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From Atomistic Model to the Peierls–Nabarro Model with γ-surface for Dislocations

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Abstract

The Peierls–Nabarro (PN) model for dislocations is a hybrid model that incorporates the atomistic information of the dislocation core structure into the continuum theory. In this paper, we study the convergence from a full atomistic model to the PN model with γ-surface for the dislocation in a bilayer system. We prove that the displacement field and the total energy of the dislocation solution of the PN model are asymptotically close to those of the full atomistic model. Our work can be considered as a generalization of the analysis of the convergence from atomistic model to Cauchy–Born rule for crystals without defects.

1. Introduction

Dislocations are line defects and the primary carriers of plastic deformation in crystals. They are essential in the understanding of mechanical and plastic properties of crystalline materials [32]. Models at different length, and time scales have been developed to characterize the behaviors of dislocations and properties of the materials. Atomistic models and first principles calculations are able to capture detailed information of dislocations, however, they are computationally time-consuming and are limited to domains of small size over short time scales. On the other hand, the continuum theory of dislocations based on linear elasticity theory applies to much larger domains; although this theory is accurate outside the dislocation core region (of a few lattice constants size), it breaks down inside the dislocation core where the atomic structure is heavily distorted. The Peierls–Nabarro (PN) model [45,52] is a hybrid model that incorporates in the continuum model the dislocation core structure informed by atomistic or first principles calculations. Ever since its development, this model and its generalizations have been widely employed in the investigation of dislocation-core related properties [6,11–15,22,31,34–37,40,41,43,44,46,54–66,68–70].

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In the classical PN model [45,52], the slip plane of a straight edge or screw dislocation divides the crystal into two half-space elastic continua reconnected by a nonlinear potential force incorporating the atomistic effect. The nonlinear potential force is described based on the relative displacement (disregistry) across the slip plane in the direction of Burgers vector of the dislocation. The total energy consists of two half-space elastic energies and a misfit energy that leads to the nonlinear potential force across the slip plane. The misfit energy in the classical PN model is approximated by a sinusoidal function of the disregistry. The dislocation configuration is regarded as the minimizer of the total energy subject to the constraint of the Burgers vector of the dislocation. Such a hybrid model is able to give fairly good results of the dislocation core structure, the non-singular stress field and the total energy, as well as the Peierls stress and the Peierls energy for the motion of the dislocation.

Vitek [59] introduced the concept of the generalized stacking fault energy (or the γ-surface), which is expressed in terms of the disregistry vector (relative displacement vector) across the slip plane. For a given disregistry vector, the value of the γ-surface is defined as the energy increment per unit area (after relaxation) when the two half-spaces of the crystal have a uniform relative shift across the slip plane by this disregistry vector, which can be calculated by atomistic models. The γ-surface does not only provide a more realistic nonlinear potential than the sinusoidal form used in the original works of Peierls and Nabarro [45,52], but also enables vector-valued disregistry function across the slip plane than the scalar disregistry function in the original PN model. Thus it is able to describe the partial dissociation of perfect dislocations [59,60]. The γ-surfaces can be calculated using the empirical potentials as in the original work of Vitek [59]. Recently, the γ-surfaces are also obtained more accurately by using the first principles calculations (e.g. [6,31,34,37,70]). The method of γ-surface has become an important tool for the study of dislocations and plastic properties in crystals.

Besides the incorporation of γ-surfaces, a considerable number of generalizations of the classical PN model in other aspects have also been developed in the past seventy years. These generalizations further considered elastic anisotropy [22,54,68], the lattice discreteness and Peierls stress [6,37,43,56,57,63,64], nonlocal misfit energy [41,55] and gradient energy [40,61], and dislocation cross-slip [36,65]. Generalized PN models have also been developed for curved dislocations [35,44,68,69] and within the phase field framework for curved dislocations [58]. Models within the PN framework have also been proposed for grain boundaries [11,12,57,62], twin boundary junctions [15], and bilayer graphene and other bilayer materials [13,14,70]. Asymptotic analysis [67] and rigorous analysis [8,9,17,18,21,27,30,42,48–51] have also been performed for the convergence and properties from the PN models to models of discrete dislocations, dislocation distributions and plasticity at larger length and time scales.

Despite the wide range of generalizations and applications of the PN models, there is not much mathematical understanding and rigorous analysis on the atomistic foundation of these models. An attempt was made by El Hajj et al. [21] (theorem) and Fino et al. [23] (full proof) to prove the convergence from the nearest neighbor Frenkel–Kontorova model [24] on squared lattice to the PN model

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using viscosity solutions. Such a Frenkel–Kontorova model is a simplified, special atomistic model compared with the atomistic models used in molecular dynamics / molecular static (MD/MS) simulations, and some important aspects of the derivation of the PN models from those atomistic models used in MD/MS simulations still need rigorous justification. For example, in their convergence theorem established based on the nearest neighbor Frenkel–Kontorova model [21,23], the γ-surface is identical to nearest neighbor interaction potential across the slip plane in the atomistic model, whereas in a real crystalline material, the range of the interaction between atoms is larger than the nearest neighbors and rigorous analysis is still needed for the derivation of the γ-surface in the PN model from atomistic models in real MD/MS simulations. Moreover, their convergence proof is based on the framework of viscosity solution as the ratio of the length of the Burgers vector vs the dislocation core width (denoted by ε) goes to 0. However, in a real crystal, the dislocation core width is a finite multiple of the length of the Burgers vector.

In this paper, we perform a rigorous analysis for the convergence from atomistic model to the PN model with γ-surface, in the regime where the lattice constant (or equivalently, the length of the Burgers vector of the dislocation) is much smaller than the dislocation core width (i.e., their ratio $\varepsilon \ll 1$). In the atomistic model used in our convergence proof, each atom interacts with all other atoms via an interatomic potential whose effective interaction range is much larger than the nearest neighbor interaction. Such atomistic models are commonly used in MD/MS simulations. As a result, the decomposition of the total energy into the elastic energy and misfit energy (expressed in terms of the γ-surface) in the framework of the PN models is rigorously justified based on this general atomistic model. Our proof is a variant of the proof for the convergence of nonlinear numerical schemes, which enables us to obtain the convergence rate of $O(\varepsilon^2)$. In our proof, we focus on the one-dimensional form of the generalized PN model recently developed for the inter-layer dislocations in a bilayer system [13,14]. Note that in the generalized PN model in Refs. [13,14], dislocations are lines lying between the two layers in a bilayer system, which are different from the dislocations as point defects in a monolayer graphene studied by Ariza et al. [1,2] using a discrete dislocation dynamics model.

Our work can also be considered as an extension of the analysis of the convergence issue of Cauchy–Born rule [3,4] for elastic media without dislocations and other defects, see, e.g. [3,5,7,19,20,25,38,39,47] for the recent progress. The major difficulty in the analysis of the PN model lies in the fact that due to the presence of the dislocation, the displacement vector across the slip plane of the dislocation is no longer continuous, which is unlike in the Cauchy–Born rule where the displacement and its gradient are always continuous. Such a discontinuity in the PN model is handled by the γ-surface, and our work successfully establishes the convergence from atomistic model to the PN model under the one-dimensional setting. Our proof is inspired by the work of E and Ming [20], in which the stability and convergence of the Cauchy–Born rule were rigorously analyzed for states close to perfect lattices. More precisely, we show that the dislocation solution and the associated energy of the PN model is an approximation of the dislocation solution using the full atomistic model. An important assumption in our analysis is that the ratio of the lattice constant to the dislocation core size is small, which is valid

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in the bilayer graphene due to the strong intra-layer atomic interaction and weak inter-layer atomic interaction [13,14].

Our convergence result is based on the consistency, the linear stability, and a fixed point argument. Infinite interaction range causes difficulties in estimating the truncation error and proving the compactness for the fixed point iteration. This is solved by detailed estimates on the decaying of the derivatives of the pair potentials and the PN solution. Another difficulty is that the stability of the atomistic dislocation solution cannot be directly obtained from that of a perfect lattice because the disregistry might be as large as a (half) Burger vector. This is different from the situation in the Cauchy–Born rule [20], where both atomistic and continuous configurations are perturbed from a common equilibrium state. To overcome this, we first prove the stability for the PN solution using the standard techniques in elliptic partial differential equations. Consequently, we obtain the first positive eigenvalue of the linearized PN operator at the PN solution. The stability of the atomistic model is then achieved by controlling the stability gap between two models. Such stability of a dislocation core still lacks systematic study in the literature. An attempt was made by Hudson and Ortner [33] for an atomistic model with nearest neighbor interaction. They obtained the stability of a screw dislocation under anti-plane deformation in the sense that the dislocation solution is a global minimizer of the total energy with given total Burgers vector. To avoid the lattice periodic translation invariant, they fixed the dislocation center. Although we also fix the center of dislocation, our proofs of stabilities are quite different from theirs. In particular, we consider both atomistic and continuum models for edge dislocation, and the stabilities are proved in a continuum-to-atomistic way, as shown above. Again, in the stability analysis of our atomistic model, the infinite-ranged pair potentials lead to an issue in estimating double infinite summations, which is overcome by various summability lemmas obtained in this paper.

There is an extensive literature on the convergence issue of dislocation models using the language of Γ-convergence [10,16,26,28,53]. To the best of our knowledge, they all study the upscaling from the discrete dislocation theory to the dislocation density theory in much larger scales than our situation here. In contrast to these works focusing on many dislocations to dislocation density and neglect the details of the core structure, our work looks into a single dislocation core structure and provide a quantitative error estimate for displacement in the PN dislocation solution with respect to the atomistic dislocation solution. In particular, we obtain the misfit potential in the continuum model from atomistic model according to the exact definition of γ surface instead of a phenomenological quadratic or sinusoidal approximation.

The present paper is organized as follows. We present the atomistic model and the PN model, and state the main results of this paper in Sect. 2. Section 3 provides some preliminary results for the rest of the analysis. In Sect. 4, we deal with the consistency issue of the PN model based on asymptotic analysis of the atomistic model. In Sect. 5, we focus on the existence and stability of the PN model. Section 6 is concerned with the stability of atomistic model. In Sect. 7, we collect the previous results to prove the existence of the atomistic solution which is close to the continuum solution in the asymptotic sense. Finally, our key assumption on

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the smallness of ε is validated in the appendix using data based on first principle calculations.

2. Models and Main Results

In this paper, we study the one-dimensional form of the generalized PN model recently developed for the inter-layer dislocations in a bilayer system (see the related bilayer graphene model in [13]). That is, the dislocation is straight and the structure of the bilayer system is uniform in the direction of the dislocation. We focus on an edge dislocation between a planar bilayer system and neglect the buckling effect [13]. This is a reasonably simplified scenario, for instance, when the bilayer is bonded by a substrate such that the buckling is limited. In fact, comparing to in-plane displacement, the out-of-plane displacement affects only slightly the structure of an edge dislocation. As a result, we only study the displacement within the slip plane. The dislocation solutions are local minimizers of the total energy in the atomistic model and the PN model, respectively, subject to the constraint of the total Burgers vector. We will show that the dislocation solution of the PN model is an approximation of the dislocation solution using the atomistic model.

2.1. Atomistic Model

In the one-dimensional setting, the bilayer system atoms along the x axis. The two atomic layers are located at $y = \pm\frac{1}{2}d$, respectively, where d is the distance between two layers. For a perfect bilayer system without dislocation, the atoms are located at $\Gamma_{\mathrm{a}}^{\pm} = \{\mathbf{x}_i^{\pm} = (x_i^{\pm}, \pm\frac{1}{2}d) : i \in \mathbb{Z}\}$, where $x_i^{+} = ia - \frac{1}{2}a$, $x_i^{-} = ia$, and a is the lattice constant, see Fig. 1a. This perfect lattice is the reference state of the dislocation to be described below.

Suppose that there is a dislocation centered at the origin $(0, 0)$ with Burgers vector $\mathbf{b} = (a, 0)$. This dislocation is an edge dislocation. The dislocation structure is described by using the perfect lattice above as the reference state, and the atomic sites are $\Gamma_{\mathrm{a}}'^{\pm} = \{\mathbf{x}_i'^{\pm} = (x_i'^{\pm}, \pm\frac{1}{2}d) : i \in \mathbb{Z}\}$, where $x_i'^{+} = x_i^{+} + u_i^{+} = ia - \frac{1}{2}a + u_i^{+}$ and $x_i'^{-} = x_i^{-} + u_i^{-} = ia + u_i^{-}$. The displacement field $u = \{u_i^{+}, u_i^{-}\}_{i\in\mathbb{Z}}$ of this edge dislocation satisfies the boundary conditions at $\pm\infty$:

$$\lim_{i\to-\infty} (u_i^{+} - u_i^{-}) = 0, \quad \lim_{i\to+\infty} (u_i^{+} - u_i^{-}) = a. \tag{1}$$

To fix the center of the dislocation at $(0, 0)$, we also assume

$$u_0^{+} - u_0^{-} = a/2. \tag{2}$$

See the atomic configuration of this dislocation shown in Fig. 1b. Here we only consider the horizontal displacement, and the vertical displacement that is normal to the bilayer is neglected due to the non-buckling case.

Suppose that the system is described by pairwise potentials. The interaction is $V\left(\frac{|\mathbf{x}_j'^{\pm} - \mathbf{x}_i'^{\pm}|}{a}\right) = V\left(\frac{x_j'^{\pm} - x_i'^{\pm}}{a}\right)$ for atoms $\mathbf{x}_j'^{\pm}$ and $\mathbf{x}_i'^{\pm}$ in the same layer; while it is

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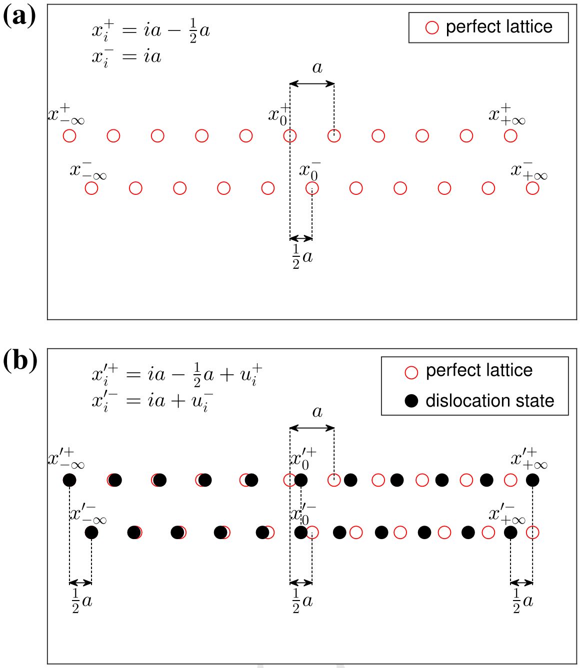

Fig. 1. **a** Perfect lattice. **b** Configuration of an edge dislocation (compared with the reference state)

$V_{\text{inter}}\left(\frac{|\mathbf{x}_j'^+ - \mathbf{x}_i'^-|}{a}\right)$ for atoms $\mathbf{x}_j'^+$ and $\mathbf{x}_i'^-$ from different layers. When the distance d between two layers is fixed, we have $|\mathbf{x}_j'^+ - \mathbf{x}_i'^-| = \sqrt{(x_j'^+ - x_i'^-)^2 + d^2}$ and the interlayer potential only depends on the horizontal distance $|x_j'^+ - x_i'^-|$. We define

$$V_d\left(\frac{x_j'^+ - x_i'^-}{a}\right) := V_{\text{inter}}\left(\frac{|\mathbf{x}_j'^+ - \mathbf{x}_i'^-|}{a}\right) = V_{\text{inter}}\left(\frac{\sqrt{(x_j'^+ - x_i'^-)^2 + d^2}}{a}\right). \tag{3}$$

The total energy of the atomistic model is given by

$$\begin{aligned} E_{\text{a}}[u] = \frac{1}{2}\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}^*}\Bigg\{&\left[V\left(\frac{x_{i+s}'^+ - x_i'^+}{a}\right) - V(s)\right] \\ &+ \left[V\left(\frac{x_{i+s}'^- - x_i'^-}{a}\right) - V(s)\right]\Bigg\} \\ &+ \sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\left[V_d\left(\frac{x_{i+s}'^+ - x_i'^-}{a}\right) - V_d\left(s - \frac{1}{2}\right)\right] \end{aligned}$$

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$$= \frac{1}{2}\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}^*}\left[V\left(s+\frac{u_{i+s}^+-u_i^+}{a}\right)+V\left(s+\frac{u_{i+s}^--u_i^-}{a}\right)-2V(s)\right]$$

$$+\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\left[V_d\left(s-\frac{1}{2}+\frac{u_{i+s}^+-u_i^-}{a}\right)-V_d\left(s-\frac{1}{2}\right)\right]. \tag{4}$$

Recall that the state of perfect lattice is used as the reference state.

The atomic sites of the edge dislocation is determined by minimizing the total energy in Eq. (4) subject to the displacement conditions in Eqs. (1) and (2).

2.2. *Peierls–Nabarro (PN) Model*

In the PN model, we consider an edge dislocation with Burgers vector $\mathbf{b} = (a, 0)$ centered at the origin of the xy plane in the bilayer system $\Gamma_{\text{PN}}^+ \cup \Gamma_{\text{PN}}^-$, where $\Gamma_{\text{PN}}^\pm = \left\{\mathbf{x}^\pm = (x'^\pm, \pm\frac{1}{2}d) : x'^\pm = x + u^\pm(x), x \in \mathbb{R}\right\}$. As in the atomistic model, we only consider the displacement within its own layer (i.e., the x direction), and call it the horizontal displacement. The vertical displacement that is normal to the bilayer is neglected. Here $u^+(x)$ and $u^-(x)$ are the horizontal displacements along the two layers Γ_{PN}^+ and Γ_{PN}^-, respectively.

As in the classical PN model [45,52], the disregistry (relative displacement) $\phi(x)$ between the two layers is

$$\phi(x) = u^+(x) - u^-(x). \tag{5}$$

The disregistry $\phi(x)$ of this edge dislocation satisfies the boundary conditions

$$\lim_{x\to-\infty}\phi(x) = 0, \quad \lim_{x\to+\infty}\phi(x) = a. \tag{6}$$

We also assume that

$$\phi(0) = a/2 \tag{7}$$

In order to fix the center of the dislocation at $x = 0$. Note that the horizontal displacement is not continuous in the y direction, and the discontinuity is described by the disregistry function $\phi(x)$. The disregistry function $\phi(x)$ also describes the structure of the dislocation; more precisely, $\phi(x)$ is the distribution of the Burgers vector.

In the framework of the PN model [45,52] with γ-surface [59], the total energy of the bilayer system is divided into two parts: an elastic energy due to the intra-layer elastic interaction and a misfit energy due to the nonlinear interaction between the two layers, which is

$$E_{\text{PN}}[u] = E_{\text{elas}}[u] + E_{\text{mis}}[\phi]. \tag{8}$$

Here $E_{\text{elas}}[u]$ is the elastic energy due to the intra-layer elastic interaction in the two layers

$$E_{\text{elas}}[u] = \int_{\mathbb{R}}\left(\frac{1}{2}\alpha|\nabla u^+|^2 + \frac{1}{2}\alpha|\nabla u^-|^2\right)\mathrm{d}x, \tag{9}$$

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where α is the elastic modulus. Note that in each layer, the elastic energy density is $\frac{1}{2}\alpha|\nabla u^{\pm}|^2$. The energy $E_{\text{mis}}[\phi]$ is the misfit energy due to the nonlinear interaction between the two layers

$$E_{\text{mis}}[\phi] = \int_{\mathbb{R}} \gamma(\phi)\,\mathrm{d}x, \tag{10}$$

where the density of this misfit energy $\gamma(\phi)$ is the γ-surface (or the generalized stacking fault energy) [59] that is defined as the energy increment per unit length when there is a uniform shift of ϕ between the two layers. Especially, when $\phi = ia$, $i \in \mathbb{Z}$, the shifted system still has the perfect lattice structure, and $\gamma(\phi) = 0$. In summary, the energy density of the PN model is

$$W_{\text{PN}}\left(\phi, \nabla u^+, \nabla u^-\right) = \frac{1}{2}\alpha|\nabla u^+|^2 + \frac{1}{2}\alpha|\nabla u^-|^2 + \gamma(\phi). \tag{11}$$

The γ-surface $\gamma(\phi)$ accounts for the nonlinear interaction between the two layers with displacement discontinuity ϕ between them. Using its definition, the γ-surface can be calculated from the atomistic model in Sect. 2.1 by

$$\gamma(\phi) = \frac{1}{a}\sum_{s\in\mathbb{Z}}\left[V_d\left(s - \frac{1}{2} + \frac{\phi}{a}\right) - V_d\left(s - \frac{1}{2}\right)\right]. \tag{12}$$

The constant α in the elastic energy in Eq. (9) can also be calculated from the atomistic model in Sect. 2.1 by

$$\alpha = \frac{1}{2a}\sum_{s\in\mathbb{Z}^*} V''(s)|s|^2. \tag{13}$$

The purpose of this paper is to establish the convergence from the atomistic model in Sect. 2.1 to the PN model in Eqs. (8)–(10). As a result, the decomposition of the total energy into the elastic energy and misfit energy (expressed in terms of the γ-surface) in the framework of the PN models is rigorously justified based on the atomistic model. Especially, here the γ-surface in Eq. (12) is calculated from the atomistic model following the definition introduced by Vitek [59], and we rigorously prove its convergence to the continuum form. Recall that the sinusoidal potential in the classical PN model [45,52] and some other simplified forms of multi-well potentials in later generalization and analysis (such as the piecewise quadratic potential) only reflect the lattice periodicity across the slip plane in a phenomenological way.

This PN model for the bilayer material contains the essential features of the PN models with γ-surface. That is, the system is considered as two elastic continua connected by a misfit energy expressed in terms of the γ-surface that accounts for the nonlinear interaction between the two elastic continua. Note that for a dislocation in $\mathbb{R}^3$, as in the classical PN model [45,52] with the γ-surface [59] and later generalizations as reviewed in the introduction section, the three-dimensional space is divided by the slip plane of the dislocation into two half-space elastic continua, and they are connected by a misfit energy expressed in terms of the γ-surface across the slip plane. The total energy is $E_{\text{PN}} = E_{\text{elas}} + E_{\text{mis}}$, where

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$E_{\text{elas}} = \int_{\mathbb{R}^3\setminus\{z=0\}} \sum_{i,j=1}^{3} \frac{1}{2}\sigma_{ij}\epsilon_{ij}\mathrm{d}x\mathrm{d}y\mathrm{d}z$ and $E_{\text{mis}} = \int_{\mathbb{R}^2} \gamma(\phi(x, y))\mathrm{d}x\mathrm{d}y$. Here the xy plane is the slip plane of the dislocation, and $\frac{1}{2}\sigma_{ij}\epsilon_{ij}$ is the (linear) elastic energy density, σ_{ij} and ϵ_{ij} are the stress and strain tensors, respectively, and $\gamma(\phi)$ is the γ-surface. Generalization can also be made to replace the energy of linear elasticity in the PN model by the energy of Cauchy–Born nonlinear elasticity.

2.3. Weak Interlayer Interaction and Rescaling

For a bilayer system, the van der Waals-like interaction between the two layers is weak compared to the strong interlayer covalent-bond interaction in each layer [13]. That is, $V_d \ll V$ in the atomistic model. We write the relationship as

$$V_d = O(\varepsilon^2)V, \tag{14}$$

where ε is some dimensionless small parameter to be defined below. Recall that in the PN model for the bilayer system, the elastic energy E_{elas} is due to the interlayer interaction and the misfit energy E_{mis} comes from the interaction between the two layers. The dimensionless small parameter ε is defined based on the PN model as follows.

For most parts of the system, the atoms are away from the dislocation, and their atomistic structure is close to that of the stable perfect lattice. For example, when $\phi/a \ll 1$ in the PN model in Sect. 2.3, which happens on the negative part of the x axis away from the origin, the energy density in the PN model in Eq. (11) is approximated well by a quadratic form:

$$W_{\text{PN}}\left(\phi, \nabla u^+, \nabla u^-\right) \approx \frac{1}{2}\alpha|\nabla u^+|^2 + \frac{1}{2}\alpha|\nabla u^-|^2 + \frac{1}{2}\gamma''(0)\phi^2 \tag{15}$$

$$= \frac{1}{2}\alpha|\nabla u^+|^2 + \frac{1}{2}\alpha|\nabla u^-|^2 + \frac{1}{2}a^2\gamma''(0)\left(\frac{\phi}{a}\right)^2. \tag{16}$$

In fact, when $\phi/a \ll 1$, $\gamma(\phi)$ should reduce to the elastic energy density per unit length in the linear elasticity theory ([32] Sect. 1–2), which gives $\gamma''(0) = (a/d)\mu > 0$, where μ is the shear modulus of the crystal. We remark that a similar quadratic form works for the positive part, with the last term in Eq. (16) replaced by $\frac{1}{2}a^2\gamma''(0)\left(\frac{\phi-a}{a}\right)^2$.

The ratio of the coefficients $\frac{a^2\gamma''(0)}{\alpha}$ is a dimensionless constant that characterizes the relative strength of the inter-layer interaction versus the intra-layer interaction. Recall that the parameter α is expressed in terms of quantities in the atomistic model as in Eq. (13). Using the atomistic expression of $\gamma(\phi)$ in Eq. (12), we have

$$\gamma''(0) = \frac{1}{a^3}\sum_{s\in\mathbb{Z}} V_d''\left(s - \frac{1}{2}\right). \tag{17}$$

As suggested by Eqs. (13), (17) and (14), we define the dimensionless parameter

$$\varepsilon = \sqrt{\frac{a^2\gamma''(0)}{\alpha}}, \tag{18}$$

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and assume that

$$\varepsilon \ll 1. \tag{19}$$

A validation of this assumption based on values of atomistic and first principles calculations [13,70] is given in the Appendix.

Using a/ε as the unit length for the spatial variable x and a as the unit length for the displacements in the PN model, we have the following rescaled quantities:

$$\tilde{x} = \frac{\varepsilon x}{a}, \quad \tilde{u}^{\pm} = \frac{u^{\pm}}{a}, \quad \tilde{\phi} = \frac{\phi}{a}. \tag{20}$$

Accordingly, the variables and functionals related to energy densities are rescaled to

$$\tilde{\alpha} = a\alpha, \quad \tilde{\gamma}(\tilde{\phi}) = a\gamma(\phi), \tag{21}$$

$$\tilde{W}_{\mathrm{PN}}(\tilde{\phi}, \nabla_{\tilde{x}}\tilde{u}^{+}, \nabla_{\tilde{x}}\tilde{u}^{-}) = \varepsilon^{-1} W_{\mathrm{PN}}(\phi, \nabla u^{+}, \nabla u^{-}), \tag{22}$$

$$\tilde{E}_{\mathrm{PN}}[u] = \varepsilon^{-1} E_{\mathrm{PN}}[u], \quad \tilde{E}_{\mathrm{a}}[u] = \varepsilon^{-1} E_{\mathrm{a}}[u]. \tag{23}$$

Using these rescaled variables, the total energy in the PN model can be written as

$$\begin{aligned} \tilde{E}_{\mathrm{PN}}[u] &= \int_{\mathbb{R}} \tilde{W}_{\mathrm{PN}}(\tilde{\phi}, \nabla_{\tilde{x}}\tilde{u}^{+}, \nabla_{\tilde{x}}\tilde{u}^{-})\, \mathrm{d}\tilde{x} \\ &= \int_{\mathbb{R}} \left\{ \frac{1}{2}\tilde{\alpha}|\nabla_{\tilde{x}}\tilde{u}^{+}|^2 + \frac{1}{2}\tilde{\alpha}|\nabla_{\tilde{x}}\tilde{u}^{-}|^2 + \tilde{\gamma}(\tilde{\phi}) \right\} \mathrm{d}\tilde{x}, \end{aligned} \tag{24}$$

where

$$\tilde{\alpha} = \sum_{s\in\mathbb{Z}^*} \frac{1}{2} V''(s)|s|^2, \tag{25}$$

$$\tilde{\gamma}(\tilde{\phi}) = \sum_{s\in\mathbb{Z}} \left[U\left(s - \frac{1}{2} + u^{+} - u^{-}\right) - U\left(s - \frac{1}{2}\right) \right]. \tag{26}$$

Here, following Eq. (14), we define in the atomistic model that

$$U = \varepsilon^{-2} V_d, \tag{27}$$

so that $U = O(1)V$.

Finally, using Eq. (27), the total energy in the atomistic model can be written as

$$\begin{aligned} \tilde{E}_{\mathrm{a}}[u] = \frac{\varepsilon^{-1}}{2} \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}^*} \left[V\left(s + (\tilde{u}^{+}_{i+s} - \tilde{u}^{+}_{i})\right) + V\left(s + (u^{-}_{i+s} - u^{-}_{i})\right) - 2V(s) \right] \\ + \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} \left[U\left(s - \frac{1}{2} + (u^{+}_{i+s} - u^{-}_{i})\right) - U\left(s - \frac{1}{2}\right) \right]. \end{aligned} \tag{28}$$

For simplicity of notation, frow now on, we will use variables without $\sim$ in the PN model after the above rescaling.

We remark that $E_{\mathrm{PN}}[u]$ is independent of ε, and hence $E_{\mathrm{PN}}[u] = O(1)$. The first and the second variations of atomistic and continuum models are denoted as $\delta E_{\mathrm{a}}[u]$, $\delta^2 E_{\mathrm{a}}[u]$, $\delta E_{\mathrm{PN}}[u]$, and $\delta^2 E_{\mathrm{PN}}[u]$, respectively. Their explicit form are given in Proposition 11.

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2.4. Assumptions and Notations

For readers' convenience, we first collect assumptions and fix notations.

Assumption. Here is the collection of our assumptions which are physically reasonable and will be discussed in details later.

A1 (weak inter-layer interaction) $\varepsilon \ll 1$.
A2 (symmetry) $V(x) = V(-x)$ and $U(x) = U(-x)$.
A3 (regularity) $V \in C^4(\mathbb{R}\backslash\{0\})$ and $U \in C^4(\mathbb{R})$.
A4 (fast decay) there exist $\beta > 0$ and $\theta > 0$, such that

$$|V^{(k)}(x)| \le \beta |x|^{-k-4-\theta}, \;\; |x| \ge \tfrac{1}{2}, \;\; k = 0, 1, \ldots, 4, \tag{29}$$

$$|U^{(k)}(x)| \le \beta |x|^{-k-2-\theta}, \;\; |x| > 0, \;\; k = 0, 1, \ldots, 4. \tag{30}$$

A5 (elasticity constant) $\alpha > 0$.
A6 (γ-surface) $\arg\min_{\phi\in\mathbb{R}} \gamma(\phi) = \mathbb{Z}$ and $\gamma''(0) > 0$.
A7 (small stability gap) $\varDelta < \frac{1}{3}\kappa$, where

$$\varDelta = \lim_{\varepsilon\to 0} \sup_{\|f\|_{X_\varepsilon}=1} \left\langle \delta^2 E_{\mathrm{PN}}[0]\bar{f}, \bar{f}\right\rangle_0 - \left\langle \delta^2 E_{\mathrm{a}}[0] f, f\right\rangle_\varepsilon, \tag{31}$$

$$\kappa = \inf_{\|f\|_{X_0}=1} \langle \delta^2 E_{\mathrm{PN}}[v] f, f\rangle_0. \tag{32}$$

with v being the dislocation solution of the PN model (cf. Theorem 1). The operators and functional spaces here will be defined in Eqs. (34)–(47).

We remark that in our bilayer system setting, A1–A7 are all satisfied. In particular, a verification of Assumption A1 is provided in the Appendix, where we show that $\varepsilon \approx 0.0475 \ll 1$ based on the data from Refs. [13,70].

In general, Assumptions A2–A4 are satisfied by most pair potentials, such as the Lennard–Jones potential, the Morse potential, etc.. The physical meaning of Assumptions A5–A6 is that the perfect lattice structure without defects is the unique global minimizer of the total energy and is strictly stable (cf. the discussion after Eq. (16)).

For Assumption A7, we remark that $\varDelta \ge 0$ (cf. Proposition 7) characterizes the stability gap between atomistic model ($\delta^2 E_{\mathrm{a}}[0]$) and PN model ($\delta^2 E_{\mathrm{PN}}[0]$) at perfect lattice, while $\kappa > 0$ (only depends on α, β, θ, and $\gamma''(0)$, cf. Proposition 3) depicts the stability of the dislocation solution of the PN model. We also provide an explicit formula for $\varDelta$ (cf. Proposition 6). The following are two examples where A7 holds:

Example 1. (nearest neighbor interaction) Let V be nearest neighbor interaction, i.e., $V(s) = 0$ for $|s| \ge 2$. Then $\varDelta = 0$ and Assumption A7 holds. (cf. Proposition 8).

Example 2. (Lennard–Jones potential) Let V be Lennard–Jones (m, n) potential, i.e.,

$$V(x) = V_{\mathrm{LJ}}(x) = -\left(\frac{r_0}{|x|}\right)^m + \left(\frac{r_0}{|x|}\right)^n, \;\; 1 < m < n, \;\; x \ne 0, \tag{33}$$

where r_0 is some characteristic distance. Then $\varDelta = 0$ and Assumption A7 holds. (cf. Proposition 10).

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Notations. In the proofs, we do not intend to optimize the constants, and hence we frequently use C to be an ε-independent constant, which may be different from line to line.

For convenience, we introduce the difference operators $D_s^{\pm}$ for f defined on $\varepsilon\mathbb{Z}$ or $\mathbb{R}$:

$$D_s^+ f(x) = \frac{f(x+\varepsilon s) - f(x)}{\varepsilon}, \quad D_s^- f(x) = \frac{f(x) - f(x-\varepsilon s)}{\varepsilon}, \ s \in \mathbb{Z}. \tag{34}$$

Moreover, we denote $Df = D_1^+ f$ and $D^k f = (D_1^+)^k f$ for $k \in \mathbb{N}$. For function f defined on $\varepsilon\mathbb{Z}$, we denote

$$f_i = f(\varepsilon i), \ i \in \mathbb{Z}. \tag{35}$$

Next, we introduce discrete Sobolev spaces $H_\varepsilon^k = H_\varepsilon^k(\varepsilon\mathbb{Z}) = \{f : \|f\|_{\varepsilon,k} < \infty\}$, $k \in \mathbb{N}$, where the H_ε^k norm is defined as follows:

$$\|f\|_{\varepsilon,k}^2 = \varepsilon \sum_{0 \le j \le k} \sum_{i \in \mathbb{Z}} |D^j f_i|^2. \tag{36}$$

Due to the convention, we denote $L_\varepsilon^2 = H_\varepsilon^0$ with norm $\|\cdot\|_\varepsilon = \|\cdot\|_{\varepsilon,0}$. We refer the readers to Lemma 4 for relations and properties of these spaces. For $f, g \in L_\varepsilon^2$, their inner products is given by

$$(f, g)_\varepsilon = \varepsilon \sum_{i \in \mathbb{Z}} f_i g_i. \tag{37}$$

If $f^\pm, g^\pm \in L_\varepsilon^2$, then we write $f = (f^+, f^-) \in L_\varepsilon^2$, $D^k f = (D^k f^+, D^k f^-)$ and define

$$\|f\|_{\varepsilon,k}^2 = \|f^+\|_{\varepsilon,k}^2 + \|f^-\|_{\varepsilon,k}^2, \tag{38}$$

$$(f, g)_\varepsilon = (f^+, g^+)_\varepsilon + (f^-, g^-)_\varepsilon. \tag{39}$$

Similarly, if $f^\pm, g^\pm \in L^2$, we write $f = (f^+, f^-) \in L^2$, $\nabla^k f = (\nabla^k f^+, \nabla^k f^-)$ and define

$$\|f\|_{H^k}^2 = \|f^+\|_{H^k}^2 + \|f^-\|_{H^k}^2, \tag{40}$$

$$(f, g)_0 = (f^+, g^+)_0 + (f^-, g^-)_0. \tag{41}$$

We use the notation $\|\cdot\|$ and $(\cdot,\cdot)_0$ to denote the L^2 norm and L^2 inner product, respectively. The uniform norms on $\varepsilon\mathbb{Z}$ is given by $\|f\|_{L_\varepsilon^\infty} = \sup_{i\in\mathbb{Z}} |f_i|$.

If $f = (f^+, f^-) \in L_\varepsilon^2$, we define its linear interpolation $\bar{f} = (\bar{f}^+, \bar{f}^-) \in L^2$:

$$\bar{f}^\pm(x) = \frac{(i+1)\varepsilon - x}{\varepsilon} f_i^\pm + \frac{x - i\varepsilon}{\varepsilon} f_{i+1}^\pm \text{ for } i\varepsilon \le x < (i+1)\varepsilon. \tag{42}$$

We define the jump of $f = (f^+, f^-)$ in y direction

$$f^\perp(x) = f^+(x) - f^-(x) \text{ and } f_i^\perp = f_i^+ - f_i^-. \tag{43}$$

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Note that the jump $u^\perp = \phi$ is the disregistry for the displacement of the PN model.

Throughout this paper, the evaluations $f^\pm(0)$ are always in the trace sense. We define the following functional spaces for the analysis of both models:

$$X_0 = \left\{ f = (f^+, f^-) : \|f\|_{X_0} < \infty,\ f^\pm(0) = 0 \right\}, \tag{44}$$

$$X_\varepsilon = \left\{ f = (f^+, f^-) : \|f\|_{X_\varepsilon} < \infty,\ f_0^\pm = 0 \right\}, \tag{45}$$

where $\|f\|_{X_0} = (f, f)_{X_0}^{1/2}$ and $\|f\|_{X_\varepsilon} = (f, f)_{X_\varepsilon}^{1/2}$ with the following inner products

$$(f, g)_{X_0} = (\nabla f^+, \nabla g^+)_0 + (\nabla f^-, \nabla g^-)_0 + (f^\perp, g^\perp)_0, \tag{46}$$

$$(f, g)_{X_\varepsilon} = (Df^+, Dg^+)_\varepsilon + (Df^-, Dg^-)_\varepsilon + (f^\perp, g^\perp)_\varepsilon. \tag{47}$$

It is easy to check that X_0 and X_ε are both Hilbert spaces with respect to inner products $(\cdot,\cdot)_{X_0}$ and $(\cdot,\cdot)_{X_\varepsilon}$. We remark that $\|f\|_{X_0}^2 = \|\nabla f\|^2 + \|f^\perp\|^2$ and $\|f\|_{X_\varepsilon}^2 = \|Df\|_\varepsilon^2 + \|f^\perp\|_\varepsilon^2$. We use notations $\langle\cdot,\cdot\rangle_0$ and $\langle\cdot,\cdot\rangle_\varepsilon$ for pairings on $X_0^* \times X_0$ and $X_\varepsilon^* \times X_\varepsilon$, respectively. The following linear subspace of X_ε will be useful in the proofs:

$$M_\varepsilon = \{ f = (f^+, f^-) \in X_\varepsilon : f_i^+ = -f_i^- = -f_{-i}^+,\ i \in \mathbb{Z} \}. \tag{48}$$

Let $u^0 = (u^{0+}, u^{0-})$ and $u^\varepsilon = (u^{\varepsilon+}, u^{\varepsilon-})$, where

$$u^{0+}(x) = \begin{cases} 0, & x < -\frac{1}{4}, \\ x + \frac{1}{4}, & -\frac{1}{4} \le x \le \frac{1}{4}, \\ \frac{1}{2}, & x > \frac{1}{4} \end{cases} \tag{49}$$

$$u^{0-}(x) = -u^{0+}(x),\ x \in \mathbb{R}, \tag{50}$$

$$u_i^{\varepsilon\pm} = u^{0\pm}(\varepsilon i),\ i \in \mathbb{Z}. \tag{51}$$

Then we define the lifts of X_0 and X_ε, i.e., the affine space over X_0 and X_ε, as follows:

$$\bar{X}_0 = \left\{ u = (u^+, u^-) : u - u^0 \in X_0 \right\}, \tag{52}$$

$$\bar{X}_\varepsilon = \left\{ u = (u^+, u^-) : u - u^\varepsilon \in X_\varepsilon \right\}. \tag{53}$$

Finally, we define solution spaces for our problems as follows:

$$S_0 = \left\{ u = (u^+, u^-) \in \bar{X}_0 : \lim_{x\to-\infty} u^\perp(x) = 0,\ \lim_{x\to+\infty} u^\perp(x) = 1 \right\}, \tag{54}$$

$$S_\varepsilon = \left\{ u = (u^+, u^-) \in \bar{X}_\varepsilon : \lim_{i\to-\infty} u_i^\perp = 0,\ \lim_{i\to+\infty} u_i^\perp = 1 \right\}. \tag{55}$$

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2.5. Main Results

For the PN model, we solve the minimization problem for $v = (v^+, v^-) \in S_0$:

$$\inf_{u \in S_0} E_{\mathrm{PN}}[u]. \tag{56}$$

The Euler–Lagrange equation of this minimization problem reads as

$$\begin{cases} \delta E_{\mathrm{PN}}[u] = 0, \\ \lim_{x \to -\infty} u^{\perp}(x) = 0, \ \lim_{x \to +\infty} u^{\perp}(x) = 1, \ u^{\pm}(0) = \pm\frac{1}{4}. \end{cases} \tag{57}$$

For the atomistic model, we solve the minimization problem for $v^\varepsilon = (v^{\varepsilon,+}, v^{\varepsilon,-}) \in S_\varepsilon$:

$$\inf_{u \in S_\varepsilon} E_{\mathrm{a}}[u]. \tag{58}$$

The Euler–Lagrange equation of this minimization problem reads as

$$\begin{cases} \delta E_{\mathrm{a}}[u] = 0, \\ \lim_{i \to -\infty} u_i^{\perp} = 0, \ \lim_{i \to +\infty} u_i^{\perp} = 1, \ u_0^{\pm} = \pm\frac{1}{4}. \end{cases} \tag{59}$$

We extend the domain of $E_{\mathrm{a}}[\cdot]$ (respectively, $E_{\mathrm{PN}}[\cdot]$) to $\bar{X}_\varepsilon$ (respectively, $\bar{X}_0$). Thus $E_{\mathrm{a}}[u] = +\infty$ is allowed. Actually, this corresponds to the case that two atoms have the same location.

The main results of this paper are

Theorem 1. (Existence for PN model) *If Assumptions A1–A6 in* Sect. 2.4 *hold, then the PN problem* (57) *has a unique solution* $v = (v^+, v^-)$ *and* $v \in S_0$ *is the* X_0*-global minimizer of the energy functional* (24). *Moreover,* $v^+(x) = -v^-(x)$ *for all* $x \in \mathbb{R}$, *and* $v^+(\cdot)$ *is strictly increasing and smooth (at least* C^5*) with* $\|v\|_{W^{5,\infty}} \le C$ *and* $\|\nabla v\|_{W^{4,1}} \le C$.

Theorem 2. (Existence for atomistic model; Convergence) *If Assumptions A1–A7 in* Sect. 2.4 *hold, then there exists an* $\varepsilon_0 > 0$ *such that for any* $0 < \varepsilon < \varepsilon_0$, *the atomistic problem* (59) *has a solution* $v^\varepsilon = (v^{\varepsilon,+}, v^{\varepsilon,-})$ *and* $v^\varepsilon \in S_\varepsilon$ *is a* X_ε*-local minimizer of the energy functional* (28). *Furthermore,* $\|v^\varepsilon - v\|_{X_\varepsilon} \le C\varepsilon^2$, *where* v *is the dislocation solution of the PN model in Theorem* 1.

A constant C in these theorems may depend on $\alpha, \beta, \theta, \Delta$, and $\gamma''(0)$, but it is independent of ε. Thanks to the convergence of displacement, we have the following important corollary for convergence of energy:

Corollary 1. (Convergence of energy) *If Assumptions A1–A7 hold, then there exists an* $\varepsilon_0 > 0$ *such that for any* $0 < \varepsilon < \varepsilon_0$ *we have*

$$\left| E_{PN}[v] - E_a[v^\varepsilon] \right| \le C\varepsilon^2, \tag{60}$$

where v *and* v^ε *are the solutions of the PN model and the atomistic model, respectively, in Theorems* 1 *and* 2.

Note that E_{PN} is of order $O(1)$ in this corollary, and hence the relative error is of order $O(\varepsilon^2)$. Before the rescaling, E_{PN} is of order $O(\varepsilon)$ and the relative error is still of order $O(\varepsilon^2)$.

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3. Preliminaries

We provide some preliminary results in this section, including some lemmas characterizing the properties of pair potentials and γ-surface. For simplicity of notation, we set, for $k = 0, 1, 2, \dots$

$$V_{k,s} = \operatorname*{ess\,sup}_{|\xi - s| \le \frac{1}{2}|s|} |\nabla^k V(\xi)|, \ \ s \in \mathbb{Z}^* \tag{61}$$

$$U_{k,s} = \operatorname*{ess\,sup}_{|\xi - s + \frac{1}{2}| \le 1} |\nabla^k U(\xi)|, \ \ s \in \mathbb{Z}, \tag{62}$$

$$v_{k,s,i} = \operatorname*{ess\,sup}_{\varepsilon(i-|s|) \le x \le \varepsilon(i+|s|)} \left|\nabla^k v^+(x)\right|, \ \ i, s \in \mathbb{Z}. \tag{63}$$

Roughly speaking, $V_{k,s}$ (or $U_{k,s}$, respectively) is a bound for $\nabla^k V(\xi)$ (or $\nabla^k U(\xi)$, respectively) nearby $\xi = s$, and $v_{k,s,i}$ is a bound for ∇v in $\varepsilon|s|$-neighbor nearby $x = \varepsilon i$. These quantities may appear in proofs from time to time.

First, we study the regularity of γ-surface and summability of pair potentials in our models.

Lemma 1. (fast decay and summability) *Suppose that Assumptions A3–A4 hold. Then there exists a constant $C = C(\beta, \theta)$ satisfying the summability conditions*

$$\textstyle\sum_{s\in\mathbb{Z}^*} |s|^{k+3} V_{k,s} \le C, \ \ k = 0, 1, \dots, 4, \tag{64}$$
$$\textstyle\sum_{s\in\mathbb{Z}} |s|^{k+1} U_{k,s} \le C, \ \ k = 0, 1, \dots, 4. \tag{65}$$

Proof. By defintion Eq. (61) and Assumption A4, we have $V_{k,s} \le C(\frac{1}{2}|s|)^{-k-4-\theta}$. Therefore, for $k = 0, 1, \dots, 4$

$$\sum_{s\in\mathbb{Z}^*} |s|^{k+3} V_{k,s} \le \sum_{s\in\mathbb{Z}^*} 2^{k+4+\theta} C|s|^{-1-\theta} \le C.$$

It is similar to show these properties for U. □

Lemma 2. (regularity of γ-surface) *Suppose that Assumptions A3–A4 hold. Then there exist $C = C(\beta, \theta)$ and $\varepsilon_0 = \varepsilon_0(\beta, \theta)$ such that for any $0 < \varepsilon < \varepsilon_0$, we have*

$$\gamma \in C^4(\mathbb{R}) \text{ and } \|\nabla^k \gamma\|_{L^\infty} \le C \text{ for } k = 0, 1, \cdots, 4. \tag{66}$$

Proof. Assumption A3 with Lemma 1 implies that $\gamma \in C^4(\mathbb{R})$ and

$$\nabla^k \gamma(\xi) = \sum_{s\in\mathbb{Z}} U^{(k)}\left(s - \frac{1}{2} + \xi\right), \ \ k = 1, 2, \cdots, 4. \tag{67}$$

Let n be the nearest integer of ξ. By Lemma 1 again, we have $|\nabla^k \gamma(\xi)| \le \sum_{s\in\mathbb{Z}} U_{k,s+n} \le C$. If $k = 0$, then $|\gamma(\xi)| \le \sum_{s\in\mathbb{Z}} (U_{0,s+n} + U_{0,s}) \le C$. □

Remark 1. This regularity of γ-surface is indispensable and it essentially relies on the regularity and summability of the pair potential V_d (or U). Consequently, a smooth dislocation solution depends on the regularity of V_d (or U).

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Lemma 3. (symmetry and local stability of γ-surface) *Suppose that Assumptions A2–A4 and A6 hold. Then we have the following properties of the γ-surface*

$$\begin{array}{ll} \textit{(periodicity)} & \gamma(\xi+1)=\gamma(\xi),\ \ \xi\in\mathbb{R}, \\ \textit{(symmetry)} & \gamma(\xi)=\gamma(-\xi),\ \ \xi\in\mathbb{R}, \\ \textit{(local stability)} & \gamma(\xi)\ge\frac{1}{4}\gamma''(0)\xi^2,\ \ |\xi|\le C, \end{array} \tag{68}$$

for some constant $C=C(\beta,\theta,\gamma''(0))$.

Proof. By the proof of Lemma 2, the series in the definition $\gamma(\xi)=\sum_{s\in\mathbb{Z}}[U(s-\frac{1}{2}+\xi)-U(s-\frac{1}{2})]$ is absolutely summable and its sum is irrelevant to the summation order. In particular, we have $\sum_{s\in\mathbb{Z}}[U(s+\frac{1}{2}+\xi)-U(s)]=\sum_{s\in\mathbb{Z}}[U(s-\frac{1}{2}+\xi)-U(s)]$. That is $\gamma(\xi+1)=\gamma(\xi)$.

Next, the symmetry $\gamma(\xi)=\gamma(-\xi)$ follows immediately from Assumption A2.

The Taylor expansion of γ near 0 leads to $\gamma(\xi)=\gamma(0)+\gamma'(0)\xi+\frac{1}{2}\gamma''(\xi_1)\xi^2$, where ξ_1 is between 0 and ξ. Note that $\gamma(0)=0$. The symmetry and the fact that $\gamma\in C^4$ imply that $\gamma'(0)=0$. By the assumption $\gamma''(0)>0$ in A6 and the continuity of γ'', we have $\gamma(\xi)=\frac{1}{2}\gamma''(\xi_1)\xi^2\ge\frac{1}{4}\gamma''(0)\xi^2$ for sufficiently small ξ. □

Remark 2. Recall that the γ-surface $\gamma(\phi)$ is defined in Eq. (12) from the atomistic model following the definition of Vitek [59]. The sinusoidal interplanar potential function in the classical PN model: $\gamma_{\text{cl-PN}}(\phi)=\frac{\mu b^2}{4\pi^2 d}\left(1-\cos\frac{2\pi\phi}{b}\right)$, where d is the interplanar distance, b is the length of the Burgers vector and μ is the shear modulus, is a phenomenological potential that satisfies the main features of a γ-surface summarized in Eq. (68).

4. Existence and Stability of the PN Model

In this section, we study the dislocation solution of the PN model, in particular, its existence and stability.

For the existence, we rewrite our one-step minimization problem (56) into a two-step minimization problem: first minimizing $u=(u^+,u^-)$ with fixed $u^\perp=\phi$, then minimizing the energy with respect to ϕ. This two-step procedure becomes a routine since the original works of Peierls and Nabarro [45,52], however, the equivalence lacks a rigorous proof. Here we provide a detailed discussion on the relation of these two minimization problems. We use our bilayer system setting in order to be consistent with this work. The equivalence result and its proof can both be straightforwardly extended to the general PN model (e.g., in three dimension and for curved dislocations).

We define the function space for disregistry ϕ:

$$\Phi_0=\left\{\phi:\phi-\phi^0\in H^1,\lim_{x\to-\infty}\phi(x)=0,\lim_{x\to+\infty}\phi(x)=1,\phi(0)=\tfrac{1}{2}\right\}, \tag{69}$$

$$\phi^0(x)=\begin{cases}0, & x<-\frac{1}{4},\\ 2x+\frac{1}{2}, & -\frac{1}{4}\le x\le\frac{1}{4},\\ 1, & x>\frac{1}{4}.\end{cases} \tag{70}$$

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It is easy to check that for any $u \in S_0$, we have $\phi := u^{\perp} \in \Phi_0$. In particular, $\phi^0 = u^{0,\perp} \in \Phi_0$.

In our bilayer system, the two-step minimization reads as:

(i) given $\phi \in \Phi_0$, find $u_\phi = (u_\phi^+, u_\phi^-) \in S_0$ with $u_\phi^{\perp} = \phi$ such that

$$E_{\mathrm{elas}}[u_\phi] = \inf_{u \in S_0,\ u^{\perp}=\phi} E_{\mathrm{elas}}[u], \tag{71}$$

and denote $E_{\mathrm{elas}}^{II}[\phi] = \inf_{u \in S_0,\ u^{\perp}=\phi} E_{\mathrm{elas}}[u]$;

(ii) find $\phi^* \in \Phi_0$ such that

$$E_{\mathrm{PN}}^{II}[\phi^*] = \inf_{\phi \in \Phi_0} E_{\mathrm{PN}}^{II}[\phi], \tag{72}$$

where the total energy functional in this two-step minimization problem is defined as

$$E_{\mathrm{PN}}^{II}[\phi] = E_{\mathrm{elas}}^{II}[\phi] + E_{\mathrm{mis}}[\phi]. \tag{73}$$

To make it clear, we list the relationship between the various functionals in these minimization problems. The one-step minimization problem (56) reads as:

$$\inf_{u \in S_0} E_{\mathrm{PN}}[u] = \inf_{u \in S_0, u^{\perp}=\phi} \{E_{\mathrm{elas}}[u] + E_{\mathrm{mis}}[\phi]\};$$

the two-step minimization problem (71)–(72) reads as:

$$\begin{aligned}\inf_{\phi \in \Phi_0} E_{\mathrm{PN}}^{II}[\phi] &= \inf_{\phi \in \Phi_0} \left\{E_{\mathrm{elas}}^{II}[\phi] + E_{\mathrm{mis}}[\phi]\right\}\\ &= \inf_{\phi \in \Phi_0} \left\{\left(\inf_{u \in S_0, u^{\perp}=\phi} E_{\mathrm{elas}}[u]\right) + E_{\mathrm{mis}}[\phi]\right\}.\end{aligned}$$

We remark that, in general (PN models), $E_{\mathrm{elas}}^{II}[\phi]$ always exists, even if the optimal displacement u may not exist (in S_0) for some given disregistry ϕ with the consistency condition $u^{\perp} = \phi$. In many applications such as the original PN model, there is an explicit solution for the step (i) problem (71). It follows that one simply needs to solve the step (ii) problem (72). This is a great advantage to use this two-step minimization model.

The following proposition establishes the equivalence between these minimization problems:

Proposition 1. (equivalence between two minimization problems) *We suppose that $E_{PN}[u^0] < +\infty$. Then the two-step minimization problem (71)–(72) is equivalent to the one-step minimization problem (56) in the following senses:*

1. *$m^I = m^{II}$, where $m^I = \inf_{u \in S_0} E_{PN}[u]$ and $m^{II} = \inf_{\phi \in \Phi_0} E_{PN}^{II}[\phi]$.*
2. *Given any minimizing sequence $\{u^i\}_{i=1}^{\infty}$ of problem (56), then $\{\phi^i := u^{i,\perp}\}_{i=1}^{\infty}$ is a minimizing sequence of problem (72). Conversely, given any minimizing sequence $\{\phi^i\}_{i=1}^{\infty}$ of problem (72), there exists a sequence $\{u^i\}_{i=1}^{\infty}$ with $u^{i,\perp} = \phi^i$, $i \in \mathbb{N}$ such that $\{u^i\}_{i=1}^{\infty}$ is a minimizing sequence of problem (56).*

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3. *If u^* is a minimizer of problem (56), $\phi^* := u^{*,\perp}$ is a minimizer of problem (72). Conversely, if ϕ^* is a minimizer of problem (72) and u^* solves*

$$E_{elas}[u^*] = \inf_{u\in S_0,\ u^\perp=\phi^*} E_{elas}[u], \tag{74}$$

then u^* is a minimizer of problem (56). In particular, if the minimizer u^* in (74) is unique, then u^* and ϕ^* has a one-to-one correspondence.

Remark 3. Condition (74) means $E_{\mathrm{elas}}[u^*] = E^{II}_{\mathrm{elas}}[\phi^*]$. For most applications, including our case $E_{\mathrm{elas}}[u] = \int_{\mathbb{R}} \frac{1}{2}\alpha(|\nabla u^+|^2 + |\nabla u^-|^2)\mathrm{d}x$, the minimizer $u^* \in S_0$ satisfying Eq. (74) exists, and it is unique.

Proof. By Assumption A6, $\gamma(x) \geq \gamma(0) = 0$ for all $x \in \mathbb{R}$. Thus $E_{\mathrm{mis}}[\phi] \geq 0$. Obviously, $E_{\mathrm{elas}}[u] \geq 0$ and $E^{II}_{\mathrm{elas}}[\phi] \geq 0$ for any $u \in S_0$ and $\phi \in \Phi_0$, respectively. Hence m^I and m^{II} are bounded below by 0. In addition, they are prevented from being $+\infty$ due to the assumption $E_{\mathrm{PN}}[u^0] < +\infty$.

1. If $\{u^i\}_{i=1}^\infty$ is a minimizing sequence of problem (56), then $\lim_{i\to+\infty} E_{\mathrm{PN}}[u^i] = m^I$. For all i,

$$m^{II} \leq E^{II}_{\mathrm{PN}}[u^{i,\perp}] \leq E_{\mathrm{PN}}[u^i]. \tag{75}$$

Taking the limit $i \to +\infty$, we obtain $m^{II} \leq m^I$.

Conversely, if $\{\phi^i\}_{i=1}^\infty$ a minimizing sequence of problem (72), then we have $\lim_{i\to+\infty} E^{II}_{\mathrm{PN}}[\phi^i] = m^{II}$. For any i, there exist $u^i \in S_0$ with $u^{i,\perp} = \phi^i$ such that $E_{\mathrm{elas}}[u^i] \leq i^{-1} + E^{II}_{\mathrm{elas}}[\phi^i]$. Then

$$m^I \leq E_{\mathrm{PN}}[u^i] \leq i^{-1} + E^{II}_{\mathrm{PN}}[\phi^i]. \tag{76}$$

Taking the limit $i \to +\infty$, we obtain $m^I \leq m^{II}$. Hence $m^I = m^{II}$.

2. If $\{u^i\}_{i=1}^\infty$ is a minimizing sequence of problem (56), then we set $\phi^i = u^{i,\perp}$ for all $i \in \mathbb{N}$. Thus $\lim_{i\to} E^{II}_{\mathrm{PN}}[\phi^i] = m^{II}$ follows from Eq. (75) and $m^I = m^{II}$. Conversely, if $\{\phi^i\}_{i=1}^\infty$ a minimizing sequence of problem (72), then we choose $u^i \in S_0$ with $u^{i,\perp} = \phi^i$ such that $E_{\mathrm{elas}}[u^i] \leq i^{-1} + E^{II}_{\mathrm{elas}}[\phi^i]$. Thus $\lim_{i\to+\infty} E_{\mathrm{PN}}[u^i] = m^I$ follows from Eq. (76) and $m^I = m^{II}$.
3. If $E_{\mathrm{PN}}[u^*] = m^I$, then $E^{II}_{\mathrm{PN}}[u^{*,\perp}] \leq E_{\mathrm{PN}}[u^*] = m^I = m^{II}$. Conversely, if $E^{II}_{\mathrm{PN}}[\phi^*] = m^{II}$ and $E_{\mathrm{elas}}[u^*] = \inf_{u\in S_0,\ u^\perp=\phi^*} E_{\mathrm{elas}}[u]$, then

$$E_{\mathrm{PN}}[u^*] = E_{\mathrm{elas}}[u^*] + E_{\mathrm{mis}}[u^{*,\perp}] = E^{II}_{\mathrm{elas}}[\phi^*] + E_{\mathrm{mis}}[\phi^*] = E^{II}_{\mathrm{PN}}[\phi^*] = m^I.$$

□

Now we prove Theorem 1 by solving the two-step minimization. The first step is explicitly solvable. Next, we prove the existence and other properties of the minimizer ϕ.

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Proof of Theorem 1.

1. Two-step minimization problem. Recall that $E_{\text{elas}}[u] = \int_{\mathbb{R}} \frac{1}{2}\alpha \left(|\nabla u^+|^2 + |\nabla u^-|^2\right) \mathrm{d}x$. For any $\phi \in \Phi_0$, we have

$$\arg \min_{u \in S_0, u^{\perp}=\phi} E_{\text{elas}}[u] = \arg \min_{u \in S_0} \int_{\mathbb{R}} \frac{1}{2}\alpha \left(|\nabla u^+|^2 + |\nabla u^+ - \nabla\phi|^2\right) \mathrm{d}x$$
$$= \left(\frac{1}{2}\phi, -\frac{1}{2}\phi\right).$$

Moreover, $E^{II}_{\text{elas}}[\phi] = E_{\text{elas}}[(\frac{1}{2}\phi, -\frac{1}{2}\phi)] = \frac{1}{4}\int_{\mathbb{R}} \alpha|\nabla\phi|^2 \mathrm{d}x$. By Proposition 1, we only need to minimize the following energy $E^{II}_{\text{PN}}[\phi]$ in terms of disregistry $\phi \in \Phi_0$:

$$E^{II}_{\text{PN}}[\phi] = \int_{\mathbb{R}} \left(\frac{1}{4}\alpha|\nabla\phi|^2 + \gamma(\phi)\right) \mathrm{d}x. \tag{77}$$

2. Existence, uniqueness, and symmetry. Define $\Gamma(\xi) = \int_0^{\xi} \sqrt{\alpha\gamma(\eta)}\mathrm{d}\eta$ for $\xi \in \mathbb{R}$. Recall that $\gamma(\cdot)$ is nonnegative, bounded, and continuous. Hence $\Gamma(\xi)$ is well-defined and $\nabla\Gamma(\xi) = \sqrt{\alpha\gamma(\xi)}$. Note that $\Gamma(0) = 0$ and $\Gamma(1) = \int_0^1 \sqrt{\alpha\gamma(\eta)}\mathrm{d}\eta$. Applying the AM-GM inequality to Eq. (77), we have

$$E^{II}_{\text{PN}}[\phi] \geq \int_{\mathbb{R}} |\nabla\phi(x)|\sqrt{\alpha\gamma(\phi(x))}\mathrm{d}x$$
$$= \int_{\mathbb{R}} |\nabla\Gamma(\phi(x))|\mathrm{d}x$$
$$\geq \lim_{x\to+\infty} \Gamma(\phi(x)) - \lim_{x\to-\infty} \Gamma(\phi(x))$$
$$= \int_0^1 \sqrt{\alpha\gamma(\eta)}\mathrm{d}\eta.$$

For the first step, the equality holds if and only if $\frac{1}{2}\sqrt{\alpha}|\nabla\phi| = \sqrt{\gamma \circ \phi}$. Therefore $\inf_{\phi\in\Phi_0} E^{II}_{\text{PN}}[\phi] = \int_0^1 \sqrt{\alpha\gamma(\eta)}\mathrm{d}\eta$. Moreover, $\phi^* \in \Phi_0$ is a minimizer if and only if $\frac{1}{2}\sqrt{\alpha}|\nabla\phi(x)| = \sqrt{\gamma(\phi(x))}$ for a.e. $x \in \mathbb{R}$ and $\nabla\phi(x)$ does not change sign for a.e. $x \in \mathbb{R}$. Obviously, $\nabla\phi(x) \geq 0$ for a.e. $x \in \mathbb{R}$. Thus the minimizer $\phi^* \in \Phi_0$ is the solution of the differential equation

$$\nabla\phi(x) = \frac{2}{\sqrt{\alpha}}\sqrt{\gamma(\phi(x))}, \quad \phi(0) = \frac{1}{2}, \tag{78}$$

with boundary conditions $\lim_{x\to-\infty} \phi^*(x) = 0$, and $\lim_{x\to+\infty} \phi^*(x) = 1$. Note that $\sqrt{\gamma(x)}$ is uniformly Lipschitz due to the fact that γ behaves quadratically near $\mathbb{Z}$ (because γ attains its minimum value 0 at integer values). The initial value problem (78) has a unique classical (differentiable) solution on $\mathbb{R}$. We denote this solution as $\phi^*(x), x \in \mathbb{R}$. It will be checked that $\phi^* \in \Phi_0$ in the next step. Therefore the minimization problem (24) has a unique global minimizer. Recall that $\gamma \in C^4$ (cf. Lemma 2). Thus ϕ^* is C^5 by Eq. (78). Moreover, it is the unique solution of the Euler–Lagrange equation

$$-\frac{1}{2}\alpha\nabla^2\phi^* - \gamma'(\phi^*) = 0. \tag{79}$$

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3. Strictly increasing, boundary conditions, and exponential decay. We claim that $\phi^*(x) \notin \mathbb{Z}$ for all $x \in \mathbb{R}$. Indeed, if $\phi^*(x_0) = n$ for some $x_0 \in \mathbb{R}$ and $n \in \mathbb{Z}$, then $\nabla(\phi^* - n) = \frac{2}{\sqrt{\alpha}}\sqrt{\gamma(\phi^* - n)}$ due to Lemma 3 and Eq. (78). Using the Lipschitz property of $\sqrt{\gamma}$, $|\nabla(\phi^* - n)| \le C|\phi^* - n|$. Gronwall's inequality with $\phi^*(x_0) - n = 0$ implies that $\phi^*(x) = n$ for all $x \in \mathbb{R}$. This contradicts with $\phi^*(0) = \frac{1}{2}$. Thus $\phi^*(x) \notin \mathbb{Z}$ for all $x \in \mathbb{R}$. As a result, we obtain that $0 < \phi^*(x) < 1$ and $\nabla\phi^*(x) > 0$ for all $x \in \mathbb{R}$.

Next, we prove that the boundary conditions are satisfied. Since ϕ^* strictly increasing and bounded, the limit $M := \lim_{x\to+\infty}\phi^*(x)$ exists. Obviously, $M \le 1$. If $M < 1$, we have $m' := \min_{\xi\in[\frac{1}{2},M]}\frac{2}{\sqrt{\alpha}}\sqrt{\gamma(\xi)} > 0$ due to Assumption A6. Thus $\nabla\phi^*(x) \ge m' > 0$ for all $x \ge 0$. This leads to $\lim_{x\to+\infty}\phi^*(x) = +\infty$ which contradicts with the boundedness of ϕ^*. Therefore we must have $\lim_{x\to+\infty}\phi^*(x) = 1$. Similarly, we have $\lim_{x\to-\infty}\phi^*(x) = 0$.

By Lemma 3, we have $\gamma(1-\phi^*(x)) \ge \frac{1}{4}\gamma''(0)(1-\phi^*(x))^2$ for $\phi^*(x) \ge 1 - c_0$, where $c_0 = c_0(\beta, \theta, \gamma''(0))$. Since $\lim_{x\to+\infty}\phi^*(x) = 1$, there exists a constant $K > 0$ such that $\phi^*(x) \ge 1 - c_0$ for $x > K$. These with Eq. (78) leads to

$$\begin{aligned}\nabla(1-\phi^*(x)) = -\frac{2}{\alpha}\sqrt{\gamma(1-\phi^*(x))} &\le -\frac{2}{\alpha}\sqrt{\frac{1}{4}\gamma''(0)(1-\phi^*(x))^2}\\ &\le -C(1-\phi^*(x))\end{aligned}$$

for all $x > K$ and some $C > 0$. By Gronwall's inequality, we have for $x \ge K$

$$1 - \phi^*(x) \le (1-\phi^*(K))\exp(-C(x-K)) \le C'\exp(-Cx).$$

By choosing a larger constant C', the exponential decay estimate holds for all $x \ge 0$: $1 - \phi^*(x) \le C'\exp(-C|x|)$. Similarly, we have $\phi^*(x) \le C'\exp(-C|x|)$ for $x \le 0$.

4. Regularity. Note that $\|\phi^*\|_{L^\infty} \le 1$ and $\|\nabla\phi^*\|_{L^\infty} = \frac{2}{\sqrt{\alpha}}\|\sqrt{\gamma}\|_{L^\infty} < \infty$. Since $\nabla\phi^* > 0$, we have $\|\nabla\phi^*\|_{L^1} = \int_{-\infty}^{\infty}\nabla\phi^*(x) = 1$. Next $\nabla^2\phi^* = -\frac{2}{\alpha}\gamma'(\phi^*)$. Thus $\nabla^2\phi^* \in L^\infty$ by Lemma 2. Note that $|\gamma'(\phi^*)| \le |\gamma'(0) + \gamma''(\xi)\phi^*| \le C|\phi^*|$ and $|\gamma'(\phi^*)| \le |\gamma'(1) + \gamma''(\xi)(\phi^* - 1)| \le C|1 - \phi^*|$. Then

$$\begin{aligned}\|\nabla^2\phi^*\|_{L^1} &\le \frac{2}{\alpha}\int_{-\infty}^{\infty}|\gamma'(\phi^*(x))|\mathrm{d}x\\ &\le C\int_{-\infty}^{0}|\phi^*(x)|\mathrm{d}x + C\int_0^{\infty}|1-\phi^*(x)|\mathrm{d}x < C,\end{aligned}$$

where the last inequality is due to the exponential decay property of $\phi^*(x)$. By direct calculations, we have

$$\begin{aligned}\nabla^3\phi^* &= -\frac{2}{\alpha}\gamma''(\phi^*)\nabla\phi^*,\\ \nabla^4\phi^* &= -\frac{2}{\alpha}\left[\gamma'''(\phi^*)(\nabla\phi^*)^2 + \gamma''(\phi^*)\nabla^2\phi^*\right],\\ \nabla^5\phi^* &= -\frac{2}{\alpha}\left[\gamma^{(4)}(\phi^*)(\nabla\phi^*)^3 + 3\gamma'''(\phi^*)\nabla\phi^*\nabla^2\phi^* + \gamma''(\phi^*)\nabla^3\phi^*\right].\end{aligned}$$

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Here we are implicitly using (79) and the chain rule, which is permissible since $\gamma \in C^4$. Recall that $\gamma^{(k)} \in L^\infty$ for $k = 2, 3, 4$ (cf. Lemma 2). This with $\nabla\phi^* \in L^\infty$ and $\nabla^2\phi^* \in L^\infty$ leads to $\nabla^k\phi^* \in L^\infty$ for $k = 3, 4, 5$, successively. Then the boundedness $\gamma^{(k)} \in L^\infty$, $k = 2, 3, 4$ with $\nabla\phi^* \in L^1$ and $\nabla\phi^* \in L^\infty$ leads to $\nabla^k\phi^* \in L^1$ for $k = 3, 4, 5$, successively.

5. Dislocation solution v. Now we summarize the above properties of ϕ^*. The dislocation solution $v = (\frac{1}{2}\phi^*, -\frac{1}{2}\phi^*)$ is the unique solution of the PN problem (57) and $v \in S_0$ is the unique X_0-global minimizer of the energy functional (24). Moreover, v is symmetric $v^+(x) = -v^-(x)$ for all $x \in \mathbb{R}$ and $v^+(\cdot) \in C^5$ is strictly increasing with $\|v\|_{W^{5,\infty}} \le C$ and $\|\nabla v\|_{W^{4,1}} \le C$. □

A corollary of Theorem 1 shows the symmetry property of $v^\pm$.

Corollary 2. *Let $v = (v^+, v^-)$ be the dislocation solution of the PN model in Theorem 1. Then v has the symmetry with respect to x: $v^+(x) + v^+(-x) = \frac{1}{2}$ and $v^-(x) + v^-(-x) = -\frac{1}{2}$, $x \in \mathbb{R}$.*

Proof. By the symmetry and periodicity of γ-surface (cf. Lemma 3), we have $\gamma(\frac{1}{2} + \xi) = \gamma(\xi - \frac{1}{2}) = \gamma(\frac{1}{2} - \xi)$ for all $\xi \in \mathbb{R}$. Recall that $\sqrt{\gamma(x)}$ is uniformly Lipschitz due to the fact that γ behaves quadratically near $\mathbb{Z}$. Then it is easy to see the solution of the differential equation $\nabla\phi^* = \sqrt{\frac{4}{\alpha}\gamma(\phi^*)}$ with initial value $\phi^*(0) = \frac{1}{2}$ satisties $\phi^*(x) - \frac{1}{2} = \frac{1}{2} - \phi^*(-x)$ for $x \ge 0$. This with the fact that $v = (\frac{1}{2}\phi^*, -\frac{1}{2}\phi^*)$ completes the proof. □

Due to the translation invariance, the second variation of energy at the dislocation solution $\delta^2 E_{\mathrm{PN}}[v]$ has a zero eigenvalue. The following proposition guarantees that this zero eigenvalue is simple (in other words, the eigenfunctions corresponding to zero eigenvalue form a one-dimension linear space):

Proposition 2. (zero eigenvalue is simple) *Suppose that Assumptions A1–A6 hold. Let v be the dislocation solution of the PN model in Theorem 1. If $f \in C^2 \cap X_0$ and f solves $\delta^2 E_{PN}[v]f = 0$, then $f = A\nabla v$ for some constant A.*

Proof. Let $g = \nabla v$. Thus we have

$$
\begin{aligned}
&-\alpha\nabla^2 f^\pm \pm \gamma''(v^\perp)(f^+ - f^-) = 0,\\
&-\alpha\nabla^2 g^\pm \pm \gamma''(v^\perp)(g^+ - g^-) = \nabla\left[-\alpha\nabla^2 v^\pm \pm \gamma'(v^\perp)\right] = 0.
\end{aligned}
$$

The first equation implies $\nabla^2 f^+(x) = -\nabla^2 f^-(x)$ for all $x \in \mathbb{R}$. Thus, for all $x \in \mathbb{R}$, $\nabla f^+(x) + \nabla f^-(x) = \lim_{x\to+\infty}[\nabla f^+(x) + \nabla f^-(x)] = 0$ because $f \in C^2 \cap X_0$. Then for all $x \in \mathbb{R}$, we have $f^+(x) + f^-(x) = f^+(0) + f^-(0) = 0$ where the last equality is also due to $f \in X_0$. Now we have $f^+ - f^- = 2f^+ = -2f^-$ and

$$-\alpha\nabla^2 f^\pm + 2\gamma''(v^\perp) f^\pm = 0, \tag{80}$$

$$-\alpha\nabla^2 g^\pm + 2\gamma''(v^\perp) g^\pm = 0. \tag{81}$$

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Eliminating the $\gamma''(v^\perp)$ term leads to

$$-\alpha g^\pm \nabla^2 f^\pm + \alpha f^\pm \nabla^2 g^\pm = 0 \text{ or } \alpha \nabla \left(g^\pm \nabla f^\pm - f^\pm \nabla g^\pm \right) = 0.$$

Thus $g^\pm \nabla f^\pm - f^\pm \nabla g^\pm$ is a constant. From the proof of Theorem 1, we know that $\|g\|_{L^\infty} \le C$ and $\|\nabla g\|_{L^\infty} \le C$. Recall that $f \in C^2 \cap X_0$ and $f^+ = -f^-$. We obtain that $g^\pm(x)\nabla f^\pm(x) - f^\pm(x)\nabla g^\pm(x) = \lim_{x\to+\infty}[g^\pm(x)\nabla f^\pm(x) - f^\pm(x)\nabla g^\pm(x)] = 0$ for all $x \in \mathbb{R}$. By strictly monotonicity of $v^\pm$ (cf. Theorem 1), we have $g^\pm = \nabla v^\pm \ne 0$. Thus $(g^\pm)^2 \nabla \left(\frac{f^\pm}{g^\pm}\right) = g^\pm \nabla f^\pm - f^\pm \nabla g^\pm = 0$. Therefore $f = Ag = A\nabla v$ for some constant A. □

Remark 4. The physical meaning of Proposition 2 is that the dislocation solution v, satisfying the boundary conditions but not the center condition, is invariant under translation. Indeed, let us consider an infinitesimal translation $\mathrm{d}x$ of the dislocation solution. The translated displacement field is $v(x+\mathrm{d}x)$ and hence the perturbation is $v(x+\mathrm{d}x) - v(x) = (\nabla v)\mathrm{d}x$. This perturbation mode is exactly the eigenfunction, in the previous proposition, corresponding to the zero eigenvalue.

Now we are ready to obtain the stability result of the PN model. Later (cf. Proposition 9 in Sect. 6), we will see that the stability of the atomistic model can be achieved by this PN stability with the small stability gap Assumption A7.

Proposition 3. (stability of PN model) *Suppose that Assumptions A1–A6 hold. Let v be the dislocation solution of the PN model in Theorem 1. There exists a constant $\kappa = \kappa(\alpha, \beta, \theta, \gamma''(0)) > 0$ such that for $f \in X_0$, we have*

$$\left\langle \delta^2 E_{PN}[v] f, f \right\rangle_0 \ge \kappa \|f\|^2_{X_0}. \tag{82}$$

Proof. We prove the statement by contradiction. Suppose there exists a sequence $\{f^n\}_{n=1}^\infty$ satisfying the following conditions:

$$\|f^n\|_{X_0} = 1 \quad \text{and} \quad \tfrac{1}{n}\|f^n\|^2_{X_0} > \left\langle \delta^2 E_{\mathrm{PN}}[v] f^n, f^n \right\rangle_0 = I[f^n], \tag{83}$$

where the functional $I[f] = \int_{\mathbb{R}} \left\{ \alpha|\nabla f^+|^2 + \alpha|\nabla f^-|^2 + \gamma''(v^\perp)(f^\perp)^2 \right\} \mathrm{d}x$.

From the proof of the Theorem 1, we know that $v^\perp = \phi^*$ is strictly increasing on $\mathbb{R}$ with $\lim_{x\to-\infty}\phi^*(x) = 0$ and $\lim_{x\to+\infty}\phi^*(x) = 1$. This with Assumption A6 and Lemma 3 implies that $\gamma''(v^\perp(x)) \ge \frac{1}{2}\gamma''(0) > 0$ on $\mathbb{R}\backslash(-K, K)$ for some $K < \infty$. Define

$$I_K[f] := \int_{-K}^{K} \{\alpha|\nabla f^+|^2 + \alpha|\nabla f^-|^2 + \gamma''(v^\perp)(f^\perp)^2\}\mathrm{d}x$$

$$I_{K^c}[f] := \int_{\mathbb{R}\backslash(-K,K)} \{\alpha|\nabla f^+|^2 + \alpha|\nabla f^-|^2 + \gamma''(v^\perp)(f^\perp)^2\}\mathrm{d}x.$$

The uniformly boundedness $\|f^n\|_{X_0} = 1$ implies that there exists a subsequence (still denoted as $\{f^n\}_{n=1}^\infty$) with $f^* \in X_0$ satisfying (1) $\nabla f^{n,\pm} \to \nabla f^{*,\pm}$ weakly in L^2, (2) $f^{n,\perp} \to f^{*,\perp}$ weakly in $L^2(\mathbb{R})$, and (3) $f^{n,\perp} \to f^{*,\perp}$ strongly in $L^2((-K, K))$. The statements (1) and (3) imply that the functional $I_K[f]$ is weak

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lower semi-continuous: $\liminf_{n\to\infty} I_K[f^n] \geq I_K[f]$ for any $f^n \to f$ weakly in $H^1((-K,K))$. For $x \in \mathbb{R}\backslash(-K,K)$, the integrand $\gamma''(v^\perp)(f^\perp)^2$ in $I_{K^c}[f]$ is convex since $\gamma''(v^\perp(x)) > 0$. By convexity, the functional $I_{K^c}[f]$ is weak lower semi-continuous. Therefore $I[f] = I_K[f] + I_{K^c}[f]$ is weak lower semi-continuous. By weak lower semi-continuity, $0 = \frac{1}{n}\|f^n\|_{X_0}^2 \geq \liminf_{n\to+\infty} I[f^n] \geq I[f^*]$. Since v minimizes the energy E_{PN}, we have $I[f^*] \geq 0$. Thus f^* minimizes the functional $I[f]$ and hence solves Euler–Lagrange equation in the weak sense

$$-\alpha\nabla^2 f^{*,\pm} \pm \gamma''(v^\perp) f^{*,\perp} = 0.$$

Note that $\gamma''(v^\perp)$ is continuous by Lemma 2 and Theorem 1. We apply the Schauder estimate and obtain $f^{*,\pm} \in C^{2,\delta}_{\mathrm{loc}}(\mathbb{R})$ [29]. Proposition 2 implies $f^* = A\nabla v$. Note that $A\nabla v^\perp(0) = f^{*,\perp}(0) = 0$ and $\nabla v^\perp(0) \neq 0$. Then $A = 0$ and $f^{*,\pm} \equiv 0$. Notice that $H^1(\mathbb{R})$ can be embedded in $C^{0,\frac{1}{2}}(\mathbb{R})$. Utilizing Arzela–Ascoli theorem, we obtain $f^{n,\perp} \to f^{*,\perp} \equiv 0$ uniformly on $(-K,K)$. Therefore

$$\begin{aligned}
\lim_{n\to\infty} I[f^n] \geq& -\sup_{x\in\mathbb{R}} |\gamma''(v^\perp(x))| \lim_{n\to\infty} \int_{-K}^{K} (f^{n,\perp})^2 \mathrm{d}x \\
&+\alpha \lim_{n\to\infty} \int_{\mathbb{R}} \left\{ |\nabla f^{n,+}|^2 + |\nabla f^{n,-}|^2 \right\} \mathrm{d}x \\
&+ \lim_{n\to\infty} \int_{\mathbb{R}\backslash(-K,K)} \gamma''(v^\perp)(f^{n,\perp})^2 \mathrm{d}x \\
\geq& \min\left\{\alpha, \frac{1}{2}\gamma''(0)\right\} \\
&\cdot \lim_{n\to\infty} \left\{ \int_{\mathbb{R}} \left(|\nabla f^{n,+}|^2 + |\nabla f^{n,-}|^2 \right) \mathrm{d}x + \int_{\mathbb{R}\backslash(-K,K)} (f^{n,\perp})^2 \mathrm{d}x \right\} \\
=& \min\left\{\alpha, \frac{1}{2}\gamma''(0)\right\} > 0.
\end{aligned}$$

This is in contradiction with $\lim_{n\to\infty} I[f^n] \leq \lim_{n\to\infty} \frac{1}{n}\|f^n\|_{X_0}^2 = 0$. Hence the original statement holds. □

5. Consistency of the PN Model

In this section, the force consistency is obtained at the dislocation solution of the PN model. More precisely, the force in the atomistic model is $O(\varepsilon^2)$-close to its counterpart in the PN model, provided that the displacement of the atomistic model is exactly the dislocation solution in Theorem 1. This asymptotic analysis is not only formal but also rigorous in the sense that we estimate the truncation error in X_ε norm.

Here we first provide several lemmas connecting the discrete Sobolev spaces.

Lemma 4. (property of discrete Sobolev norms) *For $k \in \mathbb{N}$, we have*

$$\|f\|_\varepsilon \leq \|f\|_{\varepsilon,k} \leq 2^{k+1} \max\{1, \varepsilon^{-k}\} \|f\|_\varepsilon. \tag{84}$$

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Proof. By definition, we have $\|f\|_\varepsilon^2 \le \|f\|_{\varepsilon,k}^2$ and

$$\|D^j f\|_\varepsilon^2 \le 4\varepsilon^{-2}\|D^{j-1} f\|_\varepsilon^2 \le 2^{2j}\varepsilon^{-2j}\|f\|_\varepsilon^2$$

for $j = 1, \cdots, k$. Then $\|f\|_{\varepsilon,k}^2 \le \sum_{j=0}^{k} 2^{2j}\varepsilon^{-2j}\|f\|_\varepsilon^2 \le 2^{2k+2}\max\{1, \varepsilon^{-2k}\}\|f\|_\varepsilon^2$. □

Lemma 5. (property of M_ε) *The linear space M_ε is a Hilbert space with inner product $(\cdot,\cdot)_{X_\varepsilon}$. Moreover, we have $M_\varepsilon \subset H_\varepsilon^1$ and for $f \in M_\varepsilon$*

$$\|f\|_{\varepsilon,1}^2 \le \|f\|_{X_\varepsilon}^2 \le 2\|f\|_{\varepsilon,1}^2. \tag{85}$$

Proof. The Hilbert space is easy to check. And Eq. (85) follows from $\|f^\perp\|_\varepsilon^2 = 2\|f\|_\varepsilon^2$ for $f \in M_\varepsilon$. □

Lemma 6. (property of finite difference operator $D_s^\pm$) *If $s \in \mathbb{Z}^*$ and $f \in L_\varepsilon^2$, then*

$$\|D_s^\pm f\|_\varepsilon \le |s|\|Df\|_\varepsilon. \tag{86}$$

Proof. Without loss of generality, we suppose $s > 0$ and prove the result for $D_s^+ f$. By the Cauchy–Schwarz inequality, we have

$$(D_s^+ f_i^\pm)^2 = \left(\sum_{j=i}^{i+s-1} Df_j^\pm\right)^2 \le s\sum_{j=i}^{i+s-1}(Df_j^\pm)^2.$$

Then $\|D_s^+ f\|_\varepsilon^2 \le s^2\|Df\|_\varepsilon^2$ follows from this. □

The following summability lemma is quite helpful in estimating the truncation errors (cf. Proposition 4):

Lemma 7. (summability of v) *Let v be the dislocation solution of the PN model in Theorem 1. Given $k = 1, 2, \cdots, 4$ and $s \in \mathbb{Z}^*$, $\varepsilon \le 1$, we have*

$$\varepsilon\sum_{i\in\mathbb{Z}} v_{k,s,i} \le C|s| \text{ and } \|v_{k,s}\|_\varepsilon^2 \le C|s|, \tag{87}$$

where $C = C(\|\nabla v\|_{W^{k,1}}, \|v\|_{W^{k,\infty}})$ is independent of s. (cf. Eq. (63) for the definition of $v_{k,s,i}$.)

Proof. Without loss of generality, we suppose that $s > 0$. For each $i \in \mathbb{Z}$, there exists some ξ_i with $\varepsilon(i-s) \le \xi_i \le \varepsilon(i+s)$ satisfying $v_{k,s,i} = |\nabla^k v^+(\xi_i)|$. Note that $\sum_{i\in\mathbb{Z}} v_{k,s,i} = \sum_{j=0}^{2s-1}\sum_{n\in\mathbb{Z}} v_{k,s,2ns+j}$. Then for each $j \in \{0, 1, 2, \cdots, 2s-1\}$, we have

$$2s\varepsilon\sum_{n\in\mathbb{Z}} v_{k,s,2ns+j} \le \sum_{n\in\mathbb{Z}}\int_{\varepsilon(2(n-1)s+j)}^{\varepsilon(2ns+j)} |\nabla^k v^+(\xi_{2ns+j}) - \nabla^k v^+(x)|$$
$$+|\nabla^k v^+(x)|\mathrm{d}x$$

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$$\leq \sum_{n\in\mathbb{Z}} \int_{\varepsilon(2(n-1)s+j)}^{\varepsilon(2ns+j)} \left(\int_x^{\xi_{2ns+j}} |\nabla^{k+1} v^+(\xi)| \mathrm{d}\xi \right) \mathrm{d}x$$

$$+\|\nabla^k v^+\|_{L^1}$$

$$\leq 2s\varepsilon \|\nabla^{k+1} v^+\|_{L^1} + \|\nabla^k v^+\|_{L^1}.$$

Recall that $\|v^+\|_{W^{5,\infty}} \leq C$ and $\|\nabla v^+\|_{W^{4,1}} \leq C$ from Theorem 1. Hence we have $\varepsilon \sum_{i\in\mathbb{Z}} v_{k,s,i} \leq 2s\varepsilon\|\nabla^{k+1} v^+\|_{L^1} + \|\nabla^k v^+\|_{L^1} \leq 2s\|\nabla v^+\|_{W^{k,1}} \leq C|s|$. Obviously, we have $\operatorname{ess\,sup}_{i\in\mathbb{Z}} v_{k,s,i} \leq \|v^+\|_{W^{k,\infty}} \leq C|s|$. Equation (87) follows from this. □

Proposition 4. (consistency of PN model) *Suppose that Assumptions A1–A6 hold. Let v be the dislocation solution of the PN model in Theorem 1, then there exist C and ε_0 such that for $0 < \varepsilon < \varepsilon_0$ and $f \in M_\varepsilon$ we have*

$$|\langle \delta E_a[v], f\rangle_\varepsilon| \leq C\varepsilon^2 \|f\|_{X_\varepsilon}. \tag{88}$$

Here C and ε_0 depend on α, β, θ, and $\gamma''(0)$.

Proof. 1. Since v is the solution of the PN model and $f_i^+ = -f_i^-$, we have

$$0 = \sum_{\pm} \{-\alpha\nabla^2 v_i^\pm \pm \gamma'(v_i^+ - v_i^-)\} f_i^\pm$$

$$= -\sum_{s\in\mathbb{Z}^*} \sum_{\pm} \frac{1}{2} V''(s) s^2 \nabla^2 v_i^\pm f_i^\pm$$

$$+\sum_{s\in\mathbb{Z}} U'\left(s - \frac{1}{2} + v_i^+ - v_i^-\right)(f_i^+ - f_i^-).$$

From the proof of Lemma 7, we have $-\alpha\nabla^2 v^\pm \in L^2_\varepsilon$ and hence $\gamma'(v^+ - v^-) \in L^2_\varepsilon$. Note that $f^\pm \in L^2_\varepsilon$. The series in $\sum_\pm\{-\alpha\nabla^2 v_i^\pm \pm \gamma'(v_i^+ - v_i^-)\} f_i^\pm$ is absolutely summable. Thus, we can rewrite that $\langle \delta E_{\mathrm{a}}[v], f\rangle_\varepsilon = R_{\mathrm{elas}} + R_{\mathrm{mis}}$, where

$$R_{\mathrm{elas}} = -\sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}^*} \sum_{\pm} \frac{1}{2} \left\{ D_s^-[V'(s + \varepsilon D_s^+ v_i^\pm)] - \varepsilon V''(s) s^2 \nabla^2 v_i^\pm \right\} f_i^\pm,$$

$$R_{\mathrm{mis}} = \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} \left[U'\left(s - \frac{1}{2} + v_{i+s}^+ - v_i^-\right)(f_{i+s}^+ - f_i^-)\right.$$

$$\left. - U'\left(s - \frac{1}{2} + v_i^+ - v_i^-\right)(f_i^+ - f_i^-)\right]$$

$$= \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} \frac{1}{2} \left[U'\left(s - \frac{1}{2} + v_{i+s}^+ - v_i^-\right)(f_{i+s}^+ - f_i^-)\right.$$

$$+ U'\left(s - \frac{1}{2} + v_i^+ - v_{i-s}^-\right)(f_i^+ - f_{i-s}^-)$$

$$\left. - 2U'\left(s - \frac{1}{2} + v_i^+ - v_i^-\right)(f_i^+ - f_i^-)\right].$$

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2. Estimate $|R_{\rm elas}|$. Rewrite $R_{\rm elas}$ as

$$R_{\rm elas} = -\,\varepsilon^{-1}\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}^*}\frac{1}{2}\Big\{\varepsilon D_s^-[V'(s+\varepsilon D_s^+ v_i^+)] - \varepsilon D_s^-[V'(s-\varepsilon D_s^+ v_i^+)] \\ -2\varepsilon^2 V''(s)s^2\nabla^2 v_i^+\Big\} f_i^+,$$

where we have used the fact that $\nabla^2 v_i^+ f_i^+ = \nabla^2 v_i^- f_i^-$. This is because $v^+ = -v^-$ and $f_i^+ = -f_i^-$. Using the Taylor expansion for $V'(\cdot)$ at $V'(s)$, we have

$$\begin{aligned}
&\varepsilon D_s^-[V'(s+\varepsilon D_s^+ v_i^+)] - \varepsilon D_s^-[V'(s-\varepsilon D_s^+ v_i^+)]\\
&\quad = V'(s+v_{i+s}^+ - v_i^+) - V'(s+v_i^+ - v_{i-s}^+) - V'(s - v_{i+s}^+ + v_i^+)\\
&\qquad + V'(s - v_i^+ + v_{i-s}^+)\\
&\quad = 2(\varepsilon D_s^+ v_i^+ + \varepsilon D_{-s}^+ v_i^+)V''(s) + \varepsilon^3[(D_s^+ v_i^+)^3 + (D_{-s}^+ v_i^+)^3]V^{(4)}(\xi)
\end{aligned}$$

for some ξ. Note that $\varepsilon D_s^+ v_i^+ + \varepsilon D_{-s}^+ v_i^+ = v_{i+s}^+ + v_{i-s}^+ - 2v_i^+$. Thus $|\varepsilon D_s^+ v_i^+ + \varepsilon D_{-s}^+ v_i^+ - \varepsilon^2 s^2 \nabla^2 v_i^+| \le \frac{1}{12}\varepsilon^4 s^4 v_{4,s,i}$ and

$$\begin{aligned}
\varepsilon^3|(D_s^+ v_i^+)^3 + (D_{-s}^+ v_i^+)^3| &\le \varepsilon^3 |D_s^+ v_i^+ + D_{-s}^+ v_i^+|\cdot 3s^2\|\nabla v\|_{L^\infty}^2\\
&\le 3\varepsilon^4 s^4 v_{2,s,i}\|\nabla v\|_{L^\infty}^2,
\end{aligned}$$

where we have used the identity $a^3+b^3 = (a+b)(a^2-ab+b^2)$ and the fact that $|D_{\pm s}^+ v_i^+| \le |s|\|\nabla v\|_{L^\infty}$. Hence

$$\begin{aligned}
&\left|\varepsilon D_s^-[V'(s+\varepsilon D_s^+ v_i^+)] - \varepsilon D_s^-[V'(s-\varepsilon D_s^+ v_i^+)] - 2\varepsilon^2 V''(s)s^2\nabla^2 v_i^+\right|\\
&\quad \le 3(1+\|\nabla v\|_{L^\infty}^2)(v_{2,s,i}+v_{4,s,i})\varepsilon^4(s^4 V_{2,s} + s^4 V_{4,s}).
\end{aligned}$$

Therefore

$$\begin{aligned}
|R_{\rm elas}| &\le \varepsilon^2\frac{3}{2}(1+\|\nabla v\|_{L^\infty}^2)\sum_{s\in\mathbb{Z}^*}(s^4 V_{2,s} + s^4 V_{4,s})\varepsilon\sum_{i\in\mathbb{Z}}(v_{2,s,i}+v_{4,s,i})|f_i^+|\\
&\le C\varepsilon^2\sum_{s\in\mathbb{Z}^*}(|s|^5 V_{2,s} + |s|^5 V_{4,s})\|f\|_{X_\varepsilon}\\
&\le C\varepsilon^2\|f\|_{X_\varepsilon},
\end{aligned}$$

where the second and the third inequalities are due to Lemmas 7 and 1, respectively.

3. Estimate $|R_{\rm mis}|$. Rewrite $R_{\rm mis} = R_{\rm mis,1} + R_{\rm mis,2}$, where

$$R_{\rm mis,1} = \varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\frac{1}{2}\left[U'\left(s-\frac{1}{2}+v_{i+s}^+ - v_i^-\right) + U'\left(s-\frac{1}{2}+v_i^+ - v_{i-s}^-\right)\right. \\ \left. -2U'\left(s-\frac{1}{2}+v_i^+ - v_i^-\right)\right](f_i^+ - f_i^-),$$

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$$R_{\text{mis},2} = \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} \frac{1}{2} \left[U'\left(s - \frac{1}{2} + v^+_{i+s} - v^-_i\right)(f^+_{i+s} - f^+_i) + U'\left(s - \frac{1}{2} + v^+_i - v^-_{i-s}\right)(f^-_i - f^-_{i-s}) \right].$$

Since $f \in M_\varepsilon$, we have $f^+ = -f^-$ and

$$R_{\text{mis},2} = \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} \frac{1}{2} \left[U'\left(s - \frac{1}{2} + v^+_{i+s} - v^-_i\right)(f^+_{i+s} - f^+_i + f^-_{i+s} - f^-_i) \right] = 0.$$

Thanks to the symmetry of v, we have $U'(s - \frac{1}{2} + v^+_i - v^-_{i-s}) = U'(s - \frac{1}{2} + v^+_{i-s} - v^-_i)$. Applying Taylor expansion, we have

$$\begin{aligned}
&\left| U'\left(s - \frac{1}{2} + v^+_{i+s} - v^-_i\right) + U'\left(s - \frac{1}{2} + v^+_{i-s} - v^-_i\right) - 2U'\left(s - \frac{1}{2} + v^+_i - v^-_i\right) \right| \\
&\le |v^+_{i+s} + v^+_{i-s} - 2v^+_i| \left| U''\left(s - \frac{1}{2} + v^+_i - v^-_i\right) \right| + \frac{1}{2}(|v^+_{i+s} - v^+_i|^2 + |v^+_{i-s} - v^+_i|^2) U_{3,s} \\
&\le \varepsilon^2 s^2 U_{2,s} v_{2,s,i} + \varepsilon^2 \|\nabla v\|_{L^\infty} s^2 U_{3,s} v_{1,s,i},
\end{aligned}$$

where in the last inequality we have used $|v^+_{i\pm s} - v^+_i|^2 = \varepsilon^2 |D^+_{\pm s} v^+_i|^2 \le \varepsilon^2 s^2 \|\nabla v\|_{L^\infty} v_{1,s,i}$. Thus by Lemmas 1 and 7, we obtain

$$\begin{aligned}
|R_{\text{mis}}| = |R_{\text{mis},1}| &\le \varepsilon^2 (1 + \|\nabla v\|_{L^\infty}) \sum_{s\in\mathbb{Z}} \left(s^2 U_{2,s} + s^2 U_{3,s}\right) \varepsilon \times \sum_{i\in\mathbb{Z}} (v_{2,s,i} + v_{1,s,i}) |f^+_i| \\
&\le C\varepsilon^2 \sum_{s\in\mathbb{Z}} \left(|s|^3 U_{2,s} + |s|^3 U_{3,s}\right) \|f\|_{X_\varepsilon} \\
&\le C\varepsilon^2 \|f\|_{X_\varepsilon}.
\end{aligned}$$

□

6. Stability of the Atomistic Model

In this section, the linear stability analysis is applied to the atomistic model. We will first study this stability at the dislocation solution of the PN model v, then extend it to displacement field u which is sufficient close to v.

We start with the following key observation: with or without a dislocation, the stability gap between the atomistic and PN models remains the same, up to an $O(\varepsilon)$ truncation error.

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Proposition 5. (stability gap with/without dislocation) *Suppose that Assumptions A1–A6 hold. Let v be the dislocation solution of the PN model in Theorem 1. Then there exists an $\varepsilon_0 > 0$ such that for $0 < \varepsilon < \varepsilon_0$ and $f \in X_\varepsilon$ we have*

$$\left\langle \delta^2 E_a[v] f, f \right\rangle_\varepsilon - \left\langle \delta^2 E_{\mathrm{PN}}[v] \bar{f}, \bar{f} \right\rangle_0 = \left\langle \delta^2 E_a[0] f, f \right\rangle_\varepsilon - \left\langle \delta^2 E_{\mathrm{PN}}[0] \bar{f}, \bar{f} \right\rangle_0 + O(\varepsilon) \| f \|^2_{X_\varepsilon}. \tag{89}$$

Proof. 1. Recall second variations (116) at continuum dislocation solution v

$$\left\langle \delta^2 E_{\mathrm{a}}[v] f, f \right\rangle_\varepsilon = \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}^*} \sum_{\pm} \frac{1}{2} V''(s + \varepsilon D_s^+ v_i^\pm) \left(D_s^+ f_i^\pm \right)^2 + \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} U'' \left(s - \frac{1}{2} + v_{i+s}^+ - v_i^- \right) (f_{i+s}^+ - f_i^-)^2,$$

$$\left\langle \delta^2 E_{\mathrm{a}}[0] f, f \right\rangle_\varepsilon = \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}^*} \sum_{\pm} \frac{1}{2} V''(s) \left(D_s^+ f_i^\pm \right)^2 + \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} U'' \left(s - \frac{1}{2} \right) (f_{i+s}^+ - f_i^-)^2,$$

$$\left\langle \delta^2 E_{\mathrm{PN}}[v] \bar{f}, \bar{f} \right\rangle_0 = \sum_{i\in\mathbb{Z}} \int_{\varepsilon i}^{\varepsilon(i+1)} \left\{ \alpha |\nabla \bar{f}^+|^2 + \alpha |\nabla \bar{f}^-|^2 + \gamma''(v^+ - v^-)(\bar{f}^\perp)^2 \right\} \mathrm{d}x,$$

$$\left\langle \delta^2 E_{\mathrm{PN}}[0] \bar{f}, \bar{f} \right\rangle_0 = \sum_{i\in\mathbb{Z}} \int_{\varepsilon i}^{\varepsilon(i+1)} \left\{ \alpha |\nabla \bar{f}^+|^2 + \alpha |\nabla \bar{f}^-|^2 + \gamma''(0)(\bar{f}^\perp)^2 \right\} \mathrm{d}x,$$

where $\alpha = \sum_{s\in\mathbb{Z}^*} \frac{1}{2} V''(s) s^2$ and $\gamma''(\xi) = \sum_{s\in\mathbb{Z}} U''(s - \frac{1}{2} + \xi)$. Then

$$\left\langle \delta^2 E_{\mathrm{a}}[v] f, f \right\rangle_\varepsilon - \left\langle \delta^2 E_{\mathrm{a}}[0] f, f \right\rangle_\varepsilon - \left\langle \delta^2 E_{\mathrm{PN}}[v] \bar{f}, \bar{f} \right\rangle_0 + \left\langle \delta^2 E_{\mathrm{PN}}[0] \bar{f}, \bar{f} \right\rangle_0 = \sum_{k=1}^{5} R_k,$$

where

$$R_1 = \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}^*} \sum_{\pm} \frac{1}{2} \left[V''(s + \varepsilon D_s^+ v_i^\pm) - V''(s) \right] (D_s^+ f_i^\pm)^2,$$

$$R_2 = \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} \left[U'' \left(s - \frac{1}{2} + v_{i+s}^+ - v_i^- \right) - U'' \left(s - \frac{1}{2} + v_i^+ - v_i^- \right) \right] \times (f_{i+s}^+ - f_i^-)^2,$$

$$R_3 = \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} \left[U'' \left(s - \frac{1}{2} + v_i^+ - v_i^- \right) - U'' \left(s - \frac{1}{2} \right) \right] \times \left[(f_{i+s}^+ - f_i^-)^2 - (f_i^+ - f_i^-)^2 \right],$$

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$$R_4 = \sum_{i\in\mathbb{Z}} \int_{\varepsilon i}^{\varepsilon(i+1)} \sum_{s\in\mathbb{Z}} \Bigg[U''\left(s - \frac{1}{2} + v_i^+ - v_i^-\right) - U''\left(s - \frac{1}{2} + v^+ - v^-\right)\Bigg] (f_i^+ - f_i^-)^2 \mathrm{d}x,$$

$$R_5 = \sum_{i\in\mathbb{Z}} \int_{\varepsilon i}^{\varepsilon(i+1)} \sum_{s\in\mathbb{Z}} \Bigg[U''\left(s - \frac{1}{2} + v^+ - v^-\right) - U''\left(s - \frac{1}{2}\right)\Bigg] \cdot \Big[(f_i^+ - f_i^-)^2 - (\bar{f}^+ - \bar{f}^-)^2 \Big] \mathrm{d}x.$$

Here $v^\pm = v^\pm(x)$. It remains to show $R_i = O(\varepsilon)\|f\|_{X_\varepsilon}^2$ for $i = 1, 2, \cdots, 5$.

2. We estimate R_i, $i = 1, 2, \cdots, 5$.

(1) For sufficiently small ε, we have $|V''(s + \varepsilon D_s^+ v_i^\pm) - V''(s)| \le V_{3,s}|v_{i+s}^\pm - v_i^\pm| \le \varepsilon \|\nabla v\|_{L^\infty} V_{3,s}|s|$. Using Lemmas 6 and 1, we have

$$|R_1| \le \frac{1}{2}\varepsilon \|\nabla v\|_{L^\infty} \sum_{s\in\mathbb{Z}^*} V_{3,s}|s| \|D_s^+ f\|_\varepsilon^2$$
$$\le \frac{1}{2}\varepsilon \|\nabla v\|_{L^\infty} \|Df\|_\varepsilon^2 \sum_{s\in\mathbb{Z}^*} V_{3,s}|s|^3 \le O(\varepsilon)\|f\|_{X_\varepsilon}^2.$$

(2) Next, $(f_{i+s}^+ - f_i^-)^2 \le 2(f_{i+s}^+ - f_i^+)^2 + 2(f_i^\perp)^2 = 2\varepsilon^2 (D_s^+ f_i^+)^2 + 2(f_i^\perp)^2$. Thus by Lemma 6,

$$\sum_{i\in\mathbb{Z}} (f_{i+s}^+ - f_i^-)^2 \le 2\varepsilon s^2 \|Df^+\|_\varepsilon^2 + 2\varepsilon^{-1}\|f^\perp\|_\varepsilon^2 \le \varepsilon^{-1}(2s^2 + 2)\|f\|_{X_\varepsilon}^2.$$

Note that

$$\left| U''\left(s - \frac{1}{2} + v_{i+s}^+ - v_i^-\right) - U''\left(s - \frac{1}{2} + v_i^+ - v_i^-\right) \right|$$
$$\le U_{3,s}|v_{i+s}^+ - v_i^+|$$
$$\le \varepsilon \|\nabla v^+\|_{L^\infty} U_{3,s}|s|.$$

Therefore

$$|R_2| \le \varepsilon^2 \|\nabla v^+\|_{L^\infty} \sum_{s\in\mathbb{Z}} U_{3,s}|s| \sum_{i\in\mathbb{Z}} (f_{i+s}^+ - f_i^-)^2$$
$$\le \varepsilon \|\nabla v^+\|_{L^\infty} \|f\|_{X_\varepsilon}^2 \sum_{s\in\mathbb{Z}} U_{3,s}|s|(2s^2 + 2) \le O(\varepsilon)\|f\|_{X_\varepsilon}^2.$$

(3) Next, we have for $\varepsilon \le 1$

$$\sum_{i\in\mathbb{Z}} |(f_{i+s}^+ - f_i^-)^2 - (f_i^+ - f_i^-)^2|$$
$$\le \sum_{i\in\mathbb{Z}} (f_{i+s}^+ - f_i^+)^2 + \sum_{i\in\mathbb{Z}} 2|f_{i+s}^+ - f_i^+| \cdot |f_i^+ - f_i^-|$$

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$$
\begin{aligned}
&\le \varepsilon^2 \sum_{i\in\mathbb{Z}} |D_s^+ f_i^+|^2 + \varepsilon \sum_{i\in\mathbb{Z}} |D_s^+ f_i^+|^2 + \varepsilon \sum_{i\in\mathbb{Z}} |f_i^\perp|^2 \\
&\le (\varepsilon+1)s^2 \|Df^+\|_\varepsilon^2 + \|f^\perp\|_\varepsilon^2 \\
&\le (2s^2+1)\|f\|_{X_\varepsilon}^2,
\end{aligned} \tag{90}
$$

where we have used Lemma 6. Note that $|U''(s-\frac{1}{2}+v_i^+-v_i^-)-U''(s-\frac{1}{2})| \le \|v^\perp\|_{L^\infty} U_{3,s}$. Therefore

$$
\begin{aligned}
|R_3| &\le \varepsilon \|v^\perp\|_{L^\infty} \sum_{s\in\mathbb{Z}} U_{3,s} \sum_{i\in\mathbb{Z}} |(f_{i+s}^+ - f_i^-)^2 - (f_i^+ - f_i^-)^2| \\
&\le \varepsilon \|v^\perp\|_{L^\infty} \|f\|_{X_\varepsilon}^2 \sum_{s\in\mathbb{Z}} U_{3,s}(2s^2+1) \le O(\varepsilon)\|f\|_{X_\varepsilon}^2.
\end{aligned}
$$

(4) We have $|U''(s-\frac{1}{2}+v_i^+-v_i^-)-U''(s-\frac{1}{2}+v^+-v^-)| \le 2\varepsilon\|\nabla v\|_{L^\infty} U_{3,s}$ for $i\varepsilon \le x < (i+1)\varepsilon$. Note that $\sum_{i\in\mathbb{Z}} \int_{\varepsilon i}^{\varepsilon(i+1)} (f_i^+ - f_i^-)^2 \mathrm{d}x = \|f^\perp\|_\varepsilon^2$. Thus

$$
|R_4| \le 2\varepsilon \|\nabla v\|_{L^\infty} \|f^\perp\|_\varepsilon^2 \sum_{s\in\mathbb{Z}} U_{3,s} \le O(\varepsilon)\|f\|_{X_\varepsilon}^2.
$$

(5) Finally, we have $|U''(s-\frac{1}{2}+v_i^+-v_i^-)-U''(s-\frac{1}{2})| \le \|v^\perp\|_{L^\infty} U_{3,s}$. Note that $|f_i^\perp - \bar{f}^\perp| = \frac{x-i\varepsilon}{\varepsilon}|f_{i+1}^\perp - f_i^\perp| = (x-i\varepsilon)|Df_i^+ - Df_i^-| \le (x-i\varepsilon)\cdot(|Df_i^+|+|Df_i^-|)$ and $|\bar{f}^\perp| \le |f_i^\perp|+|f_{i+1}^\perp|$ for $i\varepsilon \le x < (i+1)\varepsilon$. Hence

$$
\begin{aligned}
|(f_i^\perp)^2 - (\bar{f}^\perp)^2| &\le |f_i^\perp - \bar{f}^\perp| \cdot (|f_i^\perp| + |\bar{f}^\perp|) \\
&\le 2(x-i\varepsilon)(|Df_i^+| + |Df_i^-|)\cdot(|f_i^\perp| + |f_{i+1}^\perp|).
\end{aligned}
$$

Then

$$
\begin{aligned}
&\sum_{i\in\mathbb{Z}} \int_{\varepsilon i}^{\varepsilon(i+1)} |(f_i^\perp)^2 - (\bar{f}^\perp)^2| \mathrm{d}x \\
&\le \varepsilon^2 \sum_{i\in\mathbb{Z}} (|Df_i^+| + |Df_i^-|)\cdot(|f_i^\perp| + |f_{i+1}^\perp|) \\
&\le \varepsilon(\|Df^+\|_\varepsilon + \|Df^-\|_\varepsilon)\|f^\perp\|_\varepsilon \\
&\le 2\varepsilon\|f\|_{X_\varepsilon}^2.
\end{aligned} \tag{91}
$$

Therefore,

$$
|R_5| \le 2\varepsilon \|v^\perp\|_{L^\infty} \|f\|_{X_\varepsilon}^2 \sum_{s\in\mathbb{Z}} U_{3,s} \le O(\varepsilon)\|f\|_{X_\varepsilon}^2.
$$

□

The next lemma reveals the relation between a function in X_ε and its extension.

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Lemma 8. (linear interpolation) *If $f \in X_\varepsilon$, then its extension $\bar{f} \in X_0$ (cf. Eq. (42)). Moreover, we have*

$$\|Df\|_\varepsilon^2 + \tfrac{1}{3}\|f^\perp\|_\varepsilon^2 \le \|\bar{f}\|_{X_0}^2 \le \|f\|_{X_\varepsilon}^2. \tag{92}$$

Proof. By definition, we have $\nabla \bar{f}^\pm(x) = Df_i^\pm$ for $i\varepsilon \le x < (i+1)\varepsilon$, and hence $\|\nabla \bar{f}\|^2 = \|Df\|_\varepsilon^2$. Direct calculation leads to $\|\bar{f}^\perp\|^2 = \varepsilon \sum_{i\in\mathbb{Z}} \frac{1}{3}[(f_i^\perp)^2 + f_i^\perp f_{i+1}^\perp + (f_{i+1}^\perp)^2]$. Thus $\frac{1}{3}\|f^\perp\|_\varepsilon^2 \le \|\bar{f}^\perp\|^2 \le \|f^\perp\|_\varepsilon^2$. Equation (92) follows these immediately. □

Proposition 6. (explicit formula for Δ) *Suppose that Assumptions A1–A6 hold. Let v be the dislocation solution of the PN model in Theorem 1. Then there exists an $\varepsilon_0 > 0$ such that for $0 < \varepsilon < \varepsilon_0$ and $f \in X_\varepsilon$ we have*

$$\left\langle \delta^2 E_a[0]f, f \right\rangle_\varepsilon - \left\langle \delta^2 E_{PN}[0]\bar{f}, \bar{f} \right\rangle_0 \ge -\Delta \|f\|_{X_\varepsilon}^2 + O(\varepsilon)\|f\|_{X_\varepsilon}^2. \tag{93}$$

Moreover, Δ can be calculated by

$$\Delta = \sup_{\|f\|_{X_\varepsilon}=1} \left\{ \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\ge 2} \sum_{\pm} V''(s) \left[\left(D_s^+ f_i^\pm\right)^2 - s^2 (Df_i^\pm)^2 \right] \right\}. \tag{94}$$

Proof. By direct calculations, we have

$$\begin{aligned}
&\left\langle \delta^2 E_{\mathrm{a}}[0]f, f \right\rangle_\varepsilon - \left\langle \delta^2 E_{\mathrm{PN}}[0]\bar{f}, \bar{f} \right\rangle_0 \\
&= \varepsilon \sum_{i\in\mathbb{Z}} \left[\sum_{\pm} \sum_{s\in\mathbb{Z}^*} \frac{1}{2} V''(s) \left(D_s^+ f_i^\pm\right)^2 + \sum_{s\in\mathbb{Z}} U''\left(s - \frac{1}{2}\right) (f_{i+s}^+ - f_i^-)^2 \right] \\
&\quad - \sum_{i\in\mathbb{Z}} \int_{\varepsilon i}^{\varepsilon(i+1)} \left[\sum_{\pm} \sum_{s\in\mathbb{Z}^*} \frac{1}{2} V''(s) s^2 |\nabla \bar{f}^\pm|^2 - \sum_{s\in\mathbb{Z}} U''\left(s - \frac{1}{2}\right) (\bar{f}^\perp)^2 \right] \mathrm{d}x.
\end{aligned}$$

Let

$$\tilde{R}_1 = \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} U''\left(s - \frac{1}{2}\right) \left[(f_{i+s}^+ - f_i^-)^2 - (f_i^+ - f_i^-)^2 \right],$$

$$\tilde{R}_2 = \sum_{i\in\mathbb{Z}} \int_{\varepsilon i}^{\varepsilon(i+1)} \sum_{s\in\mathbb{Z}} U''\left(s - \frac{1}{2}\right) \left[(f_i^\perp)^2 - (\bar{f}^\perp)^2 \right] \mathrm{d}x.$$

Recalling Eqs. (90) and (91), we have

$$|\tilde{R}_1| \le \varepsilon \|f\|_{X_\varepsilon}^2 \sum_{s\in\mathbb{Z}} U_{2,s}(2s^2 + 1) \le O(\varepsilon)\|f\|_{X_\varepsilon}^2,$$

$$|\tilde{R}_2| \le 2\varepsilon \|f\|_{X_\varepsilon}^2 \sum_{s\in\mathbb{Z}} U_{2,s} \le O(\varepsilon)\|f\|_{X_\varepsilon}^2.$$

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Note that $\nabla \bar{f}^{\pm}(x) = Df_i^{\pm}$ for $i\varepsilon \le x < (i+1)\varepsilon$. Recall the definition (31). Therefore,

$$\begin{aligned} \Delta &= \lim_{\varepsilon\to 0} \sup_{\|f\|_{X_\varepsilon}=1} \left\langle \delta^2 E_{\mathrm{PN}}[0]\bar{f}, \bar{f}\right\rangle_0 - \left\langle \delta^2 E_{\mathrm{a}}[0] f, f\right\rangle_\varepsilon \\ &= \lim_{\varepsilon\to 0} \sup_{\|f\|_{X_\varepsilon}=1} \left\{ \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}^*} \sum_{\pm} \frac{1}{2} V''(s) \left[\left(D_s^+ f_i^{\pm}\right)^2 - s^2 (Df_i^{\pm})^2 \right] - \tilde{R}_1 - \tilde{R}_2 \right\} \\ &= \sup_{\|f\|_{X_\varepsilon}=1} \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\ge 2} \sum_{\pm} V''(s) \left[\left(D_s^+ f_i^{\pm}\right)^2 - s^2 (Df_i^{\pm})^2 \right], \end{aligned}$$

where we have used the symmetry of V (Assumption A2) in the last step. □

Proposition 7. ($\Delta \ge 0$) *The stability gap* (94) *is non-negative:* $\Delta \ge 0$.

Proof. By Lemma 1, we have $\sum_{s\ge 2} |V''(s)| s^2 \le \sum_{s\in\mathbb{Z}^*} V_{2,s} s^2 < C$. Then for any $M \in \mathbb{N}^*$, there exists a $t \in \mathbb{N}^*$ such that $\sum_{s\ge t+1} |V''(s)| s^2 < \frac{1}{M}$. For $s \ge 2$, by the Cauchy–Schwarz inequality, we obtain

$$\sum_{i\in\mathbb{Z}} (D_s^+ f_i^{\pm})^2 \le \sum_{i\in\mathbb{Z}} s \sum_{j=i}^{i+s-1} (Df_j^{\pm})^2 = s^2 \sum_{i\in\mathbb{Z}} (Df_i^{\pm})^2. \tag{95}$$

We define g as follows: $g_i = (2\varepsilon Mt)^{-1/2}$ for $1 \le i \le Mt$ and $g_i = 0$ otherwise. Obviously, $\|g\|_\varepsilon^2 = \frac{1}{2}$. Note that if we define $Df^{\pm} = g$, then $\|f\|_{X_\varepsilon} = \|Df\|_\varepsilon = 1$. Therefore

$$\Delta \ge \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\ge 2} 2V''(s) \left[(g_i + \cdots + g_{i+s-1})^2 - s^2 g_i^2 \right].$$

If $2 \le s \le t$, then $(g_i + \cdots + g_{i+s-1})^2 - s^2 g_i^2 = 0$ for $i \notin T$, where $T = \{-s+2, -s+2, \cdots, 0\} \cup \{Mt - s + 2, Mt - s + 3, \cdots, Mt\}$. For $i \in T$, we have $|(g_i + \cdots + g_{i+s-1})^2 - s^2 g_i^2| \le s^2 (2\varepsilon Mt)^{-1}$. Note that $|T| = 2(s-1)$. Thus for any $2 \le s \le t$, we have $\varepsilon \sum_{i\in\mathbb{Z}} \left[(g_i + \cdots + g_{i+s-1})^2 - s^2 g_i^2 \right] \ge -\varepsilon 2(s-1) s^2 (2\varepsilon Mt)^{-1} \ge -\frac{s^3}{Mt} \ge -\frac{s^2}{M}$. If $s \ge t+1$, Eq. (95) implies that $\varepsilon \sum_{i\in\mathbb{Z}} [(g_i + \cdots + g_{i+s-1})^2 - s^2 g_i^2] \ge -\varepsilon \sum_{i\in\mathbb{Z}} s^2 g_i^2 = -\frac{s^2}{2}$.

Therefore,

$$\begin{aligned} \Delta &\ge \varepsilon \sum_{i\in\mathbb{Z}} \left\{ \sum_{s=2}^{t} + \sum_{s=t+1}^{\infty} \right\} 2V''(s) \left[(g_i + \cdots + g_{i+s-1})^2 - s^2 g_i^2 \right] \\ &\ge -\sum_{s=2}^{t} 2|V''(s)| \frac{s^2}{M} - \sum_{s=t+1}^{\infty} 2|V''(s)| \frac{s^2}{2} \\ &\ge -\frac{1+2C}{M}. \end{aligned}$$

Letting M go to infinity, we obtain $\Delta \ge 0$. □

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Proposition 8. *Suppose that Assumptions A1–A6 hold. If* $V''(s) \le 0$ *for all* $|s| \ge 2$*, then* $\varDelta = 0$*, and thence* $\kappa > 3\varDelta$*. In particular, if* $V(\cdot)$ *is a nearest neighbor potential then* $\kappa > 3\varDelta = 0$*.*

Proof. Equation (95) and $V''(s) \le 0$ imply that $V''(s)\sum_{i\in\mathbb{Z}}\left[\left(D_s^+ f_i^{\pm}\right)^2 - s^2(Df_i^{\pm})^2\right] \le 0$ for $|s| \ge 2$. Hence $\varDelta \le 0$. According to Proposition 7, we have $\varDelta = 0$. □

Proposition 9. (stability of atomistic model) *Suppose that Assumptions A1–A7 hold. Let* v *be the dislocation solution of the PN model in Theorem 1. There exist* C *and* ε_0 *such that for* $0 < \varepsilon < \varepsilon_0$ *and* $f \in X_\varepsilon$ *we have*

$$\left\langle \delta^2 E_a[v]f, f\right\rangle_\varepsilon \ge C\|f\|^2_{X_\varepsilon}. \tag{96}$$

Here C *and* ε_0 *depend on* α*,* β*,* θ*,* $\gamma''(0)$*, and* $\varDelta$*.*

Proof. By Proposition 3 and Lemma 8, we have $\left\langle \delta^2 E_{\rm PN}[v]\bar f, \bar f\right\rangle_0 \ge \kappa\|\bar f\|^2_{X_0} \ge \frac{1}{3}\kappa\|f\|^2_{X_\varepsilon}$. Therefore, by Propositions 5 and 6, we have

$$\begin{aligned}\left\langle \delta^2 E_{\rm a}[v]f, f\right\rangle_\varepsilon &= \left\langle \delta^2 E_{\rm PN}[v]\bar f, \bar f\right\rangle_0 + \left\langle \delta^2 E_{\rm a}[0]f, f\right\rangle_\varepsilon \\ &\quad -\left\langle \delta^2 E_{\rm PN}[0]\bar f, \bar f\right\rangle_0 + O(\varepsilon)\|f\|^2_{X_\varepsilon} \\ &\ge \tfrac{1}{3}\kappa\|f\|^2_{X_\varepsilon} - \varDelta\|f\|^2_{X_\varepsilon} + O(\varepsilon)\|f\|^2_{X_\varepsilon} \\ &\ge C\|f\|^2_{X_\varepsilon}\end{aligned}$$

for sufficiently small ε. Here we have utilized the Assumption A7: $\varDelta < \frac{1}{3}\kappa$. □

We finish this section with a detailed verification on the stability condition of Lennard–Jones (m, n) potential. The commonly used case is $(m, n) = (6, 12)$.

Proposition 10. *Let* $V(\cdot)$ *be Lennard–Jones* (m, n) *potential, i.e.,*

$$V(x) = V_{LJ}(x) = -\left(\frac{r_0}{|x|}\right)^m + \left(\frac{r_0}{|x|}\right)^n, \quad 1 < m < n, \;\; x \ne 0, \tag{97}$$

where r_0 *is some characteristic distance. Then* $\varDelta = 0$*, provided* ε *is sufficiently small.*

Proof. We first remark that r_0 is not arbitrary but related to the minimal distance $s_0 = 1$ (the rescaled lattice constant). Note that $s_0 = 1$ solves

$$\frac{\partial}{\partial s_0}\left(\sum_{k\in\mathbb{Z}^*} V(ks_0) + \sum_{k\in\mathbb{Z}} V_d\left(ks_0 - \frac{1}{2}s_0\right)\right) = 0. \tag{98}$$

Recall that $V_d = \varepsilon^2 U$. Thus

$$\sum_{k\in\mathbb{Z}^*} kV'(k) + \varepsilon^2\sum_{k\in\mathbb{Z}}\left(k - \frac{1}{2}\right)U'\left(k - \frac{1}{2}\right) = 0. \tag{99}$$

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By Lemma 1, we have $|\sum_{k\in\mathbb{Z}}(k-\frac{1}{2})U'(k-\frac{1}{2})| \le \sum_{s\in\mathbb{Z}}(|s|+1)U_{1,s} \le C$. Then

$$0 = \sum_{k\in\mathbb{Z}^*} kV'(k) + O(\varepsilon^2) = \sum_{k\in\mathbb{Z}^*}\left[m\frac{r_0^m}{k^m} - n\frac{r_0^n}{k^n}\right] + O(\varepsilon^2)$$
$$= 2m\zeta(m)r_0^m - 2n\zeta(n)r_0^n + O(\varepsilon^2),$$

where the zeta function $\zeta(t) = \sum_{k=1}^{\infty} k^{-t}$, $t > 1$. Therefore, for sufficient small ε, we have

$$r_0^{n-m} = \frac{m\zeta(m)}{n\zeta(n)} + O(\varepsilon^2).$$

For $s \ge 2$, we have

$$V''(s) = m(m+1)\frac{r_0^m}{s^{m+2}}\left[-1 + \frac{n(n+1)r_0^{n-m}}{m(m+1)s^{n-m}}\right]$$
$$\le m(m+1)\frac{r_0^m}{s^{m+2}}\left[-1 + \frac{n(n+1)}{m(m+1)}\cdot\frac{\frac{m\zeta(m)}{n\zeta(n)} + O(\varepsilon^2)}{2^{n-m}}\right].$$

It can be shown that $\frac{(n+1)\zeta(m)}{(m+1)\zeta(n)} < 2^{n-m}$. Hence $V''(s) \le 0$, $s \ge 2$ for sufficiently small ε. By Proposition 8, we obtain $\Delta = 0$. □

7. Existence of the Atomistic Model and Convergence

In this section, we show that the atomistic model has a solution v^ε which is $O(\varepsilon^2)$ away from the PN solution v in terms of the metric induced by X_ε norm. Let us first provide the following lemma which makes use of the continuity of $\langle\delta^2 E_{\mathrm{a}}[\cdot]f, g\rangle_\varepsilon$ at v:

Lemma 9. *Suppose that Assumptions A1–A6 hold. Let v be the dislocation solution of the PN model in Theorem 1. There exist constants ε_0 and C such that for $0 < \varepsilon < \varepsilon_0$ and $u, u' \in \bar{X}_\varepsilon$ satisfying $\|u - v\|_{X_\varepsilon} \le \varepsilon$ and $\|u' - v\|_{X_\varepsilon} \le \varepsilon$ we have*

$$|\left\langle\left(\delta^2 E_a[u] - \delta^2 E_a[u']\right) f, g\right\rangle_\varepsilon| \le C\varepsilon^{-1/2}\|u - u'\|_{X_\varepsilon}\|f\|_{X_\varepsilon}\|g\|_{X_\varepsilon} \quad (100)$$

for all $f, g \in X_\varepsilon$. Here ε_0 and C depend on α, β, θ, $\gamma''(0)$, and Δ.

Proof. Note that $\|D_s^+(u-v)\|_{L_\varepsilon^\infty} \le |s|\|D(u-v)\|_{L_\varepsilon^\infty} \le |s|\varepsilon^{-1/2}\|u-v\|_{X_\varepsilon} \le |s|\varepsilon^{1/2}$. This with $\|D_s^+ v\|_{L_\varepsilon^\infty} \le |s|\|\nabla v\|_{L^\infty} \le C|s|$ implies that $\|D_s^+ u\|_{L_\varepsilon^\infty} \le C|s|$. Similarly, we have $\|D_s^+(u'-v)\|_{L_\varepsilon^\infty} \le |s|\varepsilon^{-1/2}\|u'-v\|_{X_\varepsilon} \le |s|\varepsilon^{1/2}$, $\|D_s^+(u'-u)\|_{L_\varepsilon^\infty} \le |s|\varepsilon^{-1/2}\|u'-u\|_{X_\varepsilon} \le |s|\varepsilon^{1/2}$, and $\|D_s^+ u'\|_{L_\varepsilon^\infty} \le C|s|$. For sufficiently small ε, we have

$$|V''(s+\varepsilon D_s^+ u_i^\pm) - V''(s+\varepsilon D_s^+ u_i'^\pm)| = |V^{(3)}(\xi)||\varepsilon D_s^+(u_i'^\pm - u_i^\pm)|$$
$$\le V_{3,s}|s|\varepsilon^{1/2}\|u'-u\|_{X_\varepsilon},$$

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where $|\xi - s| \le \max\{|\varepsilon D_s^+ u_i^{\pm}|, |\varepsilon D_s^+ u_i'^{\pm}|\} \le C\varepsilon|s| \le \frac{1}{2}|s|$.

Note that $\|u^{\perp} - v^{\perp}\|_{L^\infty_\varepsilon} \le \varepsilon^{-1/2}\|u - v\|_{X_\varepsilon} \le \varepsilon^{1/2}$. This with $\|v^{\perp}\|_{L^\infty_\varepsilon} \le 1$ implies that $\|u^{\perp}\|_{L^\infty_\varepsilon} \le 1 + \varepsilon^{1/2} \le 2$. Similarly, we have $\|u'^{\perp} - v^{\perp}\|_{L^\infty_\varepsilon} \le \varepsilon^{-1/2}\|u' - v\|_{X_\varepsilon} \le \varepsilon^{1/2}$, $\|u'^{\perp} - u^{\perp}\|_{L^\infty_\varepsilon} \le 2\varepsilon^{-1/2}\|u' - u\|_{X_\varepsilon} \le 2\varepsilon^{1/2}$, and $\|u'^{\perp}\|_{L^\infty_\varepsilon} \le 2$. For sufficiently small ε, we have

$$
\begin{aligned}
&\left|U''\left(s - \frac{1}{2} + u_{i+s}^+ - u_i^-\right) - U''\left(s - \frac{1}{2} + u_{i+s}'^+ - u_i'^-\right)\right| \\
&\le |U^{(3)}(\xi)||\varepsilon D_s^+(u_i'^+ - u_i^+) + (u_i'^{\perp} - u_i^{\perp})| \\
&\le \left(\sum_{j=-|s|-2}^{|s|+2} U_{3,s+j}\right)(|s| + 2)\varepsilon^{-1/2}\|u' - u\|_{X_\varepsilon},
\end{aligned}
$$

where we have used that $|\xi - (s - \frac{1}{2})| \le \max\{|\varepsilon D_s^+ u_i'^+| + |u_i'^{\perp}|, |\varepsilon D_s^+ u_i^+| + |u_i^{\perp}|\} \le |s| + 2$ and that $\sup_{|\xi - (s-\frac{1}{2})| \le |s|+2} |U^{(3)}(\xi)| \le \sum_{j=-|s|-2}^{|s|+2} U_{3,s+j}$.

Recall Eq. (116) and hence we have

$$
\begin{aligned}
&|\left\langle\left(\delta^2 E_{\mathrm{a}}[u] - \delta^2 E_{\mathrm{a}}[u']\right) f, g\right\rangle_\varepsilon| \\
&\le \varepsilon^{1/2}\|u - u'\|_{X_\varepsilon} \cdot \frac{\varepsilon}{2} \sum_{\pm} \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}^*} V_{3,s}|s| \left|D_s^+ f_i^{\pm}\right| \cdot \left|D_s^+ g_i^{\pm}\right| \\
&\quad + \varepsilon^{-1/2}\|u - u'\|_{X_\varepsilon} \cdot \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} \left(\sum_{j=-|s|-2}^{|s|+2} U_{3,s+j}\right)(|s| + 2)\left|f_{i+s}^+ - f_i^-\right| \\
&\quad \cdot \left|g_{i+s}^+ - g_i^-\right|.
\end{aligned}
$$

Utilizing Lemmas 1 and 6, we obtain

$$
\begin{aligned}
&\frac{\varepsilon}{2} \sum_{s\in\mathbb{Z}^*} V_{3,s}|s| \sum_{i\in\mathbb{Z}} \left|D_s^+ f_i^{\pm}\right| \cdot \left|D_s^+ g_i^{\pm}\right| \le \frac{1}{2} \sum_{s\in\mathbb{Z}^*} V_{3,s}|s|^3 \|Df^{\pm}\|_\varepsilon \|Dg^{\pm}\|_\varepsilon \\
&\quad \le C\|f\|_{X_\varepsilon}\|g\|_{X_\varepsilon}, \\
&\varepsilon \sum_{s\in\mathbb{Z}} \left(\sum_{j=-|s|-2}^{|s|+2} U_{3,s+j}\right)(|s| + 2) \sum_{i\in\mathbb{Z}} \left|f_{i+s}^+ + f_i^-\right| \cdot \left|g_{i+s}^+ + g_i^-\right| \\
&\quad \le C\|f\|_{X_\varepsilon}\|g\|_{X_\varepsilon}.
\end{aligned}
$$

Finally, Eq. (100) is obtained by collecting these inequalities. □

Lemma 10. *Suppose that Assumptions A1–A7 hold. Let v be the dislocation solution of the PN model in Theorem 1. There exist constants ε_0 and C such that for $0 < \varepsilon < \varepsilon_0$ and $u \in \bar{X}_\varepsilon$ satisfying $\|u - v\|_{X_\varepsilon} \le \varepsilon$ we have*

$$
\left\langle\delta^2 E_a[u]f, f\right\rangle_\varepsilon \ge C\|f\|_{X_\varepsilon}^2 \tag{101}
$$

for all $f \in X_\varepsilon$. Here ε_0 and C depend on α, β, θ, $\gamma''(0)$, and Δ.

Proof. Thanks to Proposition 9, we know $\left\langle\delta^2 E_{\mathrm{a}}[v]f, f\right\rangle_\varepsilon \ge C\|f\|_{X_\varepsilon}^2$ for all $f \in X_\varepsilon$. It is sufficient to show that $|\left\langle\delta^2 E_{\mathrm{a}}[v]f, f\right\rangle_\varepsilon - \left\langle\delta^2 E_{\mathrm{a}}[u]f, f\right\rangle_\varepsilon| \le \frac{1}{2}C\|f\|_{X_\varepsilon}^2$. The latter can be obtained by setting $v = u'$ in Lemma 9. □

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As all preparations are complete, we provide a proof of our main theorem.

Proof of Theorem 2. By Theorem 1, we have $v \in C^5$ and $\|\nabla v\|_{W^{4,1}} \leq C$ independent of ε. Define a closed ball B of M_ε as follows:

$$B = \left\{ w \in M_\varepsilon : \|w\|_{X_\varepsilon} \leq C_B \varepsilon^2 \right\}, \tag{102}$$

where the constant C_B can be chosen properly later. Given $w \in B$, we define operator $A_w : M_\varepsilon \to M_\varepsilon$ as follows:

$$(A_w f, g)_{X_\varepsilon} = \int_0^1 \langle \delta^2 E_{\mathrm{a}}[u^t] f, g \rangle_\varepsilon \mathrm{d}t, \quad f, g \in M_\varepsilon, \tag{103}$$

where $u^t = v + tw$ for $t \in [0, 1]$. It is easy to check that this operator is well-defined and self-adjoint, i.e., $(A_w f, g)_{X_\varepsilon} = (f, A_w g)_{X_\varepsilon}$. Next, we have $\|u^t - v\|_{X_\varepsilon} = t\|w\|_{X_\varepsilon} \leq C_0 \varepsilon^2$. Then by Lemma 10, we have $\langle \delta^2 E_{\mathrm{a}}[u^t] f, f \rangle_\varepsilon \geq C\|f\|^2_{X_\varepsilon}$ for $t \in [0, 1]$ and $f \in M_\varepsilon \subset X_\varepsilon$. Thus $(A_w f, f)_{X_\varepsilon} \geq C\|f\|^2_{X_\varepsilon}$ and A_w is invertible.

By Taylor's theorem with a remainder, we have, for all $\psi \in M_\varepsilon$,

$$\begin{aligned} \langle \delta E_{\mathrm{a}}[v + w], \psi \rangle_\varepsilon &= \langle \delta E_{\mathrm{a}}[v], \psi \rangle_\varepsilon + \int_0^1 \langle \delta^2 E_{\mathrm{a}}[u^t] w, \psi \rangle_\varepsilon \mathrm{d}t \\ &= \langle \delta E_{\mathrm{a}}[v], \psi \rangle_\varepsilon + (A_w w, \psi)_{X_\varepsilon}, \end{aligned} \tag{104}$$

where $w \in B$ and $u^t = v + tw$ for $t \in [0, 1]$.

To solve the atomistic model, it is sufficient to find $w \in B$ solving

$$(A_w w, \psi)_{X_\varepsilon} = -\langle \delta E_{\mathrm{a}}[v], \psi \rangle_\varepsilon \quad \text{for all} \quad \psi \in M_\varepsilon.$$

Define a map $G : B \to M_\varepsilon$ for $w \in B$ as

$$(A_w G(w), \psi)_{X_\varepsilon} = -\langle \delta E_{\mathrm{a}}[v], \psi \rangle_\varepsilon \quad \text{for all} \quad \psi \in M_\varepsilon. \tag{105}$$

Next, we check that $G(B) \subset B$ for properly chosen C_B. Indeed, by Lemma 10 and the consistency (Proposition 4), we have

$$\begin{aligned} C\|G(w)\|^2_{X_\varepsilon} &\leq (A_w G(w), G(w))_{X_\varepsilon} \\ &\leq |\langle \delta E_{\mathrm{a}}[v], G(w) \rangle_\varepsilon| \\ &\leq O(\varepsilon^2)\|G(w)\|_{X_\varepsilon}. \end{aligned}$$

Thus we can choose a constant C_B such that $\|G(w)\|_{X_\varepsilon} \leq C_B \varepsilon^2$ and $G(B) \subset B$.

We are going to apply the contraction mapping theorem to G. Obviously, B is a non-empty complete metric space with metric $d(u, v) = \|u - v\|_{X_\varepsilon}$. To guarantee the existence (and uniqueness) of a fixed point in B, it remains to show that $G : B \to B$ is a contraction mapping, i.e., $\|G(w) - G(w')\|_{X_\varepsilon} \leq L\|w - w'\|_{X_\varepsilon}$ for any $w, w' \in B$ and for some Lipschitz constant $L < 1$.

Note that $(G(w), \psi)_{X_\varepsilon} = -\langle \delta E_{\mathrm{a}}[v], A_w^{-1} \psi \rangle_\varepsilon$ and $(G(w'), \psi)_{X_\varepsilon} = -\langle \delta E_{\mathrm{a}}[v], A_{w'}^{-1} \psi \rangle_\varepsilon$ for all $\psi \in M_\varepsilon$. Thus by Proposition 4, we have

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$$
\begin{aligned}
\|G(w)-G(w')\|_{X_\varepsilon}^2 &= \left|\langle \delta E_{\mathrm{a}}[v], (A_w^{-1}-A_{w'}^{-1})(G(w)-G(w'))\rangle_\varepsilon\right| \\
&= O(\varepsilon^2)\left\|(A_w^{-1}-A_{w'}^{-1})(G(w)-G(w'))\right\|_{X_\varepsilon} \\
&= O(\varepsilon^2)\left\|A_w^{-1}(A_w-A_{w'})A_{w'}^{-1}(G(w)-G(w'))\right\|_{X_\varepsilon} \\
&\le O(\varepsilon^2)\|A_w^{-1}\|_{\mathrm{op}}\cdot\|A_w-A_{w'}\|_{\mathrm{op}}\cdot\|A_{w'}^{-1}\|_{\mathrm{op}} \\
&\quad \cdot\|G(w)-G(w')\|_{X_\varepsilon},
\end{aligned}
$$

where the operator norms are defined as follows:

$$
\begin{aligned}
\|A_w^{-1}\|_{\mathrm{op}} &:= \sup_{f\in M_\varepsilon, f\neq 0}\frac{\|A_w^{-1}f\|_{X_\varepsilon}}{\|f\|_{X_\varepsilon}}, \\
\|A_w-A_{w'}\|_{\mathrm{op}} &:= \sup_{f\in M_\varepsilon, f\neq 0}\frac{\|(A_w-A_{w'})f\|_{X_\varepsilon}}{\|f\|_{X_\varepsilon}}, \\
\|A_{w'}^{-1}\|_{\mathrm{op}} &:= \sup_{f\in M_\varepsilon, f\neq 0}\frac{\|A_{w'}^{-1}f\|_{X_\varepsilon}}{\|f\|_{X_\varepsilon}}.
\end{aligned}
$$

For $f\in M_\varepsilon$, $f\neq 0$ and $w\in B$, we have

$$
C\|A_w^{-1}f\|_{X_\varepsilon}\le \frac{\langle A_wA_w^{-1}f, A_w^{-1}f\rangle_\varepsilon}{\|A_w^{-1}f\|_{X_\varepsilon}}\le \|f\|_{X_\varepsilon}.
$$

Hence

$$
\|A_w^{-1}\|_{\mathrm{op}}\le C,\ \ \|A_{w'}^{-1}\|_{\mathrm{op}}\le C.
$$

By Lemma 9, we have

$$
\begin{aligned}
\|(A_w-A_{w'})f\|_{X_\varepsilon}^2 &= \int_0^1 \langle(\delta^2E_{\mathrm{a}}[v+tw]-\delta^2E_{\mathrm{a}}[v+tw'])f, (A_w-A_{w'})f\rangle_\varepsilon \mathrm{d}t \\
&\le \int_0^1 C\varepsilon^{-1/2}\|tw-tw'\|_{X_\varepsilon}\|f\|_{X_\varepsilon}\|(A_w-A_{w'})f\|_{X_\varepsilon}\mathrm{d}t \\
&\le C\varepsilon^{-1/2}\|w-w'\|_{X_\varepsilon}\|f\|_{X_\varepsilon}\|(A_w-A_{w'})f\|_{X_\varepsilon}.
\end{aligned}
$$

Hence

$$
\|A_w-A_{w'}\|_{\mathrm{op}}\le C\varepsilon^{-1/2}\|w-w'\|_{X_\varepsilon}.
$$

Collecting these estimates, we obtain

$$
\|G(w)-G(w')\|_{X_\varepsilon}\le C\varepsilon^{-1/2}\|w-w'\|_{X_\varepsilon}C\varepsilon^2\le L\|w-w'\|_{X_\varepsilon}, \tag{106}
$$

where $L<1$ for sufficiently small ε. Therefore, G is a contraction mapping. Consequently, there exists a unique fixed point w^ε solving $(A_{w^\varepsilon}w^\varepsilon,\psi)_{X_\varepsilon} = -\langle\delta E_{\mathrm{a}}[v],\psi\rangle_\varepsilon$ for all $\psi\in M_\varepsilon$. Let $v^\varepsilon = v+w^\varepsilon$. Thus v^ε is a local minimizer of

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E_a in X_ε norm. Indeed, for any $w \in X_\varepsilon$ with $\|w\|_{X_\varepsilon} \le C_B\varepsilon^2$, we apply Lemma 10 and obtain

$$E_a[v^\varepsilon + w] - E_a[v^\varepsilon] = \int_0^1 (1-t)\langle \delta^2 E_a[v^\varepsilon + tw]w, w\rangle_\varepsilon \mathrm{d}t \ge C\|w\|_{X_\varepsilon}^2 > 0.$$

Therefore taking v^ε the Euler–Lagrange equation of the atomistic model satisfies $\|v^\varepsilon - v\|_{X_\varepsilon} \le C\varepsilon^2$. □

Proof of Corollary 1. 1. We suppose, without loss of generality, that $\varepsilon \le 1$. Since $v^+ = -v^-$, the total energy of the PN model at v reads as

$$E_{\mathrm{PN}}[v] = \int_{\mathbb{R}} \left[\alpha|\nabla v^+|^2 + \gamma(2v^+)\right] \mathrm{d}x. \tag{107}$$

Using trapezoidal rule, we have the numerical approximation of this energy

$$E_{\mathrm{PN}}^{\mathrm{app}}[v] = \varepsilon \sum_{i\in\mathbb{Z}} \left[\alpha|\nabla v_i^+|^2 + \gamma(2v_i^+)\right]. \tag{108}$$

It is sufficient to show that $\left|E_a[v^\varepsilon] - E_{\mathrm{PN}}^{\mathrm{app}}[v]\right| \le C\varepsilon^2$ and $\left|E_{\mathrm{PN}}^{\mathrm{app}}[v] - E_{\mathrm{PN}}[v]\right| \le C\varepsilon^2$.

2. Estimate $|E_a[v^\varepsilon] - E_{\mathrm{PN}}^{\mathrm{app}}[v]|$. Recall Eqs. (25) and (26). Let $E_a[v^\varepsilon] - E_{\mathrm{PN}}^{\mathrm{app}}[v] = R_{\mathrm{elas}} + R_{\mathrm{mis}}$, where

$$\begin{aligned} R_{\mathrm{elas}} &= \frac{\varepsilon^{-1}}{2}\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}^*}\Big[V(s+\varepsilon D_s^+ v_i^{\varepsilon,+}) + V(s-\varepsilon D_s^+ v_i^{\varepsilon,+}) - 2V(s) \\ &\quad -\varepsilon^2 V''(s)s^2(\nabla v_i^+)^2\Big], \\ R_{\mathrm{mis}} &= \varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\left[U\left(s-\frac{1}{2}+v_{i+s}^{\varepsilon,+}+v_i^{\varepsilon,+}\right) - U\left(s-\frac{1}{2}+2v_i^+\right)\right]. \end{aligned}$$

Let $w = v^\varepsilon - v$ on $\varepsilon\mathbb{Z}$. Thanks to Theorem 2, we have $w \in M_\varepsilon$ and $\|w\|_{X_\varepsilon} \le C\varepsilon^2$. This implies that $v^{\varepsilon,+} = -v^{\varepsilon,-}$, $\|Dw\|_{L_\varepsilon^\infty} \le C\varepsilon^{\frac{3}{2}}$, and $\|Dw\|_\varepsilon \le C\varepsilon^2$. Using Lemmas 6 and 7, we have $\|D_s^+ w\|_\varepsilon \le |s|\|Dw\|_\varepsilon \le C|s|\varepsilon^2$ and $\|D_s^+ v\|_\varepsilon \le |s|\|Dv\|_\varepsilon \le |s|\|v_{1,1}\|_\varepsilon \le C|s|$. Also notice that $\|D_s^+ v\|_{L_\varepsilon^\infty} \le |s|\|\nabla v\|_{L^\infty} \le C|s|$ and $\|D_s^+ w\|_{L_\varepsilon^\infty} \le |s|\|Dw\|_{L_\varepsilon^\infty} \le C|s|\varepsilon^{\frac{3}{2}}$. Thus

$$\|D_s^+ v^\varepsilon\|_\varepsilon \le \|D_s^+ v\|_\varepsilon + \|D_s^+ w\|_\varepsilon \le C|s|, \tag{109}$$

$$\|D_s^+ v^\varepsilon\|_{L_\varepsilon^\infty} \le \|D_s^+ v\|_{L_\varepsilon^\infty} + \|D_s^+ w\|_{L_\varepsilon^\infty} \le C|s|. \tag{110}$$

Since $\|D_s^+ w\|_\varepsilon \le C|s|\varepsilon^2$, we have $\|D_s^- D_s^+ w\|_\varepsilon \le |s|\|DD_s^+ w\|_\varepsilon \le C\varepsilon^{-1}|s|\|D_s^+ w\|_\varepsilon \le Cs^2\varepsilon$. Note that $\|D_s^- D_s^+ v\|_\varepsilon \le s^2\|v_{2,1}\|_\varepsilon \le Cs^2$. Thus

$$\|D_s^- D_s^+ v^\varepsilon\|_\varepsilon \le \|D_s^- D_s^+ w\|_\varepsilon + \|D_s^- D_s^+ v\|_\varepsilon \le Cs^2.$$

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To estimate the elastic part, we apply Taylor theorem:

$$|R_{\text{elas}}| \le \left|\frac{\varepsilon}{2}\sum_{s\in\mathbb{Z}^*} V''(s)\sum_{i\in\mathbb{Z}}\left[(D_s^+ v_i^{\varepsilon,+})^2 - (s\nabla v_i^+)^2\right]\right| + \frac{\varepsilon^3}{24}\sum_{s\in\mathbb{Z}^*} V_{4,s}\sum_{i\in\mathbb{Z}} |D_s^+ v_i^{\varepsilon,+}|^4. \tag{111}$$

For the second term on the right hand side of (111), we have

$$\begin{aligned}\frac{\varepsilon^3}{24}\sum_{s\in\mathbb{Z}^*} V_{4,s}\sum_{i\in\mathbb{Z}} |D_s^+ v_i^{\varepsilon,+}|^4 &\le C\varepsilon^2 \sum_{s\in\mathbb{Z}^*} V_{4,s} s^2 \|D_s^+ v^\varepsilon\|_\varepsilon^2 \\ &\le C\varepsilon^2 \sum_{s\in\mathbb{Z}^*} V_{4,s} s^4 \le C\varepsilon^2,\end{aligned} \tag{112}$$

where we have used Eqs. (109) and (110). We notice that $D_s^+ v_i^{\varepsilon,+} - s\nabla v_i^+ = D_s^+ w_i + D_s^+ v_i^+ - s\nabla v_i^+$ and $|D_s^+ v_i^+ - s\nabla v_i^+ - \frac{1}{2}\varepsilon s^2 \nabla^2 v_i^+| \le \frac{1}{6}\varepsilon^2 |s|^3 v_{3,s,i}$ (Recall Eq. (63)). Using Lemma 7, we have $\|v_{3,s}\|_\varepsilon \le C|s|^{1/2}$ and $\|\nabla^k v\|_\varepsilon \le \|v_{k,1}\|_\varepsilon \le C$, $k = 1, 2$. For the first term on the right hand side of Eq. (111), we have

$$\begin{aligned}&\left|\frac{\varepsilon}{2}\sum_{s\in\mathbb{Z}^*} V''(s)\sum_{i\in\mathbb{Z}}\left[(D_s^+ v_i^{\varepsilon,+})^2 - (s\nabla v_i^+)^2\right]\right| \\
&\le \left|\frac{\varepsilon}{2}\sum_{s\in\mathbb{Z}^*} V''(s)\sum_{i\in\mathbb{Z}}(D_s^+ w_i + D_s^+ v_i^+ - s\nabla v_i^+)(D_s^+ v_i^{\varepsilon,+} + s\nabla v_i^+)\right| \\
&\le \frac{1}{2}\sum_{s\in\mathbb{Z}^*} V_{2,s}\left(\|D_s^+ w\|_\varepsilon + \frac{1}{6}\varepsilon^2 |s|^3 \|v_{3,s}\|_\varepsilon\right)(\|D_s^+ v^\varepsilon\|_\varepsilon + |s|\|\nabla v\|_\varepsilon) \\
&\quad + \left|\frac{\varepsilon}{2}\sum_{s\in\mathbb{Z}^*} V''(s)\sum_{i\in\mathbb{Z}}\left(\frac{1}{2}\varepsilon s^2 \nabla^2 v_i^+\right) D_s^+ v_i^{\varepsilon,+}\right| \\
&\quad + \left|\frac{\varepsilon}{2}\sum_{s\in\mathbb{Z}^*} V''(s)\sum_{i\in\mathbb{Z}}\left(\frac{1}{2}\varepsilon s^2 \nabla^2 v_i^+\right) \nabla v_i^+\right| \\
&\le C\varepsilon^2 \sum_{s\in\mathbb{Z}^*} V_{2,s}|s|^5 + C\varepsilon^2 \sum_{s\in\mathbb{Z}^*} V_{2,s} s^4 + 0 \le C\varepsilon^2.\end{aligned} \tag{113}$$

We have used the facts that

$$\sum_{i\in\mathbb{Z}} \nabla^2 v_i^+ \nabla v_i^+ = \frac{1}{2}\sum_{i\in\mathbb{Z}}(\nabla^2 v_i^+ \nabla v_i^+ + \nabla^2 v_{-i}^+ \nabla v_{-i}^+) = 0,$$

$$\begin{aligned}\sum_{s\in\mathbb{Z}^*} V''(s) s^2 D_s^+ v_i^{\varepsilon,+} &= \frac{1}{2}\sum_{s\in\mathbb{Z}^*} V''(s) s^2 (D_s^+ v_i^{\varepsilon,+} + D_{-s}^+ v_i^{\varepsilon,+}) \\ &= \frac{\varepsilon}{2}\sum_{s\in\mathbb{Z}^*} V''(s) s^2 (D_s^- D_s^+ v_i^{\varepsilon,+}),\end{aligned}$$

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and

$$
\begin{aligned}
&\left|\frac{\varepsilon}{2}\sum_{s\in\mathbb{Z}^*}V''(s)\sum_{i\in\mathbb{Z}}\left(\frac{1}{2}\varepsilon s^2\nabla^2 v_i^+\right)D_s^+ v_i^{\varepsilon,+}\right|\\
&\quad\le\left|\frac{\varepsilon^3}{8}\sum_{s\in\mathbb{Z}^*}V''(s)s^2\sum_{i\in\mathbb{Z}}\nabla^2 v_i^+ D_s^- D_s^+ v_i^{\varepsilon,+}\right|\\
&\quad\le C\varepsilon^2\sum_{s\in\mathbb{Z}^*}V_{2,s}s^4.
\end{aligned}
$$

Next, we estimate the misfit part. Thanks to Lemma 5, we have $\|w^+\|_\varepsilon \le \|w\|_{X_\varepsilon} \le C\varepsilon^2$. Also recall that $\|v^+\|_\varepsilon \le C$. Note that $v_{i+s}^{\varepsilon,+} + v_i^{\varepsilon,+} - 2v_i^+ = w_{i+s}^+ + w_i^+ + \varepsilon D_s^+ v_i^+$ and $v_{i+s}^{\varepsilon,+} + v_i^{\varepsilon,+} - 2v_{i+s}^+ = w_{i+s}^+ + w_i^+ - \varepsilon D_s^+ v_i^+$. Since $\sum_{s\in\mathbb{Z}} U'(s-\frac{1}{2}) = 0$ and the series that follows are absolutely summable, we have

$$
\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}U'\left(s-\frac{1}{2}\right)(w_{i+s}^+ + w_i^+) = 2\sum_{i\in\mathbb{Z}}w_i^+\sum_{s\in\mathbb{Z}}U'\left(s-\frac{1}{2}\right) = 0.
$$

Now repeatedly applying the Taylor theorem to U leads to

$$
\begin{aligned}
|2R_{\text{mis}}| &= \left|\varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\left[2U\left(s-\frac{1}{2}+v_{i+s}^{\varepsilon,+}+v_i^{\varepsilon,+}\right)-U\left(s-\frac{1}{2}+2v_i^+\right)\right.\right.\\
&\quad\left.\left.-U\left(s-\frac{1}{2}+2v_{i+s}^+\right)\right]\right|\\
&\le\left|\varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\left[U'\left(s-\frac{1}{2}+2v_i^+\right)+U'\left(s-\frac{1}{2}+2v_{i+s}^+\right)\right]\right.\\
&\quad\left.\times(w_{i+s}^+ + w_i^+)\right|\\
&\quad+\left|\varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\left[U'\left(s-\frac{1}{2}+2v_i^+\right)\right.\right.\\
&\quad\left.\left.-U'\left(s-\frac{1}{2}+2v_{i+s}^+\right)\right]\varepsilon D_s^+ v_i^+\right|\\
&\quad+\left|\varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\frac{1}{2}U_{2,s}\left[(w_{i+s}^+ + w_i^+ + \varepsilon D_s^+ v_i^+)^2\right.\right.\\
&\quad\left.\left.+(w_{i+s}^+ + w_i^+ - \varepsilon D_s^+ v_i^+)^2\right]\right|\\
&\le\left|\varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}2U'\left(s-\frac{1}{2}\right)(w_{i+s}^+ + w_i^+)\right|\\
&\quad+\left|\varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}U_{2,s}(2v_i^+ + 2v_{i+s}^+)(w_{i+s}^+ + w_i^+)\right|
\end{aligned}
$$

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$$
\begin{aligned}
&+\varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} 2U_{2,s}|\varepsilon D_s^+ v_i^+|^2 + C\varepsilon^2 \\
&\leq 0 + C\varepsilon^2 + C\varepsilon^2 + C\varepsilon^2 \leq C\varepsilon^2. \qquad (114)
\end{aligned}
$$

Combining Eqs. (111), (112), (113) and (114), we obtain

$$|E_{\mathrm{a}}[v^\varepsilon] - E_{\mathrm{PN}}^{\mathrm{app}}[v]| \leq C\varepsilon^2.$$

3. Estimate $\left|E_{\mathrm{PN}}^{\mathrm{app}}[v] - E_{\mathrm{PN}}[v]\right|$. Let $g(x) = \alpha(\nabla v^+(x))^2 + \gamma(2v^+(x))$ for $x \in \mathbb{R}$. Then $g \in C^4$ and

$$
\begin{aligned}
g'(x) &= 2\alpha \nabla v^+ \nabla^2 v^+ + 2\gamma'(2v^+)\nabla v^+, \\
g''(x) &= 2\alpha(\nabla^2 v^+)^2 + 2\alpha \nabla v^+ \nabla^3 v^+ + 4\gamma''(2v^+)(\nabla v^+)^2 + 2\gamma'(2v^+)\nabla^2 v^+.
\end{aligned}
$$

By Lemma 2, we have $\|\gamma^{(k)}\|_{L^\infty} \leq C$, $k = 1, 2$. Thus

$$\max_{(i-1/2)\varepsilon \leq \xi \leq (i+1/2)\varepsilon} |g''(\xi)| \leq C\left\{(v_{2,1,i})^2 + v_{1,1,i}v_{3,1,i} + (v_{1,1,i})^2 + v_{2,1,i}\right\}.$$

Finally, we apply Lemma 7 to get

$$
\begin{aligned}
\left|E_{\mathrm{PN}}^{\mathrm{app}}[v] - E_{\mathrm{PN}}[v]\right| &\leq \sum_{i\in\mathbb{Z}} \left| \int_{(i-1)\varepsilon}^{(i+1)\varepsilon} g(x)\mathrm{d}x - \varepsilon g(i\varepsilon) \right| \\
&\leq \frac{\varepsilon^3}{3} \sum_{i\in\mathbb{Z}} \max_{(i-1/2)\varepsilon \leq \xi \leq (i+1/2)\varepsilon} |g''(\xi)| \\
&\leq C\varepsilon^3 \sum_{i\in\mathbb{Z}} \left\{(v_{2,1,i})^2 + v_{1,1,i}v_{3,1,i} + (v_{1,1,i})^2 + v_{2,1,i}\right\} \\
&\leq C\varepsilon^2.
\end{aligned}
$$

□

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Compliance with Ethical Standards

Conflict of interest The authors declare that they have no conflict of interest.

Appendix A: Variations of Energies

In this appendix, we list the explicit expressions of the variations for both models. Note that $\delta E_{\mathrm{a}}[u] \in X_\varepsilon^*$ and $\delta^2 E_{\mathrm{a}}[u] f \in X_\varepsilon^*$ for $u \in S_\varepsilon$ and $f \in X_\varepsilon$. In $\langle \delta E_{\mathrm{a}}[u], f\rangle_\varepsilon$ for $f \in X_\varepsilon$, $\langle \cdot, \cdot \rangle_\varepsilon$ is a pairing on $X_\varepsilon^* \times X_\varepsilon$.

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Proposition 11. (variations of energies) *Suppose that Assumptions A1–A6 hold.*

1. *For $u \in S_\varepsilon$ and $f, g \in X_\varepsilon$, we have*

$$
\begin{aligned}
\langle \delta E_a[u], f\rangle_\varepsilon = {} & \sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}^*}\frac{1}{2}\left[V'(s+\varepsilon D_s^+u_i^+)(D_s^+f_i^+)\right.\\
& \left.+V'(s+\varepsilon D_s^+u_i^-)(D_s^+f_i^-)\right]\\
& +\varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\left[U'\left(s-\frac{1}{2}+u_{i+s}^+-u_i^-\right)(f_{i+s}^+-f_i^-)\right], \quad (115)
\end{aligned}
$$

$$
\begin{aligned}
\left\langle \delta^2 E_a[u]f, g\right\rangle_\varepsilon = {} & \varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}^*}\frac{1}{2}[V''(s+\varepsilon D_s^+u_i^+)(D_s^+f_i^+)(D_s^+g_i^+)\\
& +V''(s+\varepsilon D_s^+u_i^-)(D_s^+f_i^-)(D_s^+g_i^-)]\\
& +\varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\left[U''\left(s-\frac{1}{2}+u_{i+s}^+-u_i^-\right)\right.\\
& \left.\times(f_{i+s}^+-f_i^-)(g_{i+s}^+-g_i^-)\right]. \quad (116)
\end{aligned}
$$

The series in (116) is absolutely summable in the following sense for sufficiently small ε:

$$
\begin{aligned}
& \varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}^*}\sum_{\pm}\frac{1}{2}\left|V''(s+\varepsilon D_s^+u_i^\pm)(D_s^+f_i^\pm)(D_s^+g_i^\pm)\right|\\
& \quad +\varepsilon\sum_{i\in\mathbb{Z}}\sum_{s\in\mathbb{Z}}\left|U''\left(s-\frac{1}{2}+u_{i+s}^+-u_i^-\right)(f_{i+s}^+-f_i^-)(g_{i+s}^+-g_i^-)\right|\\
& < \infty. \quad (117)
\end{aligned}
$$

If $f \in M_\varepsilon$ and $u = v$ is the PN solution of Theorem 1, then the series in (115) is absolutely summable in the following sense for sufficiently small ε:

$$
\begin{aligned}
& \sum_{i\in\mathbb{Z}}\left|\sum_{s\in\mathbb{Z}^*}\frac{1}{2}[V'(s+\varepsilon D_s^+u_i^+)(D_s^+f_i^+)+V'(s+\varepsilon D_s^+u_i^-)(D_s^+f_i^-)]\right|\\
& \quad +\varepsilon\sum_{i\in\mathbb{Z}}\left|\sum_{s\in\mathbb{Z}}\left[U'\left(s-\frac{1}{2}+u_{i+s}^+-u_i^-\right)(f_{i+s}^+-f_i^-)\right]\right| < \infty. \quad (118)
\end{aligned}
$$

2. *For $u \in S_0$ and $f, g \in X_0$, we have*

$$
\langle \delta E_{PN}[u], f\rangle_0 = \int_{\mathbb{R}}\left\{\alpha\nabla u^+\nabla f^+ + \alpha\nabla u^-\nabla f^- + \gamma'(u^\perp)f^\perp\right\}\mathrm{d}x, \quad (119)
$$

$$
\left\langle \delta^2 E_{PN}[u]f, g\right\rangle_0 = \int_{\mathbb{R}}\left\{\alpha\nabla f^+\nabla g^+ + \alpha\nabla f^-\nabla g^- + \gamma''(u^\perp)f^\perp g^\perp\right\}\mathrm{d}x. \quad (120)
$$

Proof. Using difference operators, the atomistic energy reads as

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$$E_{\mathrm{a}}[u] = \varepsilon^{-1} \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}^*} \frac{1}{2} \left[V\left(s + \varepsilon D_s^+ u_i^+\right) + V\left(s + \varepsilon D_s^+ u_i^-\right) - 2V(s) \right]$$
$$+ \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} \left[U\left(s - \frac{1}{2} + (u_{i+s}^+ - u_i^-)\right) - U\left(s - \frac{1}{2}\right) \right].$$

Then Eqs. (115), (116), (119) and (120) are obtained via direct calculations. For sufficiently small ε, we have

$$\text{left hand side of (117)} \leq \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}^*} \sum_{\pm} \frac{1}{2} V_{2,s} |D_s^+ f_i^\pm| |D_s^+ g_i^\pm|$$
$$+ \varepsilon \sum_{i\in\mathbb{Z}} \sum_{s\in\mathbb{Z}} U_{2,s} |f_{i+s}^+ - f_i^-| |g_{i+s}^+ - g_i^-|$$
$$\leq C,$$

where the first term is bounded by $\frac{1}{2} \sum_{s\in\mathbb{Z}^*} V_{2,s} s^2 \|Df\|_\varepsilon \|Dg\|_\varepsilon \leq C \|f\|_{X_\varepsilon} \|g\|_{X_\varepsilon} \leq C$ and the second term is bounded similarly because of Lemmas 1 and 6.

If $f \in M_\varepsilon$ and $u = v$ is the PN solution of Theorem 1, then the absolutely summability of the series in (118) is essentially shown in the proof of Proposition 4 (See the estimates of $|R_{\mathrm{elas}}|$ and $|R_{\mathrm{mis}}|$). □

We remark that the order of the double summation $\sum_i$ and $\sum_s$ can not be changed in Eq. (118); while the order of the double summation $\sum_i$ and $\sum_s$ is changeable in Eq. (117). We also remark that, at the perfect lattice (corresponding to $u \equiv 0$ which is not in S_0 or S_ε), the second variation $\delta^2 E_{\mathrm{a}}[0]$ and $\delta^2 E_{\mathrm{PN}}[0]$ can also be defined and satisfy the same formulas in Proposition 11.

Appendix B: Small Parameter ε Calculated by Atomistic and First Principles Calculations

An example of the bilayer systems is bilayer graphene. In this appendix, we calculate the small parameter ε defined in Eq. (18) in Sect. 2.3 that characterizes the strength of the weak van der Waals interlayer interaction v.s. the strong covalent-bond intralayer interaction in the bilayer graphene, using the data of atomistic and first principles calculations [13,70].

In the PN model for bilayer graphene in Ref. [13], the two dimensional γ-surface was fitted by a truncated trigonometric series as

$$\gamma_{2\mathrm{d}}(\phi, \psi) = c_0 + c_1 \left[\cos\frac{2\pi}{a}\left(\phi + \frac{\psi}{\sqrt{3}}\right) + \cos\frac{2\pi}{a}\left(\phi - \frac{\psi}{\sqrt{3}}\right) + \cos\frac{4\pi\psi}{\sqrt{3}a} \right]$$
$$+ c_2 \left[\cos\frac{2\pi}{a}\left(\phi + \sqrt{3}\psi\right) + \cos\frac{2\pi}{a}\left(\phi - \sqrt{3}\psi\right) + \cos\frac{4\pi\phi}{a} \right]$$
$$+ c_3 \left[\cos\frac{2\pi}{a}\left(2\phi + \frac{2\psi}{\sqrt{3}}\right) + \cos\frac{2\pi}{a}\left(2\phi - \frac{2\psi}{\sqrt{3}}\right) + \cos\frac{8\pi\psi}{\sqrt{3}a} \right]$$

$$
\begin{aligned}
&+c_4\left[\sin\frac{2\pi}{a}\left(\phi-\frac{\psi}{\sqrt{3}}\right)-\sin\frac{2\pi}{a}\left(\phi+\frac{\psi}{\sqrt{3}}\right)+\sin\frac{4\pi\psi}{\sqrt{3}a}\right]\\
&+c_5\left[\sin\frac{2\pi}{a}\left(2\phi-\frac{2\psi}{\sqrt{3}}\right)-\sin\frac{2\pi}{a}\left(2\phi+\frac{2\psi}{\sqrt{3}}\right)+\sin\frac{8\pi\psi}{\sqrt{3}a}\right],
\end{aligned}
$$

where $\{c_i\}_{i=1}^5$ are constants obtained by fitting the data of first principles calculations [70] as

$$
\begin{aligned}
&c_0=21.336\times10^{-3},\ \ c_1=-6.127\times10^{-3},\ \ c_2=-1.128\times10^{-3},\\
&c_3=0.143\times10^{-3},\ c_4=\sqrt{3}c_1,\ \ c_5=-\sqrt{3}c_3,
\end{aligned}
$$

where the units are $\mathrm{J/m^2}$. On the other hand, the elasticity constants of each monolayer graphene, in the unit of $\mathrm{J/m^2}$, are [13]

$$C_{11}=312.67,\ \ C_{12}=91.66,\ \ C_{44}=110.40.$$

In our one-dimensional case, $\gamma(\phi)=\gamma_{2\mathrm{d}}(\phi,0)$ and $\alpha=C_{11}$. Using the above values and Eq. (18) in Sect. 2.3, we have

$$\varepsilon=\sqrt{\frac{a^2\frac{\partial^2\gamma_{2\mathrm{d}}(0,0)}{\partial\phi^2}}{C_{11}}}\approx0.0475.$$

Thus it is reasonable to set ε as a small parameter.

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