, \boldsymbol{v}_1)\boldsymbol{u}_1 = -\mathcal{L}_1(\boldsymbol{u}_0, \boldsymbol{v}_1, \boldsymbol{v}_2) + \frac{1}{2}(\boldsymbol{p}_0 \cdot \nabla)\boldsymbol{f}, \tag{5.14}$$

$$\mathcal{L}_{\mathrm{lin}}(\boldsymbol{u}_0, \boldsymbol{v}_1)\boldsymbol{u}_2 = -\mathcal{L}_2(\boldsymbol{u}_0, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3) - \frac{\delta \mathcal{L}_1}{\delta \mathsf{A}}(\boldsymbol{u}_0, \boldsymbol{v}_1, \boldsymbol{v}_2)\boldsymbol{u}_1 - \frac{1}{2}\Big(\frac{\delta^2 \mathcal{L}_0}{\delta \mathsf{A}^2}(\boldsymbol{u}_0, \boldsymbol{v}_1)\boldsymbol{u}_1\Big)\boldsymbol{u}_1 + \frac{1}{4}(\boldsymbol{p}_0 \cdot \nabla)^2 \boldsymbol{f}, \tag{5.15}$$

where $\mathcal{L}_{\mathrm{lin}}(\cdot, \boldsymbol{v}_1)$ is the linearized operator of $\mathcal{L}_0$ for fixed $\boldsymbol{v}_1$. We next relate these equations to the Euler–Lagrange equations and show that they are solvable.

To carry out the details of this analysis, again we will work with the case when V consists of three-body interactions only. It is easy to see how the argument can be extended to the general case.

Depending on the type of atoms that participate in the interaction, we can group the terms of V into the following subsets: AAA, AAB, ABB and BBB. The AAA and

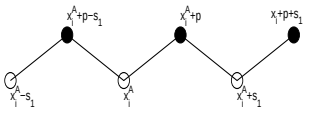

Fig. 6. A schematic illustration of the interactions between atoms on complex lattices for pair $\langle \boldsymbol{p}, \boldsymbol{p}-\boldsymbol{s} \rangle$

BBB terms are treated in the same way as for simple lattices. Hence we will restrict our attention to the *AAB* and *ABB* terms.

Fix an *A* atom at site $\boldsymbol{x}_i$. Consider its interaction with two *B* atoms at $\boldsymbol{x}_i + \boldsymbol{p}$ and $\boldsymbol{x}_i + \boldsymbol{p} - \boldsymbol{s}_1$. As in the case of simple lattice, we pair this interaction with the interactions between the atoms at *AAB*, and at *ABB* (see Fig. 6). Neglecting other terms in $\mathcal{L}_\varepsilon$, we have

$$\begin{aligned}
&\mathcal{L}_\varepsilon^A(\boldsymbol{y}_i^A, \boldsymbol{y}_i^B):\\
&= [\partial_{\alpha_1} V_{AB}(\boldsymbol{y}_i^B - \boldsymbol{y}_i^A, \boldsymbol{y}_{i-\boldsymbol{s}_1}^B - \boldsymbol{y}_i^A) - \partial_{\alpha_1} V_{AB}(\boldsymbol{y}_i^A - \boldsymbol{y}_i^B, \boldsymbol{y}_{i+\boldsymbol{s}_1}^A - \boldsymbol{y}_i^B)\\
&+ \partial_{\alpha_2} V_{AB}(\boldsymbol{y}_i^B - \boldsymbol{y}_i^A, \boldsymbol{y}_{i-\boldsymbol{s}_1}^B - \boldsymbol{y}_i^A) - \partial_{\alpha_2} V_{AB}(\boldsymbol{y}_{i-\boldsymbol{s}_1}^A - \boldsymbol{y}_{i-\boldsymbol{s}_1}^B, \boldsymbol{y}_i^A - \boldsymbol{y}_{i-\boldsymbol{s}_1}^B)],
\end{aligned}$$

where the first and third terms come from the interaction of atoms at $\boldsymbol{x}_i, \boldsymbol{x}_i + \boldsymbol{p}, \boldsymbol{x}_i + \boldsymbol{p} - \boldsymbol{s}_1$, the second term comes from the interaction of atoms at $\boldsymbol{x}_i, \boldsymbol{x}_i + \boldsymbol{p}, \boldsymbol{x}_i + \boldsymbol{s}_1$, and the last term comes from the interaction of atoms at $\boldsymbol{x}_i, \boldsymbol{x}_i + \boldsymbol{p} - \boldsymbol{s}_1, \boldsymbol{x}_i - \boldsymbol{x}_1$.

Similarly for the *B* atom at the site $\boldsymbol{x}_i + \boldsymbol{p}$, we have, corresponding to the interaction pair shown in Fig. 6:

$$\begin{aligned}
&\mathcal{L}_\varepsilon^B(\boldsymbol{y}_i^A, \boldsymbol{y}_i^B):\\
&= [\partial_{\alpha_1} V_{AB}(\boldsymbol{y}_i^A - \boldsymbol{y}_i^B, \boldsymbol{y}_{i+\boldsymbol{s}_1}^A - \boldsymbol{y}_i^B) - \partial_{\alpha_1} V_{AB}(\boldsymbol{y}_i^B - \boldsymbol{y}_i^A, \boldsymbol{y}_{i-\boldsymbol{s}_1}^B - \boldsymbol{y}_i^A)\\
&+ \partial_{\alpha_2} V_{AB}(\boldsymbol{y}_i^A - \boldsymbol{y}_i^B, \boldsymbol{y}_{i+\boldsymbol{s}_1}^A - \boldsymbol{y}_i^B) - \partial_{\alpha_2} V_{AB}(\boldsymbol{y}_{i+\boldsymbol{s}_1}^B - \boldsymbol{y}_{i+\boldsymbol{s}_1}^A, \boldsymbol{y}_i^B - \boldsymbol{y}_{i+\boldsymbol{s}_1}^A)].
\end{aligned}$$

We may rewrite $\mathcal{L}_\varepsilon^A$ and $\mathcal{L}_\varepsilon^B$ into a more compact form as

$$\begin{aligned}
\mathcal{L}_\varepsilon^A(\boldsymbol{y}_i^A, \boldsymbol{y}_i^B) = {} & \partial_{\alpha_1} V_{AB}(D_{\boldsymbol{p}}^+ \boldsymbol{y}_i^A, D_{\boldsymbol{p}-\boldsymbol{s}_1}^+ \boldsymbol{y}_i^A) + \partial_{\alpha_1} V_{AB}(D_{\boldsymbol{p}}^+ \boldsymbol{y}_i^A, D_{\boldsymbol{p}-\boldsymbol{s}_1}^+ \boldsymbol{y}_{i+\boldsymbol{s}_1}^A)\\
& + \partial_{\alpha_2} V_{AB}(D_{\boldsymbol{p}}^+ \boldsymbol{y}_i^A, D_{\boldsymbol{p}-\boldsymbol{s}_1}^+ \boldsymbol{y}_i^A)\\
& + \partial_{\alpha_2} V_{AB}(D_{\boldsymbol{p}}^+ \boldsymbol{y}_{i-\boldsymbol{s}_1}^A, D_{\boldsymbol{p}-\boldsymbol{s}_1}^+ \boldsymbol{y}_i^A),
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{L}_\varepsilon^B(\boldsymbol{y}_i^A, \boldsymbol{y}_i^B) = {} & -\partial_{\alpha_1} V_{AB}(D_{\boldsymbol{p}}^+ \boldsymbol{y}_i^A, D_{\boldsymbol{p}-\boldsymbol{s}_1}^+ \boldsymbol{y}_i^A) - \partial_{\alpha_1} V_{AB}(D_{\boldsymbol{p}}^+ \boldsymbol{y}_i^A, D_{\boldsymbol{p}-\boldsymbol{s}_1}^+ \boldsymbol{y}_{i+\boldsymbol{s}_1}^A)\\
& - \partial_{\alpha_2} V_{AB}(D_{\boldsymbol{p}}^+ \boldsymbol{y}_i^A, D_{\boldsymbol{p}-\boldsymbol{s}_1}^+ \boldsymbol{y}_{i+\boldsymbol{s}_1}^A)\\
& - \partial_{\alpha_2} V_{AB}(D_{\boldsymbol{p}}^+ \boldsymbol{y}_{i+\boldsymbol{s}_1}^A, D_{\boldsymbol{p}-\boldsymbol{s}_1}^+ \boldsymbol{y}_{i+\boldsymbol{s}_1}^A).
\end{aligned}$$

Let $\boldsymbol{\varphi}$ be a smooth periodic function, using summation by parts, we have

$$\begin{aligned}&\sum_{i=1}^{N}(\mathcal{L}_\varepsilon^A(\boldsymbol{y}_i^A,\boldsymbol{y}_i^B)+\mathcal{L}_\varepsilon^B(\boldsymbol{y}_i^A,\boldsymbol{y}_i^B))\boldsymbol{\varphi}_i\\ =&\sum_{i=1}^{N}(\partial_{\boldsymbol{\alpha}_1}V_{AB}(D_{\boldsymbol{p}}^+\boldsymbol{y}_i^A,D_{\boldsymbol{p}-\boldsymbol{s}_1}^+\boldsymbol{y}_i^A)+\partial_{\boldsymbol{\alpha}_2}V_{AB}(D_{\boldsymbol{p}}^+\boldsymbol{y}_{i-\boldsymbol{s}_1}^A,D_{\boldsymbol{p}-\boldsymbol{s}_1}^+\boldsymbol{y}_i^A))D_{\boldsymbol{s}_1}^-\boldsymbol{\varphi}_i.\end{aligned}$$

Taylor expansion at $\boldsymbol{x}_i^A$ gives

$$\begin{aligned}D_{\boldsymbol{s}_1}^-\boldsymbol{\varphi}&=(\boldsymbol{s}_1\cdot\nabla)\boldsymbol{\varphi}-\frac{1}{2}(\boldsymbol{s}_1\cdot\nabla)^2\boldsymbol{\varphi}+O(\varepsilon^3),\\ D_{\boldsymbol{p}}^+\boldsymbol{y}_i^A&=\varepsilon\boldsymbol{v}_1+\varepsilon^2\boldsymbol{v}_2+\varepsilon^3\boldsymbol{v}_3+\varepsilon^4\boldsymbol{v}_4+O(\varepsilon^5),\end{aligned}$$

and

$$D_{\boldsymbol{p}-\boldsymbol{s}_1}^+\boldsymbol{y}_i^A=-(I+\nabla\boldsymbol{u})\boldsymbol{s}_1+\varepsilon\boldsymbol{v}_1+\boldsymbol{a}_1,\qquad D_{\boldsymbol{p}}^+\boldsymbol{y}_{i-\boldsymbol{s}_1}^A=\varepsilon\boldsymbol{v}_1+\boldsymbol{b}_1,$$

where

$$\boldsymbol{a}_1=\frac{1}{2}(\boldsymbol{s}_1\cdot\nabla)^2\boldsymbol{u}-\varepsilon(\boldsymbol{s}_1\cdot\nabla)\boldsymbol{v}_1+\varepsilon^2\boldsymbol{v}_2\quad\text{and}\quad\boldsymbol{b}_1=-\varepsilon(\boldsymbol{s}_1\cdot\nabla)\boldsymbol{v}_1+\varepsilon^2\boldsymbol{v}_2.$$

The following lemma gives a characterization for the differential operators $\widetilde{\mathcal{L}}_i^A$ and $\widetilde{\mathcal{L}}_i^B$.

Lemma 5.3. *For $i\geqq 0$, the differential operators $\widetilde{\mathcal{L}}_i^A(\cdot,\boldsymbol{v}_{i+2})$ and $\widetilde{\mathcal{L}}_i^B(\cdot,\boldsymbol{v}_{i+2})$ are algebraic equations for the argument $\boldsymbol{v}_{i+2}$.*

Moreover,

$$\widetilde{\mathcal{L}}_{-1}^A(\boldsymbol{u},\boldsymbol{v})+\widetilde{\mathcal{L}}_{-1}^B(\boldsymbol{u},\boldsymbol{v})=\boldsymbol{0}\tag{5.16}$$

for any smooth functions $\boldsymbol{u}$ and $\boldsymbol{v}$.

Proof. This lemma is a tedious but straightforward calculation. We will omit the details except to say that it is useful to note the following:

$$\partial_{\boldsymbol{\alpha}_j}V_{AB}(-\boldsymbol{x},-\boldsymbol{y})=-\partial_{\boldsymbol{\alpha}_j}V_{AB}(\boldsymbol{x},\boldsymbol{y})\quad\text{for}\quad j=1,2,$$

which is a direct consequence of (2.3).

Lemma 5.4. *The differential operator $\mathcal{L}_0$ is of the form:*

$$\mathcal{L}_0(\boldsymbol{u},\boldsymbol{v}_1)=-\operatorname{div}(\partial_{\boldsymbol{\alpha}_2}V_{AB}(\varepsilon\boldsymbol{v}_1,-\boldsymbol{s}_1-(\boldsymbol{s}_1\cdot\nabla)\boldsymbol{u}+\varepsilon\boldsymbol{v}_1)\boldsymbol{s}_1).\tag{5.17}$$

Moreover, it is the variational operator for W_{CB}.

Proof. We omit the interaction between the same species. For the pair $\langle\, \boldsymbol{p}, \boldsymbol{p}-\boldsymbol{s}_1 \,\rangle$, we consider the following term in W_{CB}:

$$V_{AB}(\boldsymbol{p}, -(I+\mathsf{A})\boldsymbol{s}_1 + \boldsymbol{p}) \qquad \text{with} \quad \mathsf{A} = \nabla \boldsymbol{u}.$$

Applying (2.16) to the pair $\langle\, \boldsymbol{p}, \boldsymbol{p}-\boldsymbol{s}_1 \,\rangle$, we get the differential operator corresponding to this pair:

$$\begin{aligned}\mathcal{L}(\boldsymbol{u}, \boldsymbol{v}_1) &= -\partial^2_{\alpha_2} V_{AB}[(\boldsymbol{s}_1\cdot\nabla)^2\boldsymbol{u} - (\boldsymbol{s}_1\cdot\nabla)\boldsymbol{p}] - \partial_{\alpha_1\alpha_2} V_{AB}(\boldsymbol{s}_1\cdot\nabla)\boldsymbol{p} \\ &= -\operatorname{div}(\partial_{\alpha_2} V_{AB}(\boldsymbol{p}, -(I+\mathsf{A})\boldsymbol{s}_1 + \boldsymbol{p})\cdot \boldsymbol{s}_1),\end{aligned}$$

which is the same as the corresponding term in the equation (5.17).

Lemma 5.5. *All higher-order differential operators $\mathcal{L}_i (i \geqq 1)$ are in divergence form.*

Proof. This claim is a straightforward consequence of the fact that $\mathcal{L}^A_\varepsilon + \mathcal{L}^B_\varepsilon$ is in divergence form.

Next we consider the terms in $\mathcal{L}^A_\varepsilon - \mathcal{L}^B_\varepsilon$.

Lemma 5.6. *If* **Assumption A** *holds, then for $i = -1, 0, 1, \cdots$,*

$$\widetilde{\mathcal{L}}^A_i(\boldsymbol{u}, \boldsymbol{v}_1, \cdots, \boldsymbol{v}_{i+2}) = \boldsymbol{0} \qquad \textit{and} \qquad \widetilde{\mathcal{L}}^B_i(\boldsymbol{u}, \boldsymbol{v}_1, \cdots, \boldsymbol{v}_{i+2}) = \boldsymbol{0} \tag{5.18}$$

are solvable in terms of $\boldsymbol{v}_{i+2}$.

Proof. We only consider the interactions shown in Fig. 6.

First, we consider the $O(1/\varepsilon)$ equations. Applying (2.15) to the pair $\langle\, \boldsymbol{p}, \boldsymbol{p}-\boldsymbol{s}_1 \,\rangle$, we obtain

$$\partial_{\alpha_1} V_{AB}(\boldsymbol{p}, -(\mathsf{I}+\mathsf{A})\boldsymbol{s}_1 + \boldsymbol{p}) + \partial_{\alpha_2} V_{AB}(\boldsymbol{p}, -(\mathsf{I}+\mathsf{A})\boldsymbol{s}_1 + \boldsymbol{p}) = \boldsymbol{0},$$

which is always solvable with respect to $\boldsymbol{p}$ due to **Assumption A**. Notice that

$$\widetilde{\mathcal{L}}^A_{-1}(\boldsymbol{u}^\varepsilon, \boldsymbol{v}_1) = (\partial_{\alpha_1} + \partial_{\alpha_2}) V_{AB}(\varepsilon\boldsymbol{v}_1, -(\mathsf{I}+\nabla\boldsymbol{u})\boldsymbol{s}_1 + \varepsilon\boldsymbol{v}_1).$$

Therefore, the $O(1/\varepsilon)$ equations for A atoms are also solvable with $\boldsymbol{v}_1 = \boldsymbol{p}$. Using (5.16), we see that the other $O(1/\varepsilon)$ equations $\widetilde{\mathcal{L}}^B_{-1}(\boldsymbol{u}, \boldsymbol{v}_1) = \boldsymbol{0}$ for B atoms are also solvable with respect to $\boldsymbol{v}_1$.

In the case when $i \geqq 0$, a straightforward calculation gives that the coefficients of the argument $\boldsymbol{v}_{i+2}$ is:

$$(\partial_{\alpha_1} + \partial_{\alpha_2})^2 V_{AB}(\varepsilon\boldsymbol{v}_1, -\boldsymbol{s}_1 + (\boldsymbol{s}_1\cdot\nabla)\boldsymbol{u} + \varepsilon\boldsymbol{v}_1),$$

which is positive definite since $\boldsymbol{p}$ is a local minimizer.

From the $O(1)$ equations, it is straightforward to obtain the equations for $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$.

Lemma 5.7. *If* **Assumption A** *holds, then there exist* $\boldsymbol{u}_1, \boldsymbol{u}_2 \in X$ *that satisfies equations* (5.14) *and* (5.15)*, respectively.*

Proof. Using Lemma 5.5, we see that the right-hand side of (5.14) and (5.15) belong to Y. Next, by **Assumption A**, there exists a constant κ such that if $\|\boldsymbol{f}\|_{L^p} \leqq \kappa$, then $\mathcal{L}_{\text{lin}}$ is elliptic at $\boldsymbol{u}_0$. Therefore, there exist $\boldsymbol{u}_1, \boldsymbol{u}_2 \in X$ that satisfy the equations (5.14) and (5.15), respectively.

As a direct consequence of Lemma 5.4 and Lemma 5.7, we have

Corollary 5.2. *Define*

$$\begin{aligned} \widetilde{\boldsymbol{y}}^A &= \boldsymbol{x} + \boldsymbol{u}_0(\boldsymbol{x}) + \varepsilon \boldsymbol{u}_1(\boldsymbol{x}) + \varepsilon^2 \boldsymbol{u}_2(\boldsymbol{x}), \\ \widetilde{\boldsymbol{y}}^B &= \widetilde{\boldsymbol{y}}^A + \varepsilon \boldsymbol{v}_1(\boldsymbol{x}) + \varepsilon^2 \boldsymbol{v}_2(\boldsymbol{x}) + \varepsilon^3 \boldsymbol{v}_3(\boldsymbol{x}) + \varepsilon^4 \boldsymbol{v}_4(\boldsymbol{x}). \end{aligned} \tag{5.19}$$

If $\boldsymbol{f} \in W^{6,p}(\Omega; \mathbb{R}^d)$*, then there exists a constant* C *such that*

$$\left|\mathcal{L}_\varepsilon^A(\widetilde{\boldsymbol{y}}^A, \widetilde{\boldsymbol{y}}^B) - \boldsymbol{f}\right| \leqq C\varepsilon^3, \qquad \left|\mathcal{L}_\varepsilon^B(\widetilde{\boldsymbol{y}}^A, \widetilde{\boldsymbol{y}}^B) - \boldsymbol{f}\right| \leqq C\varepsilon^3. \tag{5.20}$$

Proof. Since $\boldsymbol{f} \in W^{6,p}(\Omega; \mathbb{R}^d)$, using Theorem 2.1, we conclude that $\boldsymbol{u}_0 \in W^{8,p}(\Omega; \mathbb{R}^d)$. Therefore, $\boldsymbol{u}_0 \in C^7(\overline{\Omega})$ by the Sobolev embedding theorem. This gives that $\widetilde{\boldsymbol{y}}^A, \widetilde{\boldsymbol{y}}^B \in C^5(\overline{\Omega})$. Therefore, using (5.14), (5.15), (5.17) and (5.12), we get

$$\left| \frac{1}{2}[\mathcal{L}_\varepsilon^A(\widetilde{\boldsymbol{y}}^A, \widetilde{\boldsymbol{y}}^B) + \mathcal{L}_\varepsilon^B(\widetilde{\boldsymbol{y}}^A, \widetilde{\boldsymbol{y}}^B)] - \boldsymbol{f} \right| \leqq C\varepsilon^3,$$

where C depends on $\|\boldsymbol{u}_0\|_{C^7(\overline{\Omega})}$.

Using Lemma 5.6 and the equations satisfied by $\boldsymbol{v}_2$, $\boldsymbol{v}_3$ and $\boldsymbol{v}_4$, we obtain

$$\left|\mathcal{L}_\varepsilon^A(\widetilde{\boldsymbol{y}}^A, \widetilde{\boldsymbol{y}}^B) - \mathcal{L}_\varepsilon^B(\widetilde{\boldsymbol{y}}^A, \widetilde{\boldsymbol{y}}^B)\right| \leqq C\varepsilon^3,$$

where C depends on $\|\boldsymbol{u}_0\|_{C^5(\overline{\Omega})}$. A combination of the above two results give (5.20).

6. Local Minimizer for the Atomistic Model

In this section, we prove Theorem 2.2 and Theorem 2.3. We will deal directly with complex lattices with two species of atoms. We assume that there are a total of $2N$ atoms, N atoms of type A, and N atoms of type B.

By translation invariance of V, we have $\mathsf{H}_{\alpha\beta}(i, j)$ depends only on the difference of i and j, namely, $\mathsf{H}_{\alpha\beta}(i, j) = \mathsf{H}_{\alpha\beta}(0, j - i)$, which immediately implies a simpler expression of the dynamical matrix D:

$$\{\mathsf{D}_{\kappa\kappa'}[n]\}_{\alpha\beta} = \sum_{j=1}^{N} \{\mathsf{H}_{\kappa\kappa'}\}_{\alpha\beta}(0, j) e^{i(\boldsymbol{x}_j + \boldsymbol{x}(\kappa) - \boldsymbol{x}(\kappa'))\cdot \boldsymbol{k}_n}.$$

It is clear that

$$\{\mathsf{H}_{\kappa\kappa'}\}_{\alpha\beta}(i,j) = \frac{1}{N}\sum_{n=1}^{N}\{\mathsf{D}_{\kappa\kappa'}[n]\}_{\alpha\beta}e^{-i(x_j^{\kappa'}-x_i^{\kappa})\cdot k_n}. \tag{6.1}$$

For any $\boldsymbol{z}\in\mathbb{R}^{N\times d}$, we have

$$\boldsymbol{z}_j = \frac{1}{N}\sum_{m=1}^{N}\hat{\boldsymbol{z}}[m]e^{-i\boldsymbol{x}_j\cdot\boldsymbol{k}_m},$$

where $\{\hat{\boldsymbol{z}}[m]\}$ are the Fourier coefficients of $\{\boldsymbol{z}\}$, defined as

$$\hat{\boldsymbol{z}}[m] := \sum_{n=1}^{N}z_n e^{i\boldsymbol{x}_n\cdot\boldsymbol{k}_m},$$

and $\{\boldsymbol{k}_m\}$ are the discrete wave vectors in the first Brillouin zone. Similarly, we may define $\hat{\boldsymbol{z}}^A[m]$ and $\hat{\boldsymbol{z}}^B[m]$.

For $\boldsymbol{z}\in\mathbb{R}^{N\times d}$, we define the discrete H^1-norm as

$$\|\boldsymbol{z}\|_1 := \Big(\frac{1}{N^2}\sum_{n=1}^{N}|\boldsymbol{k}_n|^2\,|\hat{\boldsymbol{z}}[n]|^2\Big)^{1/2}.$$

Throughout this section, we will frequently refer to the identities:

$$\sum_{\boldsymbol{x}}e^{i\boldsymbol{x}\cdot\boldsymbol{k}} = N\delta_{\boldsymbol{k},\boldsymbol{0}}, \tag{6.2}$$

and

$$\sum_{\boldsymbol{k}}e^{i\boldsymbol{x}\cdot\boldsymbol{k}} = N\delta_{\boldsymbol{x},\boldsymbol{0}}, \tag{6.3}$$

where $\boldsymbol{x}=\boldsymbol{x}^A$ or $\boldsymbol{x}=\boldsymbol{x}^B$ and $\boldsymbol{k}$ runs through all the sites in the first Brillouin zone of lattice L. We refer to [3, Appendix F] for a proof.

We first establish several inequalities concerning $\{\boldsymbol{z}\}$, which serve to give a description of the norm $\|\cdot\|_d$ defined in (2.28).

For any $\boldsymbol{z}=(\boldsymbol{z}^A,\boldsymbol{z}^B)\in\mathbb{R}^{2N\times d}$, define yet another norm

$$\|\boldsymbol{z}\|_a := \varepsilon^{d/2-1}\Big(\sum_{i=1}^{N}\sum_{|\boldsymbol{x}_{ij}^A|=\varepsilon}\big|\boldsymbol{z}_i^A-\boldsymbol{z}_j^A\big|^2+\sum_{i=1}^{N}\sum_{|\boldsymbol{x}_{ij}^B|=\varepsilon}\big|\boldsymbol{z}_i^B-\boldsymbol{z}_j^B\big|\Big)^{1/2},$$

where $\boldsymbol{x}_{ij}^{\kappa}=\boldsymbol{x}_i^{\kappa}-\boldsymbol{x}_j^{\kappa}$ with $\kappa=A,B$.

Lemma 6.1. *For any $\boldsymbol{z}=(\boldsymbol{z}^A,\boldsymbol{z}^B)\in\mathbb{R}^{2N\times d}$, there exists a constant C that only depends on the coordination number of L such that*

$$\|\boldsymbol{z}\|_a \leqq C(\|\boldsymbol{z}^A\|_1+\|\boldsymbol{z}^B\|_1). \tag{6.4}$$

Proof. We have

$$\left|\boldsymbol{z}_i^A - \boldsymbol{z}_j^A\right|^2 = \frac{1}{N^2}\sum_{n,m=1}^{N} \hat{\boldsymbol{z}}^A[n]\overline{\hat{\boldsymbol{z}}}^A[m][e^{i\boldsymbol{x}_i^A\cdot\boldsymbol{k}_{nm}} - e^{i\boldsymbol{x}_i^A\cdot\boldsymbol{k}_n}e^{-i\boldsymbol{x}_j^A\cdot\boldsymbol{k}_m} - e^{i\boldsymbol{x}_j^A\cdot\boldsymbol{k}_m}e^{-i\boldsymbol{x}_j^A\cdot\boldsymbol{k}_n} + e^{i\boldsymbol{x}_i^A\cdot\boldsymbol{k}_{nm}}].$$

We will decompose $\varepsilon^{d-2}\sum_{i=1}^{N}\sum_{\left|\boldsymbol{x}_{ij}^A\right|=\varepsilon}\left|\boldsymbol{z}_i^A - \boldsymbol{z}_j^A\right|^2$ into $I_1 + I_2 + I_3 + I_4$ according to the above expression. Using (6.2), we obtain

$$\begin{aligned} I_1 &= \frac{K\varepsilon^{d-2}}{N^2}\sum_{n,m=1}^{N} \hat{\boldsymbol{z}}^A[n]\overline{\hat{\boldsymbol{z}}}^A[m]\sum_{i=1}^{N} e^{i\boldsymbol{x}_i^A\cdot\boldsymbol{k}_{nm}} \\ &= \frac{K\varepsilon^{d-2}}{N^2}\sum_{n,m=1}^{N} \hat{\boldsymbol{z}}^A[n]\overline{\hat{\boldsymbol{z}}}^A[m]N\delta_{nm} = \frac{K\varepsilon^{d-2}}{N}\sum_{n=1}^{N}\left|\hat{\boldsymbol{z}}^A[n]\right|^2, \end{aligned}$$

where K is the coordination number of the underlying lattice. Similarly, $I_4 = I_1$. Note that

$$I_2 = -\frac{\varepsilon^{d-2}}{N^2}\sum_{i=1}^{N}\sum_{\left|\boldsymbol{x}_{ij}^A\right|=\varepsilon}\sum_{n,m=1}^{N} \hat{\boldsymbol{z}}^A[n]\overline{\hat{\boldsymbol{z}}}^A[m]e^{i\boldsymbol{x}_i^A\cdot\boldsymbol{k}_n}e^{-i(\boldsymbol{x}_i^A - \boldsymbol{x}_{ij}^A)\cdot\boldsymbol{k}_m}.$$

For any point $\boldsymbol{x}_i^A$, $\boldsymbol{x}_{ij}^A$ is the same since all atoms have the same environment. Therefore, we denote $\boldsymbol{\alpha}_j = \boldsymbol{x}_{ij}^A$. A direct manipulation leads to

$$\begin{aligned} I_2 &= -\frac{\varepsilon^{d-2}}{N^2}\sum_{i=1}^{N}\sum_{\left|\boldsymbol{x}_{ij}^A\right|=\varepsilon}\sum_{n,m=1}^{N} \hat{\boldsymbol{z}}^A[n]\overline{\hat{\boldsymbol{z}}}^A[m]e^{i\boldsymbol{x}_i^A\cdot\boldsymbol{k}_n}e^{-i(\boldsymbol{x}_i^A + \boldsymbol{\alpha}_j)\cdot\boldsymbol{k}_m} \\ &= -\frac{\varepsilon^{d-2}}{N^2}\sum_{n,m=1}^{N} \hat{\boldsymbol{z}}^A[n]\overline{\hat{\boldsymbol{z}}}^A[m]\sum_{i=1}^{N} e^{i\boldsymbol{x}_i^A\cdot\boldsymbol{k}_{nm}}\sum_{j=1}^{K} e^{-i\boldsymbol{\alpha}_j\cdot\boldsymbol{k}_m} \\ &= -\frac{\varepsilon^{d-2}}{N}\sum_{n=1}^{N}\left|\hat{\boldsymbol{z}}^A[n]\right|^2\sum_{j=1}^{K} e^{-i\boldsymbol{\alpha}_j\cdot\boldsymbol{k}_m}. \end{aligned}$$

Similarly,

$$I_3 = -\frac{\varepsilon^{d-2}}{N}\sum_{n=1}^{N}\left|\hat{\boldsymbol{z}}^A[n]\right|^2\sum_{j=1}^{K} e^{i\boldsymbol{\alpha}_j\cdot\boldsymbol{k}_m}.$$

Summing up the expression for $I_1, \cdots, I_4$, we obtain

$$\begin{aligned} \varepsilon^{d-2}\sum_{i=1}^{N}\sum_{\left|\boldsymbol{x}_{ij}^A\right|=\varepsilon}\left|\boldsymbol{z}_i^A - \boldsymbol{z}_j^A\right|^2 &= \frac{2\varepsilon^{d-2}}{N}\sum_{n=1}^{N}\left|\hat{\boldsymbol{z}}^A[n]\right|^2\sum_{j=1}^{K}(1 - \cos(\boldsymbol{\alpha}_j\cdot\boldsymbol{k}_n)) \\ &= \frac{4\varepsilon^{d-2}}{N}\sum_{n=1}^{N}\left|\hat{\boldsymbol{z}}^A[n]\right|^2\sum_{j=1}^{K}\sin^2\frac{\boldsymbol{\alpha}_j\cdot\boldsymbol{k}_n}{2}. \end{aligned}$$

Similarly,

$$\varepsilon^{d-2}\sum_{i=1}^{N}\sum_{\left|\boldsymbol{x}_{ij}^{A}\right|=\varepsilon}\left|\boldsymbol{z}_i^B-\boldsymbol{z}_j^B\right|^2=\frac{4\varepsilon^{d-2}}{N}\sum_{n=1}^{N}\left|\hat{\boldsymbol{z}}^B[n]\right|^2\sum_{j=1}^{K}\sin^2\frac{\boldsymbol{\alpha}_j\cdot\boldsymbol{k}_n}{2}.$$

From these two identities and the definition of the discrete H^1-norm $\|\boldsymbol{z}\|_1$, we have

$$\begin{aligned}\|\boldsymbol{z}\|_a^2 &\leqq \frac{\varepsilon^{d-2}}{N}\sum_{n=1}^{N}(\left|\hat{\boldsymbol{z}}^A[n]\right|^2+\left|\hat{\boldsymbol{z}}^B[n]\right|^2)\sum_{j=1}^{K}\left|\boldsymbol{\alpha}_j\cdot\boldsymbol{k}_n\right|^2\\ &\leqq C(\|\boldsymbol{z}^A\|_1^2+\|\boldsymbol{z}^B\|_1^2),\end{aligned}$$

which leads to the desired estimate (6.1).

The following simple fact is useful.

Lemma 6.2. *Given a block matrix* $\widetilde{\mathsf{A}}\in\mathbb{R}^{2d\times 2d}$

$$\widetilde{\mathsf{A}}=\begin{pmatrix}\mathsf{A}_{11} & \mathsf{A}_{12}\\ \mathsf{A}_{12}^{*} & \mathsf{A}_{22}\end{pmatrix},$$

where $\mathsf{A}_{11}\in\mathbb{R}^{d\times d}$ *and* $\mathsf{A}_{22}\in\mathbb{R}^{d\times d}$ *are positive definite. If* $\widetilde{\mathsf{A}}$ *is semi-positive definite, then for any* $\boldsymbol{w},\boldsymbol{v}\in\mathbb{R}^d$,

$$\boldsymbol{w}^T\mathsf{A}_{11}\boldsymbol{w}+\boldsymbol{v}^T\mathsf{A}_{22}\boldsymbol{v}\geqq\frac{1}{2}(\boldsymbol{w},\boldsymbol{v})^T\widetilde{\mathsf{A}}(\boldsymbol{w},\boldsymbol{v}).\tag{6.5}$$

Lemma 6.3. *Under* **Assumption A**, *for any* $\boldsymbol{z}=(\boldsymbol{z}^A,\boldsymbol{z}^B)$, *there exists a constant* λ *independent of* N *and a constant* C_1 *that depends on the coordination number of* L, Λ_2 *and the dimension* d *such that*

$$\|\,\boldsymbol{z}\,\|_d\geqq\sqrt{\lambda/2}\Lambda_2\varepsilon^{d/2-1}\|\boldsymbol{z}^A-\boldsymbol{z}^B\|_{\ell_2}-C_1(\|\boldsymbol{z}^A\|_1+\|\boldsymbol{z}^B\|_1).\tag{6.6}$$

Proof. Using the translation invariance of H_0, for any $1\leqq j\leqq 2N$, we have

$$\sum_{i=1}^{2N}\mathsf{H}_0(i,j)=\mathbf{0}.\tag{6.7}$$

Using the above identities, we get

$$\boldsymbol{z}^T\mathsf{H}_0\boldsymbol{z}=-\frac{1}{2}\sum_{i,j=1}^{2N}(\boldsymbol{z}_i-\boldsymbol{z}_j)\mathsf{H}_0(i,j)(\boldsymbol{z}_i-\boldsymbol{z}_j),$$

which can be expanded into

$$\begin{aligned}\boldsymbol{z}^T \mathsf{H}_0 \boldsymbol{z} = &-\frac{1}{2}\sum_{\kappa=A,B}\sum_{i,j=1}^{N}(\boldsymbol{z}_i^\kappa - \boldsymbol{z}_j^\kappa)\mathsf{H}_{\kappa\kappa}(i,j)(\boldsymbol{z}_i^\kappa - \boldsymbol{z}_j^\kappa)\\ &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_i^A - \boldsymbol{z}_j^B)\mathsf{H}_{AB}(i,j)(\boldsymbol{z}_i^A - \boldsymbol{z}_j^B)\\ &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_i^B - \boldsymbol{z}_j^A)\mathsf{H}_{AB}^*(i,j)(\boldsymbol{z}_i^B - \boldsymbol{z}_j^A).\end{aligned}$$

We rewrite the above equation as

$$\begin{aligned}\boldsymbol{z}^T \mathsf{H}_0 \boldsymbol{z} = &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_i^A - \boldsymbol{z}_j^A)(\mathsf{H}_{AA} + \mathsf{H}_{AB})(i,j)(\boldsymbol{z}_i^A - \boldsymbol{z}_j^A)\\ &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_i^B - \boldsymbol{z}_j^B)(\mathsf{H}_{BB} + \mathsf{H}_{AB}^*)(i,j)(\boldsymbol{z}_i^B - \boldsymbol{z}_j^B)\\ &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_j^A - \boldsymbol{z}_j^B)\mathsf{H}_{AB}(i,j)(\boldsymbol{z}_j^A - \boldsymbol{z}_j^B)\\ &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_j^A - \boldsymbol{z}_j^B)\mathsf{H}_{AB}^*(i,j)(\boldsymbol{z}_j^A - \boldsymbol{z}_j^B) + I_3, \qquad (6.8)\end{aligned}$$

where

$$\begin{aligned}I_3 = &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_i^A - \boldsymbol{z}_j^A)\mathsf{H}_{AB}(i,j)(\boldsymbol{z}_j^A - \boldsymbol{z}_j^B)\\ &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_j^A - \boldsymbol{z}_j^B)\mathsf{H}_{AB}(i,j)(\boldsymbol{z}_i^A - \boldsymbol{z}_j^A)\\ &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_i^B - \boldsymbol{z}_j^B)\mathsf{H}_{AB}^*(i,j)(\boldsymbol{z}_j^A - \boldsymbol{z}_j^B)\\ &-\frac{1}{2}\sum_{i,j=1}^{N}(\boldsymbol{z}_j^A - \boldsymbol{z}_j^B)\mathsf{H}_{AB}^*(i,j)(\boldsymbol{z}_i^B - \boldsymbol{z}_j^B).\end{aligned}$$

Using (6.7), we have

$$\sum_{i=1}^{N}[\mathsf{H}_{AA}(i,j) + \mathsf{H}_{AB}^*(i,j)] = \mathbf{0}, \quad \sum_{i=1}^{N}[\mathsf{H}_{AB}(i,j) + \mathsf{H}_{BB}(i,j)] = \mathbf{0},$$

which implies

$$\begin{aligned}\boldsymbol{z}^T \mathsf{H}_0 \boldsymbol{z} = \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)\left\{\sum_{j=1}^{N}(\mathsf{H}_{AA}(i,j)+\mathsf{H}_{BB}(i,j))\right\}(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)\\ -\frac{1}{2}\Big[\sum_{i,j=1}^{N}(\boldsymbol{z}_i^A - \boldsymbol{z}_j^A)(\mathsf{H}_{AA}+\mathsf{H}_{AB}+\mathsf{H}_{AB}^*)(i,j)(\boldsymbol{z}_i^A - \boldsymbol{z}_j^A)\\ -\sum_{i,j=1}^{N}(\boldsymbol{z}_i^B - \boldsymbol{z}_j^B)\mathsf{H}_{BB}(i,j)(\boldsymbol{z}_i^B - \boldsymbol{z}_j^B)\Big] + I_3 =: I_1 + I_2 + I_3.\end{aligned}$$

Using (6.1), we have

$$\sum_{j=1}^{N}(\mathsf{H}_{AA}(i,j)+\mathsf{H}_{BB}(j,i)) = \frac{1}{N}\sum_{n=1}^{N}(\mathsf{D}_{AA}+\mathsf{D}_{BB})[n]. \tag{6.9}$$

Using (6.5) with $\boldsymbol{w} = \boldsymbol{v} = \boldsymbol{z}_i^A - \boldsymbol{z}_i^B$, for each i and n, we have

$$\begin{aligned}&(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)^T(\mathsf{D}_{AA}+\mathsf{D}_{BB})[n](\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)\\ &\geqq \frac{1}{2}(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B, \boldsymbol{z}_i^A - \boldsymbol{z}_i^B)^T\mathsf{D}[n](\boldsymbol{z}_i^A - \boldsymbol{z}_i^B, \boldsymbol{z}_i^A - \boldsymbol{z}_i^B).\end{aligned}$$

For each fixed n, we let $Q[n]$ be a $2d \times 2d$ matrix consisting of the normalized eigenvectors of the eigenvalue problem:

$$\mathsf{D}[n]Q_i[n] = \widetilde{\omega}_i^2[n]Q_i[n] \qquad 1 \leqq i \leqq 2d,$$

where $Q_i[n]$ is the $i-$th column of $Q[n]$. Let $Q_i[n] = (Q_i^A[n], Q_i^B[n])^T$. Combining the above two equations, we get

$$I_1 \geqq \frac{1}{N}\sum_{n=1}^{N}\sum_{i=1}^{N}\sum_{j=1}^{2d}\widetilde{\omega}_j^2[n]\left|(Q_i^A[n]+Q_i^B[n])\cdot(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)\right|^2. \tag{6.10}$$

Using (6.5) again with $\boldsymbol{w} = \boldsymbol{z}_i^A - \boldsymbol{z}_i^B$ and $\boldsymbol{v} = \boldsymbol{z}_i^B - \boldsymbol{z}_i^A$, for each i and n, we have

$$\begin{aligned}&(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)\cdot(\mathsf{D}_{AA}+\mathsf{D}_{BB})[n]\cdot(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)\\ &\geqq \frac{1}{2}(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B, \boldsymbol{z}_i^B - \boldsymbol{z}_i^A)^T\cdot\mathsf{D}[n]\cdot(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B, \boldsymbol{z}_i^B - \boldsymbol{z}_i^A).\end{aligned}$$

Repeating the above procedure, we get another lower-bound for I_1:

$$I_1 \geqq \frac{1}{N}\sum_{n=1}^{N}\sum_{i=1}^{N}\sum_{j=1}^{2d}\widetilde{\omega}_j^2[n]\left|(Q_i^A[n]-Q_i^B[n])\cdot(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)\right|^2. \tag{6.11}$$

A combination of (6.10) and (6.11) gives

$$I_1 \geqq \frac{1}{N}\sum_{n=1}^{N}\sum_{i=1}^{N}\sum_{j=1}^{2d}\widetilde{\omega}_j^2[n]\left(\left|Q_j^A[n]\cdot(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)\right|^2 + \left|Q_j^B[n]\cdot(\boldsymbol{z}_i^A - \boldsymbol{z}_i^B)\right|^2\right).$$

Next we claim that there exists a constant λ independent of N such that

$$I_1 \geqq \lambda \Lambda_2^2 \varepsilon^{-2} \|\boldsymbol{z}^A - \boldsymbol{z}^B\|_{\ell_2}^2. \tag{6.12}$$

For a fixed n, the optical branch, for example, is $j = 1, \cdots, d$. Therefore,

$$I_1 \geqq \frac{1}{N} \sum_{n=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{d} \widetilde{\omega}_j^2[n] (\left| Q_j^A[n] \cdot (\boldsymbol{z}_i^A - \boldsymbol{z}_i^B) \right|^2 + \left| Q_j^B[n] \cdot (\boldsymbol{z}_i^A - \boldsymbol{z}_i^B) \right|^2).$$

As to $d = 1$, using the fact that the eigenvector $Q_j[n]$ is normalized, we have

$$\left| Q_j^A[n] \cdot (\boldsymbol{z}_i^A - \boldsymbol{z}_i^B) \right|^2 + \left| Q_j^B[n] \cdot (\boldsymbol{z}_i^A - \boldsymbol{z}_i^B) \right|^2 = \left| \boldsymbol{z}_i^A - \boldsymbol{z}_i^B \right|^2,$$

which gives

$$I_1 \geqq \frac{1}{N} \sum_{n=1}^{N} \sum_{i=1}^{N} \widetilde{\omega}^2[n] \left| \boldsymbol{z}_i^A - \boldsymbol{z}_i^B \right|^2. \tag{6.13}$$

As to $d = 3$, we claim there exists a constant λ_1 independent of j and N such that

$$\begin{aligned} &\sum_{n=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{d} \widetilde{\omega}_j^2[n] (\left| Q_j^A[n] \cdot (\boldsymbol{z}_i^A - \boldsymbol{z}_i^B) \right|^2 + \left| Q_j^B[n] \cdot (\boldsymbol{z}_i^A - \boldsymbol{z}_i^B) \right|^2) \\ &\geqq \lambda_1 \sum_{n=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{d} \widetilde{\omega}_j^2[n] \left| \boldsymbol{z}_i^A - \boldsymbol{z}_i^B \right|^2. \end{aligned} \tag{6.14}$$

Denote by $\boldsymbol{w} = (\boldsymbol{z}_i^A - \boldsymbol{z}_i^B) / \left| \boldsymbol{z}_i^A - \boldsymbol{z}_i^B \right|$ and

$$F(\boldsymbol{w}) = \sum_{j=1}^{d} \widetilde{\omega}_j^2[n] (\left| Q_j^A[n] \cdot \boldsymbol{w} \right|^2 + \left| Q_j^B[n] \cdot \boldsymbol{w} \right|^2).$$

Obviously $F(\boldsymbol{w}) \geqq 0$. If $F(\boldsymbol{w}) = 0$, we have

$$Q_j^\kappa[n] \cdot \boldsymbol{w} = 0 \qquad \text{for } \kappa = \mathrm{A}, \mathrm{B},\ j = 1, 2, 3.$$

Obviously, there exist three nonzero constant ℓ_j that may depend on n such that

$$Q_j^A[n] = \ell_j Q_j^B[n] \qquad j = 1, 2, 3.$$

By the orthogonality of $\{Q_j[n]\}$, we have

$$1 + \ell_1 \ell_2 = 0 \qquad 1 + \ell_2 \ell_3 = 0 \qquad 1 + \ell_1 \ell_3 = 0.$$

This is obviously impossible. Therefore, $F(\boldsymbol{w}) > 0$ for all $\boldsymbol{w}$. Since $|\boldsymbol{w}| = 1$, there exists a constant $\lambda(n)$ such that

$$F(\boldsymbol{w}) \geqq \lambda(n).$$

This gives (6.14) with $\lambda_1 = \min_{1 \leqq n \leqq N} \lambda(n)$.

As to $d = 2$, repeating the above procedure, we have

$$Q_j^A[n] = \ell_j(n) Q_j^B[n] \quad \text{and} \quad Q_j^B[n] \cdot \boldsymbol{w} = 0 \qquad j = 1, 2,$$

and

$$\ell_1(n)\ell_2(n) = -1 \qquad \text{for } n = 1, \cdots, N.$$

For $N \geqq 2$, there always exit two linearly independent vectors $Q_j^B[n_1]$ and $Q_j^B[n_2]$ such that $Q_j^B[n_i] \cdot \boldsymbol{w} = 0$ for $i = 1, 2$, which immediately leads to $\boldsymbol{w} = \boldsymbol{0}$. This contradicts with $|\boldsymbol{w}| = 1$. Repeating the procedure for $d = 3$, we obtain (6.14) remains valid for $d = 2$.

Finally, using **Assumption A**, (6.13) and (6.14), we get (6.12) with $\lambda = \min(\lambda_1, 1)$.

Using Lemma 6.1 and the fact that the atomistic potential has finite range, we have

$$|I_2| \leqq C_2 \varepsilon^{-d} (\|\boldsymbol{z}^A\|_1^2 + \|z^B\|_1^2). \tag{6.15}$$

Similarly, we get

$$|I_3| \leqq C_3 \varepsilon^{-d/2-1} \|\boldsymbol{z}^A - \boldsymbol{z}^B\|_{\ell_2} (\|\boldsymbol{z}^A\|_1 + \|\boldsymbol{z}^B\|_1). \tag{6.16}$$

A combination of (6.12), (6.15) and (6.16) gives (6.6).

Lemma 6.4. *Under* **Assumption A**, *there exists a constant C that only depends on Λ_1, Λ_2, d and the coordination number of L such that*

$$\| \boldsymbol{z} \|_d \geqq C(\|\boldsymbol{z}^A\|_1 + \|\boldsymbol{z}^B\|_1 + \varepsilon^{d/2-1} \|\boldsymbol{z}^A - \boldsymbol{z}^B\|_{\ell_2}). \tag{6.17}$$

Proof. It is easy to see that

$$\boldsymbol{z}^T \mathsf{H}_0 \boldsymbol{z} = [\boldsymbol{z}^A]^T \mathsf{H}_{AA} \boldsymbol{z}^A + [\boldsymbol{z}^A]^T \mathsf{H}_{AB} \boldsymbol{z}^B + [\boldsymbol{z}^B]^T \mathsf{H}_{AB}^* \boldsymbol{z}^A + [\boldsymbol{z}^B]^T \mathsf{H}_{BB} \boldsymbol{z}^B.$$

Using (6.1), we express each item in terms of the dynamical matrix D.

$$\begin{aligned}
&[\boldsymbol{z}^A]^T \mathsf{H}_{AA} \boldsymbol{z}^A \\
&= \frac{1}{N^3} \sum_{i,j=1}^{N} \sum_{m=1}^{N} \hat{\boldsymbol{z}}^A[m] e^{-i\boldsymbol{x}_i^A \cdot \boldsymbol{k}_m} \sum_{n=1}^{N} \mathsf{D}_{AA}[n] e^{-i(\boldsymbol{x}_j^A - \boldsymbol{x}_i^A) \cdot \boldsymbol{k}_n} \sum_{p=1}^{N} \overline{\hat{\boldsymbol{z}}}^A[p] e^{i\boldsymbol{x}_j^A \cdot \boldsymbol{k}_p} \\
&= \frac{1}{N^3} \sum_{m,n,p=1}^{N} \hat{\boldsymbol{z}}^A[m] \mathsf{D}_{AA}[n] \overline{\hat{\boldsymbol{z}}}^A[p] \Big(\sum_{i=1}^{N} e^{-i\boldsymbol{x}_i^A \cdot \boldsymbol{k}_{mn}} \Big) \sum_{j=1}^{N} e^{-i\boldsymbol{x}_j^A \cdot \boldsymbol{k}_{np}}.
\end{aligned}$$

Using (6.2), we rewrite the above identity into

$$\begin{aligned}
[\boldsymbol{z}^A]^T \mathsf{H}_{AA} \boldsymbol{z}^A &= \frac{1}{N^3} \sum_{m,n,p=1}^{N} \hat{\boldsymbol{z}}^A[m] N \delta_{nm} \mathsf{D}_{AA}[n] \overline{\hat{\boldsymbol{z}}}^A[p] N \delta_{np} \\
&= \frac{1}{N} \sum_{n=1}^{N} \hat{\boldsymbol{z}}^A[n] \mathsf{D}_{AA}[n] \overline{\hat{\boldsymbol{z}}}^A[n].
\end{aligned}$$

Proceeding along the same line, we obtain

$$[\boldsymbol{z}^{\kappa'}]^T \mathsf{H}_{\kappa\kappa'} \boldsymbol{z}^{\kappa} = \frac{1}{N} \sum_{n=1}^{N} \hat{\boldsymbol{z}}^{\kappa}[n] \mathsf{D}_{\kappa\kappa'}[n] \overline{\hat{\boldsymbol{z}}}^{\kappa'}[n]$$

for $\kappa, \kappa' = A, B$. We thus write $\boldsymbol{z}^T \mathsf{H}_0 \boldsymbol{z}$ as

$$\boldsymbol{z}^T \mathsf{H}_0 \boldsymbol{z} = \frac{1}{N} \sum_{n=1}^{N} (\hat{\boldsymbol{z}}^A[n], \hat{\boldsymbol{z}}^B[n]) \mathsf{D}[n] (\hat{\boldsymbol{z}}^A[n], \hat{\boldsymbol{z}}^B[n]).$$

As in Lemma 6.3 and using

$$\widetilde{\omega}_a^2(n) \geqq \Lambda_1^2 |\boldsymbol{k}_n|^2 \quad \text{and} \quad \widetilde{\omega}_o^2(n) \geqq \widetilde{\omega}_a^2(n) \geqq \Lambda_1^2 |\boldsymbol{k}_n|^2 ,$$

we have

$$\begin{aligned} \hat{\boldsymbol{z}}[n]^T \mathsf{D}[n] \hat{\boldsymbol{z}}[n] &= \sum_{i=1}^{d} ((\widetilde{\omega}_a^2(n))_i + (\widetilde{\omega}_o^2(n))_i) |Q[n] \hat{\boldsymbol{z}}[n]|^2 \\ &\geqq 2\Lambda_1^2 |\boldsymbol{k}_n|^2 |Q \hat{\boldsymbol{z}}[n]|^2 = 2\Lambda_1^2 |\boldsymbol{k}_n|^2 |\hat{\boldsymbol{z}}[n]|^2 , \end{aligned} \tag{6.18}$$

where we have used the fact that Q is an orthogonal matrix. Therefore, we obtain

$$\begin{aligned} \boldsymbol{z}^T \mathsf{H}_0 \boldsymbol{z} &\geqq \frac{2\Lambda_1^2}{N} \sum_{n=1}^{N} |\boldsymbol{k}_n|^2 \left(\left| \hat{\boldsymbol{z}}^A[n] \right|^2 + \left| \hat{\boldsymbol{z}}^B[n] \right|^2 \right) \geqq 2\Lambda_1^2 N (\|\boldsymbol{z}^A\|_1^2 + \|\boldsymbol{z}^B\|_1^2) \\ &\geqq C\Lambda_1^2 \varepsilon^{-d} (\|\boldsymbol{z}^A\|_1^2 + \|\boldsymbol{z}^B\|_1^2), \end{aligned}$$

which leads to

$$\| \boldsymbol{z} \|_d^2 \geqq C\Lambda_1^2 (\|\boldsymbol{z}^A\|_1^2 + \|\boldsymbol{z}^B\|_1^2). \tag{6.19}$$

A convex combination of (6.19) and (6.6) leads to (6.17).

The identity (6.18) give an alternative characterization of $\| \cdot \|_d$ norm. In the next lemma, we will show that the right-hand side of (6.17) is actually an equivalent norm of $\| \boldsymbol{z} \|_d$.

Lemma 6.5. *If there exists a constant C independent of ε such that the optical branch of the dynamical matrix satisfies $\widetilde{\omega}_o(\boldsymbol{k}) \leqq C/\varepsilon$, then for any $\boldsymbol{z} \in \mathbb{R}^{2N \times d}$, there exists a constant C_1 such that*

$$\| \boldsymbol{z} \|_d \leqq C_1 (\|\boldsymbol{z}^A\|_1 + \|\boldsymbol{z}^B\|_1 + \varepsilon^{d/2-1} \|\boldsymbol{z}^A - \boldsymbol{z}^B\|_{\ell_2}). \tag{6.20}$$

Proof. We start with the identity (6.9) in Lemma 6.3. Using the fact that

$$(\widetilde{\omega}_a(n))_i \leqq (\widetilde{\omega}_o(n))_i \leqq C/\varepsilon$$

for $1 \leqq i \leqq d$, we have

$$I_1 \leqq C_4 \varepsilon^{-2} \|\boldsymbol{z}^A - \boldsymbol{z}^B\|_{\ell_2}^2,$$

which together with (6.15) and (6.16) leads to

$$\begin{aligned}\| \boldsymbol{z} \|_d^2 &\leqq C_4\varepsilon^{d-2}\|\boldsymbol{z}^A - \boldsymbol{z}^B\|_{\ell_2}^2 + C_2(\|\boldsymbol{z}^A\|_1^2 + \|\boldsymbol{z}^B\|_1^2) \\ &\quad + C_3\varepsilon^{d/2-1}\|\boldsymbol{z}^A - \boldsymbol{z}^B\|_{\ell_2}(\|\boldsymbol{z}^A\|_1 + \|\boldsymbol{z}^B\|_1) \\ &\leqq \max(C_4, C_2, C_3/2)(\|\boldsymbol{z}^A\|_1 + \|\boldsymbol{z}^B\|_1 + \varepsilon^{d/2-1}\|\boldsymbol{z}^A - \boldsymbol{z}^B\|_{\ell_2})^2,\end{aligned}$$

which gives (6.20) with $C_1 = \sqrt{\max(C_4, C_2, C_3/2)}$.

Next we establish a discrete *Poincaré inequality*.

Lemma 6.6. *For any $\boldsymbol{z} \in \mathbb{R}^{N\times d}$ that satisfies $\sum_{j=1}^N \boldsymbol{z}_j = \boldsymbol{0}$, there exists a constant C such that*

$$\|\boldsymbol{z}\|_{\ell_2} \leqq C\varepsilon^{-d/2}\|\boldsymbol{z}\|_1. \tag{6.21}$$

Proof. Since $\sum_{j=1}^N \boldsymbol{z}_j = \boldsymbol{0}$ and $\boldsymbol{k}_1 = \boldsymbol{0}$, $\hat{\boldsymbol{z}}[1] = \boldsymbol{0}$. Therefore, by definition,

$$\|\boldsymbol{z}\|_{\ell_2}^2 = \frac{1}{N^2}\sum_{j=1}^N\sum_{m=2}^N \hat{\boldsymbol{z}}[m]e^{-i\boldsymbol{x}_j\cdot\boldsymbol{k}_m}\sum_{m=2}^N \overline{\hat{\boldsymbol{z}}}[m]e^{i\boldsymbol{x}_j\cdot\boldsymbol{k}_m}.$$

By the Cauchy-Schwartz inequality, we have

$$\sum_{m=2}^N \hat{\boldsymbol{z}}[m]e^{-i\boldsymbol{x}_j\cdot\boldsymbol{k}_m} \leqq \Big(\sum_{m=2}^N |\hat{\boldsymbol{z}}[m]|^2\,|\boldsymbol{k}_m|^2\Big)^{1/2}\Big(\sum_{m=2}^N |\boldsymbol{k}_m|^{-2}\Big)^{1/2}.$$

Combining the above two statements, we obtain

$$\|z\|_{\ell_2}^2 \leqq \frac{1}{N}\sum_{m=2}^N |\hat{\boldsymbol{z}}[m]|^2\,|\boldsymbol{k}_m|^2\sum_{m=2}^N |\boldsymbol{k}_m|^{-2} = N\|z\|_1^2\sum_{m=2}^N |\boldsymbol{k}_m|^{-2}.$$

Since $\boldsymbol{k}_m = \sum_{j=1}^d \frac{m_j}{N_j}\boldsymbol{b}_j$, where $\{\boldsymbol{b}_j\}$ is the basis of the reciprocal lattice, we get $|\boldsymbol{k}_m| = \frac{2\pi}{\varepsilon}\Big(\sum_{j=1}^d \big|m_j/N_j\big|^2\Big)^{1/2}$. A direct calculation gives

$$\begin{aligned}\sum_{m=2}^N |\boldsymbol{k}_m|^{-2} &\leqq (\frac{\varepsilon}{2\pi})^2\sum_{m=2}^N\Big(\sum_{j=1}^d \big|m_j/N_j\big|^2\Big)^{-1} \leqq \frac{d^{-2}}{(2\pi)^2}\sum_{j=1}^d\sum_{m_j=1}^{N_j}(\varepsilon N_j/m_j)^2 \\ &\leqq C\sum_{j=1}^d\sum_{m_j=1}^{N_j} m_j^{-2} \leqq C,\end{aligned}$$

where we have used $\varepsilon N_j \leqq C$ for $1 \leqq j \leqq d$. Combining the above two inequalities and noting that $N = O(\varepsilon^{-d})$, we obtain (6.21).

Lemma 6.7. *If there exists a constant κ such that*

$$\varepsilon^d \boldsymbol{z}^T \mathsf{H}(\boldsymbol{y}_1)\boldsymbol{z} \geqq \kappa\|\boldsymbol{z}\|_d^2 \qquad \textit{for all} \quad \boldsymbol{z} = (\boldsymbol{z}^A, \boldsymbol{z}^B) \in \mathbb{R}^{2N\times d}, \tag{6.22}$$

then there exists a constant δ such that for any $\boldsymbol{y}_2$ that satisfies $\big|\boldsymbol{y}_1 - \boldsymbol{y}_2\big|_{1,\infty} \leqq \delta$, we have

$$\varepsilon^d \boldsymbol{z}^T \mathsf{H}(\boldsymbol{y}_2)\boldsymbol{z} \geqq \frac{\kappa}{2}\|\boldsymbol{z}\|_d^2 \qquad \textit{for all} \quad \boldsymbol{z} = (\boldsymbol{z}^A, \boldsymbol{z}^B) \in \mathbb{R}^{2N\times d} \tag{6.23}$$

for sufficiently small ε.

Proof. Using translation invariance, we have for any $1 \leqq i \leqq 2N$,

$$\sum_{j=1}^{2N} \mathsf{H}(i,j) = \mathbf{0},$$

which leads to

$$\boldsymbol{z}^T \mathsf{H}(\boldsymbol{y})\boldsymbol{z} = -\frac{1}{2}\sum_{i,j=1}^{2N} (\boldsymbol{z}_i - \boldsymbol{z}_j)\mathsf{H}(i,j)(\boldsymbol{y})(\boldsymbol{z}_i - \boldsymbol{z}_j).$$

Therefore, using the fact that the potential V is of finite range, and noting the basic inequality

$$\left|\boldsymbol{z}_i^A - \boldsymbol{z}_j^B\right|^2 \leqq 2\left|\boldsymbol{z}_i^A - \boldsymbol{z}_i^B\right|^2 + 2\left|\boldsymbol{z}_i^B - \boldsymbol{z}_j^B\right|^2,$$

we get

$$\begin{aligned}
&\left|\sum_{i,j=1}^{2N} (\boldsymbol{z}_i - \boldsymbol{z}_j)(\mathsf{H}(i,j)(\boldsymbol{y}_1) - \mathsf{H}(i,j)(\boldsymbol{y}_2))(\boldsymbol{z}_i - \boldsymbol{z}_j)\right| \\
&\leqq C\delta\varepsilon^{-2}\sum_{i=1}^{N}\sum_{|\boldsymbol{x}_{ij}|=\varepsilon} \left(\left|\boldsymbol{z}_i^A - \boldsymbol{z}_j^A\right|^2 + \left|\boldsymbol{z}_i^B - \boldsymbol{z}_j^B\right|^2 + \left|\boldsymbol{z}_i^A - \boldsymbol{z}_j^B\right|^2\right) \\
&\leqq C\delta\varepsilon^{-2}\sum_{i=1}^{N}\sum_{|\boldsymbol{x}_{ij}|=\varepsilon} \left(\left|\boldsymbol{z}_i^A - \boldsymbol{z}_j^A\right|^2 + \left|\boldsymbol{z}_i^B - \boldsymbol{z}_j^B\right|^2\right) + CL\delta\varepsilon^{-2}\sum_{i=1}^{N}\left|\boldsymbol{z}_i^A - \boldsymbol{z}_i^B\right|^2.
\end{aligned}$$

It follows from Lemma 6.4 that

$$\varepsilon^d \left|\boldsymbol{z}^T[\mathsf{H}(\boldsymbol{y}_2) - \mathsf{H}(\boldsymbol{y}_1)]\boldsymbol{z}\right| \leqq C\delta\|\boldsymbol{z}\|_a^2 + CL\delta\varepsilon^{d-2}\|\,\boldsymbol{z}^A - \boldsymbol{z}^B\,\|_{\ell_2}^2 \leqq C\delta\|\,\boldsymbol{z}\,\|_d^2,$$

which yields

$$\begin{aligned}
\varepsilon^d \boldsymbol{z}^T \mathsf{H}(\boldsymbol{y}_2)\boldsymbol{z} &= \varepsilon^d \boldsymbol{z}^T \mathsf{H}(\boldsymbol{y}_1)\boldsymbol{z} + \varepsilon^d \boldsymbol{z}^T[\mathsf{H}(\boldsymbol{y}_2) - \mathsf{H}(\boldsymbol{y}_1)]\boldsymbol{z} \\
&\geqq \kappa\|\boldsymbol{z}\|_d^2 - C\delta\|\boldsymbol{z}\|_d^2 \\
&\geqq (\kappa/2)\|\,\boldsymbol{z}\,\|_d^2
\end{aligned}$$

for $\delta = \kappa/(2C)$. This gives (6.23).

Lemma 6.8. *Assume that $\widetilde{\boldsymbol{y}}$ satisfies:*

1. *There exists a constant κ such that*

$$\varepsilon^d \boldsymbol{z}^T \mathsf{H}(\widetilde{\boldsymbol{y}})\boldsymbol{z} \geqq \kappa\|\boldsymbol{z}\|_d^2 \quad \textit{for all} \quad \boldsymbol{z} \in \mathbb{R}^{2N\times d}.$$

2. *There exists a constant $q > 2$ such that $\varepsilon^{d/2}\|\,T(\widetilde{\boldsymbol{y}})\,\|_{\ell_2} \leqq K_1\varepsilon^q$.*
3. *$\widetilde{\boldsymbol{y}} - \boldsymbol{x} - \widetilde{\mathsf{B}}\cdot\boldsymbol{x}$ is periodic.*

Then there exists a unique solution $\boldsymbol{y}$ that satisfies (2.22) *and*

$$\|\boldsymbol{y} - \widetilde{\boldsymbol{y}}\|_d \leqq C\varepsilon^q. \tag{6.24}$$

Proof. Write

$$T(\boldsymbol{y}) = T(\widetilde{\boldsymbol{y}}) + \int_0^1 (1-t)\mathsf{H}(\boldsymbol{y}^t)\,\mathrm{d}t \cdot (\boldsymbol{y} - \widetilde{\boldsymbol{y}}),$$

where $\boldsymbol{y}^t = t\boldsymbol{y} + (1-t)\widetilde{\boldsymbol{y}}$. Hence $\boldsymbol{y}$ is a solution of (2.22) if and only if

$$\int_0^1 (1-t)\mathsf{H}(\boldsymbol{y}^t)\,\mathrm{d}t \cdot (\boldsymbol{y} - \widetilde{\boldsymbol{y}}) = -T(\widetilde{\boldsymbol{y}}). \tag{6.25}$$

Let

$$B := \left\{ \boldsymbol{y} \in \mathcal{A} \mid \|\boldsymbol{y} - \widetilde{\boldsymbol{y}}\|_d < \varepsilon^2 \right\}.$$

We define a map $F : B \to B$ as follows. For any $\boldsymbol{y} \in B$, let $F(\boldsymbol{y})$ be the solution of the linear system

$$\int_0^1 (1-t)\mathsf{H}(\boldsymbol{y}^t)\,\mathrm{d}t \cdot (F(\boldsymbol{y}) - \widetilde{\boldsymbol{y}}) = -T(\widetilde{\boldsymbol{y}}). \tag{6.26}$$

We first show that F is well defined. Since $\|\boldsymbol{y}^t - \widetilde{\boldsymbol{y}}\|_d \leqq t\|\boldsymbol{y} - \widetilde{\boldsymbol{y}}\|_d \leqq \varepsilon^2$, we have $\left|\boldsymbol{y}^t - \widetilde{\boldsymbol{y}}\right|_{1,\infty} \leqq C\varepsilon^{2-d/2} < \delta$, if ε is sufficiently small, given that $d \leqq 3$. Using the first assumption on $\widetilde{\boldsymbol{y}}$ and Lemma 6.7, we conclude that there exists a constant κ such that

$$\varepsilon^d \boldsymbol{z}^T \mathsf{H}(\boldsymbol{y}^t)\boldsymbol{z} \geqq \frac{\kappa}{2}\|\boldsymbol{z}\|_d^2.$$

Therefore, the linear system (6.26) is solvable and F is well defined. Moreover, $F(\boldsymbol{y}) - \boldsymbol{x} - \widetilde{\mathsf{B}} \cdot \boldsymbol{x}$ is periodic.

$\boldsymbol{F}$ is also continuous since V is smooth. Using Lemma 6.6 and note that $\sum_{i=1}^{2N}[F(\boldsymbol{y})_i - \widetilde{\boldsymbol{y}}_i] = \boldsymbol{0}$, we obtain

$$\begin{aligned} \kappa\varepsilon^{-d}\|F(\boldsymbol{y}) - \widetilde{\boldsymbol{y}}\|_d^2 &\leqq \|F(\boldsymbol{y}) - \widetilde{\boldsymbol{y}}\|_{\ell_2}\|T(\widetilde{\boldsymbol{y}})\|_{\ell_2} \\ &\leqq CK_1\varepsilon^{q-d}\|F(\boldsymbol{y}) - \widetilde{\boldsymbol{y}}\|_d. \end{aligned} \tag{6.27}$$

If $\|F(\boldsymbol{y}) - \widetilde{\boldsymbol{y}}\|_d = 0$, we have $F(B) \subset B$. Otherwise, the above inequality gives

$$\|F(\boldsymbol{y}) - \widetilde{\boldsymbol{y}}\|_d \leqq C\varepsilon^q,$$

which in turn implies $F(B) \subset B$ for sufficiently small ε since $q > 2$. Now the existence of $\boldsymbol{y}$ follows from the Brouwer fixed point theorem. Moreover, we conclude that $\boldsymbol{y}$ satisfies (6.24), and the solution $\boldsymbol{y}$ is locally unique since the Hessian at $\boldsymbol{y}$ is nondegenerate.

Lemma 6.9. *There exist two constants M_1 and M_2 such that if $\|\mathsf{B}\| \leqq M_1$ and $\|\boldsymbol{f}\|_{W^{6,p}} \leqq M_2$, then there exists $\widetilde{\boldsymbol{y}}$ that satisfies the second and third conditions of Lemma 6.8 for $q = 2$.*

This is a direct consequence of Lemma 5.1 and Corollary 5.2.

Lemma 6.10. *There exist two constants M_1 and M_2 such that if $\|\mathsf{B}\| \leqq M_1$ and $\|\boldsymbol{f}\|_{W^{6,p}} \leqq M_2$, then there exist a constant κ_1 and $\widetilde{\boldsymbol{y}}$ such that*

$$\varepsilon^d \boldsymbol{z}^T \mathsf{H}(\widetilde{\boldsymbol{y}})\boldsymbol{z} \geqq \kappa_1 \|\boldsymbol{z}\|_d^2 \qquad \text{for all} \quad \boldsymbol{z} \in \mathbb{R}^{2N\times d}. \tag{6.28}$$

Proof. Define $M_1 = M_2 = \delta/(4C)$, where C is the constant that appears in the right-hand side of the following inequality. For simple lattices,

$$\begin{aligned}
\left|\widetilde{\boldsymbol{y}} - \boldsymbol{x}\right|_{1,\infty} &\leqq C\|\nabla \boldsymbol{u}_{\mathrm{CB}}\|_{L^\infty} + C\varepsilon^2\|\nabla \boldsymbol{u}_2\|_{L^\infty} \\
&\leqq C\|\nabla(\boldsymbol{u}_{\mathrm{CB}} - \mathsf{B}\cdot\boldsymbol{x})\|_{L^\infty} + C\|\mathsf{B}\| + C\varepsilon^2\|\nabla \boldsymbol{u}_2\|_{L^\infty} \\
&\leqq C\|\boldsymbol{u}_{\mathrm{CB}} - \mathsf{B}\cdot\boldsymbol{x}\|_{2,p} + C\varepsilon^2\|\boldsymbol{u}_2\|_{2,p} + C\|\mathsf{B}\| \\
&\leqq C\|\boldsymbol{f}\|_{6,p} + C\|\mathsf{B}\| \leqq C(M_1 + M_2) = \delta/2 < \delta.
\end{aligned}$$

For complex lattices, the estimate for $\left|\widetilde{\boldsymbol{y}}^A - \boldsymbol{x}^A\right|_{1,\infty}$ is the same as above. In addition,

$$\begin{aligned}
\left|\widetilde{\boldsymbol{y}}^B - \boldsymbol{x}^B\right|_{1,\infty} &\leqq \left|\widetilde{\boldsymbol{y}}^A - \boldsymbol{x}^A\right|_{1,\infty} \\
&\quad + C(\varepsilon^2\|\nabla \boldsymbol{v}_2\|_{1,\infty} + \varepsilon^3\|\nabla \boldsymbol{v}_3\|_{1,\infty} + \varepsilon^4\|\nabla \boldsymbol{v}_4\|_{1,\infty}) \\
&\leqq \left|\widetilde{\boldsymbol{y}}^A - \boldsymbol{x}^A\right|_{1,\infty} + C\|\boldsymbol{u}\|_{6,\infty} \\
&\leqq C(M_1 + M_2) + C\|\boldsymbol{f}\|_{5,p} \\
&\leqq C(2M_1 + M_2) = 3\delta/4 < \delta.
\end{aligned}$$

Note that $\boldsymbol{z}^T\mathsf{H}_0\boldsymbol{z} = \varepsilon^{-d}\|\boldsymbol{z}\|_d^2$, therefore (6.28) follows from Lemma 6.7.

Proof of Theorem 2.2 It follows from Lemma 6.8 that there exists a $\boldsymbol{y}^\varepsilon$ that satisfies (2.22) and $\|\boldsymbol{y}^\varepsilon - \widetilde{\boldsymbol{y}}\|_d \leqq C\varepsilon^3$. Therefore,

$$\|\boldsymbol{y}^\varepsilon - \boldsymbol{y}_{\mathrm{CB}}\|_d \leqq \|\boldsymbol{y}^\varepsilon - \widetilde{\boldsymbol{y}}\|_d + \|\widetilde{\boldsymbol{y}} - \boldsymbol{y}_{\mathrm{CB}}\|_d \leqq C\varepsilon^3 + C\varepsilon \leqq C\varepsilon.$$

This gives (2.27).

For any $\hat{\boldsymbol{y}} \in \mathbb{R}^{2N\times d}$ with $|\hat{\boldsymbol{y}} - \boldsymbol{y}^\varepsilon|_{1,\infty} \leqq \delta/2$, where δ is the same as in Lemma 6.7, we write

$$E(\hat{\boldsymbol{y}}) - E(\boldsymbol{y}^\varepsilon) = (\hat{\boldsymbol{y}} - \boldsymbol{y}^\varepsilon)\cdot\int_0^1 (1-t)\mathsf{H}(t\hat{\boldsymbol{y}} + (1-t)\boldsymbol{y}^\varepsilon)\,\mathrm{d}t\cdot(\hat{\boldsymbol{y}} - \boldsymbol{y}^\varepsilon).$$

Note that

$$\left|t\hat{\boldsymbol{y}} + (1-t)\boldsymbol{y}^\varepsilon - \widetilde{\boldsymbol{y}}\right|_{1,\infty} \leqq t\,|\hat{\boldsymbol{y}} - \boldsymbol{y}^\varepsilon|_{1,\infty} + \left|\boldsymbol{y}^\varepsilon - \widetilde{\boldsymbol{y}}\right|_{1,\infty} \leqq \delta/2 + C\varepsilon^{3-d/2} \leqq \delta$$

for sufficiently small ε. Using Lemma 6.7, there exists a constant C such that

$$E(\hat{\boldsymbol{y}}) - E(\boldsymbol{y}^\varepsilon) \geqq C\varepsilon^{-d}\|\hat{\boldsymbol{y}} - \boldsymbol{y}^\varepsilon\|_d^2 > 0.$$

Therefore $\boldsymbol{y}^\varepsilon$ is a discrete $W^{1,\infty}$ local minimizer. □

Proof of Theorem 2.3 The proof is essentially the same as that of Theorem 2.2. The only difference is

$$\|\boldsymbol{y}^\varepsilon - \boldsymbol{y}_{\mathrm{CB}}\|_d \leqq \|\boldsymbol{y}^\varepsilon - \widetilde{\boldsymbol{y}}\|_d + \|\widetilde{\boldsymbol{y}} - \boldsymbol{y}_{\mathrm{CB}}\|_d \leqq C\varepsilon^3 + C\varepsilon^2 \leqq C\varepsilon^2,$$

since $\boldsymbol{u}_1 = \boldsymbol{0}$ due to Lemma 5.2. This gives (2.29). □

Appendix A. Detailed asymptotic analysis for the one-dimensional model

In this appendix, we will give a detailed asymptotic analysis of the *one dimensional* model. Explicit expressions for $\mathcal{L}_0, \mathcal{L}_1$ and $\mathcal{L}_2$ that have been omitted in § 5.2 will be given here. We consider a complex lattice with two species of atoms A and B.

Considering the equilibrium equations for atoms A and B respectively

$$\mathcal{L}_\varepsilon^A(y_i^A, y_i^B) = f(x_i^A) \quad \text{and} \quad \mathcal{L}_\varepsilon^B(y_i^A, y_i^B) = f(x_i^B),$$

where

$$\begin{aligned}
\mathcal{L}_\varepsilon^A(y_i^A, y_i^B) &= V'_{AB}(y_i^B - y_i^A) - V'_{AB}(y_i^A - y_{i-1}^B) \\
&\quad + V'_{AA}(y_{i+1}^A - y_i^A) - V'_{AA}(y_i^A - y_{i-1}^A), \\
\mathcal{L}_\varepsilon^B(y_i^A, y_i^B) &= V'_{AB}(y_{i+1}^A - y_i^B) - V'_{AB}(y_i^B - y_i^A) \\
&\quad + V'_{BB}(y_{i+1}^B - y_i^B) - V'_{BB}(y_i^B - y_{i-1}^B),
\end{aligned}$$

which can be rewritten as

$$\begin{aligned}
\mathcal{L}_\varepsilon^A(y_i^A, y_i^B) &= V'_{AB}(D_p^+ y_i^A) + V'_{AB}(D_{p-\varepsilon}^+ y_i^A) + D_\varepsilon^- V_{AA}(D_\varepsilon^+ y_i^A), \\
\mathcal{L}_\varepsilon^B(y_i^A, y_i^B) &= -V'_{AB}(D_{p-\varepsilon}^+ y_{i+1}^A) - V'_{AB}(D_\varepsilon^+ y_i^A) + D_\varepsilon^- V_{BB}(D_\varepsilon^+ y_i^B).
\end{aligned}$$

Proceeding as in § 5.2, we get

$$\begin{aligned}
\widetilde{\mathcal{L}}_{-1}(u, v_1) &= 0, & \widetilde{\mathcal{L}}_0(u, v_1, v_2) &= -f', \\
\widetilde{\mathcal{L}}_1(u, v_1, v_2, v_3) &= -\frac{1}{2} f'', & \widetilde{\mathcal{L}}_2(u, v_1, v_2, v_3, v_4) &= -\frac{1}{6} f^{(3)},
\end{aligned} \tag{A.1}$$

where

$$\begin{aligned}
\widetilde{\mathcal{L}}_{-1}(u, v_1) &= 2V'_{AB}(v_1) + 2V'_{AB}(v_1 - 1 - u_x), \\
\widetilde{\mathcal{L}}_0(u, v_1, v_2) &= 2[V''_{AB}(v_1) + V''_{AB}(v_1 - 1 - u_x)]v_2 \\
&\quad - V''_{AB}(v_1 - 1 - u_x)v_{1x} \\
&\quad + \partial_x(V'_{AA}(1 + u_x) - V'_{BB}(1 + u_x)), \\
\widetilde{\mathcal{L}}_1(u, v_1, v_2, v_3) &= 2V''_{AB}(v_1) + V''_{AB}(v_1 - 1 - u_x)(b_1 + b_3) \\
&\quad + V^{(3)}_{AB}(v_1)v_2^2 + \frac{1}{2} V^{(3)}_{AB}(v_1 - 1 - u_x)(a_1^2 + a_3^2) \\
&\quad + \partial_x(V''_{BB}(1 + u_x)u_{xx}),
\end{aligned}$$

where

$$a_1 = v_2 - v_{1x} + \frac{1}{2}u_{xx}, \qquad b_1 = v_3 - v_{2x} + \frac{1}{2}v_{1xx} - \frac{1}{6}u_{xxx},$$
$$a_2 = v_{1x} + \frac{1}{2}u_{xx}, \qquad b_2 = v_{2x} + \frac{1}{2}v_{1xx} + \frac{1}{6}u_{xxx},$$
$$a_3 = v_2 - \frac{1}{2}u_{xx}, \qquad b_3 = v_3 - \frac{1}{6}u_{xxx}.$$

We omit the expression of $\widetilde{\mathcal{L}}_2$ since we do not need it to solve v_4.

In what follows, we give the explicit expressions of $\mathcal{L}_0, \mathcal{L}_1$ and $\mathcal{L}_2$. The arguments of V_{AB}, V_{AA} and V_{BB} will be omitted unless otherwise stated.

$$\begin{aligned}
\mathcal{L}_0(u, v_1) &= -\partial_x(V'_{AB} - V'_{AA} - V'_{BB}),\\
\mathcal{L}_1(u, v_1, v_2) &= -\frac{1}{2}\partial_x^2(V'_{AB} + V'_{AA} + V'_{BB})\\
&\quad - \partial_x(V''_{AB}a_1 - \frac{1}{2}V''_{AA}u_{xx} - V''_{BB}a_2),\\
\mathcal{L}_2(u, v_1, v_2, v_3) &= -\frac{1}{6}\partial_x^3(V'_{AB} - V'_{AA} - V'_{BB})\\
&\quad - \frac{1}{2}\partial_x^2(V''_{AB}a_1 + \frac{1}{2}V''_{AA}u_{xx} + V''_{BB}a_2)\\
&\quad - \partial_x[V''_{AB}b_1 + \frac{1}{2}V^{(3)}_{AB}a_1^2 - \frac{1}{6}V''_{AA}u_{xxx} - \frac{1}{8}V^{(3)}_{AA}u_{xx}^2\\
&\qquad - V''_{BB}b_2 - \frac{1}{2}V^{(3)}_{BB}a_2^2].
\end{aligned}$$

Define

$$\alpha = V''_{AB}(v_1 - 1 - u_x), \quad \beta = V''_{AB}(v_1).$$

It is easy to see that

$$\mathcal{L}_1(u, v_1, v_2) = -\partial_x((a_1 + v_{1x}/2 - u_{xx}/2)V''_{AB} + (-a_2 + u_{xx}/2)V''_{BB}).$$

Differentiating the equation $\widetilde{\mathcal{L}}_{-1}(u, v_1) = 0$, we have

$$(\alpha + \beta)v_{1x} = \alpha\, u_{xx}.$$

Solving $\widetilde{\mathcal{L}}_0(u, v_1, v_2) = -f'$, we get

$$v_2 = \frac{\alpha}{\alpha + \beta}\frac{v_{1x}}{2} - \frac{u_{xx}(V''_{AA} - V''_{BB}) - f'}{2(\alpha + \beta)}.$$

A combination of the above three equations gives

$$\mathcal{L}_1 = \partial_x\Big[\frac{V''_{AB}(v_1)}{V''_{AB}(v_1 - 1 - u_x) + V''_{AB}(v_1)}\Big(\widetilde{V}''_{AB} + V''_{AA} + V''_{BB} + f'/2\Big)\Big],$$

where

$$\widetilde{V}''_{AB} = \frac{V''_{AB}(v_1 - 1 - u_x)V''_{AB}(v_1)}{V''_{AB}(v_1 - 1 - u_x) + V''_{AB}(v_1)}.$$

Solving $\widetilde{\mathcal{L}}_1(u, v_1, v_2, v_3) = -f''/2$, we obtain

$$\begin{aligned} v_3 = {} & \frac{\alpha}{\alpha+\beta}(v_{2x}/2 - v_{1xx}/4 + u_{xxx}/6) \\ & - \frac{V^{(3)}_{AB}(v_1)}{\alpha+\beta}\frac{v_2^2}{2} - \frac{V^{(3)}_{AB}(v_1 - 1 - u_x)}{\alpha+\beta}\frac{a_1^2 + a_3^2}{4} - G, \end{aligned}$$

where $G = (\partial_x(V''_{BB}(1+u_x)u_x) + f''/4)/(\alpha+\beta)$. Substituting v_3, v_2, a_1 and a_3 into $\mathcal{L}_2$, we obtain

$$\mathcal{L}_2 = \mathcal{L}_2^1 + \mathcal{L}_2^2 + \mathcal{L}_2^3,$$

where

$$\begin{aligned} \mathcal{L}_2^1 = {} & \partial_x^2\Big(\frac{u_{xx}}{6}(V''_{AA} + V''_{BB}) + \frac{\alpha\beta}{\alpha+\beta}u_{xx}V''_{BB}\Big) \\ & + \frac{1}{24}\partial_x\Big(u_{xx}^2(V^{(3)}_{AA} + V^{(3)}_{BB}) - V''_{BB}\,G\Big), \\ \mathcal{L}_2^2 = {} & \partial_x\Big[\frac{\alpha\beta}{4(\alpha+\beta)}\Big(\frac{\alpha\beta}{(\alpha+\beta)^2}u_{xx}\Big)_x + \alpha\Big(\frac{1}{12} - \frac{1}{8}\frac{\alpha^2}{(\alpha+\beta)^2}\Big)\Big(\frac{\beta}{\alpha+\beta}\Big)_x u_{xx} \\ & - \frac{\alpha\beta}{12(\alpha+\beta)}u_{xxx} + \frac{\alpha\beta}{2(\alpha+\beta)}G_x\Big], \\ \mathcal{L}_2^3 = {} & \partial_x\Big[\Big(\frac{1}{24}\frac{\beta^2}{(\alpha+\beta)^2} - \frac{\alpha\beta^3}{8(\alpha+\beta)^4}\Big)V^{(3)}_{AB}(v_1 - 1 - u_x)u_{xx}^2 \\ & - \frac{1}{2}V^{(3)}_{AB}(v_1 - 1 - u_x)\Big(\frac{\alpha\beta^2}{(\alpha+\beta)^3}u_{xx} + \frac{\beta}{\alpha+\beta}G\Big)G \\ & + \frac{1}{2}V^{(3)}_{AB}(v_1)\Big(\frac{\alpha^3}{(\alpha+\beta)^3}u_{xx} - \frac{\alpha}{\alpha+\beta}G\Big)G\Big]. \end{aligned}$$

Next let $u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \cdots$, and substituting this ansatz into $\mathcal{L}_0, \mathcal{L}_1$ and $\mathcal{L}_2$, we obtain

$$-\partial_x(V'_{AB}(v_1 - 1 - u_{0x}) - V'_{AA}(1 + u_{0x}) - V'_{BB}(1 + u_{0x})) = f(x).$$

A straightforward calculation gives

$$\mathcal{L}_{\mathrm{lin}}(u_0, v_1)u_1 = \partial_x\Big((V''_{AB}(v_1 - 1 - u_{0x}) + V''_{AA}(1 + u_{0x}) + V''_{BB}(1 + u_{0x}))u_{1x}\Big).$$

Therefore, we obtain the equations for u_1 and u_2:

$$\begin{aligned} & \mathcal{L}_{\mathrm{lin}}(u_0, v_1)u_1 = -\mathcal{L}_1 + f'/2, \\ & \mathcal{L}_{\mathrm{lin}}(u_0, v_1)u_2 = -\mathcal{L}_2 - \frac{\delta\mathcal{L}_1}{\delta u_0} - \frac{1}{2}\Big(\frac{\delta^2\mathcal{L}_0}{\delta u_0^2}\Big)u_1 + f''/4. \end{aligned}$$

Appendix B. Elastic stiffness tensor for simple and complex lattices

Elastic stiffness tensor and the elastic modulus tensor are two different concepts. They coincide when the internal stress vanishes [27], i.e. $D_{\mathrm{A}} W_{\mathrm{CB}}(\mathbf{0}) = \mathbf{0}$.

Equation (2.17) is an explicit expression for the elastic stiffness tensor in the case of two-body potentials. Here we generalize this formula to many-body potentials. In the case of simple lattice, we have, for any $\boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^d$,

$$\begin{aligned}&\mathsf{C}(\boldsymbol{\xi}\otimes\boldsymbol{\eta},\boldsymbol{\xi}\otimes\boldsymbol{\eta})\\ &= \sum_{m=2}\sum_{\langle \boldsymbol{s}_1,\cdots,\boldsymbol{s}_{m-1}\rangle}\sum_{\substack{\langle \boldsymbol{s}_i,\boldsymbol{s}_j\rangle\\ 1\leqq i<j\leqq m-1}} ((\boldsymbol{s}_i\cdot\boldsymbol{\eta})(\boldsymbol{\xi}\cdot\partial_{\boldsymbol{\alpha}_i}) + (\boldsymbol{s}_j\cdot\boldsymbol{\eta})(\boldsymbol{\xi}\cdot\partial_{\boldsymbol{\alpha}_j}))^2 V_m,\end{aligned}$$

where $V_m = V_m(\boldsymbol{s}_1, \cdots, \boldsymbol{s}_{m-1})$. For example, if V contains only three-body potential V_3, then for any $\boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^d$,

$$\mathsf{C}(\boldsymbol{\xi}\otimes\boldsymbol{\eta},\boldsymbol{\xi}\otimes\boldsymbol{\eta}) = \sum_{\langle \boldsymbol{s}_1,\boldsymbol{s}_2\rangle} ((\boldsymbol{s}_1\cdot\boldsymbol{\eta})(\boldsymbol{\xi}\cdot\partial_{\boldsymbol{\alpha}_1}) + (\boldsymbol{s}_2\cdot\boldsymbol{\eta})(\boldsymbol{\xi}\cdot\partial_{\boldsymbol{\alpha}_2}))^2 V_3(\boldsymbol{s}_1,\boldsymbol{s}_2).$$

Next we turn to complex lattices. We first consider the one-dimensional case. Minimizing $W(A, p)$ with respect to p, we obtain $p = p(A)$. Next differentiating with respect to A, we get

$$\frac{dp}{dA} = \frac{\sum_s (V''_{AB}((1+A)s - p) - V''_{AB}((1+A)s + p))s}{\sum_s V''_{AB}((1+A)s - p) + \sum_s V''_{AB}((1+A)s + p)}.$$

Note that

$$\begin{aligned}D_A^2 W_{\mathrm{CB}}(A) &= D_A^2 W(A, p(A)) + D_{Ap}^2 W(A, p(A))\\ &= \sum_s (V''_{AA}((1+A)s) + V''_{BB}((1+A)s)\\ &\qquad + V''_{AB}((1+A)s + p) + V''_{AB}((1+A)s - p))s^2\\ &\quad + \sum_s (V''_{AB}((1+A)s + p(A)) - V''_{AB}((1+A)s - p(A)))s\frac{dp}{dA}.\end{aligned}$$

A combination of the above two identities leads to:

$$\begin{aligned}D_A^2 W_{\mathrm{CB}}(A) = &\sum_s (V''_{AA}((1+A)s) + V''_{BB}((1+A)s)\\ &+ V''_{AB}((1+A)s + p(A)) + V''_{AB}((1+A)s - p(A)))s^2\\ &- \frac{\left(\sum_s (V''_{AB}((1+A)s - p(A)) - V''_{AB}((1+A)s + p(A)))s\right)^2}{\sum_s V''_{AB}((1+A)s - p(A)) + \sum_s V''_{AB}((1+A)s + p(A))}.\end{aligned}$$

Therefore, let $p_0 = p(0)$, we have

$$\mathsf{C} = \sum_s [V''_{AA}(s) + V''_{BB}(s) + V''_{AB}(s+p_0) + V''_{AB}(s-p_0)]s^2 - \frac{\left(\sum_s [V''_{AB}(s-p_0) - V''_{AB}(s+p_0)]s\right)^2}{\sum_s V''_{AB}(s-p_0) + \sum_s V''_{AB}(s+p_0)}. \tag{B.1}$$

As to high dimensional case, we only consider the one when V is a three-body potential. Other cases can be dealt with similarly. Solving the algebraic equations (2.15), we obtain $\boldsymbol{p} = \boldsymbol{p}(\mathsf{A})$. Differentiating (2.15) with respect to A, we get

$$D_{\mathsf{A}}\boldsymbol{p} = -\mathsf{S}(\mathsf{A})^{-1} \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{i=1}^{2} \boldsymbol{K}_i(\mathsf{A})\boldsymbol{s}_i$$

with

$$\mathsf{S}(\mathsf{A}) = \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} (\partial_{\boldsymbol{\alpha}_1} + \partial_{\boldsymbol{\alpha}_2})^2 V^1_{AB}(\mathsf{A}) + \partial^2_{\boldsymbol{\alpha}_2} V^2_{AB}(\mathsf{A}) + \partial^2_{\boldsymbol{\alpha}_1} V^3_{AB}(\mathsf{A}),$$

$$\boldsymbol{K}_i(\mathsf{A}) = \sum_{j=1}^{2} \partial^2_{\boldsymbol{\alpha}_i\boldsymbol{\alpha}_j} V^1_{AB}(\mathsf{A}) + \sum_{j=1}^{2} \partial^2_{\boldsymbol{\alpha}_j\boldsymbol{\alpha}_2} V^2_{AB}(\mathsf{A}) + \sum_{j=1}^{2} \partial^2_{\boldsymbol{\alpha}_j\boldsymbol{\alpha}_1} V^3_{AB}(\mathsf{A}),$$

where

$$V^1_{AB}(\mathsf{A}) = V_{AB}((\mathsf{I}+\mathsf{A})\widetilde{\boldsymbol{s}}_1 + \boldsymbol{p}(\mathsf{A}), (\mathsf{I}+\mathsf{A})\widetilde{\boldsymbol{s}}_2 + \boldsymbol{p}(\mathsf{A})),$$
$$V^2_{AB}(\mathsf{A}) = V_{AB}((\mathsf{I}+\mathsf{A})\widetilde{\boldsymbol{s}}_1 + \boldsymbol{p}(\mathsf{A}), (\mathsf{I}+\mathsf{A})\widetilde{\boldsymbol{s}}_2),$$
$$V^3_{AB}(\mathsf{A}) = V_{AB}((\mathsf{I}+\mathsf{A})\widetilde{\boldsymbol{s}}_1, (\mathsf{I}+\mathsf{A})\widetilde{\boldsymbol{s}}_2 + \boldsymbol{p}(\mathsf{A})).$$

Therefore, we get

$$D^2_{\mathsf{A}} W_{AB} = \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} (\boldsymbol{s}_1 \cdot \partial_{\boldsymbol{\alpha}_1} + \boldsymbol{s}_2 \cdot \boldsymbol{\alpha}_2)^2 \sum_{k=1}^{3} V^k_{AB}(\mathsf{A}) - \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{i=1}^{2} \boldsymbol{K}_i(\mathsf{A})\Big(\boldsymbol{s}_i, \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{j=1}^{2} \mathsf{S}(\mathsf{A})^{-1}\boldsymbol{K}_j(\mathsf{A})\boldsymbol{s}_j\Big).$$

Define $\widetilde{V}(\mathsf{A}) = V_{AA}(\mathsf{A}) + V_{BB}(\mathsf{A}) + 2\sum_{i=1}^{3} V^i_{AB}(\mathsf{A})$. Then, we have

$$\begin{aligned} &\mathsf{C}(\boldsymbol{\xi}\otimes\boldsymbol{\eta}, \boldsymbol{\xi}\otimes\boldsymbol{\eta}) \\ &= \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \Big((\boldsymbol{\xi}\cdot\partial_{\boldsymbol{\alpha}_1})(\boldsymbol{s}_1\cdot\boldsymbol{\eta}) + (\boldsymbol{\xi}\cdot\partial_{\boldsymbol{\alpha}_2})(\boldsymbol{s}_2\cdot\boldsymbol{\eta})\Big)^2 \widetilde{V}(\boldsymbol{0}) \\ &\quad - \Big(\sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{i=1}^{2} [\boldsymbol{K}_i(\boldsymbol{0})](\boldsymbol{\xi},\boldsymbol{\xi})\boldsymbol{s}_i\cdot\boldsymbol{\eta}, \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \sum_{i=1}^{2} [\mathsf{S}(\boldsymbol{0})^{-1}\boldsymbol{K}_i(\boldsymbol{0})](\boldsymbol{\xi},\boldsymbol{\xi})\boldsymbol{s}_i\cdot\boldsymbol{\eta}\Big). \end{aligned} \tag{B.2}$$

Compare this formula with simple lattices, we see that (B.2) has the form of a Schur complement when the terms involving $\boldsymbol{p}$ are eliminated.

Appendix C. Proof of Lemma 3.1 for the complex lattice

The objective of this section is to prove Lemma 3.1 for the complex lattice, we exploit the expansion in [26, Section 12].

Using the definition of W_{CB} and Lemma 6.4, we obtain that $D^2_{\boldsymbol{p}} W(\mathbf{0}, \boldsymbol{p}_0)$ is positive definite. It remains to prove that the elastic modulus C satisfies the *Legendre-Hadamard* condition at the undeformed configuration. Denote

$$\widetilde{\mathsf{D}}_{\kappa\kappa'}[\boldsymbol{k}] = \sum_{j=1}^{N} \mathsf{H}_{\kappa\kappa'}(0, j) Q_{\kappa\kappa'}(\boldsymbol{k}, \boldsymbol{x}_j),$$

where

$$Q_{\kappa\kappa'}(\boldsymbol{k}, \boldsymbol{x}_j) = 1 + i\boldsymbol{k} \cdot (\boldsymbol{x}_j + \boldsymbol{x}(\kappa) - \boldsymbol{x}(\kappa')) + \frac{1}{2}[\boldsymbol{k} \cdot (\boldsymbol{x}_j + \boldsymbol{x}(\kappa) - \boldsymbol{x}(\kappa'))]^2.$$

For $s = 1, \cdots, d$, we define $\lambda(\boldsymbol{k}, s)$ as

$$2 \sum \mathsf{C}_{\alpha\beta\gamma\delta} k_\beta k_\delta y_\gamma(s) = \lambda(\boldsymbol{k}, s) y_\alpha(s), \tag{C.1}$$

where $\boldsymbol{y} = \{y_\alpha\} \in \mathbb{R}^d$ satisfying $\sum_\alpha y_\alpha(s) \cdot y_\alpha(s') = \delta_{ss'}$. By [26, equation (12.15)], $\lambda(\boldsymbol{k}, s)$ satisfies

$$\sum_{\kappa'} \widetilde{\mathsf{D}}_{\kappa\kappa'}[\boldsymbol{k}] \cdot \widetilde{\boldsymbol{w}}_{\kappa'}(\boldsymbol{k}, s) = \lambda(\boldsymbol{k}, s) \boldsymbol{w}_\kappa(s), \tag{C.2}$$

where $\boldsymbol{w}_\kappa(s) = \boldsymbol{y}(s)/\sqrt{2}$ for $\kappa = A, B$, and

$$\widetilde{\boldsymbol{w}}_\kappa(\boldsymbol{k}, s) = \boldsymbol{w}_\kappa(s) + |\boldsymbol{k}| \boldsymbol{w}^1_\kappa(s) + |\boldsymbol{k}|^2 \boldsymbol{w}^2_\kappa(s). \tag{C.3}$$

Scrutinizing the derivation in [26, Section 7 and Section 12], we may find that $\boldsymbol{w}^1_\kappa$ is just the scaled *shifts* between atoms A and B, and both $\boldsymbol{w}^1_\kappa$ and $\boldsymbol{w}^2_\kappa$ are linear functions of $\boldsymbol{w}_\kappa(s)$. We may write $\boldsymbol{w}^1_\kappa(s) = \varepsilon \mathsf{A}_1 \boldsymbol{w}_\kappa(s)$ and $\boldsymbol{w}^2_\kappa(s) = \varepsilon^2 \mathsf{A}_2 \boldsymbol{w}_\kappa(s)$, where A_1 and A_2 are two constant matrices whose entries are independent of ε but may depend on the potential function V. The existence of $\boldsymbol{w}_\kappa$ is a direct consequence of the translation invariance of H_0, while the existence of $\boldsymbol{w}^1_\kappa$ and $\boldsymbol{w}^2_\kappa$ follows from Lemma 6.4. Moreover, proceeding along the same line that leads to (3.4), we obtain

$$\|\mathsf{D}_{\kappa\kappa'}[\boldsymbol{k}] - \widetilde{\mathsf{D}}_{\kappa\kappa'}[\boldsymbol{k}]\| \leqq C\varepsilon |\boldsymbol{k}|^3 \qquad \kappa, \kappa' = \mathrm{A}, \mathrm{B}, \tag{C.4}$$

where C is independent of ε and $\boldsymbol{k}$.

Using the definition of D and λ, we get

$$\begin{aligned}[\widetilde{\boldsymbol{w}}(\boldsymbol{k}, s)]^T \mathsf{D}[\boldsymbol{k}] \cdot \widetilde{\boldsymbol{w}}(\boldsymbol{k}, s) - \lambda(\boldsymbol{k}, s) \left|\widetilde{\boldsymbol{w}}\right|^2 &= \lambda(\boldsymbol{k}, s) \widetilde{\boldsymbol{w}} \cdot (\widetilde{\boldsymbol{w}} - \boldsymbol{w}) \\ &\quad + [\widetilde{\boldsymbol{w}}(\boldsymbol{k}, s)]^T (\mathsf{D} - \widetilde{\mathsf{D}})[\boldsymbol{k}] \cdot \widetilde{\boldsymbol{w}}(\boldsymbol{k}, s).\end{aligned}$$

Note the expressions of $\widetilde{\boldsymbol{w}}, \boldsymbol{y}$, using (C.4) and (C.3), we have

$$\left|\omega^2(\boldsymbol{k}, s) - \lambda(\boldsymbol{k}, s)\right| \leqq C(\varepsilon |\boldsymbol{k}| \lambda(\boldsymbol{k}, s) + \varepsilon |\boldsymbol{k}|^3),$$

which in turn implies

$$(1 + C\varepsilon|\boldsymbol{k}|)\lambda(\boldsymbol{k}, s) \geqq \omega^2(\boldsymbol{k}, s) - C\varepsilon|\boldsymbol{k}|^3 .$$

Using **Assumption A**, for sufficiently small ε, we obtain

$$(1 + C\varepsilon|\boldsymbol{k}|)\lambda(\boldsymbol{k}, s) \geqq (\Lambda - C\varepsilon|\boldsymbol{k}|)|\boldsymbol{k}|^2 .$$

For sufficiently small ε and note that $\boldsymbol{k}$ is $O(1)$ for $\boldsymbol{k}$ in the first Brillouin zone, taking $C\varepsilon|\boldsymbol{k}| = \Lambda/2$, we obtain

$$\lambda(\boldsymbol{k}, s) \geqq \frac{\Lambda}{\Lambda + 2}|\boldsymbol{k}|^2 ,$$

which together with (C.1) gives **Assumption B**.

Acknowledgements. The work of E is supported in part by an NSF grant, with additional support from the project "Research Team on Complex Systems" of the Chinese Academy of Science. The work of Ming is partially supported by the National Natural Science Foundation of China under the grant 10571172 and also supported by the National Basic Research Program under the grant 2005CB321704.

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