

# CONVERGENCE FROM ATOMISTIC MODEL TO PEIERLS-NABARRO MODEL FOR DISLOCATIONS IN BILAYER SYSTEM WITH COMPLEX LATTICE\*

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**Abstract.** In this paper, we prove the convergence from the atomistic model to the Peierls–Nabarro (PN) model of two-dimensional bilayer system with complex lattice. We show that the displacement field and the total energy of the solution of the PN model converge to those of the full atomistic model with second-order accuracy  $O(\varepsilon^2)$ , where  $\varepsilon$  is a small dimensionless parameter characterizing a wide dislocation core with respect to the lattice constant. The consistency of PN model and the stability of atomistic model are essential in our proof. The main idea of our approach is to use several low-degree polynomials to approximate the energy due to atomistic interactions of different groups of atoms of the complex lattice.

**Keywords.** Dislocations; complex lattice; interpolation polynomial; Peierls–Nabarro model.

**AMS subject classifications.** 35Q70; 35Q74; 74A50; 74G10.

## 1. Introduction

Dislocations are line defects in crystalline materials [11] and the dislocation theory is essential to understand the plastic deformation properties in crystalline materials. Continuum theory of dislocations based on linear elasticity theory works well outside the dislocation core region, which is a small region of a few lattice constants size around the dislocations; however, it breaks down inside the dislocation core where the atomic structure is heavily distorted. Atomistic models and Peierls–Nabarro models [11, 16, 17, 23] are widely applied to describe dislocation-core related properties. Although atomistic models are able to describe the details in the dislocation core region well, length and time scales of atomistic simulations are limited. The Peierls–Nabarro models [16, 17] are continuum models that incorporate the atomistic structure within the dislocation core region, and can be applied to simulations of larger length and time scales. The nonlinear elastic effect associated with the dislocation core is included in a Peierls–Nabarro model by a nonlinear potential, i.e., the  $\gamma$ -surface [23], that describes the atomic interaction across the slip plane of a dislocation calculated by atomistic models or first principles calculations.

Although Peierls–Nabarro models with  $\gamma$ -surfaces have been widely applied in the materials science problems associated with dislocations (e.g., [5, 6, 12, 13, 15, 19–21, 24–27]), mathematical understandings and rigorous analysis on the accuracy of this class of models, i.e., convergence from the atomistic models, are still limited. The major challenge comes from the discontinuity in the displacement (i.e. disregistry) across the slip plane of the dislocation, the nonlinear interaction across which, is modeled on the continuum level by the  $\gamma$ -surface [23]. This situation is essentially different from the condition of the convergence from atomistic models to the Cauchy–Born rule [1] (e.g. [2, 4, 7, 10]), in which smooth elastic displacement is assumed. El Hajj, Ibrahim,

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and Monneau and Fino, Ibrahim, and Monneau [8, 9] showed convergence, using the framework of viscosity solution, from an atomistic model to the Peierls-Nabarro model on a square lattice based on a two-body potential with nearest neighbor interaction. However, the calculations of the  $\gamma$ -surfaces in real atomistic simulations are normally beyond the nearest neighbor atomic interactions. Luo, Ming, and Xiang [14] proved convergence from a full atomistic model to the Peierls-Nabarro model with  $\gamma$ -surface for the dislocation in a bilayer system. In their convergence proof, each atom interacts with all other atoms via a two-body interatomic potential whose effective interaction range is much larger than the nearest neighbor interaction, which is common in atomistic simulations. They also proved that the rate of such convergence is  $O(\varepsilon^2)$  where  $\varepsilon$  is the ratio of the length of the Burgers vector of the dislocation (the lattice constant) to the dislocation core width. These proofs are all for dislocations in crystals with simple lattices. Silicon and other covalent-bonded crystals have complex lattices (unions of simple lattices), for which two-body potentials do not work well [22] and the above proofs for convergence from atomistic models to Peierls-Nabarro models of dislocations based on two-body potentials do not apply.

In this paper, we perform a rigorous convergence proof from atomistic model of complex lattice to Peierls-Nabarro model with  $\gamma$ -surface for an inter-layer dislocation in a bilayer system. We consider bilayer graphene as the prototype. Each layer has a hexagonal lattice structure which can be considered as a union of two simple triangular lattices with a shift. In our analysis, the interaction of atoms within the same layer is modeled by a three-body potential (e.g. the Stillinger-Weber potential [22] commonly used for silicon), and the inter-layer atomic interaction is described by a two-body potential (e.g. the van der Waals-like interactions described well by the Morse potentials in graphene, boron nitride, and graphene/boron nitride bilayers [27]). We focus on a straight edge dislocation.

Our proof is a generalization of the convergence result for dislocations in simple lattice in Ref. [14] and is inspired by the work of E and Ming [7] on Cauchy-Born rule without defects, where consistency and stability properties of the atomistic and continuum models play key roles. Due to the complicated interactions on complex lattices under multi-body potentials, a major challenge in the convergence proof from atomistic model on a complex lattice to continuum model is the construction of a simple and accurate link between them. Here we propose a new approach to solve this problem. The main idea of our approach is to use several (here two) low-degree polynomials (here piecewise linear functions) to approximate the energy due to atomistic interactions among different groups of atoms on the complex lattice. This energy-based method is different from that based on Taylor expansions of displacement vectors in the force equations used in Ref. [7]. This new approach can be applied generally to continuum modeling based on atomistic structures with complex lattices.

Specifically, we follow the energy method in Ref. [14] for the link (consistency and stability) between atomistic model and the Peierls-Nabarro model. Note that energy is an important quantity for the Peierls-Nabarro model of dislocations. The energies of the atomistic model and the Peierls-Nabarro model play a critical role in the proof of stability, in which, second variations of the energies are needed. For the convergence from a simple lattice, the simple approximation of the energy by piecewise linear interpolation from the atomistic model works well [14]. However, for the bilayer complex lattice that we are considering, there two different kinds of atoms, A and B, from two simple lattices, and four kinds of interactions by the three-body potential, i.e., AAA, AAB, ABB and BBB. It is tempting to use higher-degree interpolation polynomials for

the energy of these complicated atomic interactions. However, the degrees of suitable interpolation polynomials have to be very high, leading to oscillations in the interpolation energy. Alternatively, we propose a new way to construct continuum approximation of energy from the atomistic model of complex lattice (in Section 8). The total energy on atomistic level is divided into two parts, for the atomistic interactions among two different groups of atoms on the complex lattice, respectively. For each part, we establish a piecewise linear interpolation function to approximate it. This enables simple calculations of the stability of the two models in the convergence proof. Moreover, note that in the complex lattice, although the dislocation is straight in the continuum model, the locations and displacements in the atomistic model are not the same atom by atom along the dislocation, and we need to perform an analysis in the two-dimensional slip plane instead of the one-dimensional simplification adopted in the analysis for the simple lattice in Ref. [14].

The paper is organized as follows. We present the atomistic model of complex lattice and Peierls–Nabarro model for an edge dislocation in a bilayer system in Sections 2 and 3, respectively. A small dimensionless parameter  $\varepsilon$  is defined due to the weak interlayer interaction and nondimensionalization is performed in Section 4. This small parameter  $\varepsilon$  is also the ratio of the lattice constant (the length of the Burgers vector of the dislocation) to the dislocation core width. In Section 5, we collect the notations and assumptions. The main theorems including the wellposedness of the two models and convergence from the atomistic model to the Peierls–Nabarro model with  $\gamma$ -surface, are presented in Section 6. Especially, the error of the convergence is shown to be  $O(\varepsilon^2)$ . Rigorous proofs of these theorems are presented in Sections 7–9. In particular, the two piecewise linear interpolation functions that approximate two parts of the energy of atomistic interactions on the complex lattice are defined in Section 8. A proper boundary condition of atomistic model called Atomistic Dislocation Condition (ADC) is proposed to account for the displacement condition on the dislocation in the complex lattice. With this defined energy, the consistency of Peierls–Nabarro model and the stability of atomistic model are proved by comparing the Peierls–Nabarro model with the atomistic model directly.

## 2. Atomistic model of complex lattice

In this section, we present the atomistic model in a bilayer complex lattice system (e.g. bilayer graphene), from which the convergence to the Peierls–Nabarro model with  $\gamma$ -surface for an inter-layer dislocation is proved.

In the two-dimensional setting, atoms of the bilayer system are located in the planes  $z = \pm \frac{1}{2}d$ , where  $d$  is the distance between two layers.

In a plane perpendicular to the  $z$  axis, a simple lattice takes the form

$$L(\mathbf{e}_i, \mathbf{o}) = \left\{ \mathbf{x} \mid \mathbf{x} = \sum_{i=1}^2 v^i \mathbf{e}_i + \mathbf{o}, \quad v^i \in \mathbb{Z} \right\},$$

where  $\{\mathbf{e}_i\}_{i=1}^2$  is a basis of  $\mathbb{R}^2$  and  $\mathbf{o}$  is the location of some atom of the lattice. A complex lattice is regarded as a union of simple lattices:

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

for certain integer  $k$ , and  $\mathbf{p}_1, \dots, \mathbf{p}_k$  are the shift vectors.

In particular, one graphene layer consists of two simple lattices (triangular lattices)

$A$  and  $B$  (see Figure 2.1), and can be represented by

$$\begin{aligned}
 L(\mathbf{e}_i, \mathbf{o}) &= \{ \mathbf{x} \mid v^1 \mathbf{e}_1 + v^2 \mathbf{e}_2 + \mathbf{o}, v^i \in \mathbb{Z} \} && \text{for } A, \\
 L(\mathbf{e}_i, \mathbf{p}) &= \{ \mathbf{x} \mid v^1 \mathbf{e}_1 + v^2 \mathbf{e}_2 + \mathbf{o} + \mathbf{p}, v^i \in \mathbb{Z} \} && \text{for } B, \\
 \mathbf{e}_1 &= a(1, 0), \mathbf{e}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \mathbf{o} = (0, 0), \mathbf{p} = a\left(\frac{1}{2}, \frac{\sqrt{3}}{6}\right),
 \end{aligned} \tag{2.1}$$

where  $a$  is the lattice constant.

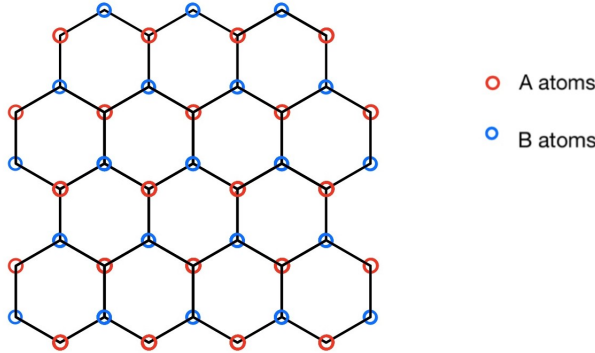


FIG. 2.1. The lattice of one graphene layer.

In this paper, we consider that a complex lattice arranged in such AB form. The layer located at  $z = \frac{1}{2}d$  is  $L = L(\mathbf{e}_i, \mathbf{o}) \cup L(\mathbf{e}_i, \mathbf{o} + \mathbf{p})$ , and that located at  $z = -\frac{1}{2}d$  is  $L = L(\mathbf{e}_i, \mathbf{o} + \mathbf{d}) \cup L(\mathbf{e}_i, \mathbf{o} + \mathbf{p} + \mathbf{d})$ , where  $\mathbf{d} = a\left(\frac{1}{2}, -\frac{\sqrt{3}}{6}\right)$  is the vector between the centers of the two layers.

Suppose that there is an edge dislocation along the  $y$  axis centered at  $z = x = 0$  with Burgers vector  $\mathbf{b} = (a, 0, 0)$ . This dislocation generates a nonzero displacement field  $\mathbf{u} = \{\mathbf{u}_s^{A+}, \mathbf{u}_s^{B+}, \mathbf{u}_s^{A-}, \mathbf{u}_s^{B-}\}$ , where  $\mathbf{s} = (x_s, y_s) \in L$  is the location of the atom in the upper layer  $z = \frac{1}{2}d$  (with superscript ‘+’) or lower layer  $z = -\frac{1}{2}d$  (with superscript ‘-’), ‘A’ or ‘B’ means that the atom is an  $A$  atom or a  $B$  atom. Here we assume that atoms in this bilayer system only have in-plane displacements, i.e.,  $\{\mathbf{u}_s^{\kappa\pm}\}$  are two-dimensional vectors. Moreover, since the dislocation is a straight edge dislocation along the  $y$  axis, the second coordinate of  $\mathbf{u}_s^{\kappa\pm}$  is 0, and we denote  $\mathbf{u}_s^{\kappa\pm} = (u_s^{\kappa\pm}, 0)$ . For this edge dislocation, the displacement field  $u_s^{\kappa\pm}$  satisfies the following conditions:

$$\lim_{x_s \rightarrow +\infty} (u_s^{A+} - u_s^{A-}) = a, \quad \lim_{x_s \rightarrow -\infty} (u_s^{A+} - u_s^{A-}) = 0, \quad u_s^{A+} = -u_s^{A-}, \tag{2.2}$$

where  $\mathbf{s} = (x_s, y_s)$  and  $\kappa = A$  or  $B$ .

The atomic interactions in the bilayer system can be divided into two parts: the intralayer interaction (covalent-bond interaction) and the inter-layer interaction (van der Waals-like interaction). For the intralayer interaction within each complex lattice layer, we focus on the three-body potential:

$$V_{\text{tot}} = \frac{1}{3!} \sum_{\substack{i,j,k, \\ i < j < k}} V_3(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k).$$

Recall that Stillinger-Weber potential [22] for the silicon crystal is the sum of interactions of two-body and three-body potentials, and the three-body potential is

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

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  $\lambda$  and  $\gamma$ ,  $\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k$  are the three different atoms in the same layer,  $\theta_{jik}$  is angle between  $\mathbf{x}_j - \mathbf{x}_i$  and  $\mathbf{x}_k - \mathbf{x}_i$  and  $r_{ij} = |\mathbf{x}_i - \mathbf{x}_j|, r_{ik} = |\mathbf{x}_i - \mathbf{x}_k|$ . In fact, this three-body potential  $V_3(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k)$  depends only on the two vectors  $\mathbf{s}_1 = \mathbf{x}_j - \mathbf{x}_i$  and  $\mathbf{s}_2 = \mathbf{x}_k - \mathbf{x}_i$ . For this reason, we assume that the three-body potential can be written in the form

$$V_3(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k) = V\left(\frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a}\right), \tag{2.3}$$

where  $\mathbf{s}_1 = \mathbf{x}_j - \mathbf{x}_i$  and  $\mathbf{s}_2 = \mathbf{x}_k - \mathbf{x}_i$ .

Therefore, with displacement field  $\mathbf{u} = \{\mathbf{u}_s^{A+}, \mathbf{u}_s^{B+}\}$ , the intralayer interactions within the upper layer  $z = +\frac{1}{2}d$  read as

$$\begin{aligned} E_{\text{a-el}}^+ = & \sum_{\mathbf{x} \in \mathbb{L}} \left\{ \frac{1}{6} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle \in \mathbb{L}^* \times \mathbb{L}^*} \left[ V\left(\frac{\mathbf{s}_1}{a} + \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{A+} - \mathbf{u}_{\mathbf{x}}^{A+}}{a}, \frac{\mathbf{s}_2}{a} + \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_2}^{A+} - \mathbf{u}_{\mathbf{x}}^{A+}}{a}\right) \right. \right. \\ & + V\left(\frac{\mathbf{s}_1}{a} + \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{B+} - \mathbf{u}_{\mathbf{x}}^{B+}}{a}, \frac{\mathbf{s}_2}{a} + \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_2}^{B+} - \mathbf{u}_{\mathbf{x}}^{B+}}{a}\right) - 2V\left(\frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a}\right) \left. \right] \\ & + \frac{1}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle \in \mathbb{L}^* \times \mathbb{L}^*} \left[ V\left(\frac{\mathbf{s}_1}{a} + \frac{\mathbf{p}}{a} + \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{B+} - \mathbf{u}_{\mathbf{x}}^{A+}}{a}, \frac{\mathbf{s}_2}{a} + \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_2}^{A+} - \mathbf{u}_{\mathbf{x}}^{A+}}{a}\right) \right. \\ & + V\left(\frac{\mathbf{s}_1}{a} - \frac{\mathbf{p}}{a} + \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{A+} - \mathbf{u}_{\mathbf{x}}^{B+}}{a}, \frac{\mathbf{s}_2}{a} + \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_2}^{B+} - \mathbf{u}_{\mathbf{x}}^{B+}}{a}\right) \\ & \left. \left. - V\left(\frac{\mathbf{s}_1}{a} - \frac{\mathbf{p}}{a}, \frac{\mathbf{s}_2}{a}\right) - V\left(\frac{\mathbf{s}_1}{a} + \frac{\mathbf{p}}{a}, \frac{\mathbf{s}_2}{a}\right) \right] \right\}, \tag{2.4} \end{aligned}$$

where

$$\mathbb{L} = L(\mathbf{e}_i, \mathbf{o}), \mathbb{L}^* = L(\mathbf{e}_i, \mathbf{o}) \setminus \{\mathbf{0}\}. \tag{2.5}$$

Note that in this formula, the summation with factor  $\frac{1}{6}$  comes from *AAA* and *BBB* types three-body interactions, and the summation with factor  $\frac{1}{2}$  comes from *AAB* and *BBA* types three-body interactions. In fact, since we use two side vectors as variables in the three-body interaction in Equation (2.3), a type *AAA* or *BBB* three-body interaction is counted 3! times in the summations: Each atom in such a three-body interaction can be used as the  $\mathbf{x} \in \mathbb{L}$  in the outer summation, and  $\langle \mathbf{s}_1, \mathbf{s}_2 \rangle, \langle \mathbf{s}_2, \mathbf{s}_1 \rangle \in \mathbb{L}^* \times \mathbb{L}^*$  in the inner summation give the same three-body interaction. Whereas for a type *AAB* (*ABB*) interaction, we collect it by using an “*A*” (“*B*”) atom as the  $\mathbf{x} \in \mathbb{L}$  in the outer summation, and each of the two “*A*” (“*B*”) atoms in the *AAB* (*ABB*) can be used as the  $\mathbf{x} \in \mathbb{L}$  in the outer summation, leading to a factor 2 for this three-body interaction. These give the summation formula in Equation (2.4). Note that this method of organizing

terms of intra-layer interactions on a complex lattice layer will be very convenient for the convergence proofs from atomistic model to the Peierls–Nabarro model in later sections.

We have a similar formula for  $E_{\text{a-el}}^-$ , i.e., the intralayer interactions within the lower layer  $z = -\frac{1}{2}d$  with displacement field  $\mathbf{u} = \{\mathbf{u}_s^{A-}, \mathbf{u}_s^{B-}\}$ , by using a different lattice

$$\mathbb{L} = L(\mathbf{e}_i, \mathbf{o} + \mathbf{d}), \mathbb{L}^* = L(\mathbf{e}_i, \mathbf{o} + \mathbf{d}) \setminus \{\mathbf{0}\}, \tag{2.6}$$

and replacing all the variables with notation “+” by those with notation “−”. The total intra layer elastic energy is

$$E_{\text{a-el}} = E_{\text{a-el}}^+ + E_{\text{a-el}}^- \tag{2.7}$$

Next, we describe the inter-layer interaction, which is a weak interaction, e.g. the van der Waals-like interaction. In [27], Morse potential is used to describe the van der Waals-like interaction, which is a two-body potential:

$$V_{\text{Morse}}(r) = D_e \left( e^{-2c(r-r_e)} - 2e^{-c(r-r_e)} \right),$$

where  $r$  is the distance between two atoms,  $r_e$  is the equilibrium bond distance,  $D_e$  is the well depth, and  $c$  controls the width of the potential. We focus on such a two-body potential for the inter-layer interaction:

$$V_{\text{inter}}(\mathbf{x}_i^+, \mathbf{x}_j^-) = V_d \left( \frac{|\mathbf{x}_i^+ - \mathbf{x}_j^-|}{a} \right), \tag{2.8}$$

where  $\mathbf{x}_i^+$  and  $\mathbf{x}_j^-$  are the locations of two atoms in the upper and lower layers, respectively, and the distance  $|\mathbf{x}_i^+ - \mathbf{x}_j^-|$  is the distance in three-dimensions.

Therefore, with displacement field  $\mathbf{u} = \{\mathbf{u}_s^{A+}, \mathbf{u}_s^{B+}, \mathbf{u}_s^{A-}, \mathbf{u}_s^{B-}\}$  in the bilayer system, the inter-layer interaction energy in the bilayer system is

$$\begin{aligned} E_{\text{a-mis}} = & \sum_{\mathbf{x} \in \mathbb{L}} \sum_{\mathbf{s} \in \mathbb{L}} \left[ V_d \left( \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{u}_{\mathbf{x}}^{A-}}{a} + \frac{\mathbf{s}}{a} - \frac{\mathbf{d}}{a} \right) - V_d \left( \frac{\mathbf{s}}{a} - \frac{\mathbf{d}}{a} \right) \right. \\ & + V_d \left( \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{u}_{\mathbf{x}}^{B-}}{a} + \frac{\mathbf{s}}{a} - \frac{\mathbf{d}+\mathbf{p}}{a} \right) - V_d \left( \frac{\mathbf{s}}{a} - \frac{\mathbf{d}+\mathbf{p}}{a} \right) \\ & + V_d \left( \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}}^{B+} - \mathbf{u}_{\mathbf{x}}^{A-}}{a} + \frac{\mathbf{s}}{a} - \frac{\mathbf{d}-\mathbf{p}}{a} \right) - V_d \left( \frac{\mathbf{s}}{a} - \frac{\mathbf{d}-\mathbf{p}}{a} \right) \\ & \left. + V_d \left( \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}}^{B+} - \mathbf{u}_{\mathbf{x}}^{B-}}{a} + \frac{\mathbf{s}}{a} - \frac{\mathbf{d}}{a} \right) - V_d \left( \frac{\mathbf{s}}{a} - \frac{\mathbf{d}}{a} \right) \right], \tag{2.9} \end{aligned}$$

where  $\mathbf{d}$  is recalled to be the vector between the centers of two layers. Here the four rows come from the  $A^+A^-$ ,  $A^+B^-$ ,  $B^+A^-$ , and  $B^+B^-$  types interactions, respectively.

Note that for simplicity of notations, we will omit  $\mathbb{L}$  and  $\mathbb{L}^*$  in the summations in later sections, e.g.,  $\sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle}$  means  $\sum_{(\mathbf{s}_1, \mathbf{s}_2) \in \mathbb{L}^* \times \mathbb{L}^*}$ .

### 3. Peierls–Nabarro model with $\gamma$ -surface

In the Peierls–Nabarro (PN) model, we may consider an edge dislocation with Burgers vector  $\mathbf{b} = (a, 0, 0)$  centered at  $x = z = 0$ , i.e., along the  $y$  axis. The locations of atoms

are  $\Gamma_{\text{PN}} = \{(\mathbf{x} + \mathbf{u}^\pm, \pm \frac{1}{2}d), \mathbf{x} \in \mathbb{R}^2\}$ . In the classical PN model, the disregistry (relative displacement)  $\phi(x)$  between the two layers is defined as

$$\phi(\mathbf{x}) = \mathbf{u}^+(\mathbf{x}) - \mathbf{u}^-(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2, \tag{3.1}$$

and satisfies the boundary conditions

$$\lim_{x \rightarrow -\infty} \phi(x, y) = \mathbf{0}, \quad \lim_{x \rightarrow +\infty} \phi(x, y) = (a, 0). \tag{3.2}$$

In addition, the dislocation is centered at  $x = z = 0$ , which means

$$\phi(0, y) = \left(\frac{1}{2}a, 0\right). \tag{3.3}$$

For the straight edge dislocation being considered, we have  $\mathbf{u}^\pm = (u^\pm, 0)$  and  $\phi = (\phi, 0)$ . In the classical PN model with  $\gamma$ -surface, the total energy of a bilayer graphene system is divided into two parts, the misfit energy (due to the interaction of two atoms from different layers) and the elastic energy (due to the interaction from the same layer).

In bilayer graphene system with  $\gamma$ -surface, the misfit energy is regarded as the interactions across the slip plane. Therefore we have the following formula by the atomistic model:

$$E_{\text{mis}}[\phi] = \int_{\mathbb{R}^2} \gamma(\phi(x, y)) \, dx \, dy, \tag{3.4}$$

where the density of this misfit energy  $\gamma(\phi)$  is the  $\gamma$ -surface [23] which is defined as the energy increment per unit area. By the definition, the  $\gamma$ -surface can be calculated in terms of the atomistic model by

$$\begin{aligned} \gamma(\phi) = & \frac{2}{\sqrt{3}a^2} \sum_{\mathbf{s}} \left[ V_{\text{d}} \left( \frac{\phi}{a} + \frac{\mathbf{s}}{a} - \frac{\mathbf{d}}{a} \right) - V_{\text{d}} \left( \frac{\mathbf{s}}{a} - \frac{\mathbf{d}}{a} \right) \right. \\ & + V_{\text{d}} \left( \frac{\phi}{a} + \frac{\mathbf{s}}{a} - \frac{\mathbf{d} + \mathbf{p}}{a} \right) - V_{\text{d}} \left( \frac{\mathbf{s}}{a} - \frac{\mathbf{d} + \mathbf{p}}{a} \right) \\ & \left. + V_{\text{d}} \left( \frac{\phi}{a} + \frac{\mathbf{s}}{a} - \frac{\mathbf{d} - \mathbf{p}}{a} \right) - V_{\text{d}} \left( \frac{\mathbf{s}}{a} - \frac{\mathbf{d} - \mathbf{p}}{a} \right) + V_{\text{d}} \left( \frac{\phi}{a} + \frac{\mathbf{s}}{a} - \frac{\mathbf{d}}{a} \right) - V_{\text{d}} \left( \frac{\mathbf{s}}{a} - \frac{\mathbf{d}}{a} \right) \right], \end{aligned} \tag{3.5}$$

The elastic energy in the PN model comes from the intralayer elastic interaction in the two layers. The elastic energy in the upper layer  $E_{\text{elas}}^+$  is

$$\begin{aligned} E_{\text{elas}}^+ &= \int_{\mathbb{R}^2} W(\nabla u^+) + W(\nabla u^-) \, dx \, dy \\ &= \int_{\mathbb{R}^2} \alpha_1 (\partial_x u^+)^2 + \alpha_2 (\partial_y u^+)^2 + \alpha_1 (\partial_x u^-)^2 + \alpha_2 (\partial_y u^-)^2 \, dx \, dy, \end{aligned} \tag{3.6}$$

where notations  $\partial_x u = \frac{\partial u}{\partial x}$ ,  $\partial_y u = \frac{\partial u}{\partial y}$ , and parameters

$$\begin{aligned} \alpha_1 = & \frac{1}{3\sqrt{3}a^2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \left\{ \left[ \partial_{ij} V \left( \frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a} \right) \right]_{11} \left( \frac{\mathbf{s}_1}{a} \cdot \mathbf{e}_x \right)^i \left( \frac{\mathbf{s}_2}{a} \cdot \mathbf{e}_x \right)^j \right. \\ & \left. + \frac{3}{2} \left[ \partial_{ij} V \left( \frac{\mathbf{s}_1 \pm \mathbf{p}}{a}, \frac{\mathbf{s}_2}{a} \right) \right]_{11} \left[ \left( \frac{\mathbf{s}_1 \pm \mathbf{p}}{a} \right) \cdot \mathbf{e}_x \right]^i \left[ \left( \frac{\mathbf{s}_2}{a} \right) \cdot \mathbf{e}_x \right]^j \right\}, \end{aligned} \tag{3.7}$$

$$\begin{aligned} \alpha_2 &= \frac{1}{3\sqrt{3}a^2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \left\{ \left[ \partial_{ij} V \left( \frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a} \right) \right]_{11} \left( \frac{\mathbf{s}_1}{a} \cdot \mathbf{e}_y \right)^i \left( \frac{\mathbf{s}_2}{a} \cdot \mathbf{e}_y \right)^j \right. \\ &\quad \left. + \frac{3}{2} \left[ \partial_{ij} V \left( \frac{\mathbf{s}_1 \pm \mathbf{p}}{a}, \frac{\mathbf{s}_2}{a} \right) \right]_{11} \left[ \left( \frac{\mathbf{s}_1 \pm \mathbf{p}}{a} \right) \cdot \mathbf{e}_y \right]^i \left[ \left( \frac{\mathbf{s}_2}{a} \right) \cdot \mathbf{e}_y \right]^j \right\}, \quad (3.8) \\ \mathbf{e}_x &= (1, 0), \quad \mathbf{e}_y = (0, 1). \end{aligned}$$

Here  $[\mathbf{A}]_{11}$  is the  $(1, 1)$ -entry of the matrix  $\mathbf{A} \in \mathbb{R}^{2 \times 2}$ , and also for simplicity of notations, for  $V(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2)$  with  $\boldsymbol{\rho}_1 = (\rho_{11}, \rho_{12})$  and  $\boldsymbol{\rho}_2 = (\rho_{21}, \rho_{22})$ , we denote

$$\begin{aligned} \partial_1 V &= \left( \frac{\partial V}{\partial \rho_{11}}, \frac{\partial V}{\partial \rho_{12}} \right)^\top, \quad \partial_2 V = \left( \frac{\partial V}{\partial \rho_{21}}, \frac{\partial V}{\partial \rho_{22}} \right)^\top, \\ \partial_{20} V &= \begin{bmatrix} \frac{\partial^2 V}{\partial \rho_{11}^2} & \frac{\partial^2 V}{\partial \rho_{11} \partial \rho_{12}} \\ \frac{\partial^2 V}{\partial \rho_{12} \partial \rho_{11}} & \frac{\partial^2 V}{\partial \rho_{12}^2} \end{bmatrix}, \quad \partial_{11} V = \begin{bmatrix} \frac{\partial^2 V}{\partial \rho_{11} \partial \rho_{21}} & \frac{\partial^2 V}{\partial \rho_{11} \partial \rho_{22}} \\ \frac{\partial^2 V}{\partial \rho_{12} \partial \rho_{21}} & \frac{\partial^2 V}{\partial \rho_{12} \partial \rho_{22}} \end{bmatrix}, \\ \partial_{02} V &= \begin{bmatrix} \frac{\partial^2 V}{\partial \rho_{21}^2} & \frac{\partial^2 V}{\partial \rho_{21} \partial \rho_{22}} \\ \frac{\partial^2 V}{\partial \rho_{22} \partial \rho_{21}} & \frac{\partial^2 V}{\partial \rho_{22}^2} \end{bmatrix}. \end{aligned}$$

In fact, by using Taylor expansion in the elastic energy in the atomistic model  $E_{\text{a-el}}^+$  in Equation (2.4), we can get the following leading order approximation of the continuum elastic energy in the upper layer:

$$\begin{aligned} E_{\text{elas}}^+ &= \frac{2}{\sqrt{3}a^4} \int_{\mathbb{R}^2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \left\{ \frac{1}{6} \partial_{ij} V \left( \frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a} \right) [(\mathbf{s}_1 \cdot \nabla) \mathbf{u}^+]^i [(\mathbf{s}_2 \cdot \nabla) \mathbf{u}^+]^j \right. \\ &\quad \left. + \frac{1}{4} \partial_{ij} V \left( \frac{\mathbf{s}_1 \pm \mathbf{p}}{a}, \frac{\mathbf{s}_2}{a} \right) [(\mathbf{s}_1 \pm \mathbf{p}) \cdot (\nabla \mathbf{u}^+)]^i [(\mathbf{s}_2) \cdot (\nabla \mathbf{u}^+)]^j \right\} dx dy. \quad (3.9) \end{aligned}$$

This leading order approximation is easily obtained by using the approximations

$$\begin{aligned} \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{A+} - \mathbf{u}_{\mathbf{x}}^{A+}}{a} &\approx \left( \frac{\mathbf{s}_1}{a} \cdot \nabla \right) \mathbf{u}^+, \quad \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{B+} - \mathbf{u}_{\mathbf{x}}^{B+}}{a} \approx \left( \frac{\mathbf{s}_1}{a} \cdot \nabla \right) \mathbf{u}^+ \\ \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{A+} - \mathbf{u}_{\mathbf{x}}^{B+}}{a} &\approx \left( \frac{\mathbf{s}_1 - \mathbf{p}}{a} \cdot \nabla \right) \mathbf{u}^+, \quad \frac{\mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{B+} - \mathbf{u}_{\mathbf{x}}^{A+}}{a} \approx \left( \frac{\mathbf{s}_1 + \mathbf{p}}{a} \cdot \nabla \right) \mathbf{u}^+, \end{aligned}$$

and symmetry of the lattice. For simplicity of notations, in Equations (3.9), we have used the expression

$$\partial_{ij} V(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2) \boldsymbol{\xi}_1 \boldsymbol{\xi}_2 := \boldsymbol{\xi}_1 \partial_{ij} V(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2) \boldsymbol{\xi}_2^\top, \quad \text{for } \boldsymbol{\xi}_i \in \mathbb{R}^2.$$

The formula of the elastic energy in the lower layer  $E_{\text{elas}}^-$  in the form of Equation (3.9) is the same except that  $\mathbf{s}_1, \mathbf{s}_2 \in \mathbb{L}^*$  with  $\mathbb{L}^*$  being defined in Equation (2.6) instead of Equation (2.5), and all the variables with notation “+” are replaced by those with notation “-”.

The two forms of elastic energy densities in Equations (3.6) and (3.9) are identical. Calculation from Equation (3.9) to Equation (3.6) will be summarized as a lemma below (Same for the calculation for the corresponding two forms of  $E_{\text{elas}}^-$ ). In the PN model part (Theorem 6.1), we use formula (3.6). In the atomistic model part (consistency of PN model and stability of atomistic model), we use formula (3.9).



LEMMA 3.1. *The two forms of elastic energy densities in Equations (3.6) and (3.9) are identical.*

*Proof.* We derive Equation (3.6) from Equation (3.9) by direct calculation. It is easy to see that the coefficients of  $(\partial_x u)^2$  and  $(\partial_y u)^2$  in Equation (3.6) are the same as those in Equation (3.9). It remains to show that there is no  $\partial_x u \partial_y u$  term in Equation (3.9), which will be done using lattice symmetry as follows.

Recall that Equation (3.9) is obtained by Taylor expansions in the elastic energy in the atomistic model in Equation (2.4). In the atomistic model, we divide the elastic interactions within this layer into four types of three-body interactions: *AAA*, *BBB*, *AAB*, and *ABB*. Recall that here we use three-body potential. The three atoms in a three-body interaction form a triangle; see Figure 3.1. Without loss of generality, suppose that the point being considered is an *A*-atom, denoted by  $T$ . In the elastic energy in the atomistic model in Equation (2.4), when  $\mathbf{x} = T$  in the outer summation, the three-body interactions in the summation includes only those of *AAA* and *AAB* types that contain the atom  $T$ ; see Figure 3.1. The interactions among such a triangle is expressed in terms of the two edge vectors  $\mathbf{s}_1$  and  $\mathbf{s}_2$  starting from the atom  $T$  as given in the inner summations in Equation (2.4). Recall that the interactions of *ABB* and *BBB* types are included in summations with a *B*-atom in the outer summation in Equation (2.4).

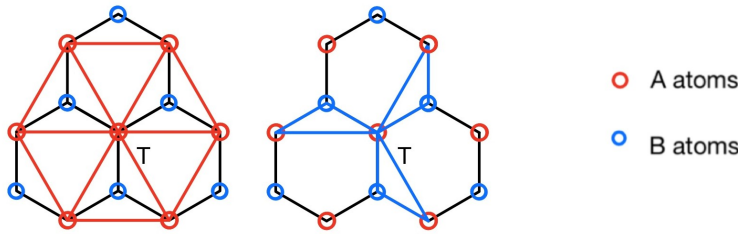


FIG. 3.1. *Different types of three-body interactions in a layer. Left: AAA, right: AAB. Types BBB and ABB are similar.*

The complex lattice being considered has 3-fold rotational symmetry, i.e., it does not change after rotations of  $2\pi/3$  and  $4\pi/3$ . For an AA edge vector starting from the atom  $T$ , e.g.,  $\mathbf{s}_1 = b_1 \mathbf{e}_1 + b_2 \mathbf{e}_2 = a \left( b_1 + \frac{1}{2} b_2, \frac{\sqrt{3}}{2} b_2 \right)$ , where  $b_1, b_2 \in \mathbb{Z}$ , it becomes  $b_2 \mathbf{e}_1 - (b_1 + b_2) \mathbf{e}_2$  and  $-(b_1 + b_2) \mathbf{e}_1 + b_1 \mathbf{e}_2$  after rotations of  $2\pi/3$  and  $4\pi/3$  around atom  $T$ , respectively.

Consider an *AAA* interaction associated with the atom  $T$ . Assume that the two AA edge vectors starting from atom  $T$  are

$$\mathbf{s}_1 = b_1 \mathbf{e}_1 + b_2 \mathbf{e}_2, \quad \mathbf{s}_2 = b_3 \mathbf{e}_1 + b_4 \mathbf{e}_2.$$

The three-body interaction among this *AAA* triangle is included in the summation in the first line in Equation (2.4). Due to the 3-fold rotational symmetry, interactions among *AAA* triangles obtained by  $2\pi/3$  and  $4\pi/3$  rotations from this one are also included in this summation.

Recall that the continuum model in Equation (3.9) is obtained by leading order approximation from the atomistic model in Equation (2.4). We divide the first term in Equation (3.9) for the *AAA* interactions into three parts that contain the terms

$\partial_{20}V\left(\frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a}\right)$ ,  $\partial_{11}V\left(\frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a}\right)$  and  $\partial_{02}V\left(\frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a}\right)$ , respectively. For the  $\partial_{20}V\left(\frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a}\right)$  term, due to the 3-fold rotational symmetry, its coefficient can be written as

$$\begin{aligned} & \lambda_1 \left\{ \left[ \left( b_1 + \frac{1}{2}b_2 \right) \partial_x u + \frac{\sqrt{3}}{2}b_2 \partial_y u \right]^2 + \left[ \left( b_2 + \frac{1}{2}b_1 \right) \partial_x u - \frac{\sqrt{3}}{2}b_1 \partial_y u \right]^2 \right. \\ & \quad \left. + \left[ \left( \frac{1}{2}b_2 - \frac{1}{2}b_1 \right) \partial_x u - \frac{\sqrt{3}}{2}(b_1 + b_2) \partial_y u \right]^2 \right\} \\ & = \lambda_{11}(\partial_x u)^2 + \lambda_{12}(\partial_y u)^2, \end{aligned}$$

where  $\lambda_1$ ,  $\lambda_{11}$ , and  $\lambda_{12}$  are independent of  $\partial_x u$  and  $\partial_y u$ . For the term  $\partial_{11}V\left(\frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a}\right)$ , for the same reason, its coefficient can be written as

$$\begin{aligned} & \lambda_2 \left\{ \left[ \left( b_1 + \frac{1}{2}b_2 \right) \partial_x u + \frac{\sqrt{3}}{2}b_2 \partial_y u \right] \left[ \left( b_4 + \frac{1}{2}b_3 \right) \partial_x u - \frac{\sqrt{3}}{2}b_3 \partial_y u \right] \right. \\ & \quad + \left[ \left( b_2 + \frac{1}{2}b_1 \right) \partial_x u - \frac{\sqrt{3}}{2}b_1 \partial_y u \right] \left[ \left( \frac{1}{2}b_4 - \frac{1}{2}b_3 \right) \partial_x u - \frac{\sqrt{3}}{2}(b_3 + b_4) \partial_y u \right] \\ & \quad \left. - \left[ \left( \frac{1}{2}b_2 - \frac{1}{2}b_1 \right) \partial_x u - \frac{\sqrt{3}}{2}(b_1 + b_2) \partial_y u \right] \left[ \left( b_3 + \frac{1}{2}b_4 \right) \partial_x u + \frac{\sqrt{3}}{2}b_4 \partial_y u \right] \right\} \\ & = \lambda_{21}(\partial_x u)^2 + \lambda_{22}(\partial_y u)^2, \end{aligned}$$

where  $\lambda_2$ ,  $\lambda_{21}$ , and  $\lambda_{22}$  are independent of  $\partial_x u$  and  $\partial_y u$ . The coefficient of  $V_{02}\left(\frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a}\right)$  is the same as that of  $\partial_{20}V\left(\frac{\mathbf{s}_1}{a}, \frac{\mathbf{s}_2}{a}\right)$  given above except that  $b_1$  and  $b_2$  are replaced by  $b_3$  and  $b_4$ .

Thus we know that the  $u_x u_y$  term vanishes in Equation (3.9) for all the *AAA* interactions. We can also show similarly that the  $\partial_x u \partial_y u$  term vanishes in Equation (3.9) for all the *AAB* interactions. A slight difference in the calculation is that for the *AB* edge vector starting from the atom, it is  $c_1 \mathbf{e}_1 + c_2 \mathbf{e}_2 + \mathbf{p}$ , where  $c_1, c_2 \in \mathbb{Z}$ , and it becomes  $c_2 \mathbf{e}_1 - (c_1 + c_2 + 1) \mathbf{e}_2 + \mathbf{p}$  and  $-(c_1 + c_2 + 1) \mathbf{e}_1 + c_1 \mathbf{e}_2 + \mathbf{p}$  after rotations of  $2\pi/3$  and  $4\pi/3$  around atom *T*.  $\square$

**4. Rescaling**

Due to the fact that the inter-layer van der Waals-like interaction is much weaker than the intra-layer covalent-bond interaction in bilayer graphene [6], i.e.,  $V_d \ll V$  in the atomistic model, we assume that

$$V_d/V = O(\varepsilon^2),$$

where  $\varepsilon$  is a small dimensionless parameter. In the PN model of bilayer graphene system, the intra-layer covalent-bond interaction gives the elastic energy  $E_{\text{elas}}$ , and the inter-layer van der Waals-like interaction gives the misfit energy  $E_{\text{mis}}$ . Following the convergence analysis for simple lattices in Ref. [14], we define the small parameter  $\varepsilon$  based on the PN model as

$$\varepsilon = \sqrt{\frac{a^2 \gamma_{xx}(\mathbf{0})}{\sqrt{\alpha_1 \alpha_2}}}, \tag{4.1}$$

and assume that

$$\varepsilon \ll 1. \tag{4.2}$$

Using  $a/\varepsilon$  as the length unit for the spatial variable  $x$  and  $a$  as the length unit for the displacement, we define the rescaled quantities:

$$\begin{aligned} \bar{x} &= \frac{\varepsilon x}{a}, \quad \bar{u}^\pm = \frac{u^\pm}{a}, \quad \bar{\phi} = \frac{\phi}{a}, \quad \bar{s}_i = \frac{s_i}{a}, \quad \bar{p} = \frac{p}{a}, \quad \bar{d} = \frac{d}{a}, \\ \bar{\alpha}_i &= a^2 \alpha_i, \quad \bar{\gamma}(\bar{\phi}) = a^2 \gamma(\phi). \end{aligned}$$

The elastic energy in the PN model in Equation (3.9) becomes

$$\begin{aligned} E_{\text{elas}}^+ &= \frac{2}{\sqrt{3}} \int_{\mathbb{R}^2} \sum_{\langle \bar{s}_1, \bar{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \left\{ \frac{1}{6} \partial_{ij} V(\bar{s}_1, \bar{s}_2) [(\bar{s}_1 \cdot \nabla) \bar{u}^+]^i [(\bar{s}_2 \cdot \nabla) \bar{u}^+]^j \right. \\ &\quad \left. + \frac{1}{4} \partial_{ij} V(\bar{s}_1 \pm \bar{p}, \bar{s}_2) [(\bar{s}_1 \pm \bar{p}) \cdot (\nabla \bar{u}^+)]^i [(\bar{s}_2) \cdot (\nabla \bar{u}^+)]^j \right\} d\bar{x} d\bar{y}, \end{aligned} \quad (4.3)$$

and similar formula for  $E_{\text{elas}}^-$ . The misfit energy in Equation (3.4) in the PN model becomes

$$E_{\text{mis}} = \int_{\mathbb{R}^2} \bar{\gamma}(\bar{\phi}) d\bar{x} d\bar{y}, \quad (4.4)$$

where

$$\begin{aligned} \bar{\gamma}(\bar{\phi}) &= \frac{2}{\sqrt{3}} \sum_{\bar{s}} \left[ U(\bar{\phi} + \bar{s} - \bar{d}) - U(\bar{s} - \bar{d}) + U(\bar{\phi} + \bar{s} - \bar{d} + \bar{p}) - U(\bar{s} - \bar{d} + \bar{p}) \right. \\ &\quad \left. + U(\bar{\phi} + \bar{s} - \bar{d} - \bar{p}) - U(\bar{s} - \bar{d} - \bar{p}) + U(\bar{\phi} + \bar{s} - \bar{d}) - U(\bar{s} - \bar{d}) \right]. \end{aligned} \quad (4.5)$$

Here, we have used the notation

$$U = \varepsilon^{-2} V_{\text{d}}. \quad (4.6)$$

Using the above notations and the intra-layer interaction energy in Equation (2.4) and the inter-layer interaction energy in Equation (2.9) in the atomistic model, the total energy in the atomistic model is

$$E_{\text{a}}[\bar{\mathbf{u}}] = \sum_{\bar{\mathbf{x}}} e_{\bar{\mathbf{x}}}[\bar{\mathbf{u}}], \quad (4.7)$$

where

$$\begin{aligned} e_{\bar{\mathbf{x}}}[\bar{\mathbf{u}}] &:= \frac{1}{6} \sum_{\langle \bar{s}_1, \bar{s}_2 \rangle} [V(\bar{s}_1 + \bar{u}_{\bar{x}+\bar{s}_1}^{A\pm} - \bar{u}_{\bar{x}}^{A\pm}, \bar{s}_2 + \bar{u}_{\bar{x}+\bar{s}_2}^{A\pm} - \bar{u}_{\bar{x}}^{A\pm}) \\ &\quad + V(\bar{s}_1 + \bar{u}_{\bar{x}+\bar{s}_1}^{B\pm} - \bar{u}_{\bar{x}}^{B\pm}, \bar{s}_2 + \bar{u}_{\bar{x}+\bar{s}_2}^{B\pm} - \bar{u}_{\bar{x}}^{B\pm}) - 2V_3(\bar{s}_1, \bar{s}_2)] \\ &\quad + \frac{1}{2} \sum_{\langle \bar{s}_1, \bar{s}_2 \rangle} [V(\bar{p} + \bar{s}_1 + \bar{u}_{\bar{x}+\bar{s}_1}^{B\pm} - \bar{u}_{\bar{x}}^{A\pm}, \bar{s}_2 + \bar{u}_{\bar{x}+\bar{s}_2}^{A\pm} - \bar{u}_{\bar{x}}^{A\pm}) \\ &\quad + V(-\bar{p} + \bar{s}_1 + \bar{u}_{\bar{x}+\bar{s}_1}^{A\pm} - \bar{u}_{\bar{x}}^{B\pm}, \bar{s}_2 + \bar{u}_{\bar{x}+\bar{s}_2}^{B\pm} - \bar{u}_{\bar{x}}^{B\pm}) - V(-\bar{p} + \bar{s}_1, \bar{s}_2) - V(\bar{p} + \bar{s}_1, \bar{s}_2)] \\ &\quad + \varepsilon^2 \sum_{\bar{s}} [U(\bar{u}_{\bar{x}+\bar{s}}^{A+} - \bar{u}_{\bar{x}}^{A-} + \bar{s} - \bar{d}) - U(\bar{s} - \bar{d}) \\ &\quad + U(\bar{u}_{\bar{x}+\bar{s}}^{A+} - \bar{u}_{\bar{s}_1}^{B-} + \bar{s} - \bar{d} + \bar{p}) - U(\bar{s} - \bar{d} + \bar{p}) \\ &\quad + U(\bar{u}_{\bar{x}+\bar{s}}^{B+} - \bar{u}_{\bar{x}}^{A-} + \bar{s} - \bar{d} - \bar{p}) - U(\bar{s} - \bar{d} - \bar{p}) \\ &\quad + U(\bar{u}_{\bar{x}+\bar{s}}^{B+} - \bar{u}_{\bar{x}}^{B-} + \bar{s} - \bar{d}) - U(\bar{s} - \bar{d})]. \end{aligned} \quad (4.8)$$

For simplicity, we will still use letters without bar for the rescaled variables in later sections.

**5. Total energy revisited and assumptions**

**5.1. Total energy revisited.** Although we are interested in a straight dislocation in the continuum model, the atomic structure is not uniform along the dislocation using the atomistic model due to the complex lattice. Therefore, we need to consider two-dimensional models for the slip plane of the dislocation instead of one-dimensional models in the convergence from the atomistic model to the continuum, PN model. We will show that the dislocation in equilibrium is a straight line in the PN model (in Theorem 6.1). Here we define the total energy in the PN model as

$$E_{\text{PN}}[\mathbf{u}] = \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R dy \int_{\mathbb{R}} W(\nabla u^+) + W(\nabla u^-) + \gamma(\phi) dx \tag{5.1}$$

where  $W(\mathbf{A})$  is defined in (3.6).

Accordingly, we redefine the total energy in the atomistic model as

$$E_a[\mathbf{u}] := \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} e_{\mathbf{x}}[\mathbf{u}], \tag{5.2}$$

where  $e_{\mathbf{x}}[\mathbf{u}]$  is defined in (4.8) (with bars being omitted for simplicity of notations, as remarked above), and  $\mathbb{L}_R$  is a truncation of  $\mathbb{L}$ :

$$\mathbb{L}_R := \{ \mathbf{s} = (x, y) \in \mathbb{L} \mid |y| \leq R \}. \tag{5.3}$$

**5.2. Notations.** We collect some notations for the rest of the paper here. First, as discussed in the previous two sections, we assume that the displacement vector is always in the  $x$  direction due to the straight edge dislocation in both the atomistic model and the PN model, and focus on the  $x$ -component of the displacement. Sometimes, when the interaction potential  $V(\cdot, \cdot)$  defined in Equation (2.3) is used, it is more convenient to use the vector displacement, and in this case, we will use the vector  $\mathbf{u} = (u, 0)$  instead of the scalar displacement component  $u$ , in both the atomistic model and the PN model.

For convenience, we denote  $\mathbb{L}_{\mathbf{p}} = \mathbb{L} \cup (\mathbb{L} + \{\mathbf{p}\})$ , where  $\mathbb{L}$  is defined in (2.5). Then we define the difference operators  $D_{\mathbf{s}}$  and  $D_{\mathbf{s}}^{\mathbf{p}}$  for  $f$  on  $\mathbb{L}_{\mathbf{p}}$ :

$$D_{\mathbf{s}} f(\mathbf{x}) = \frac{f(\mathbf{x} + \varepsilon \mathbf{s}) - f(\mathbf{x})}{\varepsilon}, \quad D_{\mathbf{s}}^{\pm \mathbf{p}} f(\mathbf{x}) = \frac{f(\mathbf{x} + \varepsilon \mathbf{s} \pm \varepsilon \mathbf{p}) - f(\mathbf{x})}{\varepsilon}, \tag{5.4}$$

where  $\mathbf{s} \in \mathbb{L}$  defined in (2.5) and  $\mathbf{p} = (\frac{1}{2}, \frac{3}{6})$ . Moreover, for functions defined on  $\mathbb{L}_{\mathbf{p}}$ , we denote

$$f_{\mathbf{s}}^A := f(\varepsilon \mathbf{s}), \quad f_{\mathbf{s}}^B := f(\varepsilon \mathbf{s} + \varepsilon \mathbf{p}). \tag{5.5}$$

Now we introduce discrete Sobolev space

$$H_{\varepsilon}^1 = H_{\varepsilon}^1(\mathbb{L}_{\mathbf{p}}) = \{ f \mid \|f\|_{1, \varepsilon} < \infty \}$$

with

$$\begin{aligned} \|f\|_{1, \varepsilon}^2 &= \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left( \sum_{\|\mathbf{s}\| \leq 1} |D_{\mathbf{s}} f_{\mathbf{x}}^A|^2 + |D_{\mathbf{s}}^{\mathbf{p}} f_{\mathbf{x}}^A|^2 + |D_{\mathbf{s}} f_{\mathbf{x}}^B|^2 + |D_{\mathbf{s}^{-\mathbf{p}}} f_{\mathbf{x}}^B|^2 \right) \\ &\quad + \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left( \sum_{\|\mathbf{s}\| \leq 1} |f_{\mathbf{s}}^B|^2 + |f_{\mathbf{s}}^A|^2 \right). \end{aligned}$$

Similarly, we define the continuum Sobolev space on  $\mathbb{R}^2$

$$H^1_\varepsilon = H^1_\varepsilon(\mathbb{R}^2) = \{f \mid \|f\|_1 \leq \infty\}$$

with

$$\|f\|_1^2 = \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R \int_{\mathbb{R}} |\partial_x f|^2 + |\partial_y f|^2 + |f|^2 dx dy.$$

For simplicity of notations, we write  $f = \{f^+, f^-\} \in H^1_\varepsilon$  if  $f^\pm \in H^1_\varepsilon$  and  $f = \{f^+, f^-\} \in H^1_\varepsilon$  if  $f^\pm \in H^1_\varepsilon$ . If  $f = \{f^+, f^-\}$ , we denote

$$f^\perp = f^+ - f^-. \tag{5.6}$$

Now we define the test function space  $X_0 \subset H^1_\varepsilon$  for the PN model on  $\{\mathbb{R}^2, \mathbb{R}^2\}$  and the test function space  $X_\varepsilon \subset H^1_\varepsilon$  for atomistic model on  $\{\mathbb{L}_p, \mathbb{L}_p\}$ :

$$X_0 = \{f \in H^1_\varepsilon \mid \|f\|_{X_0} < +\infty, f^\pm(0, y) = 0, \lim_{x \rightarrow \pm\infty} f^\pm(x, y) = 0\}, \tag{5.7}$$

where  $\|f\|_{X_0}^2 = (f, f)_{X_0}$ , and

$$\begin{aligned} (f, g)_{X_0} &= \alpha_1 [(\partial_x f^+, \partial_x g^+)_v + (\partial_x f^-, \partial_x g^-)_v] \\ &\quad + \alpha_2 [(\partial_y f^+, \partial_y g^+)_v + (\partial_y f^-, \partial_y g^-)_v] + \frac{4\sqrt{3}}{3} (f^\perp, g^\perp)_v, \end{aligned} \tag{5.8}$$

$$(f, g)_v = \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R \int_{\mathbb{R}} fg dx dy.$$

$$\begin{aligned} X_\varepsilon = \left\{ f \in H^1_\varepsilon \mid \|f\|_{X_\varepsilon} < \infty, \lim_{\mathbf{s} \cdot \mathbf{e}_1 \rightarrow \infty} f_{\mathbf{s}}^{\kappa^\pm} = 0, f_{\mathbf{s}}^{\kappa^\pm} = -f_{-\mathbf{s}}^{\kappa^\pm}, \right. \\ \left. \{f^+, f^-\} + \left\{ \frac{1}{4}, -\frac{1}{4} \right\} \text{ satisfies ADC.} \right\} \end{aligned} \tag{5.9}$$

where  $\mathbf{e}_1 = (1, 0)$ ,  $\kappa = A, B$ ,  $\|f\|_{X_\varepsilon}^2 = (f, f)_{X_\varepsilon}$ , and definition of the Atomistic Dislocation Condition (ADC) will be given in Section 9.1. We denote  $(\cdot, \cdot)_{X_\varepsilon}$  as

$$(f, g)_{X_\varepsilon} = (f^+, g^+)_a + (f^-, g^-)_a + (f^\perp, g^\perp)_\varepsilon \tag{5.10}$$

$$\begin{aligned} (f, g)_\varepsilon &= \lim_{R \rightarrow +\infty} \frac{1}{2R} \varepsilon^2 \sum_{\mathbf{x} \in \mathbb{L}_R} f_{\mathbf{x}}^A g_{\mathbf{x}}^A + f_{\mathbf{x}}^B g_{\mathbf{x}}^B \\ (f, g)_a &= (f, g)_A + (f, g)_B, \end{aligned} \tag{5.11}$$

where  $(f, g)_A$  and  $(f, g)_B$  are defined by

$$\begin{aligned} (f, g)_A &= \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\pm} \left\{ \frac{1}{6} \varepsilon^2 \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \partial_{20} V(\mathbf{s}_1, \mathbf{s}_2) (D_{\mathbf{s}_1} f_{\mathbf{x}}^{A\pm}) (D_{\mathbf{s}_1} g_{\mathbf{x}}^{A\pm}) \right. \\ &\quad \left. + \frac{1}{6} \varepsilon^2 \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \partial_{11} V(\mathbf{s}_1, \mathbf{s}_2) [(D_{\mathbf{s}_1} f_{\mathbf{x}}^{A\pm}) (D_{\mathbf{s}_2} g_{\mathbf{x}}^{A\pm}) + (D_{\mathbf{s}_2} g_{\mathbf{x}}^{A\pm}) (D_{\mathbf{s}_1} f_{\mathbf{x}}^{A\pm})] \right\} \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{6}\varepsilon^2 \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \partial_{02}V(\mathbf{s}_1, \mathbf{s}_2)(D_{\mathbf{s}_2}f_{\mathbf{x}}^{A\pm})(D_{\mathbf{s}_2}g_{\mathbf{x}}^{A\pm}) \\
 & + \varepsilon^2 \frac{1}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \partial_{20}V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2)(D_{\mathbf{s}_1}^{\mathbf{p}}f_{\mathbf{x}}^{A\pm})(D_{\mathbf{s}_1}^{\mathbf{p}}g_{\mathbf{x}}^{A\pm}) \\
 & + \varepsilon^2 \frac{1}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \partial_{11}V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2)[(D_{\mathbf{s}_1}^{\mathbf{p}}f_{\mathbf{x}}^{A\pm})(D_{\mathbf{s}_2}g_{\mathbf{x}}^{A\pm}) + (D_{\mathbf{s}_1}^{\mathbf{p}}g_{\mathbf{x}}^{A\pm})(D_{\mathbf{s}_2}f_{\mathbf{x}}^{A\pm})] \\
 & + \varepsilon^2 \frac{1}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \partial_{02}V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2)(D_{\mathbf{s}_2}^{\mathbf{p}}f_{\mathbf{x}}^{A\pm})(D_{\mathbf{s}_2}^{\mathbf{p}}g_{\mathbf{x}}^{A\pm}) \Big\}, \tag{5.12}
 \end{aligned}$$

and a similar definition is used for  $(f, g)_B$  by changing  $\mathbf{p}$  into  $-\mathbf{p}$ .

It is easy to check that  $X_0$  and  $X_\varepsilon$  are Hilbert spaces with inner products  $(\cdot, \cdot)_{X_0}$  and  $(\cdot, \cdot)_{X_\varepsilon}$ , respectively. We use the notations  $\langle \cdot, \cdot \rangle_0$  and  $\langle \cdot, \cdot \rangle_\varepsilon$  for pairing on  $X_0^* \times X_0$  and  $X_\varepsilon^* \times X_\varepsilon$ , respectively.

Finally, we define the solution spaces for the PN model and the atomistic model for an edge dislocation:

$$\begin{aligned}
 S_0 & = \{f \mid f - u_0 \in X_0\}, \\
 S_\varepsilon & = \{f \mid f - u_\varepsilon \in X_\varepsilon\}, \tag{5.13}
 \end{aligned}$$

where  $u_0 = \{u_0^+, u_0^-\}$  and  $u_\varepsilon = \{u_\varepsilon^+, u_\varepsilon^-\}$

$$\begin{aligned}
 u_0^+(\mathbf{x}) & = u_0^+(x, y) = \frac{1}{2\pi} \arctan x + \frac{1}{4}, \\
 u_0^-(\mathbf{x}) & = u_0^-(x, y) = -\frac{1}{2\pi} \arctan x - \frac{1}{4}, \\
 (u_\varepsilon^\pm)_{\mathbf{s}}^A & = u_0^\pm(\varepsilon \mathbf{s}), \quad (u_\varepsilon^\pm)_{\mathbf{s}}^B = u_0^\pm(\varepsilon \mathbf{s} + \varepsilon \mathbf{p}). \tag{5.14}
 \end{aligned}$$

These definitions are adopted to accommodate the boundary conditions in Equation (3.1)–(3.3) and Equation (2.2) for the edge dislocation in the PN model and the atomistic model.

In the proof of stability in Section 9, we divide the energy in each of the atomistic model and the PN model into two parts:

$$\begin{aligned}
 E_a^A[\mathbf{u}] & = \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left\{ \frac{1}{6} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} [V(\mathbf{s}_1 + \mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{A\pm} - \mathbf{u}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \mathbf{u}_{\mathbf{x}+\mathbf{s}_2}^{A\pm} - \mathbf{u}_{\mathbf{x}}^{A\pm})] \right. \\
 & + \frac{1}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} [V(\mathbf{p} + \mathbf{s}_1 + \mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{B\pm} - \mathbf{u}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \mathbf{u}_{\mathbf{x}+\mathbf{s}_2}^{A\pm} - \mathbf{u}_{\mathbf{x}}^{A\pm})] \\
 & - \frac{1}{3} [V(\mathbf{s}_1, \mathbf{s}_2) - V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2)] + \varepsilon^2 \sum_{\mathbf{s}} [U(\mathbf{u}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{u}_{\mathbf{x}}^{A-} + \mathbf{s} - \mathbf{d}) \\
 & \left. + U(\mathbf{u}_{\mathbf{x}+\mathbf{s}}^{B+} - \mathbf{u}_{\mathbf{x}}^{A-} + \mathbf{s} - \mathbf{p} - \mathbf{d}) - U(\mathbf{s} - \mathbf{d}) - U(\mathbf{s} - \mathbf{p} - \mathbf{d}) \right\}, \tag{5.15}
 \end{aligned}$$

$$\begin{aligned}
 E_a^B[\mathbf{u}] & = \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left\{ \frac{1}{6} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} [V(\mathbf{s}_1 + \mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{B\pm} - \mathbf{u}_{\mathbf{x}}^{B\pm}, \mathbf{s}_2 + \mathbf{u}_{\mathbf{x}+\mathbf{s}_2}^{B\pm} - \mathbf{u}_{\mathbf{x}}^{B\pm})] \right. \\
 & \left. + \frac{1}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} [V(-\mathbf{p} + \mathbf{s}_1 + \mathbf{u}_{\mathbf{x}+\mathbf{s}_1}^{A\pm} - \mathbf{u}_{\mathbf{x}}^{B\pm}, \mathbf{s}_2 + \mathbf{u}_{\mathbf{x}+\mathbf{s}_2}^{B\pm} - \mathbf{u}_{\mathbf{x}}^{B\pm})] \right\}
 \end{aligned}$$

$$\begin{aligned}
& -\frac{1}{3}V(\mathbf{s}_1, \mathbf{s}_2) - V(-\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2)] + \varepsilon^2 \sum_{\mathbf{s}} [U(\mathbf{u}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{u}_{\mathbf{x}}^{B-} + \mathbf{s} - \mathbf{p} - \mathbf{d}) \\
& - U(\mathbf{s} - \mathbf{p} - \mathbf{d}) + U(\mathbf{u}_{\mathbf{x}+\mathbf{s}}^{B+} - \mathbf{u}_{\mathbf{x}}^{B-} + \mathbf{s} - \mathbf{d}) - U(\mathbf{s} - \mathbf{d})], \tag{5.16}
\end{aligned}$$

$$\begin{aligned}
E_{\text{PN}}^A[\mathbf{u}] &= \lim_{R \rightarrow +\infty} \frac{1}{\sqrt{3}R} \int_{-R}^R \int_{\mathbb{R}} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \left\{ \frac{1}{12} \partial_{ij} V(\mathbf{s}_1, \mathbf{s}_2) [(\mathbf{s}_1 \cdot \nabla) \mathbf{u}^\pm]^i \right. \\
& \cdot [(\mathbf{s}_2 \cdot \nabla) \mathbf{u}^\pm]^j + \frac{1}{4} \partial_{ij} V(\mathbf{s}_1 + \mathbf{p}, \mathbf{s}_2) [(\mathbf{s}_1 + \mathbf{p}) \cdot (\nabla \mathbf{u}^\pm)]^i [(\mathbf{s}_2) \cdot (\nabla \mathbf{u}^\pm)]^j \left. \right\} \\
& + \sum_{\mathbf{s}} [U(\phi + \mathbf{s} - \mathbf{d}) + U(\phi + \mathbf{s} + \mathbf{p} - \mathbf{d}) - U(\mathbf{s} - \mathbf{d}) - U(\mathbf{s} + \mathbf{p} - \mathbf{d})] \, d\mathbf{x} \, d\mathbf{y}, \tag{5.17}
\end{aligned}$$

$$\begin{aligned}
E_{\text{PN}}^B[\mathbf{u}] &= \lim_{R \rightarrow +\infty} \frac{1}{\sqrt{3}R} \int_{-R}^R \int_{\mathbb{R}} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \left\{ \frac{1}{12} \partial_{ij} V(\mathbf{s}_1, \mathbf{s}_2) [(\mathbf{s}_1 \cdot \nabla) \mathbf{u}^\pm]^i \right. \\
& \cdot [(\mathbf{s}_2 \cdot \nabla) \mathbf{u}^\pm]^j + \frac{1}{4} \partial_{ij} V(\mathbf{s}_1 - \mathbf{p}, \mathbf{s}_2) [(\mathbf{s}_1 - \mathbf{p}) \cdot (\nabla \mathbf{u}^\pm)]^i [(\mathbf{s}_2) \cdot (\nabla \mathbf{u}^\pm)]^j \left. \right\} \\
& + \sum_{\mathbf{s}} [U(\phi + \mathbf{s} - \mathbf{d}) + U(\phi + \mathbf{s} - \mathbf{p} - \mathbf{d}) - U(\mathbf{s} - \mathbf{d}) - U(\mathbf{s} - \mathbf{p} - \mathbf{d})] \, d\mathbf{x} \, d\mathbf{y}. \tag{5.18}
\end{aligned}$$

The way we divide the energy, in both the atomistic model and the PN model, into two parts is that we put  $AAA$ ,  $AAB$  interactions (intralayer interactions) and interactions between  $A+$ ,  $A-$  and  $B+$ ,  $A-$  (inter-layer interactions) into the A part, and the rest of interactions are divided into the B parts.

Accordingly, we define  $\gamma$ -surface in  $E_{\text{PN}}^A[\mathbf{u}]$  as  $\gamma_A(\phi)$  and  $\gamma$ -surface in  $E_{\text{PN}}^B[\mathbf{u}]$  as  $\gamma_B(\phi)$ :

$$\begin{aligned}
\gamma_A(\phi) &:= \sum_{\mathbf{s}} U(\phi + \mathbf{s} - \mathbf{d}) + U(\phi + \mathbf{s} + \mathbf{p} - \mathbf{d}) - U(\mathbf{s} - \mathbf{d}) - U(\mathbf{s} + \mathbf{p} - \mathbf{d}) \\
\gamma_B(\phi) &:= \sum_{\mathbf{s}} U(\phi + \mathbf{s} - \mathbf{d}) + U(\phi + \mathbf{s} - \mathbf{p} - \mathbf{d}) - U(\mathbf{s} - \mathbf{d}) - U(\mathbf{s} - \mathbf{p} - \mathbf{d}). \tag{5.19}
\end{aligned}$$

**5.3. Assumptions.** Next we collect the assumptions that will be used in the proofs:

**A1** (weak inter-layer interaction):  $\varepsilon \ll 1$ .

**A2** (symmetry):  $U(-\mathbf{x}) = U(\mathbf{x})$  and  $V(\mathbf{s}_1, \mathbf{s}_2) = V(-\mathbf{s}_1, -\mathbf{s}_2)$ .

**A3** (regularity):  $U(\mathbf{x}) \in C^5(\mathbb{R} \setminus \{0\})$  and  $V(\mathbf{s}_1, \mathbf{s}_2) \in C^5(\mathbb{R}^2 \setminus \{|\mathbf{s}_1| = 0 \text{ or } |\mathbf{s}_2| = 0\})$ .

**A4** (fast decay): There are constants  $\theta > 0$  and  $C > 0$  such that:

$$\begin{aligned}
|U^{(k)}(\mathbf{x})| &\leq C|\mathbf{x}|^{-k-4-\theta}, \quad |\mathbf{x}| > 0, \\
|V^\beta(\mathbf{s}_1, \mathbf{s}_2)| &\leq C|\mathbf{s}_1|^{-\beta_1-6-\theta} |\mathbf{s}_2|^{-\beta_2-6-\theta}, \quad |\mathbf{s}_1|, |\mathbf{s}_2| > |\mathbf{p}|,
\end{aligned}$$

where  $\beta = (\beta_1, \beta_2)$  and  $V^\beta(\mathbf{s}_1, \mathbf{s}_2) = \partial_{\mathbf{s}_1}^{\beta_1} \partial_{\mathbf{s}_2}^{\beta_2} V(\mathbf{s}_1, \mathbf{s}_2)$ .

**A5** (elasticity constant):  $\alpha_1 > 0$  and  $\alpha_2 > 0$ .

**A6** ( $\gamma$ -surface):  $\nabla^2 \gamma(\mathbf{0})$  is a positive-definite matrix and  $\arg \min_{\phi \in \mathbb{R}^2} = \mathbb{L}$ , where  $\mathbb{L} = L(\mathbf{e}_i, \mathbf{o})$ .

**A7** (stability division):  $\bar{\vartheta} \geq \frac{1}{3}\vartheta$ , where

$$\begin{aligned} \bar{\vartheta} &= \min \left\{ \inf_{\|\mathbf{f}\|_{x_0}=1} \langle \delta^2 E_{\text{PN}}^A[\mathbf{v}]\mathbf{f}, \mathbf{f} \rangle_0, \inf_{\|\mathbf{f}\|_{x_0}=1} \langle \delta^2 E_{\text{PN}}^B[\mathbf{v}]\mathbf{f}, \mathbf{f} \rangle_0 \right\} \\ \vartheta &= \inf_{\|\mathbf{f}\|_{x_0}=1} \langle \delta^2 E_{\text{PN}}[\mathbf{v}]\mathbf{f}, \mathbf{f} \rangle_0, \end{aligned} \tag{5.20}$$

where  $\mathbf{v}$  is the solution of Peierls–Nabarro model (Equations (6.1)) and  $E_{\text{PN}}^A[\mathbf{v}]$  (Equation (5.17)),  $E_{\text{PN}}^B[\mathbf{v}]$  (Equation (5.18)) are a division of  $E_{\text{PN}}^A[\mathbf{v}]$ .

**A8** (small stability gap):  $\Delta < \min\{\frac{1}{3}, \frac{1}{3}\bar{\vartheta}\}$ , where  $\Delta = \max\{\Delta_A, \Delta_B\}$  and

$$\begin{aligned} \Delta_A &= \lim_{\varepsilon \rightarrow 0} \sup_{\|\mathbf{f}\|_{x_\varepsilon}=1} \langle \delta^2 E_{\text{PN}}^A[\mathbf{0}]\mathbf{f}_A, \mathbf{f}_A \rangle_0 - \langle \delta^2 E_a^A[\mathbf{0}]\mathbf{f}, \mathbf{f} \rangle_0 \\ \Delta_B &= \lim_{\varepsilon \rightarrow 0} \sup_{\|\mathbf{f}\|_{x_\varepsilon}=1} \langle \delta^2 E_{\text{PN}}^B[\mathbf{0}]\mathbf{f}_B, \mathbf{f}_B \rangle_0 - \langle \delta^2 E_a^B[\mathbf{0}]\mathbf{f}, \mathbf{f} \rangle_0, \end{aligned} \tag{5.21}$$

where  $\mathbf{f}_A$  and  $\mathbf{f}_B$  are the interpolations of complex lattice to be defined in Section 9.2.

For Assumption 1, as an example,  $\varepsilon \approx 0.0475 \ll 1$  in bilayer graphene, as shown in the Appendix of Ref. [14].

Assumptions A2–A4 are satisfied by most pair potentials, such as the Lennard–Jones potential, the Morse potential, the Stillinger–Weber potential. As for Assumption A5–A6, the physical meaning is that a perfect lattice without defects is a stable global minimizer of total energy.

For Assumption A7, we remark that  $\vartheta > 0$  (Proposition 7.1) describes the stability of the dislocation solution of Peierls–Nabarro model. If  $\delta^2 E_{\text{PN}}^A[\mathbf{u}] = \delta^2 E_{\text{PN}}^B[\mathbf{u}]$ , we obtain  $\frac{1}{2}\vartheta = \bar{\vartheta}$ . We notice the elastic energy parts in  $\delta^2 E_{\text{PN}}^A[\mathbf{u}]$  and  $\delta^2 E_{\text{PN}}^B[\mathbf{u}]$  are same:

$$\begin{aligned} & \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \partial_{ij} V(\mathbf{s}_1 - \mathbf{p}, \mathbf{s}_2) [(\mathbf{s}_1 - \mathbf{p}) \cdot (\nabla \mathbf{u}^\pm)]^i [(\mathbf{s}_2) \cdot (\nabla \mathbf{u}^\pm)]^j \\ &= \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \partial_{ij} V(-\mathbf{s}_1 - \mathbf{p}, -\mathbf{s}_2) [(-\mathbf{s}_1 - \mathbf{p}) \cdot (\nabla \mathbf{u}^\pm)]^i [(-\mathbf{s}_2) \cdot (\nabla \mathbf{u}^\pm)]^j \\ &= \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \partial_{ij} V(\mathbf{s}_1 + \mathbf{p}, \mathbf{s}_2) [(\mathbf{s}_1 + \mathbf{p}) \cdot (\nabla \mathbf{u}^\pm)]^i [(\mathbf{s}_2) \cdot (\nabla \mathbf{u}^\pm)]^j. \end{aligned}$$

Here the first equality is due to  $\mathbf{s}_1$  and  $\mathbf{s}_2$  traversing all values of  $\mathbb{L}^*$  and the second equality is due to  $V(\mathbf{s}_1, \mathbf{s}_2) = V(-\mathbf{s}_1, -\mathbf{s}_2)$ . Therefore the elastic constant in  $\delta^2 E_{\text{PN}}^A[\mathbf{u}]$  is the equal to the elastic constant in  $\delta^2 E_{\text{PN}}^B[\mathbf{u}]$ . The misfit energy parts in  $\delta^2 E_{\text{PN}}^A[\mathbf{u}]$  and  $\delta^2 E_{\text{PN}}^B[\mathbf{u}]$  are different since  $\mathbf{d} \neq \mathbf{0}$  (the vector between the centers of two layers), i.e.,  $\gamma_A''(\phi) \neq \gamma_B''(\phi)$  (Equations (5.19)). However, we notice that

$$\begin{aligned} & \gamma_A''(\phi) - \frac{1}{2}\gamma''(\phi) \\ &= \sum_{\mathbf{s}} \frac{1}{2} [U''(\phi + \mathbf{s} + \mathbf{p} - \mathbf{d}) - U''(\phi + \mathbf{s} - \mathbf{p} - \mathbf{d})] \\ &\approx \sum_{\mathbf{s}} \mathbf{p} \cdot U^{(3)}(\phi + \mathbf{s} - \mathbf{d}). \end{aligned} \tag{5.22}$$

Due to Assumption A4,  $U^{(3)}$  is smaller than  $U''$ . Therefore,  $\gamma_A''(\phi)$  and  $\gamma_B''(\phi)$  are close to  $\frac{1}{2}\gamma''(\phi)$  and  $\delta^2 E_{\text{PN}}^A[\mathbf{u}]$  and  $\delta^2 E_{\text{PN}}^B[\mathbf{u}]$  are close to  $\frac{1}{2}\delta^2 E_{\text{PN}}[\mathbf{u}]$ . Therefore, Assumption A7 is reasonable.



For Assumption A8, we remark that  $\Delta_A$  ( $\Delta_B$ ) characterizes the stability gap between atomistic model  $\delta^2 E_a^A[\mathbf{0}]$  ( $\delta^2 E_a^B[\mathbf{0}]$ ) and PN model  $\delta^2 E_{PN}^A[\mathbf{0}]$  ( $\delta^2 E_{PN}^B[\mathbf{0}]$ ) at the perfect lattice. We also provide an explicit formula for  $\delta^2 E_a^A[\mathbf{0}]$  in Lemma 9.3. In Remark 9.1, we show  $\Delta_A = 0$  and Assumption A7 holds when we consider nearest neighbor potential.

**6. Main results**

Based on the energies of the PN model (5.1) and the atomistic model (5.2), we obtain the following two Euler–Lagrange equations.

The Euler–Lagrange equation of the PN model reads as

$$\begin{cases} \delta E_{PN}[\mathbf{u}] = 0 \\ \mathbf{u} = (u, 0) \\ \lim_{x \rightarrow -\infty} u^\perp(x, y) = 0, \quad \lim_{x \rightarrow +\infty} u^\perp(x, y) = 1, \\ u^+(0, y) = \frac{1}{4}. \end{cases} \tag{6.1}$$

The Euler–Lagrange equation of the atomistic model reads as

$$\begin{cases} \delta E_a[\mathbf{u}] = 0 \\ \mathbf{u} = (u, 0) \\ u_s^{\kappa+} = -u_s^{\kappa-} \\ u_s^{\kappa\pm} + u_{-s}^{\kappa\pm} = \pm \frac{1}{2} \\ u \text{ satisfies Atomistic Dislocation Condition (ADC),} \\ \lim_{s \cdot \mathbf{e}_1 \rightarrow +\infty} (u_s^\kappa)^\perp = 1, \quad \lim_{s \cdot \mathbf{e}_1 \rightarrow -\infty} (u_s^\kappa)^\perp = 0, \end{cases} \tag{6.2}$$

where  $\kappa = A, B$  and Atomistic Dislocation Condition (ADC) will be defined in Section 9.1.

**THEOREM 6.1** (Existence of PN model). *If Assumptions A2–A5 hold, the PN system (6.1) has a unique solution  $\mathbf{v} = (v, 0) \in S_0$ ,  $v = \{v^+, v^-\}$ ,  $v^+ = -v^-$  and  $v^\pm(x, y) + v^\pm(-x, -y) = \pm \frac{1}{2}$ , which is also the  $X_0$ -global minimizer of the total energy of (5.1). Furthermore, we have  $v_y^+(x, y) = 0, v_x^+(x, y) > 0$  for all  $x, y$  and  $v^+(\cdot, y) \in W^{5,\infty}(\mathbb{R})$  and  $v^+(\cdot, y) \in W^{4,1}(\mathbb{R})$  for all  $y$ .*

**THEOREM 6.2** (Existence of atomistic model and convergence). *If Assumptions A1–A8 hold, there exists an  $\varepsilon_0$  such that for any  $0 < \varepsilon < \varepsilon_0$ , the atomistic model problem (6.2) has a unique  $\mathbf{v}^\varepsilon \in S_\varepsilon$ , which is also an  $X_\varepsilon$ -local minimizer of the total energy (5.2). Furthermore,  $\|\mathbf{v}^\varepsilon - \mathbf{v}\|_{X_\varepsilon} \leq C\varepsilon^2$ , where  $\mathbf{v}$  is the solution of PN model.*

**COROLLARY 6.1** (Convergence of Energy). *If Assumptions A1–A8 hold, there is an  $\varepsilon_0$  such that for any  $0 < \varepsilon < \varepsilon_0$ , we have*

$$|E_{PN}[\mathbf{v}] - E_a[\mathbf{v}^\varepsilon]| \leq C\varepsilon^2, \tag{6.3}$$

where  $\mathbf{v}$  and  $\mathbf{v}^\varepsilon$  are the solutions, respectively, of the PN model and the atomistic model in Theorems 6.1 and 6.2.

**7. Proof of Theorem 6.1**

In this section, we prove Theorem 6.1. We first prove that  $v^+ = -v^-$  and  $\partial_y v^\pm = 0$  for all  $(x, y) \in \mathbb{R}^2$ . Therefore, we can reduce the two-dimensional problem to a one-dimensional problem, and then the solution existence of the two-dimensional PN model follows the solution existence of the one-dimensional PN model proved in Ref. [14].

Since the solution of the PN model (6.1) is the global minimizer of the associated energy, we divide the one-step minimization into a two-step minimization:

- (1) Given  $\phi \in \Phi$ , find  $u_\phi = \{u_\phi^+, u_\phi^-\}$ , where  $u_\phi \in S_0$  with  $u_\phi^\perp = \phi$  such that

$$E_{\text{elas}}[u_\phi] = \inf_{u \in S_0, u^\perp = \phi} E_{\text{elas}}[u]$$

and we define  $E_{\text{elas}}^{II}[\phi] = \inf_{u \in S_0, u^\perp = \phi} E_{\text{elas}}[u]$ .

- (2) Find  $\phi^* \in \Phi$  such that

$$E_{\text{PN}}^{II}[\phi^*] = \inf_{\phi^* \in \Phi} E_{\text{PN}}^{II}[\phi] = E_{\text{elas}}^{II}[\phi] + E_{\text{mis}}[\phi].$$

Here

$$\Phi := \left\{ \phi \in C^5(\mathbb{R}^2) \mid \left\{ \phi - \frac{2}{\pi} \arctan x + 1, -\phi + \frac{2}{\pi} \arctan x - 1 \right\} \in X_0 \right\}.$$

Similar to Proposition 1 in Ref. [14], we have the follow lemma:

LEMMA 7.1. *Suppose that  $E_{\text{PN}}[u] < \infty$ . Then the two-step minimization problem is equivalent to the one-step minimization problem.*

*Proof.* The rigorous proof is given in [14, Proposition 1]. □

We also need the following two lemmas for the proof of Theorem 6.1. Lemma 7.2 is from Ref. [18], and the proof of Lemma 7.3 is similar to that of [14, Lemma 3].

LEMMA 7.2 ([18]). *Suppose that the curve  $\gamma: (x, y, z) = (f(s), g(s), h(s))$ ,  $s \in \mathbb{R}$ , is smooth, and  $f'^2 + g'^2 \neq 0$ , if the Jacobian determinant in*

$$P_0 = (x_0, y_0, z_0) = (f(s_0), g(s_0), h(s_0))$$

*is non-zero, i.e.,*

$$J = \begin{vmatrix} f'(s_0) & g'(s_0) \\ a(x_0, y_0, z_0) & b(x_0, y_0, z_0) \end{vmatrix} \neq 0,$$

*and  $a(P_0), b(P_0), c(P_0)$  are smooth near  $\gamma$ . Then the Cauchy initial value problem:*

$$\begin{cases} a(x, y, u)\partial_x u + b(x, y, u)\partial_y u = c(x, y, u) \\ u(f(s), g(s)) = h(s). \end{cases}$$

*has a unique solution near  $P_0$ .*

LEMMA 7.3. *Suppose  $U(\mathbf{x}) = U(-\mathbf{x})$ , then we obtain*

- (1)  $\gamma(\boldsymbol{\xi}) \geq \frac{1}{4} \gamma_{xx}(\mathbf{0}) |\boldsymbol{\xi}|^2, |\boldsymbol{\xi}| \leq C,$
- (2)  $\gamma(\mathbf{e}_1 + \boldsymbol{\xi}) = \gamma(\boldsymbol{\xi}),$
- (3)  $\gamma(\boldsymbol{\xi}_1) = \gamma(\boldsymbol{\xi}_2)$  when  $\boldsymbol{\xi}_1, \boldsymbol{\xi}_2$  are symmetric with respect to the  $y$ -axis, (7.1)

where  $C$  depends on  $\gamma_{xx}(\mathbf{0})$  and  $\mathbf{e}_1 = (1, 0)$ .

*Proof. (Proof of Theorem 6.1.)* Due to Lemma 3.1, we can rescale  $y$  to  $\bar{y}$ :

$$\bar{y} = \sqrt{\frac{\alpha_1}{\alpha_2}} y, \tag{7.2}$$

where  $\alpha_1$  and  $\alpha_2$  are defined in Lemma 3.1. To simplify the notation, we denote  $\bar{y}$  as  $y$  and  $\gamma(\xi) := \gamma((\xi, 0))$  in this proof. Furthermore, we notice (7.2) does not change the boundary condition of the PN model. Thus we define

$$\alpha := \frac{1}{2} \sqrt{\alpha_1 \alpha_2}.$$

In the PN model, the elastic energy is given by

$$E_{\text{elas}} = \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R \int_{\mathbb{R}} \frac{1}{2} \alpha (|\nabla u^+|^2 + |\nabla u^-|^2) dx dy.$$

We then divide the one-step minimization problem into a two-step minimization problem by Lemma 7.1. For any  $\phi \in \Phi$ , we have

$$\begin{aligned} & \arg \min_{u \in S_0, u^\pm = \phi} E_{\text{elas}}[u] \\ &= \arg \min_{u \in S_0} \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R \int_{\mathbb{R}} \frac{1}{2} \alpha (|\nabla u^+|^2 + |\nabla u^+ - \nabla \phi|^2) dx dy. \end{aligned} \tag{7.3}$$

Due to symmetry of quadratic functions, we have

$$\arg \min_{u \in S_0, u^\pm = \phi} E_{\text{elas}}[u] = \left\{ \frac{1}{2} \phi, -\frac{1}{2} \phi \right\}.$$

By Lemma 7.1, we further minimize the following energy  $E_{\text{PN}}^{II}[\phi]$ :

$$\begin{aligned} E_{\text{PN}}^{II}[\phi] &= \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R \int_{\mathbb{R}} \left( \frac{1}{4} \alpha |\nabla \phi|^2 + \gamma(\phi) \right) dx dy \\ &\geq \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R \int_{\mathbb{R}} |\nabla \phi(x, y)| \sqrt{\alpha \gamma(\phi(x, y))} dx dy \\ &= \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R \int_{\mathbb{R}} |\nabla \Gamma(\phi(x, y))| dx dy \\ &\geq \left| \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R \int_{\mathbb{R}} \nabla \Gamma(\phi(x, y)) dx dy \right| \\ &= \left| \left( \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{-R}^R \left[ \lim_{x \rightarrow +\infty} \Gamma(\phi(x, y)) - \lim_{x \rightarrow -\infty} \Gamma(\phi(x, y)) \right] dy, \right. \right. \\ &\quad \left. \left. \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{\mathbb{R}} [\Gamma(\phi(x, R)) - \Gamma(\phi(x, -R))] dx \right) \right| \\ &= \left| \left( \int_0^1 \sqrt{\alpha \gamma(\eta)} d\eta, \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{\mathbb{R}} [\Gamma(\phi(x, R)) - \Gamma(\phi(x, -R))] dx \right) \right| \\ &\geq \int_0^1 \sqrt{\alpha \gamma(\eta)} d\eta, \end{aligned} \tag{7.4}$$

where  $\Gamma(\xi) = \int_0^\xi \sqrt{\alpha \gamma(\eta)} d\eta$  for  $\xi \in \mathbb{R}$ . Note that the first inequality holds if and only if  $\frac{1}{2} \sqrt{\alpha} |\nabla \phi| = \sqrt{\gamma \circ \phi}$ . The second inequality holds if and only if there exists a constant  $\lambda$ , s.t  $\partial_x g = \lambda \partial_y g$  or  $\partial_y g = 0$  in  $\mathbb{R} \times (-R, R)$  for all  $R$ , where  $g = \Gamma(\phi(x, y))$ , and  $g(0, y) = \int_0^{\frac{1}{2}} \sqrt{\alpha \gamma(\eta)} d\eta$ .

Due to Lemma 7.2, we can solve this partial differential equation of first order by the method of characteristics, except  $\partial_y g = 0$ .

(1)  $\lambda \partial_x g = \partial_y g, \lambda \neq 0$ , i.e.,

$$J = \begin{vmatrix} 0 & 1 \\ \lambda & -1 \end{vmatrix} \neq 0.$$

Thus this problem is equivalent to

$$\begin{cases} \frac{dx}{dt} = \lambda, & \frac{dy}{dt} = -1, & \frac{dz}{dt} = 0 \\ (x, y, z)|_{t=0} = (0, s, \int_0^{\frac{1}{2}} \sqrt{\alpha\gamma(\eta)} d\eta). \end{cases}$$

Thus we get  $g \equiv \int_0^{\frac{1}{2}} \sqrt{\alpha\gamma(\eta)} d\eta$  near  $\{0\} \times (-R, R)$ , which is contradictory because the dislocation solution near  $x=0$  is not the constant solution.

(2)  $\partial_x g = 0, \lambda = 0$ , i.e.,

$$J = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \neq 0.$$

Thus we can also have  $g \equiv \int_0^{\frac{1}{2}} \sqrt{\alpha\gamma(\eta)} d\eta$  near  $\{0\} \times (-R, R)$ , which is contradictory.

(3)  $\partial_y g = 0, \lambda = 0$ , i.e.,

$$J = \begin{vmatrix} 0 & 1 \\ 0 & 1 \end{vmatrix} = 0,$$

which can let the second inequality hold its equality. Hence  $g = \int_0^{\phi(x,y)} \sqrt{\alpha\gamma(\eta)} d\eta$ ,  $\partial_y g = 0$  is equal to  $\partial_y \phi(x, y) = 0$  near  $\{0\} \times (-R, R)$ . Due to the arbitrariness of  $R$  and extension theorem, we have  $\partial_y \phi(x, y) = 0$  in  $\mathbb{R}^2$ .

In addition, the third inequality holds its equality if and only if

$$\lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{\mathbb{R}} [\Gamma(\phi(x, R)) - \Gamma(\phi(x, -R))] dx = 0,$$

which holds when  $\partial g = 0$ .

To summarize, we have  $E_{PN}^{II}[\phi] \geq \int_0^1 \sqrt{\alpha\gamma(\eta)} d\eta$ , and the equality holds if and only if

$$\begin{cases} \frac{1}{2} \sqrt{\alpha} |\nabla \phi| = \sqrt{\gamma \circ \phi} \\ \partial_y \phi(x, y) = 0. \end{cases} \tag{7.5}$$

We have shown that  $\phi(x, y)$  only depends on  $x$  when  $u$  is the  $X_0$ -global minimizer of the energy of  $E_{PN}$  and  $\partial_x \phi \geq 0$  is obvious. Thus we can only consider the following equation:

$$\frac{d\phi}{dx} = \frac{2}{\sqrt{\alpha}} \sqrt{\gamma(\phi)}, \quad \phi(0) = \frac{1}{2}. \tag{7.6}$$

Now we have reduced the two-dimensional problem to a one-dimensional problem. Then Theorem 6.1 follows from Lemma 7.3 and [14, Theorem 1]. □

In the proof of Theorem 6.1, we reduce a two-dimensional problem to a one-dimensional problem. Thus we can get the stability of the solution of the PN model from [14]:

PROPOSITION 7.1. *Let  $\mathbf{v}$  be the dislocation solution of the PN model, then there exists  $\vartheta > 0$  such that for any  $\mathbf{f} \in X_0$ , we have*

$$\langle \delta^2 E_{PN}[\mathbf{v}]\mathbf{f}, \mathbf{f} \rangle_0 \geq \vartheta \|\mathbf{f}\|_X^2. \tag{7.7}$$

*Proof.* Thanks to [14, Proposition 3], for all  $y \in \mathbb{R}$ ,  $v(\cdot, y)$  satisfies:

$$\begin{aligned} & \int_{\mathbb{R}} \alpha_1 (\partial_x f^+(x, y))^2 + \alpha_2 (\partial_y f^+(x, y))^2 + 2\gamma''(2v)(f^+(x, y))^2 dx \\ & \geq \vartheta(y) \left[ \int_{\mathbb{R}} \alpha_1 (\partial_x f^+(x, y))^2 + \alpha_2 (\partial_y f^+(x, y))^2 + \frac{8\sqrt{3}}{3} (f^+(x, y))^2 dx \right], \end{aligned} \tag{7.8}$$

where  $\vartheta(y)$  is the constant depending on  $y$ . Due to the uniformity of  $v$  in  $y$ -direction,  $\vartheta(y)$  is also uniform in  $y$ -direction. Thus we calculate the average value of both sides in (7.8) along  $y$ -direction and obtain (7.7).  $\square$

**8. Consistency of the PN model**

In this section, we prove the consistency of the PN model.

For simplicity of notations, we introduce some notations:

$$U_{k, \mathbf{s}} := \sup_{|\boldsymbol{\xi} - \mathbf{s}| \leq 1} |\nabla^k U(\boldsymbol{\xi})|, \quad \mathbf{s} \in \mathbb{L}, \tag{8.1}$$

$$V_{\beta, \mathbf{s}_1, \mathbf{s}_2} := \sup_{|\boldsymbol{\xi}_i - \mathbf{s}_i| \leq 1} |\nabla^\beta V(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2)|, \quad i = 1, 2, \quad \beta \in \mathbb{Z}^2, \tag{8.2}$$

$$\mathbf{v}_{k, \mathbf{s}_1, \mathbf{s}_2} := \sup_{|\mathbf{x} - \mathbf{s}_1| < |\mathbf{s}_2|} |\nabla^\beta v(x, y)|, \quad |\beta| = k,$$

where  $\mathbf{v} = (v, 0)$ .

LEMMA 8.1. *Suppose that Assumptions A2–A4 hold and  $k = 1, 2, \dots, 5$ . Then there exist constants  $H_1, H_2$  such that*

$$\sum_{\mathbf{s}} |\mathbf{s}|^{k+1} U_{k, \mathbf{s}} \leq H_1, \quad \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} |\mathbf{s}_1|^{a_1} |\mathbf{s}_2|^{a_2} V_{\alpha, \mathbf{s}_1, \mathbf{s}_2} \leq H_2, \tag{8.3}$$

where  $a_i \leq |\beta_i| + 4$  and  $\beta_i$  is defined in A4 for  $i = 1, 2$ .

*Proof.* Without loss of generality, we just prove

$$\sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} |\mathbf{s}_1|^{a_1} |\mathbf{s}_2|^{a_2} V_{\alpha, \mathbf{s}_1, \mathbf{s}_2} \leq H_2.$$

As for A4, we have

$$\begin{aligned} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} |\mathbf{s}_1|^{a_1} |\mathbf{s}_2|^{a_2} V_{\alpha, \mathbf{s}_1, \mathbf{s}_2} & \leq \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} |\mathbf{s}_1|^{a_1} |\mathbf{s}_2|^{a_2} |\mathbf{s}_1|^{-a_1 - 2 - \theta} |\mathbf{s}_2|^{-a_2 - 2 - \theta} \\ & \leq \sum_{\mathbf{s}_1} |\mathbf{s}_1|^{-2 - \theta} \sum_{\mathbf{s}_2} |\mathbf{s}_2|^{-2 - \theta} \leq H_2. \end{aligned}$$

$\square$

LEMMA 8.2. *Suppose that A1–A5 hold, then for  $k \leq 4$ , we have*

$$\varepsilon^2 \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \mathbf{v}_{k, \mathbf{x}, \mathbf{s}} \leq C|\mathbf{s}|,$$

where  $\mathbf{v}$  is the dislocation solution in Theorem 6.1.

*Proof.* Since in Theorem 6.1, we have proved  $\partial_y v^\pm = 0$  and  $\mathbf{v} = (v, 0)$ . Thus the two-dimensional problem can be reduced into a one-dimensional problem. Thanks to [14, Lemma 7], we have proved Lemma 8.2.  $\square$

In the following analysis of the paper, the constant  $C$  may be different from line to line.

PROPOSITION 8.1. *Suppose that Assumptions A1–A6 hold. Let  $\mathbf{v}$  be the dislocation solution of the PN model in Theorem 6.1, then there exist  $C$  and  $\varepsilon_0$ , when  $0 < \varepsilon < \varepsilon_0$  and  $\mathbf{f} \in X_\varepsilon$  we have*

$$\left| \langle \delta E_a[\mathbf{v}] - \delta E_{PN}[\mathbf{v}], \mathbf{f} \rangle_\varepsilon \right| = \left| \langle \delta E_a[\mathbf{v}], \mathbf{f} \rangle_\varepsilon \right| \leq C\varepsilon^2 \|\mathbf{f}\|_{X_\varepsilon}, \tag{8.4}$$

where  $C$  is independent on  $\varepsilon$ .

*Proof.* As for the  $\left| \langle \delta E_a[\mathbf{v}] - \delta E_{PN}[\mathbf{v}], \mathbf{f} \rangle_\varepsilon \right|$ , there are two parts, elastic energy parts and misfit energy parts. Furthermore, for the elastic energy parts, it can be divided into four parts, *AAA*, *AAB*, *ABB* and *BBB*. For the *AAA* and *BBB* parts, they are simple lattice cases, which have been proved in [14] (second-order accuracy). The remaining question is to estimate the *AAB* and *ABB* parts:

$$\begin{aligned} R_{\text{elas}} &= \lim_{R \rightarrow +\infty} \frac{1}{4R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \left\{ \left[ \partial_1 V(\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm}) \right] \right. \\ &\quad \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm} + \left[ \partial_2 V(\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm}) \right] \varepsilon D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm} \\ &\quad \left[ \partial_1 V(-\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{-\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{B\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{B\pm}) \right] \varepsilon D_{\mathbf{s}_1}^{-\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{B\pm} \\ &\quad \left. + \left[ \partial_2 V(-\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{-\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{B\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{B\pm}) \right] \varepsilon D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{B\pm} \right\} \\ &\quad + \frac{\varepsilon^2}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{s}_1 + \mathbf{p}, \mathbf{s}_2) [(\mathbf{s}_1 + \mathbf{p}) \cdot (\nabla)]^i (\mathbf{s}_2 \cdot \nabla)^j \mathbf{v}_{\mathbf{x}}^{A\pm} \mathbf{f}_{\mathbf{x}}^{A\pm} \\ &\quad + \frac{\varepsilon^2}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{s}_1 + \mathbf{p}, \mathbf{s}_2) [(\mathbf{s}_1 + \mathbf{p}) \cdot (\nabla)]^i (\mathbf{s}_2 \cdot \nabla)^j \mathbf{v}_{\mathbf{x}}^{B\pm} \mathbf{f}_{\mathbf{x}}^{B\pm}. \end{aligned} \tag{8.5}$$

The first four terms are from  $\delta E_a[\mathbf{v}]$  and the last two terms are from  $\delta E_{PN}[\mathbf{v}]$ .

As for the misfit energy parts, there are four parts,  $A^+A^-$  (the inter-layer interactions between the atoms  $A$  in the upper layer and the atoms  $A$  in the lower layer),  $A^+B^-$ ,  $B^+A^-$  and  $B^+B^-$ .  $A^+A^-$  and  $B^+B^-$  are the simple lattice cases. Therefore we restrict our attention to  $A^+B^-$  and  $B^+A^-$ . We estimate  $B^+A^-$  only:

$$\begin{aligned} R_{\text{mis}} &= \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} \left[ U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_{\mathbf{x}+\mathbf{s}}^{B+} - \mathbf{v}_{\mathbf{x}}^{A-}) (\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{B+} - \mathbf{f}_{\mathbf{x}}^{A-}) \right. \\ &\quad + U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_{\mathbf{x}}^{B+} - \mathbf{v}_{\mathbf{x}-\mathbf{s}}^{A-}) (\mathbf{f}_{\mathbf{x}}^{B+} - \mathbf{f}_{\mathbf{x}-\mathbf{s}}^{A-}) \\ &\quad - U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_{\mathbf{x}}^{A+} - \mathbf{v}_{\mathbf{x}}^{A-}) (\mathbf{f}_{\mathbf{x}}^{A+} - \mathbf{f}_{\mathbf{x}}^{A-}) \\ &\quad \left. - U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_{\mathbf{x}}^{B+} - \mathbf{v}_{\mathbf{x}}^{B-}) (\mathbf{f}_{\mathbf{x}}^{B+} - \mathbf{f}_{\mathbf{x}}^{B-}) \right]. \end{aligned} \tag{8.6}$$

The first two terms are from  $\delta E_a[\mathbf{v}]$  and the last two terms are from  $\delta E_{PN}[\mathbf{v}]$ .

- (1)  $R_{\text{elas}}$ : Here we show  $R_{\text{elas}}$  is the sum of  $\varepsilon^4$  order terms. In other words, we show  $\varepsilon$ ,  $\varepsilon^2$  and  $\varepsilon^3$  order terms disappear in  $R_{\text{elas}}$ . Without loss of generality, we consider one term from the  $AAB$  interactions in the atomistic model:

$$\lim_{R \rightarrow +\infty} \frac{1}{4R} \sum_{\mathbf{x} \in \mathbb{L}_R \langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum [\partial_1 V(\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm})] \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm}.$$

Due to Lemma 3.1, we notice the pairwise  $AB$  has rotational symmetry:

$$\begin{aligned} & \lim_{R \rightarrow +\infty} \frac{1}{4R} \sum_{\mathbf{x} \in \mathbb{L}_R \langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum [\partial_1 V(\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm})] \mathbf{f}_{\mathbf{x}}^{A\pm} \\ &= \lim_{R \rightarrow +\infty} \frac{1}{12R} \sum_{\mathbf{x} \in \mathbb{L}_R \langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum \left[ \partial_1 V(\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm}) \right. \\ & \quad + \partial_1 V(\mathbf{p} + \mathbf{s}_{11} + \varepsilon D_{\mathbf{s}_{11}}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_{21} + \varepsilon D_{\mathbf{s}_{21}} \mathbf{v}_{\mathbf{x}}^{A\pm}) \\ & \quad \left. + \partial_1 V(\mathbf{p} + \mathbf{s}_{12} + \varepsilon D_{\mathbf{s}_{12}}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_{22} + \varepsilon D_{\mathbf{s}_{22}} \mathbf{v}_{\mathbf{x}}^{A\pm}) \right] \mathbf{f}_{\mathbf{x}}^{A\pm} \end{aligned} \tag{8.7}$$

where the definitions of  $\mathbf{s}_{11}$ ,  $\mathbf{s}_{12}$ ,  $\mathbf{s}_{21}$  and  $\mathbf{s}_{22}$  are from Lemma 3.1 (by rotation of  $2\pi/3$  and  $4\pi/3$  for  $\mathbf{s}_1$  and  $\mathbf{s}_2$ ). Thanks to  $\mathbf{f}_{\mathbf{x}}^{A+} = -\mathbf{f}_{\mathbf{x}}^{A-}$  and  $\mathbf{v}_{\mathbf{x}}^{A+} = -\mathbf{v}_{\mathbf{x}}^{A-}$ , there are no even order terms in the Taylor expansion at  $(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2)$ :

$$\begin{aligned} & \lim_{R \rightarrow +\infty} \frac{1}{4R} \sum_{\mathbf{x} \in \mathbb{L}_R \langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum [\partial_1 V(\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm})] \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm} \\ &= \lim_{R \rightarrow +\infty} \frac{1}{6R} \sum_{\mathbf{x} \in \mathbb{L}_R \langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum \left\{ \partial_{20} V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) \varepsilon (D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A+} + D_{\mathbf{s}_{11}}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A+} + D_{\mathbf{s}_{12}}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A+}) \right. \\ & \quad + \partial_{11} V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) (\varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A+} + \varepsilon D_{\mathbf{s}_{21}} \mathbf{v}_{\mathbf{x}}^{A+} + \varepsilon D_{\mathbf{s}_{22}} \mathbf{v}_{\mathbf{x}}^{A+}) \\ & \quad + \varepsilon^3 \sum_{\mathbf{t}} \partial_{\mathbf{t}} V(\boldsymbol{\xi}) \binom{3}{t_1} \left[ (D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A+})^{t_1} (D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A+})^{t_2} + (D_{\mathbf{s}_{11}}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A+})^{t_1} (D_{\mathbf{s}_{21}} \mathbf{v}_{\mathbf{x}}^{A+})^{t_2} \right. \\ & \quad \left. \left. + (D_{\mathbf{s}_{21}}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A+})^{t_1} (D_{\mathbf{s}_{22}} \mathbf{v}_{\mathbf{x}}^{A+})^{t_2} \right] \right\} \mathbf{f}_{\mathbf{x}}^{A+}, \end{aligned} \tag{8.8}$$

where  $\boldsymbol{\xi}$  is a four-dimensional vector,

$$t \in \{ \mathbf{t} = (t_1 + 1, t_2) \mid t_1, t_2 \in \mathbb{N}, t_1 \geq 0, t_2 \geq 0, t_1 + t_2 = 3 \}.$$

Due to the calculation in Lemma 3.1 (the symmetry of  $\mathbf{s}_i$ ,  $\mathbf{s}_{i1}$ ,  $\mathbf{s}_{i2}$ ), we know that  $\varepsilon$  terms vanish in (8.8). Furthermore,  $\varepsilon^2$  terms vanish in  $R_{\text{elas}}$  since the formula of elastic energy in the PN model is from the second-order terms of the atomistic model (the definition of (3.9)). In other words, the definition of elastic energy in the Peierls–Nabarro model is to collect all the second-order terms of intralayer interactions in the atomistic model. Hence the second-order terms in  $R_{\text{elas}}$  disappear naturally. The remaining problem is to show that the  $\varepsilon^3$  terms vanish in  $R_{\text{elas}}$ . For  $O(\varepsilon^4)$  terms, the sum of them is  $O(\varepsilon^2)$  as shown by (8.13). But by direct calculation, the symmetry of  $\mathbf{s}_i$ ,  $\mathbf{s}_{i1}$ ,  $\mathbf{s}_{i2}$  cannot derive the disappearance of  $\varepsilon^3$ . However, for each  $\varepsilon^3$  term in (8.7), we are able to find similar terms in the  $ABB$  part. Now we restrict our attention to the  $O(\varepsilon^3)$  terms in

$$\partial_{20} V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) (\varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A+} + \varepsilon D_{\mathbf{s}_{11}}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A+} + \varepsilon D_{\mathbf{s}_{12}}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A+}) \mathbf{f}_{\mathbf{x}}^{A+}, \tag{8.9}$$

which can be denoted as

$$\partial_{20}V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2)|\mathbf{s}_1|^3 \varepsilon^3 (\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{A+}) \mathbf{f}_x^{A+}, \tag{8.10}$$

where  $\mathbf{h}$  is a constant vector and  $\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{A+}$  is a two-dimensional vector. In addition, in the  $ABB$  part, a similar term is

$$\partial_{20}V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2)|\mathbf{s}_1|^3 \varepsilon^3 (-\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{B+}) \mathbf{f}_x^{B+}. \tag{8.11}$$

The reason why the direction of corresponding item is  $-\mathbf{h}$  is shown in Figure 8.1. As in Figure 8.1, three red lines are interactions in  $AAB$  (8.7) part and three blue lines are interactions in  $ABB$  part and they are center symmetry of  $\mathbf{x} + \frac{1}{2}\mathbf{p}$  from each other. Combining those two terms, we have

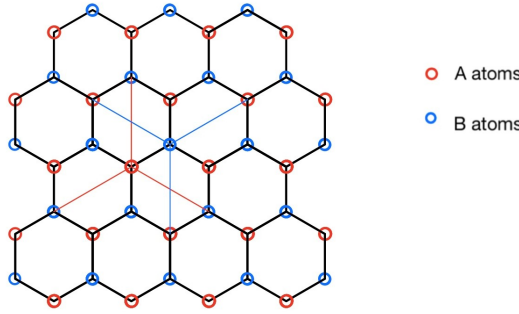


FIG. 8.1. Similar terms in the interactions in  $ABB$  part.

$$\begin{aligned} & \left| \partial_{20}V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) \varepsilon^3 [(-\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{B+}) \mathbf{f}_x^{B+} + (\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{A+}) \mathbf{f}_x^{A+}] \right| \\ \leq & \left| \partial_{20}V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) \varepsilon^3 |\mathbf{s}_1|^3 [(-\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{B+}) \mathbf{f}_x^{B+} + (\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{A+}) \mathbf{f}_x^{A+}] \right| \\ & + \left| \partial_{20}V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) \varepsilon^3 |\mathbf{s}_1|^3 [(-\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{A+}) \mathbf{f}_x^{B+} + (\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{A+}) \mathbf{f}_x^{A+}] \right| \\ \leq & \left| \partial_{20}V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) \varepsilon^4 |\mathbf{s}_1|^3 [Cv_{4,\mathbf{x},\mathbf{s}_1} \mathbf{f}_x^{B+} + (\mathbf{h} \cdot \nabla^3 \mathbf{v}_x^{A+}) D_0^p \mathbf{f}_x^{A+}] \right|. \end{aligned} \tag{8.12}$$

Similar property can be used for other  $\varepsilon^3$  terms. Thus we notice  $\varepsilon^3$  terms reduce to  $\varepsilon^4$  terms in  $R_{\text{elas}}$ . As for the  $O(\varepsilon^4)$  terms, we have

$$\begin{aligned} & \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{\mathbf{x} \in \mathbb{L}_R} C \varepsilon^4 V_{(t_1+1, t_2), \mathbf{s}_1, \mathbf{s}_2} |\mathbf{s}_1|^{t_1} |\mathbf{s}_2|^{t_2} \mathbf{v}_{4,\mathbf{x},\mathbf{s}_2} \mathbf{f}_x^{A+} \\ \leq & \varepsilon^2 \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} V_{(t_1, t_2), \mathbf{s}_1, \mathbf{s}_2} |\mathbf{s}_1|^{t_1} |\mathbf{s}_2|^{t_2+1} \|\mathbf{f}\|_{X_\varepsilon} \\ \leq & C \varepsilon^2 \|\mathbf{f}\|_{X_\varepsilon}, \end{aligned} \tag{8.13}$$

where the last two inequalities are from Lemma 8.1, Lemma 8.2 and  $t_1 + t_2 = 3$ . Thus  $R_{\text{elas}}$  is an  $O(\varepsilon^2)$  term.

(2)  $R_{\text{mis}}$ : We divide  $R_{\text{mis}}$  into two parts:

$$\begin{aligned} R_{\text{mis},1} = & \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_s \left[ U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_{\mathbf{x}+\mathbf{s}}^{B+} - \mathbf{v}_x^{A-}) \right. \\ & \left. + U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_x^{B+} - \mathbf{v}_{\mathbf{x}-\mathbf{s}}^{A-}) - U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_x^{A+} - \mathbf{v}_x^{A-}) \right] \end{aligned}$$



$$\begin{aligned}
 & -U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{B+}-\mathbf{v}_x^{B-})\Big](\mathbf{f}_x^{A+}-\mathbf{f}_x^{B-}) \\
 R_{\text{mis},2} = & \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} \left[ U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{B+}-\mathbf{v}_{\mathbf{x}}^{A-})(\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{B+}-\mathbf{f}_{\mathbf{x}}^{B+}) \right. \\
 & + U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{B+}-\mathbf{v}_{\mathbf{x}-\mathbf{s}}^{A-})(\mathbf{f}_x^{A-}-\mathbf{f}_{\mathbf{x}-\mathbf{s}}^{A-}) \\
 & - U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{A+}-\mathbf{v}_x^{A-})(\mathbf{f}_x^{A+}-\mathbf{f}_x^{B+}) \\
 & \left. - U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{B+}-\mathbf{v}_x^{B-})(\mathbf{f}_x^{A-}-\mathbf{f}_x^{B-}) \right]. \tag{8.14}
 \end{aligned}$$

As for  $R_{\text{mis},1}$ , we apply Taylor expansion at  $U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{B+}-\mathbf{v}_x^{A-})$  and obtain

$$\begin{aligned}
 R_{\text{mis},1} \leq & \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} \left[ U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{B+}-\mathbf{v}_x^{A-}) \right. \\
 & \times |\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{B+}+\mathbf{v}_{\mathbf{x}-\mathbf{s}}^{A+}-\mathbf{v}_x^{A+}-\mathbf{v}_x^{B+}|(\mathbf{f}_x^{A+}-\mathbf{f}_x^{B-}) \\
 & \left. + U_{3,\mathbf{s}}(|\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{B+}-\mathbf{v}_x^{B+}|^2+|\mathbf{v}_x^{A+}-\mathbf{v}_{\mathbf{x}-\mathbf{s}}^{A+}|^2+2|\mathbf{v}_x^{A+}-\mathbf{v}_x^{B+}|^2) \times (\mathbf{f}_x^{A+}-\mathbf{f}_x^{B-}) \right]. \tag{8.15}
 \end{aligned}$$

Due to

$$\begin{aligned}
 |\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{B+}+\mathbf{v}_{\mathbf{x}-\mathbf{s}}^{A+}-\mathbf{v}_x^{A+}-\mathbf{v}_x^{B+}| & = |\varepsilon(\mathbf{s}+\mathbf{p}) \cdot \nabla \mathbf{v}_x^{A+}-\varepsilon(\mathbf{s}+\mathbf{p}) \cdot \nabla \mathbf{v}_x^{B+}+O(\varepsilon)| \\
 & = |\varepsilon^2(\mathbf{s}+\mathbf{p}) \cdot \nabla^2 \mathbf{v}_x^{A+} \cdot (-\mathbf{p})+O(\varepsilon^2)| \\
 |\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{B+}-\mathbf{v}_x^{B+}|^2 & = \varepsilon^2|\mathbf{s} \cdot \nabla \mathbf{v}_x^{B+}+O(\varepsilon)|^2, \tag{8.16}
 \end{aligned}$$

each term in  $R_{\text{mis},1}$  is a  $\varepsilon^4$  term. Similar to (8.13), we know  $R_{\text{mis},1}$  is a  $\varepsilon^2$  term. For  $R_{\text{mis},2}$ , due to the symmetry of  $\mathbf{f}$  and  $\mathbf{v}$ , we obtain

$$\begin{aligned}
 R_{\text{mis},2} = & \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} \left[ U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{B+}-\mathbf{v}_x^{A-}) \right. \\
 & \left. - U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_{\mathbf{x}+2\mathbf{s}}^{B+}-\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{A-}) \right](\mathbf{f}_{2\mathbf{s}+\mathbf{x}}^{B+}-\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{A+}) \\
 & - \left[ U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{A+}-\mathbf{v}_x^{A-})-U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{B+}-\mathbf{v}_x^{B-}) \right] \times (\mathbf{f}_x^{A+}-\mathbf{f}_x^{B+}) \\
 = & \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} U_{2,\mathbf{s}}(-\varepsilon \nabla \mathbf{s} \cdot \mathbf{v}_{\mathbf{x}+\mathbf{s}}^{B+}-\varepsilon \mathbf{s} \cdot \nabla \mathbf{v}_x^{A+}+O(\varepsilon))(\varepsilon D_{\mathbf{s}}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}+\mathbf{s}}^{A+}) \\
 & - U_{2,\mathbf{s}}(2\varepsilon \mathbf{p} \cdot \nabla \mathbf{v}_x^{A+}+O(\varepsilon))(\varepsilon D_{\mathbf{0}}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}+\mathbf{s}}^{A+}). \tag{8.17}
 \end{aligned}$$

Therefore, each term in  $R_{\text{mis},2}$  is the  $\varepsilon^4$  terms. Similar to (8.13), we know  $R_{\text{mis},1}$  is a  $\varepsilon^2$  term. □

In the proof of the consistency, we assume the symmetry of  $\mathbf{f}$  and  $\mathbf{v}$ . However, we can remove this assumption. For an example, in  $R_{\text{mis},1}$ ,

$$\begin{aligned}
 & \varepsilon^2 \sum_{\mathbf{s}} -U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{A+}-\mathbf{v}_x^{A-})(\mathbf{f}_x^{A+}-\mathbf{f}_x^{B+}) \\
 & - U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{B+}-\mathbf{v}_x^{B-})(\mathbf{f}_x^{A-}-\mathbf{f}_x^{B-}) \\
 = & \varepsilon^2 \sum_{\mathbf{s}} -\left[ U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{A+}-\mathbf{v}_x^{A-})-U'(s+\mathbf{p}-\mathbf{d}+\mathbf{v}_x^{B+}-\mathbf{v}_x^{B-}) \right]
 \end{aligned}$$

$$\times (\mathbf{f}_x^{A+} - \mathbf{f}_x^{B+}) - U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_x^{B+} - \mathbf{v}_x^{B-})(\mathbf{f}_x^{A-} - \mathbf{f}_x^{B-} + \mathbf{f}_x^{A+} - \mathbf{f}_x^{B+}).$$

We already know the first term is a second order term due to Equations (8.17). The second term is a new term since we do not assume the symmetry of  $\mathbf{f}$ . However, we denote  $\mathbf{f}_x^{A+} + \mathbf{f}_x^{A-} = \varepsilon \bar{D}_0 \mathbf{f}_x^{A+}$ . Hence, we obtain

$$\begin{aligned} & \varepsilon^2 \sum_s -U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_x^{B+} - \mathbf{v}_x^{B-})(\mathbf{f}_x^{A-} - \mathbf{f}_x^{B-} + \mathbf{f}_x^{A+} - \mathbf{f}_x^{B+}) \\ &= \varepsilon^2 \sum_s -U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_x^{B+} - \mathbf{v}_x^{B-})(\varepsilon \bar{D}_0 \mathbf{f}_x^{A+} - \varepsilon \bar{D}_0 \mathbf{f}_x^{B+}). \end{aligned}$$

Similarly, we can obtain

$$\varepsilon^2 \sum_s -U'(\mathbf{s} + \mathbf{p} - \mathbf{d} + \mathbf{v}_x^{A+} - \mathbf{v}_x^{A-})(\varepsilon \bar{D}_0 \mathbf{f}_x^{B+} - \varepsilon \bar{D}_0 \mathbf{f}_x^{A+})$$

from  $R_{\text{mis},2}$ . Then we combine them and find that each term is still a  $\varepsilon^4$  term.

REMARK 8.1. In this paper, we consider a complex-lattice bilayer system that consists of same type of atoms. Our method can be extended to complex-lattice bilayer systems in which  $A$  and  $B$  atoms are different, e.g. the boron nitride systems. However, the accuracy of the PN model in those systems will be  $O(\varepsilon)$  instead of  $O(\varepsilon^2)$ . In the consistency proof shown above in this paper, the  $\varepsilon^3$  order terms are canceled due to symmetry of  $A$  and  $B$  atoms (Figure 8.1). For the boron nitride system, the coefficients in Equations (8.10) and (8.11) will be different, hence the  $\varepsilon^3$  order terms cannot be canceled and the accuracy of PN model in such a case will be only  $O(\varepsilon)$ .

**9. Stability of the atomistic model and proof of Theorem 6.2**

In this section, we prove stability of the atomistic model for the complex lattice. Since we already have stability of the Peierls–Nabarro model, our method is to show that the gap between  $\delta^2 E_{\text{PN}}[v]$  and  $\delta^2 E_a[v]$  is small. Here we are not able to prove the stability directly as the consistency because we do not know the exact value of  $\delta^2 E_{\text{PN}}[v]$  in the discrete space. More precisely, in the consistency of the Peierls–Nabarro model, we know  $\delta E_{\text{PN}}[v] = 0$  because  $v$  is the solution of the Peierls–Nabarro model; whereas for  $\delta^2 E_{\text{PN}}[v]$ , we just know it is positive (stability of Peierls–Nabarro model Proposition 7.1) in the continuum space.

Therefore, we construct interpolation polynomials on the complex lattice in order to estimate the energies of the two models and to compare two models. However, there are four kinds of intralayer interactions (elastic energy) and four kinds of interlayer interactions (misfit energy). It is difficult to describe the complex lattice by a single interpolation polynomial. Even if we establish a single interpolation polynomial for complex lattice, the order of the polynomial will be very high and the resulting energy will have unphysical oscillations. In order to solve this problem, we construct two interpolation polynomials to describe the energy on the complex lattice, and each polynomial describes a part of the interactions in the atomistic model.

**9.1. Atomistic dislocation condition (ADC).** In this subsection, we introduce the Atomistic Dislocation Condition (ADC).

We focus on the upper layer. Consider an A atom located on  $\{x=0\}$  as shown in Figure 9.1. By assumption, the  $x$ -component of the displacement of this atom is  $\frac{1}{4}$ . If on the crystallographic line where atoms have the same  $y$  coordinate, there is no

atom at  $x=0$ , e.g., atoms B and C in Figure 9.1, we assume that the average of the displacement about the two atoms is  $\frac{1}{4}$ . That is,

$$u_A = \frac{1}{4}, \quad \text{or} \quad \frac{u_C + u_B}{2} = \frac{1}{4}, \tag{9.1}$$

for all atoms on or near  $x=0$ . More precisely, if there is an atom located at  $x=0$  on a crystallographic line with the same  $y$  coordinate, the first equation in (9.1) holds; while if there no atom located at  $x=0$  on a crystallographic line with the same  $y$  coordinate, the second equation in (9.1) holds; see Figure 9.1. If the atomistic displacement field on the discrete space satisfies this assumption, we say that the atomistic model satisfies **Atomistic Dislocation Condition (ADC)**.

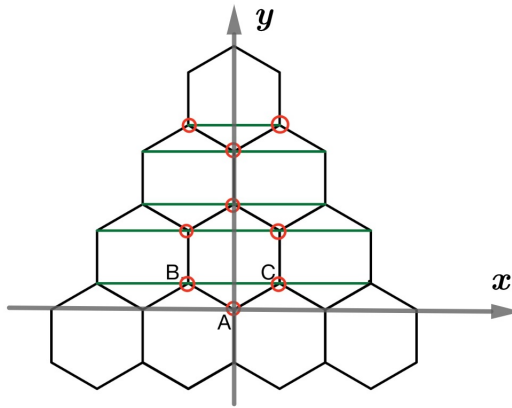


FIG. 9.1. Atomistic Dislocation Condition (ADC).

**9.2. Interpolation polynomials of complex lattice.** In this subsection, we construct interpolation polynomials for estimating the energy of the atomistic model with complex lattice, which enables us to prove the stability of atomistic model by comparing the atomistic model and the PN model directly.

Now we construct the interpolation polynomials for a test function  $f \in X_\epsilon$ . Two different interpolation polynomials are constructed on the complex lattice based on the two kind of atoms, A and B, and the four kinds of intralayer interactions, AAA, AAB and BBB, BBA. Here we focus on the intralayer interactions because the interlayer interactions can be handled in a relatively easier way.

We first consider the AAA and AAB interactions. By connecting the neighboring A atoms,  $\mathbb{R}^2$  plane is divided into triangles; see Figure 9.2(a). As shown in Figure 9.2(b), there are only two kind of triangles, whose three vertices are A atoms (AAA interactions) and two A atoms and one B atom (AAB interactions), respectively.

For each triangle, we construct the linear Lagrange interpolation for the interaction energy. Thus we get a piecewise linear interpolating function in  $\mathbb{R}^2$ . Below we give a brief introduction to linear Lagrange interpolation on a triangle. More details can be found, e.g. in [3].

Suppose  $T(x, y) = Ax + By + C$  is an interpolation polynomial in each equilateral triangle. We denote three vertices in the equilateral triangle as  $(x_1, y_1)$ ,  $(x_2, y_2)$  and

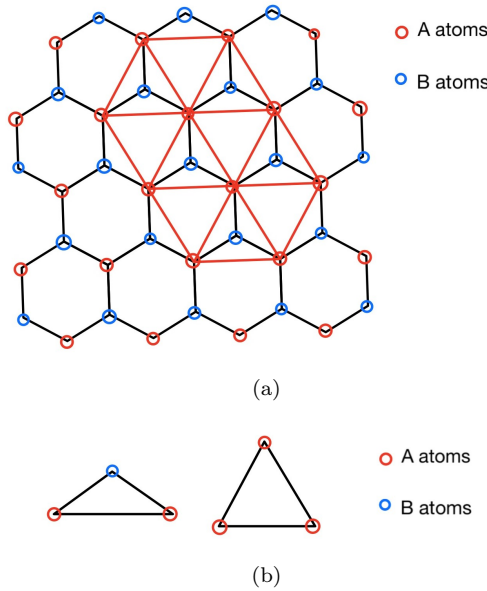


FIG. 9.2. (a) AAA and AAB interactions using a single interpolation polynomial. (b) Two kinds of triangles.

$(x_3, y_3)$ , and the value of  $f$  in these three vertices as  $T_1, T_2$  and  $T_3$ . By these notations,

$$\begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix} \begin{bmatrix} C \\ A \\ B \end{bmatrix}.$$

Solving this linear system, we obtain

$$\begin{aligned} A &= [(y_3 - y_1) \cdot (T_2 - T_1) - (y_2 - y_1) \cdot (T_3 - T_1)] / \Delta, \\ B &= [(x_2 - x_1) \cdot (T_3 - T_1) - (x_3 - x_1) \cdot (T_2 - T_1)] / \Delta, \\ \Delta &= (x_2 - x_1) \cdot (y_3 - y_1) - (x_3 - x_1) \cdot (y_2 - y_1). \end{aligned} \tag{9.2}$$

Here  $\Delta$  is twice the area of the triangle.

Now we prove that the piecewise linear function belongs to  $X_0$ .

LEMMA 9.1. *Suppose  $\mathbf{f} = \{\mathbf{f}^+, \mathbf{f}^-\} \in X_\varepsilon$ . We can find a piecewise linear function  $\mathbf{f}_A = \{\mathbf{f}_A^+, \mathbf{f}_A^-\} \in X_0$ , such that  $\mathbf{f} = \mathbf{f}_A$  on  $\mathbb{L}_p$ .*

*Proof.* Without loss of generality, we consider  $f^+ \in X_\varepsilon$ , where  $\mathbf{f}^+ = (f^+, 0)$ . Since  $\mathbb{R}^2$  is divided into triangles as shown in Figure 9.2(a) and each triangle has an interpolation polynomial, we define  $f_A^+$  in  $\mathbb{R}^2$  by combining all the interpolation polynomials, and  $f_A^+$  is a linear function on each triangle. Since the values of  $f_A^+$  on the boundary of triangles come from linear combination of the values at two vertices, we know that the two interpolation polynomials on the two neighboring triangles have the same value on the boundary where they meet. Thus  $f_A^+$  is well-defined. Moreover, since  $f_A^+$  is continuous in each triangle,  $f_A^+ \in C(\mathbb{R}^2)$ .

Finally, we prove that  $f_A^+$  satisfies the boundary conditions of  $X_0$ . Since  $f_A^+ + \frac{1}{4}$  defined on  $\mathbb{L}_p$  satisfies ADC in Equation (9.1), we know that for a triangle that contains

the  $y$ -axis, e.g., the triangle ABC in Figure 9.1, we have

$$f_A^+|_A = 0, \quad \frac{f_A^+|_B + f_A^+|_C}{2} = 0.$$

By direct calculation like (9.2), we have  $f_A^+(0, y) = 0$  inside this triangle. Therefore,

$$f_A^+(0, y) = 0 \text{ for all } y \in \mathbb{R}.$$

□

Similarly, another linear interpolating function can be constructed based on the ABB and BBB interactions. In this case, the  $\mathbb{R}^2$  plane is divided into triangles by connecting neighboring B atoms.

**9.3. Stability of the atomistic model.** In this part, we prove the stability of the atomistic model, which means we are going to prove

$$\langle \delta^2 E_a[\mathbf{v}]\mathbf{f}, \mathbf{f} \rangle_\varepsilon \geq C \|\mathbf{f}\|_{X_\varepsilon}^2, \tag{9.3}$$

for  $C > 0$  and  $\mathbf{f} \in X_\varepsilon$ . In addition, we get that (9.3) is still valid when  $\mathbf{u}$  is close to  $\mathbf{v}$ , where  $\mathbf{v}$  is the solution of the PN model. The method that we use is energy estimate by two interpolation polynomials defined in Section 9.2.

First we prove the stability gap between  $E_a^A[\mathbf{v}]$  and  $E_{PN}^A[\mathbf{v}]$  based on the interpolation polynomials.

**LEMMA 9.2.** *Suppose that A1–A6 hold, and  $\mathbf{v}$  is the dislocation solution of the PN model in Theorem 6.1. Then there exist constants  $\varepsilon_0$  and  $C$ , such that for  $0 < \varepsilon < \varepsilon_0$  and  $\mathbf{f} \in X_\varepsilon$ , we have*

$$\begin{aligned} & \langle \delta^2 E_a^A[\mathbf{v}]\mathbf{f}, \mathbf{f} \rangle_\varepsilon - \langle \delta^2 E_{PN}^A[\mathbf{v}]\mathbf{f}_A, \mathbf{f}_A \rangle_0 \\ &= \langle \delta^2 E_a^A[\mathbf{0}]\mathbf{f}, \mathbf{f} \rangle_\varepsilon - \langle \delta^2 E_{PN}^A[\mathbf{0}]\mathbf{f}_A, \mathbf{f}_A \rangle_0 + O(\varepsilon) \|\mathbf{f}\|_{X_\varepsilon}^2. \end{aligned} \tag{9.4}$$

*Proof.* By direct calculation, we have

$$\begin{aligned} & \langle \delta^2 E_a^A[\mathbf{v}]\mathbf{f}, \mathbf{f} \rangle_\varepsilon \\ &= \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left\{ \frac{\varepsilon^2}{6} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm}) \right. \\ & \quad (D_{\mathbf{s}_1} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \\ & \quad + \frac{\varepsilon^2}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^p \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm}) \\ & \quad (D_{\mathbf{s}_1}^p \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \\ & \quad + \varepsilon^2 \sum_{\mathbf{s}} [U''(\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{v}_{\mathbf{x}}^{A-} + \mathbf{s} - \mathbf{d})(\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{f}_{\mathbf{x}}^{A-})^2 \\ & \quad \left. + U''(\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{v}_{\mathbf{x}}^{B-} + \mathbf{s} - \mathbf{p} - \mathbf{d})(\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{f}_{\mathbf{x}}^{B-})^2 \right] \Big\}, \end{aligned} \tag{9.5}$$

$$\begin{aligned} & \langle \delta^2 E_a^A[\mathbf{0}]\mathbf{f}, \mathbf{f} \rangle_\varepsilon \\ &= \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left\{ \frac{\varepsilon^2}{6} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{s}_1, \mathbf{s}_2) (D_{\mathbf{s}_1} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \right. \end{aligned}$$

$$\begin{aligned}
 & + \frac{\varepsilon^2}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) (D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \\
 & + \varepsilon^2 \sum_{\mathbf{s}} [U''(\mathbf{s} - \mathbf{d})(\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{f}_{\mathbf{x}}^{A-})^2 + U''(\mathbf{s} - \mathbf{p} - \mathbf{d})(\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{f}_{\mathbf{x}}^{B-})^2] \Big\}, \tag{9.6}
 \end{aligned}$$

$$\begin{aligned}
 & \langle \delta^2 E_{\text{PN}}^A[\mathbf{v}] \mathbf{f}_A, \mathbf{f}_A \rangle_0 \\
 & = \lim_{R \rightarrow +\infty} \frac{1}{R} \int_{-R}^R \int_{\mathbb{R}} [\alpha_1 (\partial_x \mathbf{f}_A^+)^2 + \alpha_2 (\partial_y \mathbf{f}_A^+)^2 + 2\nabla^2 \gamma_A(\phi)(\mathbf{f}_A^+)^2] dx dy, \tag{9.7}
 \end{aligned}$$

$$\begin{aligned}
 & \langle \delta^2 E_{\text{PN}}^A[\mathbf{0}] \mathbf{f}_A, \mathbf{f}_A \rangle_0 \\
 & = \lim_{R \rightarrow +\infty} \frac{1}{R} \int_{-R}^R \int_{\mathbb{R}} [\alpha_1 (\partial_x \mathbf{f}_A^+)^2 + \alpha_2 (\partial_y \mathbf{f}_A^+)^2 + 2\nabla^2 \gamma_A(\mathbf{0})(\mathbf{f}_A^+)^2] dx dy. \tag{9.8}
 \end{aligned}$$

We divide (9.4) into following five parts,  $R_i, i = 1, 2, \dots, 5$ . The remaining problem is to show that these five parts are  $O(\varepsilon)$ .

(1)

$$\begin{aligned}
 R_1 = & \varepsilon^2 \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left\{ \frac{1}{6} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \right. \\
 & \partial_{ij} V(\mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm}) (D_{\mathbf{s}_1} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \\
 & + \frac{1}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm}) \\
 & (D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \\
 & - \frac{1}{6} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{s}_1, \mathbf{s}_2) (D_{\mathbf{s}_1} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \\
 & \left. - \frac{1}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) (D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \right\}. \tag{9.9}
 \end{aligned}$$

Without loss of generality, we just calculate the complex lattice parts with  $i = 2, j = 0$ :

$$\begin{aligned}
 & \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} [\varepsilon^2 \partial_{20} V(\mathbf{p} + \mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{v}_{\mathbf{x}}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm}) \\
 & - \partial_{20} V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2)] (D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm})^2 \\
 & \leq \varepsilon^3 \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} (V_{(3,0), \mathbf{p} + \mathbf{s}_1, \mathbf{s}_2} + V_{(2,1), \mathbf{p} + \mathbf{s}_1, \mathbf{s}_2}) (\mathbf{v}_{1, \mathbf{x}, \mathbf{s}_1}^{\mathbf{p}} + \mathbf{v}_{1, \mathbf{x}, \mathbf{s}_1}) (D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm})^2 \\
 & \leq C\varepsilon \|\mathbf{f}\|_{\varepsilon}^2, \tag{9.10}
 \end{aligned}$$

where the reason is the same as (8.13).

(2)

$$\begin{aligned}
 R_2 = & \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} [U''(\mathbf{v}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{v}_{\mathbf{x}}^{A-} + \mathbf{s} - \mathbf{d})(\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{f}_{\mathbf{x}}^{A-})^2 \\
 & + U''(\mathbf{v}_{\mathbf{s}+\mathbf{x}}^{B+} - \mathbf{v}_{\mathbf{x}}^{A-} + \mathbf{s} - \mathbf{p} - \mathbf{d})(\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{B+} - \mathbf{f}_{\mathbf{x}}^{A-})^2]
 \end{aligned}$$

$$\begin{aligned}
 & -U''(\mathbf{v}_x^{A+} - \mathbf{v}_x^{A-} + \mathbf{s} - \mathbf{d})(\mathbf{f}_{x+\mathbf{s}}^{A+} - \mathbf{f}_x^{A-})^2 \\
 & -U''(\mathbf{v}_x^{A+} - \mathbf{v}_x^{A-} + \mathbf{s} - \mathbf{p} - \mathbf{d})(\mathbf{f}_{x+\mathbf{s}}^{B+} - \mathbf{f}_x^{A-})^2].
 \end{aligned} \tag{9.11}$$

Without loss of generality, we just calculate the complex lattice parts:

$$\begin{aligned}
 & \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{x \in \mathbb{L}_R} \sum_{\mathbf{s}} [U''(\mathbf{v}_{s+\mathbf{x}}^{B+} - \mathbf{v}_x^{A-} + \mathbf{s} + \mathbf{p}) \\
 & \quad - U''(\mathbf{v}_x^{A+} - \mathbf{v}_x^{A-} + \mathbf{s} + \mathbf{p})](\mathbf{f}_{x+\mathbf{s}}^{B+} - \mathbf{f}_x^{A-})^2 \\
 & \leq \varepsilon \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{x \in \mathbb{L}_R} \varepsilon^2 \sum_{\mathbf{s}} U_{3,\mathbf{s}+\mathbf{p}}(\varepsilon D_{\mathbf{s}} \mathbf{f}_x^{B+} + \mathbf{f}_x^{B+} + \mathbf{f}_x^{A+})^2 \\
 & \leq C\varepsilon \|\mathbf{f}\|_{\varepsilon}^2,
 \end{aligned} \tag{9.12}$$

where the reason is the same as (8.13).

(3)

$$\begin{aligned}
 R_3 = & \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{x \in \mathbb{L}_R} \sum_{\mathbf{s}} \left\{ [U''(\mathbf{v}_x^{A+} - \mathbf{v}_x^{A-} + \mathbf{s} - \mathbf{d}) - U''(\mathbf{s} - \mathbf{d})] \right. \\
 & [(\mathbf{f}_{x+\mathbf{s}}^{A+} - \mathbf{f}_x^{A-})^2 - (\mathbf{f}_x^{A+} - \mathbf{f}_x^{A-})^2] \\
 & \quad + [U''(\mathbf{v}_x^{A+} - \mathbf{v}_x^{A-} + \mathbf{s} + \mathbf{p} - \mathbf{d}) - U''(\mathbf{s} + \mathbf{p} - \mathbf{d})] \\
 & \left. [(\mathbf{f}_{x+\mathbf{s}}^{B+} - \mathbf{f}_x^{A-})^2 - (\mathbf{f}_x^{A+} - \mathbf{f}_x^{A-})^2] \right\}.
 \end{aligned} \tag{9.13}$$

By the same way in  $R_2$ , we have

$$R_3 \leq C\varepsilon \|\mathbf{f}\|_{\varepsilon}^2.$$

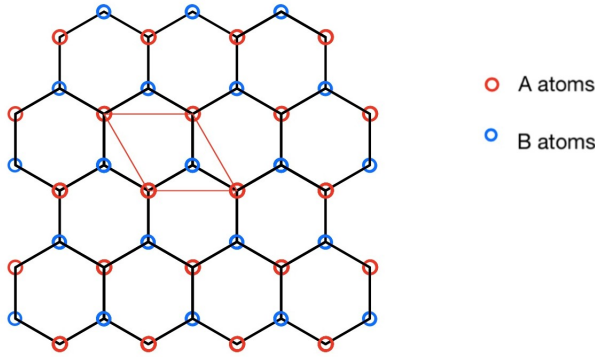


FIG. 9.3. Tessellation of  $\mathbb{R}^2$ .

(4) The next two terms,  $R_4$  and  $R_5$ , will be compared with the continuum model. We divide  $\mathbb{R}^2$  using parallelograms as shown in Figure 9.3. For each parallelogram, there is a B atom. When the label of B atom is  $\mathbf{s}$ , we denote this parallelogram as  $P_{\mathbf{s}}$ .

$$R_4 = \sum_{\mathbf{s}} \sum_x \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{P_x \cap (-R,R) \times \mathbb{R}} \sum_{\mathbf{s}} \left\{ [U''(\mathbf{s} + \mathbf{v}_x^{A+} - \mathbf{v}_x^{A-} - \mathbf{d}) \right.$$

$$\begin{aligned}
 & -U''(\mathbf{s} + \mathbf{v}^+ - \mathbf{v}^- - \mathbf{d}) (\mathbf{f}_x^{A+} - \mathbf{f}_x^{A-})^2 + [U''(\mathbf{s} + \mathbf{p} + \mathbf{v}_x^{A+} - \mathbf{v}_x^{A-} - \mathbf{d}) \\
 & - U''(\mathbf{s} + \mathbf{p} + \mathbf{v}^+ - \mathbf{v}^- - \mathbf{d})] (\mathbf{f}_x^{A+} - \mathbf{f}_x^{A-})^2 \} dx dy. \tag{9.14}
 \end{aligned}$$

Since

$$\left| U''(\mathbf{s} + \mathbf{p} + \mathbf{v}_x^{A+} - \mathbf{v}_x^{A-} - \mathbf{d}) - U''(\mathbf{s} + \mathbf{p} + \mathbf{v}^+ - \mathbf{v}^- - \mathbf{d}) \right| \leq \varepsilon U_{3, \mathbf{s} + \mathbf{p}} \|\nabla \mathbf{v}\|_\infty,$$

we can get

$$R_4 \leq C\varepsilon \|\mathbf{f}\|_\varepsilon^2. \tag{9.15}$$

(5)

$$\begin{aligned}
 R_5 = & \sum_{\mathbf{s}} \sum_{\mathbf{x}} \lim_{R \rightarrow +\infty} \frac{1}{2R} \int_{P_{\mathbf{x}} \cap (-R, R) \times \mathbb{R}} \sum_{\mathbf{s}} \left\{ [U''(\mathbf{s} + \mathbf{v}^+ - \mathbf{v}^-) \right. \\
 & - U''(\mathbf{s})] [(\mathbf{f}_x^{A+} - \mathbf{f}_x^{A-})^2 - (\mathbf{f}_A^+ - \mathbf{f}_A^-)^2] \\
 & + [U''(\mathbf{s} + \mathbf{p} + \mathbf{v}^+ - \mathbf{v}^-) \\
 & \left. - U''(\mathbf{s} + \mathbf{p})] [(\mathbf{f}_x^{A+} - \mathbf{f}_x^{A-})^2 - (\mathbf{f}_A^+ - \mathbf{f}_A^-)^2] \right\} dx dy. \tag{9.16}
 \end{aligned}$$

Since we have  $\mathbf{f} = \{(f^+, 0), (f^-, 0)\}$ ,

$$(\mathbf{f}_x^{A+} - \mathbf{f}_x^{A-})^2 - (\mathbf{f}_A^+ - \mathbf{f}_A^-)^2 = (f_x^{A+} + f_A^+ - f_x^{A-} - f_A^-)(f_x^{A+} - f_A^+ + f_x^{A-} + f_A^-)$$

In addition,

$$\int_{P_{\mathbf{x}}} 2f_A^+ dx dy = \frac{\sqrt{3}}{2} \varepsilon^2 \left[ \frac{1}{3} (f_{\mathbf{x} + \mathbf{e}_2 - \mathbf{e}_1}^{A+} + f_{\mathbf{x}}^{B+}) + \frac{5}{9} (f_{\mathbf{x} + \mathbf{e}_2}^{A+} + f_{\mathbf{x} + \mathbf{e}_1}^{A+}) + \frac{2}{9} f_{\mathbf{x} + \mathbf{e}_1}^{A+} \right]. \tag{9.17}$$

Therefore we can have

$$\begin{aligned}
 & \int_{P_{\mathbf{x}}} [(\mathbf{f}_x^{A+} - \mathbf{f}_x^{A-})^2 - (\mathbf{f}_A^+ - \mathbf{f}_A^-)^2] dx dy \\
 & \leq \frac{\sqrt{3}}{2} \varepsilon^3 2 (f_{\mathbf{x}}^{A+} + f_{\mathbf{x} + \mathbf{e}_2 - \mathbf{e}_1}^{A+} + f_{\mathbf{x}}^{B+} + f_{\mathbf{x} + \mathbf{e}_2}^{A+} + f_{\mathbf{x} + \mathbf{e}_1}^{A+}) \\
 & \quad \times (D_{\mathbf{e}_1 + \mathbf{e}_2} f_{\mathbf{x}}^{A+} + D_{\mathbf{e}_2} f_{\mathbf{x}}^{A+} + D_{\mathbf{e}_1} f_{\mathbf{x}}^{A+} + D_{\mathbf{0}}^p f_{\mathbf{x}}^{A+}). \tag{9.18}
 \end{aligned}$$

Thus

$$\begin{aligned}
 R_5 \leq & C\varepsilon^3 \sum_{\mathbf{s}} \sum_{\mathbf{x}} U_{3, \mathbf{s} + \mathbf{p}} 2 (f_{\mathbf{x}}^{A+} + f_{\mathbf{x} + \mathbf{e}_2 - \mathbf{e}_1}^{A+} + f_{\mathbf{x}}^{B+} + f_{\mathbf{x} + \mathbf{e}_2}^{A+} + f_{\mathbf{x} + \mathbf{e}_1}^{A+}) \\
 & \times (D_{\mathbf{e}_1 + \mathbf{e}_2} f_{\mathbf{x}}^{A+} + D_{\mathbf{e}_2} f_{\mathbf{x}}^{A+} + D_{\mathbf{e}_1} f_{\mathbf{x}}^{A+} + D_{\mathbf{0}}^p f_{\mathbf{x}}^{A+}) \\
 \leq & C\varepsilon \|\mathbf{f}\|_\varepsilon^2. \tag{9.19}
 \end{aligned}$$

□

Next we define the stability gap to prove the stability of the atomistic model.

LEMMA 9.3. *Suppose that A1–A6 hold, and  $\mathbf{v}$  is the dislocation solution of the PN model in Theorem 6.1. There exist constants  $\varepsilon_0$  and  $C$ , such that for  $0 < \varepsilon < \varepsilon_0$  and  $\mathbf{f} \in X_\varepsilon$ , we have*

$$\langle \delta^2 E_a^A[\mathbf{0}]\mathbf{f}, \mathbf{f} \rangle_\varepsilon - \langle \delta^2 E_{PN}^A[\mathbf{0}]\mathbf{f}_A, \mathbf{f}_A \rangle_0 \geq -\Delta_A \|\mathbf{f}\|_{X_\varepsilon}^2 + O(\varepsilon) \|\mathbf{f}\|_{X_\varepsilon}^2,$$



where  $\Delta_A$  is as shown in the proof.

*Proof.* Thanks to (9.6) and (9.8), we only need to calculate the following parts:

$$\begin{aligned}
 R_{g1} &= \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left\{ \frac{\varepsilon^2}{6} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{s}_1, \mathbf{s}_2) (D_{\mathbf{s}_1} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm})^j \right. \\
 &\quad \left. + \frac{\varepsilon^2}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) (D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \right\} \\
 &\quad - \lim_{R \rightarrow +\infty} \frac{1}{R} \int_{-R}^R \int_{\mathbb{R}} [\alpha_1 (f_A)_x^2 + \alpha_2 (f_B)_y^2] dx dy. \tag{9.20}
 \end{aligned}$$

$$\begin{aligned}
 R_{g2} &= \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left\{ \varepsilon^2 \sum_{\mathbf{s}} [U''(\mathbf{s} - \mathbf{d}) (\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{f}_{\mathbf{x}}^{A-})^2 + U''(\mathbf{s} - \mathbf{p} - \mathbf{d}) \right. \\
 &\quad \left. \times (\mathbf{f}_{\mathbf{x}+\mathbf{s}}^{B+} - \mathbf{f}_{\mathbf{x}}^{A-})^2 \right\} - \lim_{R \rightarrow +\infty} \frac{1}{R} \int_{-R}^R \int_{\mathbb{R}} 2\nabla^2 \gamma(\mathbf{0}) \mathbf{f}_A^2 dx dy. \tag{9.21}
 \end{aligned}$$

Due to (9.15) and (9.19), we have

$$R_{g2} \leq C\varepsilon \|\mathbf{f}\|_{X_\varepsilon}^2.$$

By the the definition of  $\mathbf{f}_A$  and (9.2), we have

$$\begin{aligned}
 R_{g1} &= \lim_{R \rightarrow +\infty} \frac{1}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle \setminus A_1} \sum_{i+j=2} \binom{2}{i} \left[ \frac{\varepsilon^2}{6} \partial_{ij} V(\mathbf{s}_1, \mathbf{s}_2) (D_{\mathbf{s}_1} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{v}_{\mathbf{x}}^{A\pm})^j \right. \\
 &\quad \left. + \frac{\varepsilon^2}{2} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle \setminus A_2} \sum_{i+j=2} \binom{2}{i} \partial_{ij} V(\mathbf{p} + \mathbf{s}_1, \mathbf{s}_2) (D_{\mathbf{s}_1}^{\mathbf{p}} \mathbf{f}_{\mathbf{x}}^{A\pm})^i (D_{\mathbf{s}_2} \mathbf{f}_{\mathbf{x}}^{A\pm})^j \right] \\
 &\quad - \lim_{R \rightarrow +\infty} \frac{1}{4\sqrt{3}R} \int_{-R}^R \int_{\mathbb{R}} \sum_{i+j=2} \binom{2}{i} \\
 &\quad \left\{ \frac{1}{3} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle \setminus A_1} \partial_{ij} V(\mathbf{s}_1, \mathbf{s}_2) [(\mathbf{s}_1) \cdot (\nabla \mathbf{f}_A^\pm)]^i [(\mathbf{s}_2) \cdot (\nabla \mathbf{f}_A^\pm)]^j - \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle \setminus A_2} \right. \\
 &\quad \left. \partial_{ij} V(\mathbf{s}_1 + \mathbf{p}, \mathbf{s}_2) [(\mathbf{s}_1 + \mathbf{p}) \cdot (\nabla \mathbf{f}_A^\pm)]^i [(\mathbf{s}_2) \cdot (\nabla \mathbf{f}_A^\pm)]^j \right\} dx dy, \tag{9.22}
 \end{aligned}$$

where

$$\begin{aligned}
 A_1 &:= \{(\mathbf{e}_1, \mathbf{e}_2), (-\mathbf{e}_1, \mathbf{e}_2 - \mathbf{e}_1), (\mathbf{e}_1 - \mathbf{e}_2, -\mathbf{e}_2)\}, \\
 A_2 &:= \{(\mathbf{0}, \mathbf{e}_2), (\mathbf{0}, \mathbf{e}_1), (-\mathbf{e}_2, -\mathbf{e}_2), (-\mathbf{e}_2, -\mathbf{e}_2 + \mathbf{e}_1), \\
 &\quad (-\mathbf{e}_1, -\mathbf{e}_1), (-\mathbf{e}_1, -\mathbf{e}_1 + \mathbf{e}_2)\}. \tag{9.23}
 \end{aligned}$$

Since  $\mathbf{f}_A$  is defined by  $\mathbf{f}$ ,  $R_{g1}$  is the function of  $\mathbf{f}$ . We define  $\Delta_A$ :

$$\Delta_A := - \lim_{\varepsilon \rightarrow 0} \sup_{\|\mathbf{f}\|_{X_\varepsilon} = 1} R_{g1}. \tag{9.24}$$

This completes the proof. □

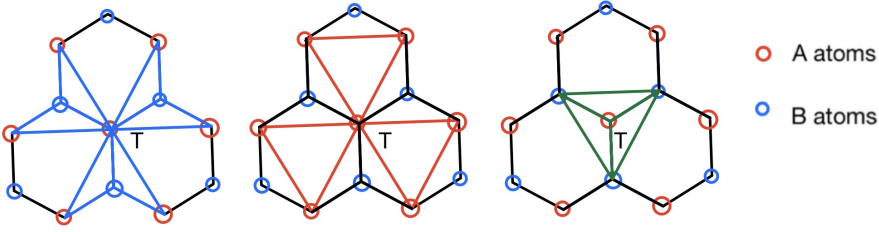


FIG. 9.4. Interpolation polynomial for nearest interaction.

REMARK 9.1. In **A8** and Lemma 9.3, we assume that  $\Delta_A$  is small, it means that we assume the “nearest” interactions dominate the elastic energy. Definition of the “nearest” interactions on the complex lattice is illustrated in Figure 9.4. For the A atom,  $T$ , there are 12 triangles containing  $T$ : six blue triangles, three red triangles and three green triangles (coming from the B part). In Figure 9.4, the blue triangles are for the  $AAB$  interactions, and the red triangles are for the  $AAA$  interactions. In addition, in the part B, there are three  $ABB$  interactions containing  $T$ . In other words, if we consider those 12 interactions as nearest interactions in elastic energy,  $\Delta_A = 0$  can be obtained. Hence we define it as **interpolation polynomial for nearest interaction**.

LEMMA 9.4. Suppose that A1–A6 hold,  $f \in X_\varepsilon$ . There exist constants  $\varepsilon_0$  and  $C$ , such that for  $0 < \varepsilon < \varepsilon_0$ ,

$$(1 - \Delta_A - C\varepsilon)\|f\|_{X_\varepsilon}^2 \leq \|f_A\|_{X_0}^2 \leq (1 + \Delta_A + C\varepsilon)\|f\|_{X_\varepsilon}^2, \tag{9.25}$$

where the  $f_A$  defined in Lemma 9.1.

*Proof.*

$$\begin{aligned} \left| \|f_A\|_{X_0}^2 - \|f\|_{X_\varepsilon}^2 \right| &= \left| R_{g1} + \frac{4\sqrt{3}}{3} \|f_A^\perp\|_v^2 - \|f^\perp\|_\varepsilon^2 \right| \\ &\leq |-\Delta_A + C\varepsilon| \|f\|_{X_\varepsilon}^2, \end{aligned} \tag{9.26}$$

where the last inequality is due to Lemma 9.3. □

PROPOSITION 9.1. Suppose that A1–A8 hold, and  $v$  is the dislocation solution of the PN model in Theorem 6.1. There exist constants  $\varepsilon_0$  and  $C > 0$ , such that for  $0 < \varepsilon < \varepsilon_0$  and  $f \in X_\varepsilon$ , we have

$$\langle \delta^2 E_a[v]f, f \rangle_\varepsilon \geq C \|f\|_{X_\varepsilon}^2.$$

*Proof.* By Lemmas 9.2, 9.3, 9.4 and Proposition 7.1, we have

$$\begin{aligned} \langle \delta^2 E_a^A[v]f, f \rangle_\varepsilon &\geq \langle \delta^2 E_{PN}^A[v]f_A, f_A \rangle_0 - \Delta_A \|f\|_{X_\varepsilon}^2 + C\varepsilon \|f\|_{X_\varepsilon}^2 \\ &\geq \bar{\vartheta} \|f_A\|_{X_0}^2 - \Delta_A \|f\|_{X_\varepsilon}^2 + C\varepsilon \|f\|_{X_\varepsilon}^2 \geq [\bar{\vartheta}(1 - \Delta_A) - \Delta_A - C\varepsilon] \|f\|_{X_\varepsilon}^2 \\ &\geq \frac{1}{4} \bar{\vartheta} \|f\|_{X_\varepsilon}^2, \end{aligned} \tag{9.27}$$

where the last inequality is due to A6. Similar property can be obtained in  $\delta^2 E_a^B[v]$  part. Therefore we obtain

$$\langle \delta^2 E_a[v]f, f \rangle_\varepsilon = \langle \delta^2 E_a^A[v]f, f \rangle_\varepsilon + \langle \delta^2 E_a^B[v]f, f \rangle_\varepsilon \geq \frac{1}{2} \bar{\vartheta} \|f\|_{X_\varepsilon}^2 \geq \frac{1}{6} \vartheta \|f\|_{X_\varepsilon}^2. \tag{9.28}$$

□

Now that we have consistency of the PN model (Proposition 8.1) and stability of the atomistic model (Proposition 9.1), we can prove Theorem 6.2 similarly as in [14].

LEMMA 9.5. *Suppose that Assumptions A1–A6 hold. Let  $\mathbf{v}$  be the dislocation solution in the PN model. There exist constants  $\varepsilon_0$  and  $C$ , such that for  $0 < \varepsilon < \varepsilon_0$  and  $\mathbf{u}, \mathbf{u}' \in S_\varepsilon$  satisfying  $\|\mathbf{u} - \mathbf{v}\|_{X_\varepsilon} \leq \varepsilon^2$  and  $\|\mathbf{u}' - \mathbf{v}\|_{X_\varepsilon} \leq \varepsilon^2$ , we have*

$$|\langle (\delta^2 E_{PN}[\mathbf{u}] - \delta^2 E_a[\mathbf{u}']) \mathbf{f}, \mathbf{g} \rangle_\varepsilon| \leq C \varepsilon^{-1} \|\mathbf{u} - \mathbf{u}'\|_{X_\varepsilon} \|\mathbf{f}\|_{X_\varepsilon} \|\mathbf{g}\|_{X_\varepsilon} \tag{9.29}$$

for all  $\mathbf{f}, \mathbf{g} \in X_\varepsilon$  and  $C$  is independent of  $\varepsilon$ .

*Proof.* By definition of the norm in  $X_\varepsilon$ , we have for all  $\mathbf{x} \in \mathbb{L}$ :

$$|D_{\mathbf{s}_1}(\mathbf{u}_\mathbf{x}^{A\pm} - \mathbf{v}_\mathbf{x}^{A\pm})| = \varepsilon^{-1} |D_{\mathbf{s}_1} \varepsilon(\mathbf{u}_\mathbf{x}^{A\pm} - \mathbf{v}_\mathbf{x}^{A\pm})| \leq \varepsilon^{-1} \|\mathbf{u} - \mathbf{v}\|_{X_\varepsilon}.$$

Therefore we can get

$$\|D_{\mathbf{s}_1}(\mathbf{u} - \mathbf{v})\|_{L^\infty_\varepsilon} \leq \varepsilon^{-1} \|\mathbf{u} - \mathbf{v}\|_{X_\varepsilon} \leq 1.$$

Furthermore, we can get  $\|D_{\mathbf{s}_1} \mathbf{u}\|_{L^\infty_\varepsilon} \leq C$  since  $\|D_{\mathbf{s}_1} \mathbf{v}\|_{L^\infty_\varepsilon} \leq \|\nabla \mathbf{v}\|_\infty \leq C$ . Similarly,

$$\|D_{\mathbf{s}_1}(\mathbf{u} - \mathbf{u}')\|_{L^\infty_\varepsilon} \leq \varepsilon^{-1} \|\mathbf{u} - \mathbf{u}'\|_{X_\varepsilon} \leq 1.$$

Similar property can be obtain in  $D_{\mathbf{s}_1}^{\pm p}$ .

As for operator  $V$ , we can have

$$\begin{aligned} & \sum_{\mathbf{s}} |\partial_{ij} V(\mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1} \mathbf{u}_\mathbf{x}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} \mathbf{u}_\mathbf{x}^{A\pm}) \\ & \quad - \partial_{ij} V(\mathbf{s}_1 + \varepsilon D_{\mathbf{s}_1} (\mathbf{u}')_\mathbf{x}^{A\pm}, \mathbf{s}_2 + \varepsilon D_{\mathbf{s}_2} (\mathbf{u}')_\mathbf{x}^{A\pm})| \\ & \leq \sum_{\mathbf{s}} (V_{(i,j+1), \mathbf{s}_1, \mathbf{s}_2} + V_{(i+1,j), \mathbf{s}_1, \mathbf{s}_2}) \varepsilon [ |(D_{\mathbf{s}_2} + D_{\mathbf{s}_1})(\mathbf{u}_\mathbf{x}^{A\pm} - (\mathbf{u}')_\mathbf{x}^{A\pm})| ] \\ & \leq C \|\mathbf{u}' - \mathbf{u}\|_{X_\varepsilon}, \end{aligned} \tag{9.30}$$

where  $\varepsilon$  is sufficiently small. Hence, we obtain

$$\begin{aligned} |\langle (\delta^2 E_{\text{elas}}[\mathbf{u}] - \delta^2 E_{\text{a-el}}[\mathbf{u}']) \mathbf{f}, \mathbf{g} \rangle_\varepsilon| & \leq C \|\mathbf{u}' - \mathbf{u}\|_{X_\varepsilon} (\mathbf{f}, \mathbf{g})_{X_\varepsilon} \\ & \leq C \|\mathbf{u} - \mathbf{u}'\|_{X_\varepsilon} \|\mathbf{f}\|_{X_\varepsilon} \|\mathbf{g}\|_{X_\varepsilon}. \end{aligned} \tag{9.31}$$

For the  $\gamma$ -surface, we use this notation in the proof:

$$U_{k, \mathbf{s}, h} = \sup_{|\boldsymbol{\xi} - \mathbf{s} + \frac{1}{2}| \leq h} |U^{(k)}(\boldsymbol{\xi})|,$$

where  $k=0, 1, 2, 3$ . We can prove the same property of  $U_{k, \mathbf{s}, h}$  as in the proof of Lemma 8.1:

$$\text{For all } h > 0, \text{ there exists } H > 0, \text{ such that } \sum_{\mathbf{s}} U_{k, \mathbf{s}, h} |\mathbf{s}|^{k+1} \leq H. \tag{9.32}$$

Since  $\mathbf{u}, \mathbf{u}' \in S_\varepsilon$ , we can get  $\|\mathbf{u}\|_\infty < \infty, \|\mathbf{u}'\|_\infty < \infty$ . Thus we can denote  $r = \|\mathbf{u}\|_\infty + \|\mathbf{u}'\|_\infty$  and get

$$\sum_{\mathbf{s}} |U'''(\mathbf{s} + \mathbf{u}_{\mathbf{x}+\mathbf{s}_2}^{A+} - \mathbf{u}_\mathbf{x}^{A-} - \mathbf{d}) - U'''(\mathbf{s} + (\mathbf{u}')_{\mathbf{x}+\mathbf{s}_2}^{A+} - (\mathbf{u}')_\mathbf{x}^{A-} - \mathbf{d})|$$

$$\begin{aligned} &\leq \sum_s U_{3,s,r} |\varepsilon^{-1} D_{s_2} (\mathbf{u}_x^{A+} - \mathbf{u}'_x{}^{A+}) + (\mathbf{u}_x^{\perp A+} - \mathbf{u}'_x{}^{\perp A+})| \\ &\leq C\varepsilon^{-1} \|\mathbf{u}' - \mathbf{u}\|_{X_\varepsilon}. \end{aligned} \tag{9.33}$$

Therefore, we get

$$\begin{aligned} |\langle (\delta^2 E_{\text{mis}}[\mathbf{u}] - \delta^2 E_{\text{a-mis}}[\mathbf{u}']) \mathbf{f}, \mathbf{g} \rangle_\varepsilon| &\leq C\varepsilon^{-1} \|\mathbf{u}' - \mathbf{u}\|_{X_\varepsilon} (\mathbf{f}, \mathbf{g})_{X_\varepsilon} \\ &\leq C\varepsilon^{-1} \|\mathbf{u} - \mathbf{u}'\|_{X_\varepsilon} \|\mathbf{f}\|_{X_\varepsilon} \|\mathbf{g}\|_{X_\varepsilon}. \end{aligned} \tag{9.34}$$

Finally, we can get Lemma 9.5 by direct calculation. □

**PROPOSITION 9.2.** *Suppose that Assumptions A1–A8 hold. Let  $\mathbf{v}$  be the dislocation solution in the PN model. There exist constants  $\varepsilon_0$  and  $C$ , such that for  $0 < \varepsilon < \varepsilon_0$  and  $\mathbf{u} \in S_\varepsilon$  satisfying  $\|\mathbf{u} - \mathbf{v}\|_{X_\varepsilon} \leq \varepsilon^2$ , we have for  $\mathbf{f} \in X_\varepsilon$*

$$\langle \delta^2 E_a[\mathbf{u}] \mathbf{f}, \mathbf{f} \rangle_\varepsilon \geq C \|\mathbf{f}\|_{X_\varepsilon}^2, \tag{9.35}$$

where  $C$  is independent of  $\varepsilon$ .

*Proof.* Let  $\mathbf{u}' = \mathbf{v}$  and  $\mathbf{g} = \mathbf{f}$  in Lemma 9.5, we have

$$|\langle (\delta^2 E_a[\mathbf{u}] - \delta^2 E_a[\mathbf{v}]) \mathbf{f}, \mathbf{f} \rangle_\varepsilon| \leq C\varepsilon \|\mathbf{f}\|_{X_\varepsilon}^2.$$

By Proposition 9.1, we have  $\langle \delta^2 E_a[\mathbf{u}] \mathbf{f}, \mathbf{f} \rangle_\varepsilon \geq C \|\mathbf{f}\|_{X_\varepsilon}^2$  for a sufficiently small  $\varepsilon$ . □

**9.4. Proof of Theorem 6.2 and Corollary 6.1.**

*Proof. (Proof of Theorem 6.2.)* First, we define a closed subset  $B$  of  $X_\varepsilon$  with an uncertain constant  $C_B$ , which will be defined later:

$$B = \{\boldsymbol{\psi} \in X_\varepsilon : \|\boldsymbol{\psi}\|_{X_\varepsilon} \leq C_B \varepsilon^2\}. \tag{9.36}$$

We define the operator  $A_\boldsymbol{\psi} : X_\varepsilon \rightarrow X_\varepsilon$  following:

$$(A_\boldsymbol{\psi} \mathbf{f}, \mathbf{g})_{X_\varepsilon} = \int_0^1 \langle \delta^2 E_a[\mathbf{u}^t] \mathbf{f}, \mathbf{g} \rangle_\varepsilon dt, \quad \mathbf{f}, \mathbf{g} \in X_\varepsilon, \tag{9.37}$$

where  $\mathbf{u}^t = \mathbf{v} + t\boldsymbol{\psi}$  for  $t \in [0, 1]$ . Next, we prove that for every  $\boldsymbol{\psi}$ ,  $A_\boldsymbol{\psi}$  is invertible. Thanks to Lax–Milgram Theorem, we only need to prove the following three parts:

- (i)  $A_\boldsymbol{\psi}$  is well-defined and  $(A_\boldsymbol{\psi} \mathbf{f}, \mathbf{g})_{X_\varepsilon}$  is bi-linear.
- (ii) There is a constant  $c > 0$  such that for every  $\mathbf{f}, \mathbf{g} \in X_\varepsilon$ ,

$$(A_\boldsymbol{\psi} \mathbf{f}, \mathbf{g})_{X_\varepsilon} \leq c \|\mathbf{f}\|_{X_\varepsilon} \|\mathbf{g}\|_{X_\varepsilon}.$$

- (iii) There is a constant  $C > 0$  such that for every  $\mathbf{f} \in X_\varepsilon$ ,

$$(A_\boldsymbol{\psi} \mathbf{f}, \mathbf{f})_{X_\varepsilon} \geq C \|\mathbf{f}\|_{X_\varepsilon}^2.$$

For (i) and (ii), it is easy to check from the definition of  $A_\boldsymbol{\psi}$ . For (iii), for every  $t$ , we have  $\|\mathbf{u}^t - \mathbf{v}\|_{X_\varepsilon} \leq t \|\boldsymbol{\psi}\|_{X_\varepsilon} \leq C_B \varepsilon^2$ . Hence, from Proposition 9.2, we have  $\langle \delta^2 E_a[\mathbf{u}^t] \mathbf{f}, \mathbf{f} \rangle_\varepsilon \geq C \|\mathbf{f}\|_{X_\varepsilon}^2$ . Thus we can get  $(A_\boldsymbol{\psi} \mathbf{f}, \mathbf{f})_{X_\varepsilon} \geq C \|\mathbf{f}\|_{X_\varepsilon}^2$ . By the above analysis,  $A_\boldsymbol{\psi}$  is invertible.

By the Newton–Leibniz formula, we have

$$\begin{aligned} \langle \delta E_a[\mathbf{v} + \mathbf{w}], \mathbf{f} \rangle_\varepsilon - \langle \delta E_a[\mathbf{v}], \mathbf{f} \rangle_\varepsilon &= \int_0^1 \langle \delta^2 E_a[\mathbf{u}^t] \mathbf{w}, \mathbf{f} \rangle_\varepsilon dt \\ &= (A_{\mathbf{w}} \mathbf{w}, \mathbf{f})_{X_\varepsilon}, \end{aligned}$$

where  $\mathbf{w} \in B$ .

If  $\mathbf{v} + \mathbf{w}$  solves the atomistic model, we can get a  $\mathbf{w}$  to solve

$$(A_{\mathbf{w}} \mathbf{w}, \mathbf{f})_{X_\varepsilon} = -\langle \delta E_a[\mathbf{v}], \mathbf{f} \rangle_\varepsilon \text{ for all } \mathbf{f} \in X_\varepsilon. \tag{9.38}$$

Next we define a map  $G : B \rightarrow X_\varepsilon$  for  $\mathbf{w} \in B$  as

$$(A_{\mathbf{w}} G(\mathbf{w}), \mathbf{f})_{X_\varepsilon} = -\langle \delta E_a[\mathbf{v}], \mathbf{f} \rangle_\varepsilon \text{ for all } \mathbf{f} \in X_\varepsilon. \tag{9.39}$$

Now we prove that  $G$  is a contraction mapping.

(i) Find a proper  $C_B$  in the definition of  $B$  to make  $G(B) \subset B$ . Since  $(A_\psi \mathbf{f}, \mathbf{f})_{X_\varepsilon} \geq C \|\mathbf{f}\|_{X_\varepsilon}^2$  and by Proposition 8.1, we have

$$\begin{aligned} C \|G(\mathbf{w})\|_{X_\varepsilon}^2 &\leq (A_{\mathbf{w}} G(\mathbf{w}), G(\mathbf{w}))_{X_\varepsilon} \\ &\leq |\langle \delta E_a[\mathbf{v}], G(\mathbf{w}) \rangle_\varepsilon| \\ &\leq \varepsilon^2 \|G(\mathbf{w})\|_{X_\varepsilon}. \end{aligned} \tag{9.40}$$

Thus we can choose a proper  $C_B$  from (9.40).

(ii) Show that  $\|G(\mathbf{w}) - G(\mathbf{w}')\|_{X_\varepsilon} \leq L \|\mathbf{w} - \mathbf{w}'\|_{X_\varepsilon}$  for any  $\mathbf{w}', \mathbf{w} \in B$  and  $L < 1$ .

Here we have

$$\begin{aligned} \|G(\mathbf{w}) - G(\mathbf{w}')\|_{X_\varepsilon}^2 &= (G(\mathbf{w}) - G(\mathbf{w}'), G(\mathbf{w}) - G(\mathbf{w}'))_{X_\varepsilon} \\ &= |\langle \delta E_a[\mathbf{v}], (A_{\mathbf{w}}^{-1} - A_{\mathbf{w}'}^{-1})(G(\mathbf{w}) - G(\mathbf{w}')) \rangle_\varepsilon| \\ &= C\varepsilon^2 \|(A_{\mathbf{w}}^{-1} - A_{\mathbf{w}'}^{-1})(G(\mathbf{w}) - G(\mathbf{w}'))\|_{X_\varepsilon} \\ &= C\varepsilon^2 \|A_{\mathbf{w}}^{-1}(A_{\mathbf{w}} - A_{\mathbf{w}'})A_{\mathbf{w}'}^{-1}(G(\mathbf{w}) - G(\mathbf{w}'))\|_{X_\varepsilon} \\ &\leq C\varepsilon^2 \|A_{\mathbf{w}}^{-1}\|_{\text{op}} \cdot \|A_{\mathbf{w}} - A_{\mathbf{w}'}\|_{\text{op}} \cdot \|A_{\mathbf{w}'}^{-1}\|_{\text{op}} \\ &\quad \cdot \|G(\mathbf{w}) - G(\mathbf{w}')\|_{X_\varepsilon}, \end{aligned}$$

where  $\|\cdot\|_{\text{op}}$  is norm of operator.

Thanks to

$$C \|A_{\mathbf{w}}^{-1} \mathbf{f}\|_{X_\varepsilon} \leq \frac{(A_{\mathbf{w}} A_{\mathbf{w}}^{-1} \mathbf{f}, A_{\mathbf{w}}^{-1} \mathbf{f})_{X_\varepsilon}}{\|A_{\mathbf{w}}^{-1} \mathbf{f}\|_{X_\varepsilon}} \leq \|\mathbf{f}\|_{X_\varepsilon},$$

we have

$$\|A_{\mathbf{w}}^{-1}\|_{\text{op}} \leq C^{-1}, \|A_{\mathbf{w}'}^{-1}\|_{\text{op}} \leq C^{-1}. \tag{9.41}$$

By Lemma 9.5, we have

$$\begin{aligned} &\|(A_{\mathbf{w}} - A_{\mathbf{w}'} ) \mathbf{f}\|_{X_\varepsilon}^2 \\ &= \int_0^1 \langle (\delta^2 E_a[\mathbf{v} + t\mathbf{w}] - \delta^2 E_a[\mathbf{v} + t\mathbf{w}']) \mathbf{f}, (A_{\mathbf{w}} - A_{\mathbf{w}'} ) \mathbf{f} \rangle_\varepsilon dt \\ &\leq \int_0^1 C\varepsilon^{-1} \|t\mathbf{w} - t\mathbf{w}'\|_{X_\varepsilon} \|\mathbf{f}\|_{X_\varepsilon} \|(A_{\mathbf{w}} - A_{\mathbf{w}'} ) \mathbf{f}\|_{X_\varepsilon} dt \\ &\leq C\varepsilon^{-1} \|\mathbf{w} - \mathbf{w}'\|_{X_\varepsilon} \|\mathbf{f}\|_{X_\varepsilon} \|(A_{\mathbf{w}} - A_{\mathbf{w}'} ) \mathbf{f}\|_{X_\varepsilon} \end{aligned}$$

Therefore

$$\|A_{\mathbf{w}} - A_{\mathbf{w}'}\|_{\text{op}} \leq C\varepsilon^{-1} \|\mathbf{w} - \mathbf{w}'\|_{X_\varepsilon} \tag{9.42}$$

Thanks to (9.41) and (9.42), we can get:

$$\|G(\mathbf{w}) - G(\mathbf{w}')\|_{X_\varepsilon} \leq C \|\mathbf{w} - \mathbf{w}'\|_{X_\varepsilon} C\varepsilon \leq L \|\mathbf{w} - \mathbf{w}'\|_{X_\varepsilon},$$

where  $L < 1$  for sufficiently small  $\varepsilon$ .

Thus  $G$  is a contraction mapping, which means there is a unique fixed point  $\mathbf{w}_\varepsilon$ , i.e.,  $G(\mathbf{w}_\varepsilon) = \mathbf{w}_\varepsilon$ . This implies that  $\mathbf{v}^\varepsilon := \mathbf{v} + \mathbf{w}_\varepsilon$  is the solution of the atomistic model. Furthermore, by Proposition 9.1, we have that for all  $f \in X_\varepsilon$ ,

$$\begin{aligned} \langle \delta^2 E_a[\mathbf{v}^\varepsilon] \mathbf{f}, \mathbf{f} \rangle_\varepsilon &\geq C \|\mathbf{f}\|_{X_\varepsilon}^2, \\ \langle \delta E_a[\mathbf{v}^\varepsilon], \mathbf{f} \rangle_\varepsilon &= 0. \end{aligned}$$

Therefore  $\mathbf{v}^\varepsilon$  is  $X_\varepsilon$ -local minimizer of the energy. □

*Proof. (Proof of Corollary 6.1.)* We still divide the energy into two parts and consider the  $A$  part only. Denote

$$\begin{aligned} E_{\text{PN}}^{A_\varepsilon}[\mathbf{u}] &= \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\langle \mathbf{s}_1, \mathbf{s}_2 \rangle} \sum_{i+j=2} \binom{2}{i} \left\{ \frac{1}{12} \partial_{ij} V(\mathbf{s}_1, \mathbf{s}_2) [(\mathbf{s}_1 \cdot \nabla) \mathbf{u}_\mathbf{x}^\pm]^i \right. \\ &\quad \cdot [(\mathbf{s}_2 \cdot \nabla) \mathbf{u}_\mathbf{x}^\pm]^j + \frac{1}{4} \partial_{ij} V(\mathbf{s}_1 + \mathbf{p}, \mathbf{s}_2) [(\mathbf{s}_1 + \mathbf{p}) \cdot (\nabla \mathbf{u}_\mathbf{x}^\pm)]^i [(\mathbf{s}_2) \cdot (\nabla \mathbf{u}_\mathbf{x}^\pm)]^j \left. \right\} \\ &\quad + \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} [U(2\mathbf{u}_\mathbf{x} + \mathbf{s} - \mathbf{d}) + U(2\mathbf{u}_\mathbf{x} + \mathbf{s} + \mathbf{p} - \mathbf{d}) - U(\mathbf{s} - \mathbf{d}) - U(\mathbf{s} + \mathbf{p} - \mathbf{d})]. \end{aligned} \tag{9.43}$$

The first part is associated with the elastic energy, and the second part the misfit energy. It is sufficient to show  $|E_a^A[\mathbf{v}^\varepsilon] - E_a^A[\mathbf{v}]| \leq C\varepsilon^2$ ,  $|E_a^A[\mathbf{v}] - E_{\text{PN}}^{A_\varepsilon}[\mathbf{v}]| \leq C\varepsilon^2$  and  $|E_{\text{PN}}^{A_\varepsilon}[\mathbf{v}] - E_{\text{PN}}^A[\mathbf{v}]| \leq C\varepsilon^2$ .

For the first term  $|E_a^A[\mathbf{v}^\varepsilon] - E_a^A[\mathbf{v}]|$ , the difference in the elastic energy part is  $|(\mathbf{v} + \mathbf{v}^\varepsilon, \mathbf{v} - \mathbf{v}^\varepsilon)_A| + O(\varepsilon^3)$ , using definitions of  $E_a^A[\cdot]$  in Equation (5.15) and inner product  $(f, g)_A$  in Equation (5.12) and Taylor expansion. Due to the definition of  $\|\cdot\|_{X_\varepsilon}$  and boundedness of  $\mathbf{v}$  and  $\mathbf{v}^\varepsilon$ , we have  $|(\mathbf{v} + \mathbf{v}^\varepsilon, \mathbf{v} - \mathbf{v}^\varepsilon)_A| \leq C \|\mathbf{v} - \mathbf{v}^\varepsilon\|_{X_\varepsilon} \leq C\varepsilon^2$ , where the last inequality is the conclusion of Theorem 6.2. For the misfit energy part of  $|E_a^A[\mathbf{v}^\varepsilon] - E_a^A[\mathbf{v}]|$ , without loss of the generality, we consider the following error, where  $\mathbf{w}_\mathbf{x}^{A\pm} := (\mathbf{v}^\varepsilon)_\mathbf{x}^\pm - \mathbf{v}_\mathbf{x}^{A\pm}$ :

$$\begin{aligned} R_{\text{e-mis-1}} &:= \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \left| \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} [U((\mathbf{v}^\varepsilon)_{\mathbf{x}+\mathbf{s}}^{A+} - (\mathbf{v}^\varepsilon)_\mathbf{x}^{A-} + \mathbf{s} - \mathbf{d}) - U(\mathbf{w}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{w}_\mathbf{x}^{A-} + \mathbf{s} - \mathbf{d})] \right| \\ &\leq \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \left\{ \left| \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} [U'(\mathbf{w}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{w}_\mathbf{x}^{A-} + \mathbf{s} - \mathbf{d})(\mathbf{w}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{w}_\mathbf{x}^{A-})] \right| \right. \\ &\quad \left. + \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} \frac{1}{2} [U_{2,\mathbf{s}}(\mathbf{w}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{w}_\mathbf{x}^{A-})^2] \right\} \\ &\leq \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \left\{ \left| \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_{\mathbf{s}} U'(s - \mathbf{d})(\mathbf{w}_{\mathbf{x}+\mathbf{s}}^{A+} - \mathbf{w}_\mathbf{x}^{A-}) \right| \right\} \end{aligned}$$

$$\begin{aligned}
 & + \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_s \frac{1}{2} U_{2,s} |(\mathbf{v}_{\mathbf{x}+s}^{A+} - \mathbf{v}_{\mathbf{x}}^{A-})(\mathbf{w}_{\mathbf{x}+s}^{A+} - \mathbf{w}_{\mathbf{x}}^{A-})| \\
 & + \sum_{\mathbf{x} \in \mathbb{L}_R} \sum_s \frac{1}{2} [U_{2,s} (\mathbf{w}_{\mathbf{x}+s}^{A+} - \mathbf{w}_{\mathbf{x}}^{A-})^2] \Big\}. \tag{9.44}
 \end{aligned}$$

Recall that the upper bound  $U_{2,s}$  is defined in Equation (8.1). The second term in Equation (9.44) is bounded by  $C\varepsilon^2$  by Theorem 6.2 as discussed above. The last term in Equation (9.44) is  $O(\varepsilon^4)$  since  $\|w\|_{X_\varepsilon}^2 \leq C\varepsilon^4$  by Theorem 6.2. The first term in Equation (9.44) vanishes because  $\sum_{\mathbf{x} \in \mathbb{L}_R} \sum_s U'(s - \mathbf{d})(\mathbf{w}_{\mathbf{x}+s}^{A+} - \mathbf{w}_{\mathbf{x}}^{A-}) = 2 \sum_{\mathbf{x} \in \mathbb{L}_R} \mathbf{w}_{\mathbf{x}}^{A+} \sum_s U'(s - \mathbf{d}) = 0$ . Here  $\sum_s U'(s - \mathbf{d}) = 0$  because it corresponds to the state of the perfect lattice. The proof is similar for the errors between other terms in the misfit energy part in  $|E_a^A[\mathbf{v}^\varepsilon] - E_a^A[\mathbf{v}]|$ . Therefore, the misfit energy part in  $|E_a^A[\mathbf{v}^\varepsilon] - E_a^A[\mathbf{v}]|$  is also bounded by  $C\varepsilon^2$ .

For the second error bound  $|E_a^A[\mathbf{v}] - E_{\text{PN}}^{A_\varepsilon}[\mathbf{v}]| \leq C\varepsilon^2$ , the proof is similar to that for the consistency of the PN model as given in Proposition 8.1 in Section 8.

For the last error bound  $|E_{\text{PN}}^{A_\varepsilon}[\mathbf{v}] - E_{\text{PN}}^A[\mathbf{v}]| \leq C\varepsilon^2$ , similar to Lemma 3.1 in Section 3, we have

$$E_{\text{PN}}^{A_\varepsilon}[\mathbf{u}] = \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left[ \frac{1}{2} \alpha_1 (\partial_x \mathbf{u}_{\mathbf{x}}^+)^2 + \frac{1}{2} \alpha_2 (\partial_y \mathbf{u}_{\mathbf{x}}^+)^2 + \gamma_A (2\mathbf{u}_{\mathbf{x}}^+) \right]. \tag{9.45}$$

Denoting  $\mathbf{g}(\mathbf{x}) := \frac{1}{2} \alpha_1 (\partial_x \mathbf{v}^+(\mathbf{x}))^2 + \frac{1}{2} \alpha_2 (\partial_y \mathbf{v}^+(\mathbf{x}))^2 + \gamma_A (2\mathbf{v}^+(\mathbf{x}))$ , and using the parallelogram  $P_{\mathbf{x}}$  define in Figure 9.3, we have

$$\begin{aligned}
 & \left| E_{\text{PN}}^{A_\varepsilon}[\mathbf{v}] - E_{\text{PN}}^A[\mathbf{v}] \right| \\
 & \leq \frac{1}{4} \lim_{R \rightarrow +\infty} \frac{\varepsilon^2}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \int_{P_{\mathbf{x}} \cup P_{\mathbf{x}-e_1} \cup P_{\mathbf{x}-e_2} \cup P_{\mathbf{x}-e_2+e_1}} |g(\mathbf{y}) - g(\mathbf{x})| d\mathbf{y} \\
 & \leq C \lim_{R \rightarrow +\infty} \frac{\varepsilon^4}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \max_{\xi \in P_{\mathbf{x}} \cup P_{\mathbf{x}-e_1} \cup P_{\mathbf{x}-e_2} \cup P_{\mathbf{x}-e_2+e_1}} |\nabla^2 g(\xi)| \\
 & \leq C \lim_{R \rightarrow +\infty} \frac{\varepsilon^4}{2R} \sum_{\mathbf{x} \in \mathbb{L}_R} \left\{ (\mathbf{v}_{2,\mathbf{x},2e_1})^2 + \mathbf{v}_{1,\mathbf{x},2e_1} \mathbf{v}_{3,\mathbf{x},2e_1} + (\mathbf{v}_{1,\mathbf{x},2e_1})^2 + \mathbf{v}_{2,\mathbf{x},2e_1} \right\} \\
 & \leq C\varepsilon^2. \tag{9.46}
 \end{aligned}$$

The last inequality is due to Lemma 8.2 in Section 8. □

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