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CAUCHY–BORN RULE AND STABILITY OF CRYSTALLINE SOLIDS AT FINITE TEMPERATURE*

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Abstract. We study the connection between atomistic and continuum models for the elastic deformation of crystalline solids at finite temperature. We prove, under certain sharp stability conditions at zero temperature, that the solid is stable when temperature is low. This gives a criterion for the onset of instabilities of crystalline solids as temperature increases. Based on the stability conditions at both zero and finite temperature, we show that the finite temperature version of Cauchy–Born rule gives a correct nonlinear elasticity model in the sense that elastically deformed states of the atomistic model are closely approximated by solutions of the continuum model with free energy functionals obtained from the Cauchy–Born rule at finite temperature. The convergence is proved for both simple and complex lattices.

Keywords. Cauchy–Born rule; finite temperature; stability of crystalline solids; atomistic model.

AMS subject classifications. 74B20; 74E15; 74G65; 74N99.

1. Introduction

The Cauchy–Born rule is a fundamental connection between atomistic and continuum models for elastically deformed crystalline solids. It was originally proposed by Cauchy and then extended by Born and Huang [4]. According to the Cauchy–Born rule, the zero-temperature stored energy density $W_{\mathrm{CB}}(\boldsymbol{A})$ at a point in the continuum model in $\mathbb{R}^d$, where the displacement gradient is $\boldsymbol{A}\in\mathbb{R}^{d\times d}$, can be approximated by the energy of a unit cell in a uniformly deformed infinite crystalline solid with the given displacement gradient $\boldsymbol{A}$ calculated by atomistic model. Accompanied by many applications of the Cauchy–Born rule to numerical simulations and design of multiscale methods [19, 25], progress in analytic aspects of the Cauchy–Born rule have also been achieved, such as the stability of the crystalline solid [9] and the successes/failures of the rule [10]. It was investigated by Braides et al. [5] that some discrete total energy consisting of pairwise interactions Γ-converges to a continuum stored energy. After that, Blanc et al. [3] established consistency of the energy under the assumption that the atomistic displacement is smooth and follows exactly the continuum displacement field. Friesecke and Theil [14] identified parameter regimes for success and failure of the Cauchy–Born rule in the sense whether the rule provides the global minimum energy in the thermodynamic limit. Later, E and Ming [7, 8] showed that the Cauchy–Born rule is valid as long as the right unit cell is used. Their proof did not require any unnecessary assumption such as the atomistic displacement field matches its continuum analogue. Their result provides a sharp criterion for the stability of crystalline solids under stress. These analyses are based on the zero-temperature Cauchy–Born rule. We remark that Yang and E [27] generalized the Cauchy–Born rule to plates, sheets, and rods at zero

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temperature. Recently, Friedrich et al. also proved the validation of zero temperature Cauchy–Born rule in the case of carbon nanotubes in three dimensions [13].

For realistic applications, it is more reasonable to consider the temperature-related Cauchy–Born rule which was obtained by Born [4], using the Helmholtz free energy instead of the stored energy, in a similar way as the zero-temperature Cauchy–Born rule. Here the Helmholtz energy is derived from a canonical ensemble. Some studies of the finite-temperature Cauchy–Born rule can be found in [26, 28]. Among these recent progress, Yang et al. [28] derived a closed form expression for the first Piola–Kirchhoff stress, which was also validated by several numerical examples. They also developed an efficient implementation method based on Fourier transform that greatly reduces the computational cost. A significant advantage of the finite-temperature Cauchy–Born rule method is that no ensemble average needs to be taken, which avoid thousands of steps of molecular dynamics or Monte Carlo simulation in ensemble sampling. However, as far as the authors are concerned, there is no rigorous proof for the success of the Cauchy–Born rule at finite temperature and the stability condition for the crystalline solid at finite temperature is not known yet.

A successful multiscale numerical method related to the Cauchy–Born rule is the quasicontinuum (QC) method, which was introduced by Tadmor et al. [24] in order to simulate the problems in crystalline materials. This method starts with fully atomistic model and uses the Cauchy–Born rule as the approximation for the homogeneous deformed region. There are numerous related works on analysis [17, 24], applications [1, 23, 25] and extensions [15, 16, 21, 22] of this method. In particular, the temperature-related QC method was introduced in Ref. [6]. However, rigorous analyses of this method such as stability and convergence are still lacking. A related work is the convergence of a force-based hybrid method in three dimensions at zero-temperature by Lu and Ming [20]. We hope that our analysis on the finite-temperature Cauchy–Born rule will also shed some light on the analysis for temperature-related QC method and other related multiscale methods.

In this paper, we first investigate the stability of the crystalline solid at finite temperature and then prove the convergence from atomistic model to the continuum model obtained by the Cauchy–Born rule at finite temperature. We prove stability of deformed crystalline solids at finite temperature under the same stability assumption as that used in the proof of stability at zero temperature in Ref. [8], namely that the undeformed crystalline solid is stable at zero temperature (see Assumption 3.1). This stability assumption is sharp for the finite-temperature problem in the sense that it is necessary for the stability at zero temperature. Next, we show consistency of the atomistic and continuum models by detailed asymptotic analysis. Note that the finite temperature Cauchy–Born rule model contains an entropy contribution that is not present in the zero temperature model. Based on the obtained consistency and stability results, convergence from atomistic model to the finite-temperature Cauchy–Born rule is proved following the zero-temperature counterpart in Ref. [8]. More precisely, we show that the finite temperature version of Cauchy–Born rule gives a correct nonlinear elasticity model in the sense that elastically deformed states of the atomistic model are closely approximated by solutions of the continuum model with free energy functionals obtained from the Cauchy–Born rule at finite temperature. We prove the convergence for both simple and complex lattices, i.e., Bravais lattices and combinations of several Bravais lattices of the same type, respectively.

2. Atomistic model and continuum model based on Cauchy–Born rule

In this section, we first fix notation and then introduce atomistic and continuum models for simple and complex lattices.

2.1. Lattice functions and norms. We start with a simple lattice (also known as Bravais lattice) crystal which is denoted as

$$\mathbb{L}=\left\{\boldsymbol{x}\in\mathbb{R}^d\,|\,\boldsymbol{x}=\sum_{\alpha=1}^{d}\mu_\alpha\boldsymbol{a}_\alpha,\boldsymbol{\mu}=(\mu_1,\dots,\mu_d)\in\mathbb{Z}^d\right\},$$

where d is the dimension and $\{\boldsymbol{a}_\alpha\}_{\alpha=1}^d\subset\mathbb{R}^d$ are the basis vectors of $\mathbb{L}$. The reciprocal lattice $\mathbb{L}^*$ reads as

$$\mathbb{L}^*=\left\{\boldsymbol{x}\in\mathbb{R}^d\,|\,\boldsymbol{x}=\sum_{\alpha=1}^{d}\mu_\alpha\boldsymbol{b}_\alpha,\boldsymbol{\mu}=(\mu_1,\dots,\mu_d)\in\mathbb{Z}^d\right\},$$

where the reciprocal basis vectors $\{\boldsymbol{b}_\beta\}_{\beta=1}^d\subset\mathbb{R}^d$ satisfy $\boldsymbol{a}_\alpha\cdot\boldsymbol{b}_\beta=2\pi\delta_{\alpha\beta}$ and $\delta_{\alpha\beta}$ is the Kronecker delta. The unit cells of $\mathbb{L}$ and $\mathbb{L}^*$ are denoted as Γ and Γ^*, respectively, which are defined by

$$\Gamma=\left\{\boldsymbol{x}\in\mathbb{R}^d\,|\,\boldsymbol{x}=\sum_{\alpha=1}^{d}c_\alpha\boldsymbol{a}_\alpha,0\le c_\alpha<1,\alpha=1,2,\dots,d\right\},$$
$$\Gamma^*=\left\{\boldsymbol{x}\in\mathbb{R}^d\,|\,\boldsymbol{x}=\sum_{\alpha=1}^{d}c_\alpha\boldsymbol{b}_\alpha,-\frac{1}{2}\le c_\alpha<\frac{1}{2},\alpha=1,2,\dots,d\right\}.$$

In the sequel, we consider atomistic models and their continuum analogues obtained by the Cauchy–Born rule in a unit cell of the continuum model $\Omega=\Gamma\subset\mathbb{R}^d$ with the periodic boundary condition. Let $\varepsilon=\frac{1}{n}\ll1$ be the lattice constant with $n\in\mathbb{N}_+$ for convenience. The (simple) lattice system for our atomistic model is denoted as $\Omega_\varepsilon=\Omega\cap\varepsilon\mathbb{L}$. Its reciprocal lattice is $\mathbb{L}_\varepsilon^*=\mathbb{L}^*\cap(\Gamma^*/\varepsilon)$. Clearly, the number of atoms in Ω_ε is $\varepsilon^{-d}=n^d=:N$. A lattice function u defined on $\varepsilon\mathbb{L}$ is Ω_ε-*periodic* if

$$\boldsymbol{u}(\boldsymbol{x})=\boldsymbol{u}(\boldsymbol{x}')\text{ for any }\boldsymbol{x},\boldsymbol{x}'\in\varepsilon\mathbb{L},\,\boldsymbol{x}-\boldsymbol{x}'=\boldsymbol{a}_\alpha\text{ for some }\alpha\in\{1,\dots,d\}.$$

With a slight abuse of notation, we identify each Ω_ε-periodic function as its restriction on Ω_ε.

For $\boldsymbol{\mu}\in\mathbb{Z}^d$ and $\boldsymbol{s}=\sum_{\alpha=1}^d\mu_\alpha\boldsymbol{a}_\alpha$, the translation operator $T_{\varepsilon,s}$ is defined as

$$(\mathcal{T}_{\varepsilon,\boldsymbol{s}}\boldsymbol{u})(\boldsymbol{x})=\boldsymbol{u}(\boldsymbol{x}+\varepsilon\boldsymbol{s})\quad\text{for }\boldsymbol{x}\in\mathbb{R}^d.$$

We define the (forward) difference operator as

$$\mathcal{D}_{\varepsilon,\boldsymbol{s}}=\varepsilon^{-1}(\mathcal{T}_{\varepsilon,\boldsymbol{s}}-I),$$

where I is the identity operator. For a multi-index $\boldsymbol{\mu}\in\mathbb{N}_+^d$, we define $|\boldsymbol{\mu}|=\sum_{\alpha=1}^d\boldsymbol{\mu}_\alpha$ and the difference operator $\mathcal{D}_\varepsilon^{\boldsymbol{\mu}}$ is given by

$$\mathcal{D}_\varepsilon^{\boldsymbol{\mu}}=\prod_{\alpha=1}^{d}(\mathcal{D}_{\varepsilon,\boldsymbol{a}_\alpha})^{\mu_\alpha}.$$

For simplicity, we will drop the subscript ε in the notations $\mathcal{T}_{\varepsilon,\boldsymbol{s}}$, $\mathcal{D}_{\varepsilon,\boldsymbol{s}}$, and $\mathcal{D}^{\boldsymbol{\mu}}_{\varepsilon}$ when there is no confusion.

Let us introduce the norms for functions defined on Ω_ε. For $k\in\mathbb{N}$, we define the discrete Sobolev norm

$$\|\boldsymbol{u}\|^2_{H^k_\varepsilon}=\sum_{0\le|\boldsymbol{\mu}|\le k}\varepsilon^d\sum_{\boldsymbol{x}\in\Omega_\varepsilon}\|(\mathcal{D}^{\boldsymbol{\mu}}_{\varepsilon}\boldsymbol{u})(\boldsymbol{x})\|^2.$$

The corresponding function space on lattice is denoted as H^k_ε (or L^2_ε when $k=0$). The uniform norms on Ω_ε are given by

$$\|\boldsymbol{u}\|_{W^{k,\infty}_\varepsilon}=\sum_{0\le|\boldsymbol{\mu}|\le k}\max_{\boldsymbol{x}\in\Omega_\varepsilon}\|(\mathcal{D}^{\boldsymbol{\mu}}_{\varepsilon}\boldsymbol{u})(\boldsymbol{x})\|.$$

For $k=0$, we write $L^\infty_\varepsilon=W^{0,\infty}_\varepsilon$ and $\|\boldsymbol{u}\|_{L^\infty_\varepsilon}=\max_{\boldsymbol{x}\in\Omega_\varepsilon}\|\boldsymbol{u}(\boldsymbol{x})\|$. For the analysis, it is also helpful to use the semi-norm on Ω_ε:

$$|\boldsymbol{u}|_{W^{1,\infty}_\varepsilon}=\max_{|\boldsymbol{\mu}|=1}\max_{\boldsymbol{x}\in\Omega_\varepsilon}\|(\mathcal{D}^{\boldsymbol{\mu}}_{\varepsilon}\boldsymbol{u})(\boldsymbol{x})\|.$$

Clearly, for mean-zero periodic functions on Ω_ε, the seminorm $|\cdot|_{W^{1,\infty}_\varepsilon}$ is equivalent to the norm $\|\cdot\|_{W^{1,\infty}_\varepsilon}$.

For $k>d/2$, we have the following discrete Sobolev embedding inequality [12]

$$\|\boldsymbol{f}\|_{L^\infty_\varepsilon}\le C\|\boldsymbol{f}\|_{H^k_\varepsilon},$$

where C depends on k and Ω. These norms defined here may be extended to vector-valued functions as usual.

Next, we introduce the notation for products and derivatives related to matrices. Let $\boldsymbol{M}\in\mathbb{R}^{d\times d}$ be a matrix, $\boldsymbol{x}\in\mathbb{R}^d$ a (column) vector, and $g:\mathbb{R}^{d\times d}\to\mathbb{R}$ a scalar function. Then we define the vector length $\|\boldsymbol{x}\|=(\sum_{\alpha=1}^d x_\alpha^2)^{1/2}$, the Frobenius norm $\|\boldsymbol{M}\|_{\mathrm{F}}=(\sum_{\alpha=1}^d\sum_{\beta=1}^d M_{\alpha\beta}^2)^{1/2}$, and the vector-matrix product $\boldsymbol{x}\cdot\boldsymbol{M}=\boldsymbol{x}^{\intercal}\boldsymbol{M}$, i.e., $(\boldsymbol{x}\cdot\boldsymbol{M})_\beta=\sum_\alpha x_\alpha M_{\alpha\beta}$. We write the derivatives of g with respect to $\boldsymbol{M}$ as follows: $D_{\boldsymbol{M}}g=(\frac{\partial g}{\partial M_{\alpha\beta}})$, $D^2_{\boldsymbol{M}}g=(\frac{\partial^2 g}{\partial M_{\alpha\beta}\partial M_{\gamma\delta}})$, and $D^3_{\boldsymbol{M}}g=(\frac{\partial^3 g}{\partial M_{\alpha\beta}\partial M_{\gamma\delta}\partial M_{\eta\lambda}})$. For matrices $\boldsymbol{N},\boldsymbol{P},\boldsymbol{Q}\in\mathbb{R}^{d\times d}$, we denote

$$\begin{aligned}
D_{\boldsymbol{M}}g:\boldsymbol{N}&=\sum_{\alpha,\beta=1}^d\frac{\partial g}{\partial M_{\alpha\beta}}N_{\alpha\beta},\\
(D^2_{\boldsymbol{M}}g:\boldsymbol{N})_{\gamma\delta}&=\sum_{\alpha,\beta=1}^d\frac{\partial^2 g}{\partial M_{\alpha\beta}\partial M_{\gamma\delta}}N_{\alpha\beta},\quad \gamma,\delta=1,\dots,d\\
(D^2_{\boldsymbol{M}}g:\boldsymbol{N}):\boldsymbol{P}&=\sum_{\alpha,\beta,\gamma,\delta=1}^d\frac{\partial^2 g}{\partial M_{\alpha\beta}\partial M_{\gamma\delta}}N_{\alpha\beta}P_{\gamma\delta},\\
((D^3_{\boldsymbol{M}}g:\boldsymbol{N}):\boldsymbol{P})_{\eta\lambda}&=\sum_{\alpha,\beta,\gamma,\delta=1}^d\frac{\partial^3 g}{\partial M_{\alpha\beta}\partial M_{\gamma\delta}\partial M_{\eta\lambda}}N_{\alpha\beta}P_{\gamma\delta},\quad \eta,\lambda=1,\dots,d.
\end{aligned}$$

2.2. Simple lattice. To make things clear, we would like to describe the setting for simple lattice first and extend to complex lattice afterwards.

We only consider the classical empirical potentials in this work. For atoms located at $\boldsymbol{y}(\boldsymbol{x})$, $\boldsymbol{x}\in\Omega_\varepsilon$, the interaction potential energy is given by

$$\mathcal{U}_\varepsilon[\boldsymbol{y}]=\sum_{i,j}V_2(\boldsymbol{y}_i/\varepsilon,\boldsymbol{y}_j/\varepsilon)+\sum_{i,j,k}V_3(\boldsymbol{y}_i/\varepsilon,\boldsymbol{y}_j/\varepsilon,\boldsymbol{y}_k/\varepsilon)+\cdots.$$

As the previous works on the Cauchy–Born rule at zero temperature [8,20], we will also make the following assumptions on the potential function V_l for $l\geq 2$:

(1) V_l is translation invariant.

(2) V_l is invariant with respect to rigid body motion.

(3) V_l is smooth in a neighborhood of the equilibrium state.

(4) V_l has finite range and consequently we will consider only interactions that involve a finite number of atoms.

The first two are general assumptions, while the latter two are common in atomistic simulations. We will only present the results for the potentials with two-body and three-body interactions under the above conditions. Moreover, the two-body interaction can be incorporated into the three-body interaction. Thus $\mathcal{U}_\varepsilon=\sum_{i,j,k}V_3(\boldsymbol{y}_i/\varepsilon,\boldsymbol{y}_j/\varepsilon,\boldsymbol{y}_k/\varepsilon)$. Thanks to the translation invariance of potential V_3, we rewrite the three-body potential into the following form:

$$V\left(\frac{\boldsymbol{y}_j-\boldsymbol{y}_i}{\varepsilon},\frac{\boldsymbol{y}_k-\boldsymbol{y}_i}{\varepsilon}\right)=V_3\left(\boldsymbol{y}_i/\varepsilon,\boldsymbol{y}_j/\varepsilon,\boldsymbol{y}_k/\varepsilon\right),$$

Let $\boldsymbol{s}_1=\frac{\boldsymbol{x}_j-\boldsymbol{x}_i}{\varepsilon}$ and $\boldsymbol{s}_2=\frac{\boldsymbol{x}_k-\boldsymbol{x}_i}{\varepsilon}$. Then $V\left(\frac{\boldsymbol{y}_j-\boldsymbol{y}_i}{\varepsilon},\frac{\boldsymbol{y}_k-\boldsymbol{y}_i}{\varepsilon}\right)=V\left(\mathcal{D}_{\boldsymbol{s}_1}\boldsymbol{y}_i,\mathcal{D}_{\boldsymbol{s}_2}\boldsymbol{y}_i\right)$. In the sequel, we use $\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}$ to represent the summation over all possible pairs $(\boldsymbol{s}_1,\boldsymbol{s}_2)$ in the range of the potential S_{int}. Here the set S_{int} has the property that if $(\boldsymbol{s}_1,\boldsymbol{s}_2)\in S_{\text{int}}$, then $(-\boldsymbol{s}_1,-\boldsymbol{s}_2)\in S_{\text{int}}$ and $(\boldsymbol{s}_2,\boldsymbol{s}_1)\in S_{\text{int}}$. Also, we will replace $\boldsymbol{y}_i$ and $\boldsymbol{y}_j$ by $\boldsymbol{y}(\boldsymbol{x})$ and $\boldsymbol{y}(\boldsymbol{x}')$, denoting the locations of atoms labelled as $\boldsymbol{x}$ and $\boldsymbol{x}'$. For $\boldsymbol{x}\in\Omega_\varepsilon$, $(\boldsymbol{s}_1,\boldsymbol{s}_2)\in S_{\text{int}}$, we denote the above three-body potential as follows:

$$V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}](\boldsymbol{x})=V\left(\mathcal{D}_{\boldsymbol{s}_1}\boldsymbol{y}(\boldsymbol{x}),\mathcal{D}_{\boldsymbol{s}_2}\boldsymbol{y}(\boldsymbol{x})\right). \tag{2.1}$$

The partial derivatives of $V(\boldsymbol{r}_1,\boldsymbol{r}_2)$ at $\boldsymbol{r}_1=\mathcal{D}_{\boldsymbol{s}_1}\boldsymbol{y}(\boldsymbol{x})$, $\boldsymbol{r}_2=\mathcal{D}_{\boldsymbol{s}_2}\boldsymbol{y}(\boldsymbol{x})$ is denoted as follows:

$$\partial_j V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}](\boldsymbol{x})=\partial_{\boldsymbol{r}_j}V\left(\mathcal{D}_{\boldsymbol{s}_1}\boldsymbol{y}(\boldsymbol{x}),\mathcal{D}_{\boldsymbol{s}_2}\boldsymbol{y}(\boldsymbol{x})\right),\ j=1,2.$$

Higher order derivatives of $V(\boldsymbol{r}_1,\boldsymbol{r}_2)$ can be written in a similar way.

The position of an atom, $x\in\Omega_\varepsilon$, under deformation is $\boldsymbol{y}(\boldsymbol{x})=\boldsymbol{x}+\boldsymbol{u}(\boldsymbol{x})$ where $\boldsymbol{u}:\Omega_\varepsilon\to\mathbb{R}^d$ is the displacement of the atoms. As mentioned above, we extend and regard $\boldsymbol{u}$ as an Ω_ε-periodic function defined on $\varepsilon\mathbb{L}$. Without further explanation, the summation $\sum_{\boldsymbol{x}}$ always stands for $\sum_{\boldsymbol{x}\in\Omega_\varepsilon}$ in the sequel. Given $\boldsymbol{B}\in\mathbb{R}^{d\times d}$, we are interested in the vector field $\boldsymbol{y}$ with $\boldsymbol{y}-\boldsymbol{x}-\boldsymbol{x}\cdot\boldsymbol{B}$ belonging to the following space

$$\boldsymbol{X}_\varepsilon:=\left\{\boldsymbol{v}:\varepsilon\mathbb{L}\to\mathbb{R}^d\,|\,\boldsymbol{v}(\boldsymbol{x})\quad\Omega_\varepsilon\text{-periodic},\quad\sum_{\boldsymbol{x}}\boldsymbol{v}(\boldsymbol{x})=\boldsymbol{0}\right\}.$$

Clearly, $\boldsymbol{x}\cdot\boldsymbol{B}$ is the linear part of the displacement.

Atomistic Model for Simple Lattice: The atomistic problem is formulated as follows: given body force $\boldsymbol{f}:\Omega_\varepsilon\to\mathbb{R}^d$ and $\boldsymbol{B}\in\mathbb{R}^{d\times d}$, find $\boldsymbol{y}^*$ such that

$$\boldsymbol{y}^*=\arg\min_{\boldsymbol{y}-\boldsymbol{x}-\boldsymbol{x}\cdot\boldsymbol{B}\in X_\varepsilon}\mathcal{I}_\varepsilon[\boldsymbol{y}], \tag{2.2}$$

with

$$\mathcal{I}_\varepsilon[\boldsymbol{y}] = \mathcal{F}_\varepsilon[\boldsymbol{y}] - \varepsilon^d \sum_{\boldsymbol{x}} \boldsymbol{f}(\boldsymbol{x}) \cdot \boldsymbol{y}(\boldsymbol{x}), \tag{2.3}$$

$$\mathcal{F}_\varepsilon[\boldsymbol{y}] = \mathcal{U}_\varepsilon[\boldsymbol{y}] - T\mathcal{S}_\varepsilon[\boldsymbol{y}], \tag{2.4}$$

$$\mathcal{U}_\varepsilon[\boldsymbol{y}] = \varepsilon^d \sum_{\boldsymbol{x}} \sum_{\boldsymbol{s}_1, \boldsymbol{s}_2} \frac{1}{2} V_{\boldsymbol{s}_1, \boldsymbol{s}_2}[\boldsymbol{y}](\boldsymbol{x}), \tag{2.5}$$

$$\mathcal{S}_\varepsilon[\boldsymbol{y}] = -\varepsilon^d \sum_{\boldsymbol{x}} dk_{\mathrm{B}} \log \frac{\hbar(\det(\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}](\boldsymbol{x})))^{\frac{1}{2d}}}{k_{\mathrm{B}} T}. \tag{2.6}$$

where $\mathcal{F}_\varepsilon[\boldsymbol{y}]$ is the Helmholtz free energy under the (spatial) local harmonic approximation which was a spatial version of the one studied by [11] and [18], $\mathcal{U}_\varepsilon[\boldsymbol{y}]$ is the potential energy, T is the temperature, $\mathcal{S}_\varepsilon[\boldsymbol{y}]$ is the entropy, k_{B} is the Boltzmann constant, $\hbar$ is the reduced Planck constant, and $\det(\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}](\boldsymbol{x}))$ is the determinant of the local dynamical matrix $\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}](\boldsymbol{x}) \in \mathbb{R}_+^{d\times d}$ for $\boldsymbol{x} \in \Omega_\varepsilon$. In general, we define the dynamical matrix related to atoms $\boldsymbol{x}, \boldsymbol{x}' \in \Omega_\varepsilon$ as follows

$$\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}](\boldsymbol{x}, \boldsymbol{x}') = \varepsilon^{2-d} \frac{\partial^2 \mathcal{U}_\varepsilon[\boldsymbol{y}]}{\partial \boldsymbol{y}(\boldsymbol{x}) \partial \boldsymbol{y}(\boldsymbol{x}')}. \tag{2.7}$$

Here the prefactor ε^{2-d} normalizes the dynamical matrix, and $\mathcal{I}_\varepsilon[\boldsymbol{y}]$ is the free energy of the system per atom due to the normalization factor ε^d. For convenience, we write $\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}](\boldsymbol{x}) = \boldsymbol{H}_\varepsilon^0[\boldsymbol{y}](\boldsymbol{x}, \boldsymbol{x})$ for $\boldsymbol{x} \in \Omega_\varepsilon$ and $\boldsymbol{H}_\varepsilon^0 = \boldsymbol{H}_\varepsilon^0[\boldsymbol{y}]|_{\boldsymbol{y}(\boldsymbol{x}) \equiv \boldsymbol{x}}(\boldsymbol{x})$. We remark that $\boldsymbol{H}_\varepsilon^0$ is constant in $\boldsymbol{x}$ due to the lattice translation invariance.

The Euler–Lagrange equation for the atomistic problem is

$$\mathcal{L}_\varepsilon[\boldsymbol{y}](\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega_\varepsilon, \tag{2.8}$$

where $\mathcal{L}_\varepsilon[\boldsymbol{y}] = \frac{\delta \mathcal{F}_\varepsilon[\boldsymbol{y}]}{\delta \boldsymbol{y}} = \frac{\delta}{\delta y}(\mathcal{U}_\varepsilon[\boldsymbol{y}] - T\mathcal{S}_\varepsilon[\boldsymbol{y}])$.

Now we introduce the continuum model based on the Cauchy–Born rule at finite temperature. To do so, we must set up some appropriate functional spaces. For any $k \in \mathbb{N}_+$ and $p > 0$, we denote by $W^{k,p}(\Omega; \mathbb{R}^d)$ the Sobolev space of mappings $\boldsymbol{v} : \Omega \to \mathbb{R}^d$ such that $\|\boldsymbol{v}\|_{W^{k,p}} < \infty$. In addition, we denote by $W_{\#}^{k,p}(\Omega; \mathbb{R}^d)$ the Sobolev space of functions whose distributional derivatives of order less than k are Ω-periodic and in the space $L^p(\Omega; \mathbb{R}^d)$. For any $p > d$ and $m \in \mathbb{N}$, we define X and Y as follows:

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

Continuum model for simple lattice: The Cauchy–Born elasticity problem is formulated as follows: given $\boldsymbol{f} \in W^{m,p}(\Omega) \cap W_{\#}^{1,p}(\Omega)$ and $\boldsymbol{B} \in \mathbb{R}^{d\times d}$, find $\boldsymbol{u}^*$ such that

$$\boldsymbol{u}^* = \arg \min_{\boldsymbol{u} - \boldsymbol{x} \cdot \boldsymbol{B} \in X} \mathcal{I}_{\mathrm{CB}}[\boldsymbol{u}], \tag{2.9}$$

where

$$\mathcal{I}_{\mathrm{CB}}[\boldsymbol{u}] = \int_\Omega \Big(W_{\mathrm{CB}}(\nabla \boldsymbol{u}(\boldsymbol{x})) - \boldsymbol{f}(\boldsymbol{x}) \cdot \boldsymbol{u}(\boldsymbol{x}) \Big) \, \mathrm{d}\boldsymbol{x}, \tag{2.10}$$

$$W_{\mathrm{CB}}(\boldsymbol{A}) = U_{\mathrm{CB}}(\boldsymbol{A}) - TS_{\mathrm{CB}}(\boldsymbol{A}), \tag{2.11}$$

$$U_{\mathrm{CB}}(\boldsymbol{A})=\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}V(\boldsymbol{s}_1+\boldsymbol{s}_1\cdot\boldsymbol{A},\boldsymbol{s}_2+\boldsymbol{s}_2\cdot\boldsymbol{A}), \tag{2.12}$$

$$S_{\mathrm{CB}}(\boldsymbol{A})=-dk_{\mathrm{B}}\log\frac{\hbar(\det(\boldsymbol{H}^0_{\mathrm{CB}}(\boldsymbol{A})))^{\frac{1}{2d}}}{k_{\mathrm{B}}T}. \tag{2.13}$$

This finite-temperature Cauchy–Born rule was also used for the application to quasi-continuum method in [6] (see also [26]). In these formulas, $\boldsymbol{A}\in\mathbb{R}^{d\times d}$ and

$$\boldsymbol{H}^0_{\mathrm{CB}}(\boldsymbol{A})=\boldsymbol{H}^0_{\varepsilon}[\boldsymbol{y}]|_{\boldsymbol{y}(\boldsymbol{x})\equiv\boldsymbol{x}+\boldsymbol{x}\cdot\boldsymbol{A}}.$$

Here $U_{\mathrm{CB}}(\boldsymbol{A})$ is the potential energy density obtained by the classic Cauchy–Born rule, i.e., Cauchy–Born rule at zero temperature. We remark that $\boldsymbol{H}^0_{\mathrm{CB}}$ can be calculated in principle, whenever V is given. Moreover, it is smooth due to the finite range and smoothness of V.

The Euler–Lagrange equation for the Cauchy–Born elasticity model is

$$\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}](\boldsymbol{x})=\boldsymbol{f}(\boldsymbol{x}),\quad \boldsymbol{x}\in\Omega. \tag{2.14}$$

where

$$\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}](\boldsymbol{x})=-\mathrm{div}\cdot(D_{\boldsymbol{A}}W_{\mathrm{CB}}(\nabla\boldsymbol{u}(\boldsymbol{x}))).$$

Recall that $D_{\boldsymbol{A}}W_{\mathrm{CB}}(\boldsymbol{A})$ denotes differentiation of $W_{\mathrm{CB}}(\boldsymbol{A})$ with respect to $\boldsymbol{A}$. More precisely, $\{D_{\boldsymbol{A}}W_{\mathrm{CB}}(\boldsymbol{A})\}_{\alpha\beta}=\frac{\partial W_{\mathrm{CB}}(\boldsymbol{A})}{\partial A_{\alpha\beta}}$ for $\alpha,\beta=1,\ldots,d$.

2.3. Complex lattice. Let us consider a complex lattice $\tilde{\mathbb{L}}:=\mathbb{L}\cup(\mathbb{L}+\boldsymbol{p}^0)$ where $\mathbb{L}$ is a simple lattice discussed above and the shift vector $\boldsymbol{p}^0\in\Omega$. Without loss of generality, we suppose type A atoms are located at the reference simple lattice $\mathbb{L}$ if there is no deformation. Similar to the simple lattice situation, we denote $\Omega^A_\varepsilon=\Omega_\varepsilon=\Omega\cap\varepsilon\mathbb{L}$, $\Omega^B_\varepsilon=\Omega\cap\varepsilon(\mathbb{L}+\boldsymbol{p}^0)$, and $\tilde{\Omega}_\varepsilon:=\Omega\cap\varepsilon\tilde{\mathbb{L}}$. Once given a force field $\boldsymbol{f}(\boldsymbol{x})$, we are interested in the displacement fields $\boldsymbol{u}^A(\boldsymbol{x})$ and $\boldsymbol{u}^B(\boldsymbol{x})$, $\boldsymbol{x}\in\Omega_\varepsilon$ with $\boldsymbol{y}^A(\boldsymbol{x})=\boldsymbol{x}+\boldsymbol{u}^A(\boldsymbol{x})$ and $\boldsymbol{y}^B(\boldsymbol{x})=\boldsymbol{x}+\boldsymbol{u}^B(\boldsymbol{x})$, $\boldsymbol{x}\in\Omega_\varepsilon$.

Before we discuss the potentials in the complex lattice scenario, we would like to introduce some difference operators. For any function pair $\varphi=(\varphi^A,\varphi^B)$ defined on Ω_ε, we set

$$\mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}}\varphi(\boldsymbol{x})=\varepsilon^{-1}(\varphi^{\kappa}(\boldsymbol{x}+\varepsilon\boldsymbol{s})-\varphi^{\kappa'}(\boldsymbol{x})), \tag{2.15}$$

where $\kappa,\kappa'=A,B$. We remark that $\mathcal{D}^{\kappa\kappa}_{\boldsymbol{s}}\varphi=\mathcal{D}_{\boldsymbol{s}}\varphi^{\kappa}$.

Three-body interactions can be classified into four cases: AAA, BBB, BBA, and AAB. We denote the corresponding three-body potentials as V_3^{AAA}, V_3^{BBB}, V_3^{BBA}, and V_3^{AAB}. Thanks to the translation invariance, we write

$$\begin{aligned}V^{\kappa\kappa'}(\mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}_1}\boldsymbol{y}(\boldsymbol{x}),\mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}_2}\boldsymbol{y}(\boldsymbol{x}))&=V^{\kappa\kappa'}\left(\frac{\boldsymbol{y}^{\kappa}(\boldsymbol{x}+\varepsilon\boldsymbol{s}_1)-\boldsymbol{y}^{\kappa'}(\boldsymbol{x})}{\varepsilon},\frac{\boldsymbol{y}^{\kappa}(\boldsymbol{x}+\varepsilon\boldsymbol{s}_2)-\boldsymbol{y}^{\kappa'}(\boldsymbol{x})}{\varepsilon}\right)\\&:=V_3^{\kappa\kappa\kappa'}\left(\frac{\boldsymbol{y}^{\kappa'}(\boldsymbol{x})}{\varepsilon},\frac{\boldsymbol{y}^{\kappa}(\boldsymbol{x}+\varepsilon\boldsymbol{s}_1)}{\varepsilon},\frac{\boldsymbol{y}^{\kappa}(\boldsymbol{x}+\varepsilon\boldsymbol{s}_2)}{\varepsilon}\right),\end{aligned} \tag{2.16}$$

where $\kappa,\kappa'=A,B$. We remark that V^{AA}, V^{BB}, V^{AB}, and V^{BA} may be different functions. If $\boldsymbol{y}=(\boldsymbol{y}^A,\boldsymbol{y}^B)$ with $\boldsymbol{y}^A,\boldsymbol{y}^B\in X_\varepsilon$, then we simply denote $\boldsymbol{y}\in X_\varepsilon$. In the sequel, the summation $\sum_\kappa$ stands for $\sum_{\kappa=A,B}$ if there is no confusion.

Atomistic Model for Complex Lattice: The atomistic problem is formulated as follows: given $\boldsymbol{f}:\tilde{\Omega}_\varepsilon\to\mathbb{R}^d$ with $\boldsymbol{f}^A(\boldsymbol{x})=\boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{f}^B(\boldsymbol{x})=\boldsymbol{f}(\boldsymbol{x}+\varepsilon\boldsymbol{p}^0)$, $\boldsymbol{x}\in\Omega_\varepsilon$, find $\boldsymbol{y}^*=(\boldsymbol{y}^{A,*},\boldsymbol{y}^{B,*})$ such that

$$\boldsymbol{y}^*=\arg\min_{\boldsymbol{y}^\kappa-\boldsymbol{x}-\boldsymbol{x}\cdot\boldsymbol{B}\in X_\varepsilon,\kappa=A,B}\mathcal{I}_\varepsilon[\boldsymbol{y}], \tag{2.17}$$

with

$$\mathcal{I}_\varepsilon[\boldsymbol{y}]=\mathcal{F}_\varepsilon[\boldsymbol{y}]-\varepsilon^d\sum_{\boldsymbol{x},\kappa}\boldsymbol{f}^\kappa(\boldsymbol{x})\cdot\boldsymbol{y}^\kappa(\boldsymbol{x}), \tag{2.18}$$

$$\mathcal{F}_\varepsilon[\boldsymbol{y}]=\mathcal{U}_\varepsilon[\boldsymbol{y}]-T\mathcal{S}_\varepsilon[\boldsymbol{y}], \tag{2.19}$$

$$\mathcal{U}_\varepsilon[\boldsymbol{y}]=\varepsilon^d\sum_{\boldsymbol{x},\kappa,\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}V^{\kappa\kappa'}_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}](\boldsymbol{x}), \tag{2.20}$$

$$\mathcal{S}_\varepsilon[\boldsymbol{y}]=-\varepsilon^d\sum_{\boldsymbol{x},\kappa}dk_{\mathrm{B}}\log\frac{\hbar(\det\boldsymbol{H}^{0,\kappa}_\varepsilon[\boldsymbol{y}](\boldsymbol{x}))^{\frac{1}{2d}}}{k_{\mathrm{B}}T}. \tag{2.21}$$

Here the three-body potential and its derivatives are denoted as follows

$$V^{\kappa\kappa'}_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}](\boldsymbol{x})=V^{\kappa\kappa'}(\mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}_1}\boldsymbol{y}(\boldsymbol{x}),\mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}_2}\boldsymbol{y}(\boldsymbol{x})), \tag{2.22}$$

$$\boldsymbol{H}^{0,\kappa\kappa'}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}')=\varepsilon^{2-d}\frac{\partial^2\mathcal{U}_\varepsilon[\boldsymbol{y}]}{\partial\boldsymbol{y}^\kappa(\boldsymbol{x})\partial\boldsymbol{y}^{\kappa'}(\boldsymbol{x}')}, \tag{2.23}$$

$$\boldsymbol{H}^{0,\kappa}_\varepsilon[\boldsymbol{y}](\boldsymbol{x})=\boldsymbol{H}^{0,\kappa\kappa}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}), \tag{2.24}$$

where $\boldsymbol{x},\boldsymbol{x}'\in\Omega_\varepsilon$, and $\kappa,\kappa'=A,B$.

The Euler–Lagrange equations for the atomistic problem are

$$\mathcal{L}^\kappa_\varepsilon[\boldsymbol{y}](\boldsymbol{x})=\boldsymbol{f}^\kappa(\boldsymbol{x}),\quad \boldsymbol{x}\in\Omega_\varepsilon,\quad \kappa=A,B, \tag{2.25}$$

where $\mathcal{L}^\kappa_\varepsilon[\boldsymbol{y}]=\frac{\delta\mathcal{F}_\varepsilon[\boldsymbol{y}]}{\delta\boldsymbol{y}^\kappa}=\frac{\delta}{\delta\boldsymbol{y}^\kappa}(\mathcal{U}_\varepsilon[\boldsymbol{y}]-T\mathcal{S}_\varepsilon[\boldsymbol{y}])$, $\kappa=A,B$.

Continuum Model for Complex Lattice: Now we turn to the continuum model based on the finite temperature Cauchy–Born rule. The Cauchy–Born elasticity problem is formulated as follows: given $\boldsymbol{f}\in W^{m,p}(\Omega)\cap W^{1,p}_{\#}(\Omega)$ and $\boldsymbol{B}\in\mathbb{R}^{d\times d}$, find $\boldsymbol{u}^*$ such that

$$\boldsymbol{u}^*=\arg\min_{\boldsymbol{u}-\boldsymbol{x}\cdot\boldsymbol{B}\in X}\mathcal{I}_{\mathrm{CB}}[\boldsymbol{u}], \tag{2.26}$$

where $\mathcal{I}_{\mathrm{CB}}[\boldsymbol{u}]=\int_\Omega(W_{\mathrm{CB}}(\nabla\boldsymbol{u}(\boldsymbol{x}))-\boldsymbol{f}(\boldsymbol{x})\cdot\boldsymbol{u}(\boldsymbol{x}))\,\mathrm{d}\boldsymbol{x}$ has the same expression as (2.10) except the fact that the Helmholtz free energy density W_{CB} is obtained via solving an optimization problem with respect to the shift $\boldsymbol{p}$ which plays a role as the internal degree of freedom:

$$W_{\mathrm{CB}}(\boldsymbol{A})=W(\boldsymbol{A},\boldsymbol{p}(\boldsymbol{A}))=\min_{\boldsymbol{p}\in\Omega}W(\boldsymbol{A},\boldsymbol{p}). \tag{2.27}$$

Since the undeformed lattice structure is stable, it is legitimate to assume that there is a unique $\boldsymbol{p}^0\in\Omega$ such that $\boldsymbol{p}^0=\arg\min_{\boldsymbol{p}\in\Omega}W(\boldsymbol{0},\boldsymbol{p})$. Then for sufficiently small $\boldsymbol{A}$, there exists a unique $\boldsymbol{p}(\boldsymbol{A})$ such that $W_{\mathrm{CB}}(\boldsymbol{A})=W(\boldsymbol{A},\boldsymbol{p}(\boldsymbol{A}))$. In particular, $\boldsymbol{p}^0=\boldsymbol{p}(\boldsymbol{0})$. The existence and uniqueness of this minimization problem for $\boldsymbol{p}(\boldsymbol{A})$ are left to Proposition 6.4. The precise definition of the energy density for complex lattice is as follows:

$$W(\boldsymbol{A},\boldsymbol{p})=U(\boldsymbol{A},\boldsymbol{p})-TS(\boldsymbol{A},\boldsymbol{p}), \tag{2.28}$$

$$U(\boldsymbol{A},\boldsymbol{p}) = U_\varepsilon[\boldsymbol{y}]|_{\boldsymbol{y}^A(\boldsymbol{x})\equiv \boldsymbol{x}+\boldsymbol{x}\cdot\boldsymbol{A},\boldsymbol{y}^B(\boldsymbol{x})\equiv \boldsymbol{y}^A(\boldsymbol{x})+\varepsilon\boldsymbol{p}}, \tag{2.29}$$

$$S(\boldsymbol{A},\boldsymbol{p}) = -\sum_\kappa dk_{\mathrm{B}} \log \frac{\hbar(\det \boldsymbol{H}^{0,\kappa}_{\mathrm{CB}}(\boldsymbol{A},\boldsymbol{p}))^{\frac{1}{2d}}}{k_{\mathrm{B}}T}, \tag{2.30}$$

$$\boldsymbol{H}^{0,\kappa}_{\mathrm{CB}}(\boldsymbol{A},\boldsymbol{p}) = \boldsymbol{H}^{0,\kappa}_\varepsilon[\boldsymbol{y}]|_{\boldsymbol{y}^A(\boldsymbol{x})\equiv \boldsymbol{x}+\boldsymbol{x}\cdot\boldsymbol{A},\boldsymbol{y}^B(\boldsymbol{x})\equiv \boldsymbol{y}^A(\boldsymbol{x})+\varepsilon\boldsymbol{p}}, \quad \kappa = A,B. \tag{2.31}$$

Here $U(\boldsymbol{A},\boldsymbol{p})$ is derived via the classic Cauchy–Born rule at zero temperature and $\boldsymbol{H}^{0,\kappa}_{\mathrm{CB}}(\boldsymbol{A},\boldsymbol{p})$ the dynamical matrix at zero temperature for complex lattices. We also denote

$$U_{\mathrm{CB}}(\boldsymbol{A}) = U(\boldsymbol{A},\boldsymbol{p}(\boldsymbol{A})), \tag{2.32}$$

$$S_{\mathrm{CB}}(\boldsymbol{A}) = S(\boldsymbol{A},\boldsymbol{p}(\boldsymbol{A})). \tag{2.33}$$

The Euler–Lagrange equation for the Cauchy–Born elasticity model still reads as (2.14).

3. Main results

In this section, we state our main results after proposing a key assumption.

We first present the stability assumption in the complex lattice setting. Then its analogue for simple lattice can be obtained automatically as a reduced case. For any $\boldsymbol{\xi}\in\mathbb{L}^*_\varepsilon$, we define the (Fourier-transformed) dynamical matrix at zero temperature

$$\boldsymbol{D}^0(\boldsymbol{\xi}) = \begin{pmatrix} \boldsymbol{D}^{0,AA}(\boldsymbol{\xi}) & \boldsymbol{D}^{0,AB}(\boldsymbol{\xi}) \\ \boldsymbol{D}^{0,BA}(\boldsymbol{\xi}) & \boldsymbol{D}^{0,BB}(\boldsymbol{\xi}) \end{pmatrix} \tag{3.1}$$

$$\boldsymbol{D}^{0,\kappa\kappa'}(\boldsymbol{\xi}) = \varepsilon^d \sum_{\boldsymbol{x}}\sum_{\boldsymbol{x}'} \boldsymbol{H}^{0,\kappa\kappa'}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}')\Big|_{\boldsymbol{y}^A(\boldsymbol{x})\equiv\boldsymbol{x},\boldsymbol{y}^B(\boldsymbol{x})\equiv\boldsymbol{y}^A(\boldsymbol{x})+\varepsilon\boldsymbol{p}^0} \mathrm{e}^{\iota(\boldsymbol{x}'-\boldsymbol{x})\cdot\boldsymbol{\xi}}. \tag{3.2}$$

To avoid confusion, we use ι instead of i to denote the imaginary unit. Let $\{(\omega^0_{\mathrm{a},\alpha}(\boldsymbol{\xi}))^2,(\omega^0_{\mathrm{o},\alpha}(\boldsymbol{\xi}))^2\}$, $\alpha=1,\dots,d$, be the eigenvalues of $\boldsymbol{D}^0(\boldsymbol{\xi})$. Here subscripts 'a' and 'o' stand for acoustic and optic respectively.

Assumption 3.1 (stability for complex lattice at zero temperature). *There exist positive constants* Λ_1 *and* Λ_2 *such that for all* $\boldsymbol{\xi}\in\mathbb{L}^*_\varepsilon$, $\boldsymbol{D}^0(\boldsymbol{\xi})\in\mathbb{R}^{d\times d}_+$ *and* $\omega^0_{a,\alpha}(\boldsymbol{\xi})\geq\Lambda_1\varepsilon\|\boldsymbol{\xi}\|$, $\omega^0_{o,\alpha}(\boldsymbol{\xi})\geq\Lambda_2$, $\alpha=1,\dots,d$.

Note that we have normalized $\boldsymbol{H}$ in its definition. Thus Assumption 3.1 is equivalent to the one proposed in [8] for the convergence analysis of the Cauchy–Born rule at zero temperature. Hence it is the minimal requirement for the stability of the crystalline solid even for the case at zero temperature. We will show that Assumption 3.1 is not only necessary but also sufficient in the sense that it implies the stability of the crystalline solid at finite temperature (c.f. Theorem 3.3). Moreover, Assumption 3.1 is also crucial for the validity of the logarithmic function of the determinant of $\boldsymbol{H}^{0,\kappa}_\varepsilon$.

For completeness, we also present the simple lattice case. For any $\boldsymbol{\xi}\in\mathbb{L}^*_\varepsilon$, the (Fourier-transformed) dynamical matrix at zero temperature reads as

$$\boldsymbol{D}^0(\boldsymbol{\xi}) = \varepsilon^d \sum_{\boldsymbol{x}}\sum_{\boldsymbol{x}'} \boldsymbol{H}^0_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}')\Big|_{\boldsymbol{y}(\boldsymbol{x})\equiv\boldsymbol{x}} \mathrm{e}^{\iota(\boldsymbol{x}'-\boldsymbol{x})\cdot\boldsymbol{\xi}}. \tag{3.3}$$

Let $(\omega^0_\alpha(\boldsymbol{\xi}))^2$, $\alpha=1,\dots,d$, be the eigenvalues of $\boldsymbol{D}^0(\boldsymbol{\xi})$. Then Assumption 3.1 is reduced to the following case:

Assumption 3.2 (stability for simple lattice at zero temperature). *There exists a positive constant* Λ *such that for all* $\boldsymbol{\xi}\in\mathbb{L}^*_\varepsilon$, $\boldsymbol{D}^0(\boldsymbol{\xi})\in\mathbb{R}^{d\times d}_+$ *and* $\omega^0_\alpha(\boldsymbol{\xi})\geq\Lambda_1\varepsilon\|\boldsymbol{\xi}\|$, $\alpha=1,\dots,d$.

In both simple and complex lattices, we introduce the following definitions for local minimizers of the Helmholtz free energy.

DEFINITION 3.1 (minimizer for continuum model). *Given $\boldsymbol{B}\in\mathbb{R}^{d\times d}$, the function $\boldsymbol{u}^*$ with $\boldsymbol{u}^*-\boldsymbol{x}\cdot\boldsymbol{B}\in X$ is a $W^{1,\infty}$ local minimizer of $\mathcal{I}_{\mathrm{CB}}$ if and only if there exists $\delta>0$ such that*

$$\mathcal{I}_{\mathrm{CB}}[\boldsymbol{u}^*]\le\mathcal{I}_{\mathrm{CB}}[\boldsymbol{u}]$$

for all $\boldsymbol{u}-\boldsymbol{x}\cdot\boldsymbol{B}\in X$ satisfying $\|\boldsymbol{u}-\boldsymbol{u}^*\|_{W^{1,\infty}}<\delta$.

DEFINITION 3.2 (minimizer for atomistic model). *Given $\boldsymbol{B}\in\mathbb{R}^{d\times d}$, the function $\boldsymbol{y}^*$ with $\boldsymbol{y}^*-\boldsymbol{x}-\boldsymbol{x}\cdot\boldsymbol{B}\in X_\varepsilon$ is a discrete $W^{1,\infty}$ local minimizer of $\mathcal{I}_\varepsilon$ if and only if there exists $\delta>0$ such that*

$$\mathcal{I}_\varepsilon[\boldsymbol{y}^*]\le\mathcal{I}_\varepsilon[\boldsymbol{y}]$$

for all $\boldsymbol{y}-\boldsymbol{x}-\boldsymbol{x}\cdot\boldsymbol{B}\in X_\varepsilon$ satisfying $\|\boldsymbol{y}-\boldsymbol{y}^*\|_{W^{1,\infty}_\varepsilon}\le\delta$.

The main results of this paper are as follows.

THEOREM 3.1 (existence, continuum model). *If Assumption 3.1 (or Assumption 3.2 for simple lattice) holds and $p>d$, $m\ge0$, then there exist positive constants κ_1, κ_2, κ_3, and T^* such that for any $\boldsymbol{B}\in\mathbb{R}^{d\times d}$ with $\|\boldsymbol{B}\|_{\mathrm{F}}\le\kappa_1$, $f\in W^{m,p}(\Omega)\cap W^{1,p}_{\#}(\Omega)$ with $\|\boldsymbol{f}\|_{W^{m,p}}\le\kappa_2$, and $0<T<T^*$, the problem (2.14) for complex lattice (or simple lattice) has one and only one solution u_{CB} that satisfies $\|\boldsymbol{u}_{\mathrm{CB}}-\boldsymbol{x}\cdot\boldsymbol{B}\|_{W^{m+2,p}}\le\kappa_3$, and $\boldsymbol{u}_{\mathrm{CB}}$ is a $W^{1,\infty}$ local minimizer of the total energy functional (2.10) for complex lattice (or simple lattice).*

THEOREM 3.2 (existence and convergence, atomistic model). *If Assumption 3.1 holds, $p>d$, and that m is sufficiently large, then there exist positive constants κ_1, κ_2, T^*, and ε_0 such that for any $\boldsymbol{B}\in\mathbb{R}^{d\times d}$ with $\|\boldsymbol{B}\|_{\mathrm{F}}\le\kappa_1$, $\boldsymbol{f}\in W^{m,p}(\Omega)\cap W^{1,p}_{\#}(\Omega)$ with $\|\boldsymbol{f}\|_{W^{m,p}}\le\kappa_2$, $0<T<T^*$, and $0<\varepsilon<\varepsilon_0$, the problem (2.25) for complex lattice (or (2.8) for simple lattice) has one and only one solution $\boldsymbol{y}_\varepsilon$, and $\boldsymbol{y}_\varepsilon$ is a discrete $W^{1,\infty}$ local minimizer of the energy functional (2.18) for complex lattice (or (2.3) for simple lattice). Moreover, $\boldsymbol{y}_\varepsilon$ satisfies*

$$\|\boldsymbol{y}_\varepsilon-\boldsymbol{y}_{\mathrm{CB}}\|_{\mathrm{d}}\le C\varepsilon, \tag{3.4}$$

where $\boldsymbol{y}_{\mathrm{CB}}=\boldsymbol{x}+\boldsymbol{u}_{\mathrm{CB}}$ and the norm $\|\cdot\|_{\mathrm{d}}$ is defined as

$$\|\boldsymbol{z}\|_{\mathrm{d}}:=\varepsilon^{d/2-1}(\boldsymbol{z}\cdot\boldsymbol{H}^0_\varepsilon\boldsymbol{z})^{1/2}, \tag{3.5}$$

for any $\boldsymbol{z}=(\boldsymbol{z}^A,\boldsymbol{z}^B)$ defined on Ω_ε. Here $\boldsymbol{H}^0_\varepsilon=\boldsymbol{H}^0_\varepsilon[\boldsymbol{y}]|_{\boldsymbol{y}(\boldsymbol{x})=\boldsymbol{x}}(\boldsymbol{x})$ is constant in $\boldsymbol{x}$. In particular, if the lattice is simple, then the error estimate (3.4) can be improved as follows:

$$\|\boldsymbol{y}_\varepsilon-\boldsymbol{y}_{\mathrm{CB}}\|_{\mathrm{d}}\le C\varepsilon^2. \tag{3.6}$$

We remark that the constants C in (3.4) and (3.6) depend on the temperature T^*.

To prove these theorems, we require three key ingredients: consistency, stability, and a fixed-point argument. Among those, we emphasize the stability result which states the stability of the undeformed lattice structure at zero temperature implies the

stability of the slightly deformed configuration at low but finite temperature. To be precise, we have the following theorem.

THEOREM 3.3 (stability for the crystalline solid at finite temperature). *Suppose that Assumption 3.1 (or Assumption 3.2 for simple lattice) holds. Then there exist positive constants* κ_1, δ, T^*, *and* ε_0 *such that for any* $\boldsymbol{B}\in\mathbb{R}^{d\times d}$ *with* $\|\boldsymbol{B}\|_{\mathrm{F}}\le\kappa_1$, $0<T<T^*$, $0<\varepsilon<\varepsilon_0$, *and* $\boldsymbol{y}$ *defined on* Ω_ε *with* $\|\boldsymbol{y}-\boldsymbol{x}-\boldsymbol{x}\cdot\boldsymbol{B}\|_{W^{1,\infty}_\varepsilon}\le\delta$, *we have*

$$\boldsymbol{z}\cdot\boldsymbol{H}^T_\varepsilon[\boldsymbol{y}]\boldsymbol{z}\ge C\|\boldsymbol{z}\|^2_{\mathrm{d}}, \tag{3.7}$$

where for simple lattice $\boldsymbol{H}^T_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}'):=\varepsilon^{2-d}\frac{\partial^2\mathcal{F}_\varepsilon}{\partial\boldsymbol{y}(\boldsymbol{x})\partial\boldsymbol{y}(\boldsymbol{x}')}$ *and* $\boldsymbol{z}\cdot\boldsymbol{H}^T_\varepsilon[\boldsymbol{y}]\boldsymbol{z}=\sum_{\boldsymbol{x},\boldsymbol{x}'}\boldsymbol{z}(\boldsymbol{x})\cdot\boldsymbol{H}^T_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}')\boldsymbol{z}(\boldsymbol{x}')$; *for complex lattice* $\boldsymbol{H}^{T,\kappa\kappa'}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}'):=\varepsilon^{2-d}\frac{\partial^2\mathcal{F}_\varepsilon}{\partial\boldsymbol{y}^\kappa(\boldsymbol{x})\partial\boldsymbol{y}^{\kappa'}(\boldsymbol{x}')}$ *and* $\boldsymbol{z}\cdot\boldsymbol{H}^T_\varepsilon[\boldsymbol{y}]\boldsymbol{z}=\sum_{\boldsymbol{x},\boldsymbol{x}',\kappa,\kappa'}\boldsymbol{z}^\kappa(\boldsymbol{x})\cdot\boldsymbol{H}^{T,\kappa\kappa'}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}')\boldsymbol{z}^{\kappa'}(\boldsymbol{x}')$.

The remainder of this paper is organized as follows. In Section 4, we derive explicit formulas for quantities related to the Cauchy–Born rule at finite temperature. In Section 5, we prove the existence of the local minimizer for the continuum model and establish the stability of the crystalline solid at finite temperature. Finally, in Section 6, the convergence as well as the existence for atomisitic model is proved based on a detailed asymptotic analysis.

4. Preliminaries

In this section, explicit expressions are derived for $\boldsymbol{H}^0_{\mathrm{CB}}(\boldsymbol{A})$ and $\boldsymbol{H}^{0,\kappa}_{\mathrm{CB}}(\boldsymbol{A},\boldsymbol{p})$ which are crucial in defining the entropy of the continuum model via finite-temperature Cauchy–Born rule. Based on these formulas, we then obtain explicit expressions of operator $\mathcal{L}_{\mathrm{CB}}$ which are helpful for the asymptotic analysis in the next section.

To simplify the notation, we define $K(\boldsymbol{M})=\log\det(\boldsymbol{M})$, $\boldsymbol{M}\in\mathbb{R}^{d\times d}_+$. Then the atomistic entropy and the Helmholtz free energy read as

$$\begin{aligned}\mathcal{S}_\varepsilon[\boldsymbol{y}]&=-\varepsilon^d\sum_{\boldsymbol{x}}dk_{\mathrm{B}}\log\frac{\hbar(\det\boldsymbol{H}^0_\varepsilon[\boldsymbol{y}])^{\frac{1}{2d}}}{k_{\mathrm{B}}T}\\&=-\varepsilon^d\sum_{\boldsymbol{x}}\frac{1}{2}k_{\mathrm{B}}K(\boldsymbol{H}^0_\varepsilon[\boldsymbol{y}])-dk_{\mathrm{B}}\log\frac{\hbar}{k_{\mathrm{B}}T},\end{aligned} \tag{4.1}$$

$$\mathcal{F}_\varepsilon[\boldsymbol{y}]=\varepsilon^d\sum_{\boldsymbol{x}}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}V_{\boldsymbol{s}_1,\boldsymbol{s}_2}+\varepsilon^d\sum_{\boldsymbol{x}}\frac{1}{2}k_{\mathrm{B}}TK(\boldsymbol{H}^0_\varepsilon)+dk_{\mathrm{B}}T\log\frac{\hbar}{k_{\mathrm{B}}T}. \tag{4.2}$$

Similarly, the continnum Helmholtz free energy density reads as

$$W_{\mathrm{CB}}(\boldsymbol{A})=\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}V+\frac{1}{2}k_{\mathrm{B}}TK+dk_{\mathrm{B}}T\log\frac{\hbar}{k_{\mathrm{B}}T}. \tag{4.3}$$

Here and in the sequel, V is evaluated as follows

$$V=V(\boldsymbol{s}_1+\boldsymbol{s}_1\cdot\boldsymbol{A},\boldsymbol{s}_2+\boldsymbol{s}_2\cdot\boldsymbol{A}). \tag{4.4}$$

Similarly, we use the abbreviations

$$\boldsymbol{H}^0_{\mathrm{CB}}=\boldsymbol{H}^0_{\mathrm{CB}}(\boldsymbol{A}),\quad K=K(\boldsymbol{H}^0_{\mathrm{CB}}(\boldsymbol{A})). \tag{4.5}$$

In order to connect the atomistic model with the continuum model, we explicitly express macroscopic quantities $\boldsymbol{H}^0_{\mathrm{CB}}(\boldsymbol{A})$ and $\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}]$ in terms of the microscopic potential V. Let us start this with simple lattice.

LEMMA 4.1. *For simple lattice, the explicit expressions for* $\boldsymbol{H}^0_\varepsilon$ *and* $\boldsymbol{H}^0_{\mathrm{CB}}$ *are as follows:*

$$\boldsymbol{H}^0_\varepsilon[\boldsymbol{y}] = \sum_{\boldsymbol{s}_1,\boldsymbol{s}_2} \frac{1}{2}\Big[(\partial_1+\partial_2)^2 V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}] + \sum_{j=1}^{2} \partial_j^2 V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]\Big], \tag{4.6}$$

$$\boldsymbol{H}^0_{\mathrm{CB}}(\boldsymbol{A}) = \sum_{\boldsymbol{s}_1,\boldsymbol{s}_2} \Big(\partial_1^2 + \frac{1}{2}\partial_1\partial_2 + \frac{1}{2}\partial_2\partial_1 + \partial_2^2\Big)V. \tag{4.7}$$

We remark that $\partial_1\partial_2 V \neq \partial_2\partial_1 V$ and hence (4.7) can not be written as $\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}(\partial_1^2 + \partial_{12} + \partial_2^2)V$.

Proof. Equation (4.6) can be obtained by direct calculations. Therefore, we have

$$\boldsymbol{H}^0_{\mathrm{CB}}(\boldsymbol{A}) = \sum_{\boldsymbol{s}_1,\boldsymbol{s}_2} \frac{1}{2}\Big[(\partial_1+\partial_2)^2 V + \sum_{j=1}^{2}\partial_j^2 V\Big] = \sum_{\boldsymbol{s}_1,\boldsymbol{s}_2} \Big(\partial_1^2 + \frac{1}{2}\partial_1\partial_2 + \frac{1}{2}\partial_2\partial_1 + \partial_2^2\Big)V.$$

∎

PROPOSITION 4.1. *For simple lattice, we have the explicit expression for* $\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}]$*:*

$$\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}] = -\mathrm{div}\cdot\Bigg\{\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\Big[\partial_i V + k_{\mathrm{B}}T D_{\boldsymbol{M}} K : \Big(\partial_1^2 + \frac{1}{2}\partial_1\partial_2 + \frac{1}{2}\partial_2\partial_1 + \partial_2^2\Big)\partial_i V\Big]\otimes \boldsymbol{s}_i\Bigg\}, \tag{4.8}$$

where $V = V(\boldsymbol{s}_1 + \boldsymbol{s}_1\cdot\nabla\boldsymbol{u}, \boldsymbol{s}_2 + \boldsymbol{s}_2\cdot\nabla\boldsymbol{u})$ *and* $K = K(\boldsymbol{H}^0_{\mathrm{CB}}(\nabla\boldsymbol{u}))$.

Proof. Taking variation of the continuum energy, we have

$$\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}] = -\mathrm{div}\cdot\Big(D_{\boldsymbol{A}} W_{\mathrm{CB}}(\nabla\boldsymbol{u})\Big) = -\mathrm{div}\cdot\Big[D_{\boldsymbol{A}}\Big(\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}V\Big) + \frac{1}{2}k_{\mathrm{B}}T D_{\boldsymbol{A}} K\Big],$$

Note that $D_{\boldsymbol{A}} V = \sum_{i=1}^{2}\partial_i V\otimes\boldsymbol{s}_i$. This with Lemma 4.1 leads to

$$D_{\boldsymbol{A}}\boldsymbol{H}^0_{\mathrm{CB}} = \sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\Big(\partial_1^2 + \frac{1}{2}\partial_1\partial_2 + \frac{1}{2}\partial_2\partial_1 + \partial_2^2\Big)\partial_i V\otimes\boldsymbol{s}_i,$$

$$D_{\boldsymbol{A}} K = D_{\boldsymbol{M}} K : \Bigg[\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\Big(\partial_1^2 + \frac{1}{2}\partial_1\partial_2 + \frac{1}{2}\partial_2\partial_1 + \partial_2^2\Big)\partial_i V\otimes\boldsymbol{s}_i\Bigg].$$

Then Equation (4.8) follows from this. ∎

Now we consider the complex lattice. We denote the partial derivative $\partial_j V^{\kappa\kappa'}_{\boldsymbol{s}_1,\boldsymbol{s}_2} = \partial_{\boldsymbol{r}_j} V^{\kappa\kappa'}_{\boldsymbol{s}_1,\boldsymbol{s}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)$ at $\boldsymbol{r}_1 = \mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}_1}\boldsymbol{y}$, $\boldsymbol{r}_2 = \mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}_2}\boldsymbol{y}$ for $j=1,2$, $\kappa,\kappa' = A,B$. Higher order derivatives will be denoted in a similar way. Then the atomistic entropy and the Helmholtz free energy read as

$$\mathcal{F}_\varepsilon[\boldsymbol{y}] = \varepsilon^d \sum_{\boldsymbol{x},\kappa,\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}V^{\kappa\kappa'}_{\boldsymbol{s}_1,\boldsymbol{s}_2} + \varepsilon^d\sum_{\boldsymbol{x},\kappa}\frac{1}{2}k_{\mathrm{B}}TK(\boldsymbol{H}^{0,\kappa}_\varepsilon) + 2dk_{\mathrm{B}}T\log\frac{\hbar}{k_{\mathrm{B}}T}. \tag{4.9}$$

Similarly, the continnum Helmholtz free energy density is given by

$$W(\boldsymbol{A},\boldsymbol{p}) = \sum_{\kappa,\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}V^{\kappa\kappa'} + \sum_{\kappa}\frac{1}{2}k_{\mathrm{B}}TK(\boldsymbol{H}^{0,\kappa}_{\mathrm{CB}}) + 2dk_{\mathrm{B}}T\log\frac{\hbar}{k_{\mathrm{B}}T}. \tag{4.10}$$

Here and in the sequel, $V^{\kappa\kappa}$, V^{BA}, and V^{AB} are evaluated as follows

$$V^{\kappa\kappa} = V^{\kappa\kappa}(\boldsymbol{s}_1 + \boldsymbol{s}_1 \cdot \boldsymbol{A}, \boldsymbol{s}_2 + \boldsymbol{s}_2 \cdot \boldsymbol{A}), \quad \kappa = A, B, \tag{4.11}$$

$$V^{BA} = V^{BA}(\boldsymbol{s}_1 + \boldsymbol{s}_1 \cdot \boldsymbol{A} + \boldsymbol{p} \cdot \boldsymbol{A}, \boldsymbol{s}_2 + \boldsymbol{s}_2 \cdot \boldsymbol{A} + \boldsymbol{p} \cdot \boldsymbol{A}), \tag{4.12}$$

$$V^{AB} = V^{AB}(\boldsymbol{s}_1 + \boldsymbol{s}_1 \cdot \boldsymbol{A} - \boldsymbol{p} \cdot \boldsymbol{A}, \boldsymbol{s}_2 + \boldsymbol{s}_2 \cdot \boldsymbol{A} - \boldsymbol{p} \cdot \boldsymbol{A}). \tag{4.13}$$

Similarly, we use the abbreviations

$$\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa} = \boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}(\boldsymbol{A}), \quad K = K(\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}(\boldsymbol{A})), \quad \kappa = A, B. \tag{4.14}$$

LEMMA 4.2. *For complex lattice, the explicit expressions for $\boldsymbol{H}_{\varepsilon}^{0,\kappa}$ and $\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}$ are as follows:*

$$\boldsymbol{H}_{\varepsilon}^{0,\kappa}[\boldsymbol{y}] = \sum_{\kappa'} \sum_{\boldsymbol{s}_1, \boldsymbol{s}_2} \frac{1}{2} \Big[(\partial_1 + \partial_2)^2 V_{\boldsymbol{s}_1, \boldsymbol{s}_2}^{\kappa' \kappa}[\boldsymbol{y}] + \sum_{j=1}^{2} \partial_j^2 V_{\boldsymbol{s}_1, \boldsymbol{s}_2}^{\kappa\kappa'}[\mathcal{T}_{-\boldsymbol{s}_j} \boldsymbol{y}] \Big], \quad \kappa = A, B, \tag{4.15}$$

$$\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}(\boldsymbol{A}, \boldsymbol{p}) = \sum_{\kappa'} \sum_{\boldsymbol{s}_1, \boldsymbol{s}_2} \frac{1}{2} \Big[(\partial_1 + \partial_2)^2 V^{\kappa' \kappa} + (\partial_1^2 + \partial_2^2) V^{\kappa\kappa'} \Big], \quad \kappa, \kappa' = A, B. \tag{4.16}$$

More explicitly, we have

$$\boldsymbol{H}_{\mathrm{CB}}^{0,A}(\boldsymbol{A}, \boldsymbol{p}) = \sum_{\boldsymbol{s}_1, \boldsymbol{s}_2} \Big(\partial_1^2 + \frac{1}{2} \partial_1 \partial_2 + \frac{1}{2} \partial_2 \partial_1 + \partial_2^2 \Big) V^{AA} + \frac{1}{2} (\partial_1 + \partial_2)^2 V^{BA} + \frac{1}{2} (\partial_1^2 + \partial_2^2) V^{AB}, \tag{4.17}$$

$$\boldsymbol{H}_{\mathrm{CB}}^{0,B}(\boldsymbol{A}, \boldsymbol{p}) = \sum_{\boldsymbol{s}_1, \boldsymbol{s}_2} \Big(\partial_1^2 + \frac{1}{2} \partial_1 \partial_2 + \frac{1}{2} \partial_2 \partial_1 + \partial_2^2 \Big) V^{BB} + \frac{1}{2} (\partial_1 + \partial_2)^2 V^{AB} + \frac{1}{2} (\partial_1^2 + \partial_2^2) V^{BA}. \tag{4.18}$$

Proof. These expressions can be obtained by direct calculations. ∎

PROPOSITION 4.2. *For complex lattice, we have the explicit expression for $\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}]$:*

$$\begin{aligned} \mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}] = -\mathrm{div} \cdot \Bigg\{ \sum_{\kappa, \kappa'} \sum_{\boldsymbol{s}_1, \boldsymbol{s}_2} \sum_{i=1}^{2} \frac{1}{2} \Bigg[\partial_i V^{\kappa\kappa'} + \frac{1}{2} k_{\mathrm{B}} T D_{\boldsymbol{M}} K \\ : \Big((\partial_1 + \partial_2)^2 \partial_i V^{\kappa' \kappa} + (\partial_1^2 + \partial_2^2) \partial_i V^{\kappa\kappa'} \Big) \Bigg] \otimes \boldsymbol{s}_i \Bigg\}, \end{aligned} \tag{4.19}$$

where $V^{\kappa\kappa} = V^{\kappa\kappa}(\boldsymbol{s}_1 + \boldsymbol{s}_1 \cdot \nabla \boldsymbol{u}, \boldsymbol{s}_2 + \boldsymbol{s}_2 \cdot \nabla \boldsymbol{u})$, $\kappa = A, B$, $V^{BA} = V^{BA}(\boldsymbol{s}_1 + \boldsymbol{s}_1 \cdot \nabla \boldsymbol{u} + \boldsymbol{p}(\nabla \boldsymbol{u}) \cdot \nabla \boldsymbol{u}, \boldsymbol{s}_2 + \boldsymbol{s}_2 \cdot \nabla \boldsymbol{u} + \boldsymbol{p}(\nabla \boldsymbol{u}) \cdot \nabla \boldsymbol{u})$, $V^{AB} = V^{AB}(\boldsymbol{s}_1 + \boldsymbol{s}_1 \cdot \nabla \boldsymbol{u} - \boldsymbol{p}(\nabla \boldsymbol{u}) \cdot \nabla \boldsymbol{u}, \boldsymbol{s}_2 + \boldsymbol{s}_2 \cdot \nabla \boldsymbol{u} - \boldsymbol{p}(\nabla \boldsymbol{u}) \cdot \nabla \boldsymbol{u})$, *and* $K = K(\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}(\nabla \boldsymbol{u}))$.

Proof. Taking variation of the continuum energy, we have

$$\begin{aligned} \mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}] &= -\mathrm{div} \cdot \Big(D_{\boldsymbol{A}} W_{\mathrm{CB}}(\nabla \boldsymbol{u}) \Big) \\ &= -\mathrm{div} \cdot \Bigg[\sum_{\kappa, \kappa'} D_{\boldsymbol{A}} \Big(\sum_{\boldsymbol{s}_1, \boldsymbol{s}_2} \frac{1}{2} V^{\kappa\kappa'} \Big) + \frac{1}{2} k_{\mathrm{B}} T \sum_{\kappa} D_{\boldsymbol{A}} K(\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}) \Bigg]. \end{aligned}$$

Note that $D_{\boldsymbol{A}}V^{\kappa\kappa'}=\sum_{i=1}^{2}\partial_i V^{\kappa\kappa'}\otimes\boldsymbol{s}_i$. This with Lemma 4.2 leads to

$$D_{\boldsymbol{A}}\boldsymbol{H}^{0,\kappa}_{\mathrm{CB}}=\sum_{\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\Big[(\partial_1+\partial_2)^2\partial_i V^{\kappa'\kappa}+(\partial_1^2+\partial_2^2)\partial_i V^{\kappa\kappa'}\Big]\otimes\boldsymbol{s}_i,$$

$$D_{\boldsymbol{A}}K(\boldsymbol{H}^{0,\kappa}_{\mathrm{CB}})=D_{\boldsymbol{M}}K:\left\{\sum_{\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\Big[(\partial_1+\partial_2)^2\partial_i V^{\kappa'\kappa}+(\partial_1^2+\partial_2^2)\partial_i V^{\kappa\kappa'}\Big]\otimes\boldsymbol{s}_i\right\}.$$

Then Equation (4.19) follows from this. ∎

REMARK 4.1. Using our formulation, the expressions, in Lemma 4.2 and Proposition 4.2 can be straightforwardly extended to multi-species complex lattice.

5. Local minimizer for the continuum model; stability at finite temperature

In this section, we first show the existence of the solution to the continuum model. Basically, this is a standard perturbation argument. The new ingredient here is that we allow the perturbation in the form of an additive term TS_{CB}. More interestingly, the proof actually implies an estimate of the critical temperature at which the crystalline solid is unstable in the sense that various instabilities may occur.

Now we rephrase a well-known lemma, which provides us an equivalent statement of the stability condition (for the complex lattice case) to be used in the proof of Theorem 3.1.

LEMMA 5.1 (Lemma 3.1 in [8]). *If Assumption 3.1 is valid, then $U(\boldsymbol{A},\boldsymbol{p})$ satisfies the generalized Legendre–Hadamard condition at the undeformed configuration $(\boldsymbol{0},\boldsymbol{p}^{\boldsymbol{0}})$: there exist two constants C_1 and C_2, independent of ε, such that for all $\boldsymbol{\xi},\boldsymbol{\eta},\boldsymbol{\zeta}\in\mathbb{R}^d$,*

$$(\boldsymbol{\xi}\otimes\boldsymbol{\eta},\boldsymbol{\zeta})\begin{pmatrix}D^2_{\boldsymbol{A}}U(\boldsymbol{0},\boldsymbol{p}^{\boldsymbol{0}}) & D_{\boldsymbol{A}\boldsymbol{p}}U(\boldsymbol{0},\boldsymbol{p}^{\boldsymbol{0}})\\ D_{\boldsymbol{p}\boldsymbol{A}}U(\boldsymbol{0},\boldsymbol{p}^{\boldsymbol{0}}) & D^2_{\boldsymbol{p}}U(\boldsymbol{0},\boldsymbol{p}^{\boldsymbol{0}})\end{pmatrix}\begin{pmatrix}\boldsymbol{\xi}\otimes\boldsymbol{\eta}\\ \boldsymbol{\zeta}\end{pmatrix}\geq C_1\|\boldsymbol{\xi}\|^2\|\boldsymbol{\eta}\|^2+C_2\|\boldsymbol{\zeta}\|^2,\tag{5.1}$$

or equivalently, $U(\boldsymbol{A},\boldsymbol{p})$ satisfies the following conditions

- *$D^2_{\boldsymbol{p}}U(\boldsymbol{0},\boldsymbol{p}^{\boldsymbol{0}})$ is positive definite*
- *U_{CB} satisfies the Legendre–Hadamard condition at the undeformed configuration:*

$$D^2_{\boldsymbol{A}}U_{\mathrm{CB}}(\boldsymbol{0})(\boldsymbol{\xi}\otimes\eta,\boldsymbol{\xi}\otimes\boldsymbol{\eta})\geq\Lambda\|\boldsymbol{\xi}\|^2\|\boldsymbol{\eta}\|^2\quad\text{for all}\quad\boldsymbol{\xi},\boldsymbol{\eta}\in\mathbb{R}^d.\tag{5.2}$$

Proof. **(Proof of Theorem 3.1.)** First, we derive the linearized operator of $\mathcal{L}_{\mathrm{CB}}$ at u:

$$\begin{aligned}\frac{\delta\mathcal{L}_{\mathrm{CB}}}{\delta\boldsymbol{u}}[\boldsymbol{u}]\boldsymbol{v}&=-\mathrm{div}\cdot(D^2_{\boldsymbol{A}}W_{\mathrm{CB}}(\nabla\boldsymbol{u}):\nabla\boldsymbol{v})\\&=-\mathrm{div}\cdot\Big[D^2_{\boldsymbol{A}}\Big(U_{\mathrm{CB}}(\nabla\boldsymbol{u})-TS_{\mathrm{CB}}(\nabla\boldsymbol{u})\Big):\nabla\boldsymbol{v}\Big],\end{aligned}\tag{5.3}$$

where $\boldsymbol{v}\in W^{1,p}_{\#}(\Omega;\mathbb{R}^d)$ and $\boldsymbol{u}-\boldsymbol{x}\cdot\boldsymbol{B}\in X$ for some given $\boldsymbol{B}\in\mathbb{R}^{d\times d}$.

For any $p>d$, we define the map $\boldsymbol{z}:X\times Y\times\mathbb{R}\to\mathbb{R}^d$ as follows:

$$\begin{aligned}\boldsymbol{z}(\boldsymbol{v},\boldsymbol{f},T)&:=\mathcal{L}_{\mathrm{CB}}[\boldsymbol{v}+\boldsymbol{x}\cdot\boldsymbol{B}]-\boldsymbol{f}\\&=-\mathrm{div}\cdot(D_{\boldsymbol{A}}U_{\mathrm{CB}}(\nabla\boldsymbol{v}))+T\mathrm{div}\cdot(D_{\boldsymbol{A}}S_{\mathrm{CB}}(\nabla\boldsymbol{v}))-\boldsymbol{f}.\end{aligned}\tag{5.4}$$

By Lemma 5.1, we have

$$\int_\Omega \nabla \boldsymbol{v} : D_{\boldsymbol{A}}^2 U_{\mathrm{CB}}(\mathbf{0}) : \nabla \boldsymbol{v}\,\mathrm{d}\boldsymbol{x} \geq \Lambda \|\nabla \boldsymbol{v}\|_{L^2}^2 \geq C_1 \|\boldsymbol{v}\|_{H^1}^2. \tag{5.5}$$

where Λ comes from the Legendre–Hadamard condition in Lemma 5.1 and the second step is due to Poincaré's inequality. For $\kappa_1 \geq 0$, set

$$M_1(\kappa_1) := \sup_{\|\boldsymbol{A}\|_{\mathrm{F}} \leq \kappa_1} \|D_{\boldsymbol{A}}^3 U_{\mathrm{CB}}(\boldsymbol{A})\|_2 = \sup_{\|\boldsymbol{A}\|_{\mathrm{F}} \leq \kappa_1} \left(\sum_{\alpha,\beta,\gamma,\delta,\eta,\lambda=1}^{d} \left(\frac{\partial^3 U_{\mathrm{CB}}(\boldsymbol{A})}{\partial A_{\alpha\beta} \partial A_{\gamma\delta} \partial A_{\eta\lambda}} \right)^2 \right)^{1/2}, \tag{5.6}$$

$$M_2(\kappa_1) := \sup_{\|\boldsymbol{A}\|_{\mathrm{F}} \leq \kappa_1} \|D_{\boldsymbol{A}}^2 S_{\mathrm{CB}}(\boldsymbol{A})\|_\infty = \sup_{\|\boldsymbol{A}\|_{\mathrm{F}} \leq \kappa_1} \max_{\alpha,\beta,\gamma,\delta} \left| \frac{\partial^2 S_{\mathrm{CB}}(\boldsymbol{A})}{\partial A_{\alpha\beta} \partial A_{\gamma\delta}} \right|. \tag{5.7}$$

Note that $M_1(\kappa_1)$ and $M_2(\kappa_1)$ are continuous and decreasing as $\kappa_1 \to 0^+$. In particular, $\lim_{\kappa_1 \to 0^+} M_1(\kappa_1) = M_1(0) = \|D_{\boldsymbol{A}}^3 U_{\mathrm{CB}}(\mathbf{0})\|_2$ and $\lim_{\kappa_1 \to 0^+} M_2(\kappa_1) = M_2(0) = \|D_{\boldsymbol{A}}^2 S_{\mathrm{CB}}(\mathbf{0})\|_\infty$. Thus for $\|\boldsymbol{B}\|_{\mathrm{F}} \leq \kappa_1$,

$$\|D_{\boldsymbol{A}}^2 U_{\mathrm{CB}}(\boldsymbol{B}) - D_{\boldsymbol{A}}^2 U_{\mathrm{CB}}(\mathbf{0})\|_\infty \leq M_1(\kappa_1) \|\boldsymbol{B}\|_{\mathrm{F}}. \tag{5.8}$$

Note that $W_{\mathrm{CB}} = U_{\mathrm{CB}}$ for $T = 0$. Therefore

$$\int_\Omega \nabla \boldsymbol{v} : D_{\boldsymbol{A}}^2 \Big(U_{\mathrm{CB}}(\boldsymbol{B}) - T S_{\mathrm{CB}}(\boldsymbol{B}) \Big) : \nabla \boldsymbol{v}\,\mathrm{d}\boldsymbol{x} \geq (C_1 - M_1(\kappa_1)\|\boldsymbol{B}\|_{\mathrm{F}} - M_2(\kappa_1) T) \|\boldsymbol{v}\|_{H^1}^2 \geq (C_1/2) \|\boldsymbol{v}\|_{H^1}^2 \tag{5.9}$$

for $\|\boldsymbol{B}\|_{\mathrm{F}} \leq \kappa_1$ and $0 \leq T < T_0$ with some positive constants κ_1 and T_0.

Next, we fix $\boldsymbol{B}$ and T with $\|\boldsymbol{B}\|_{\mathrm{F}} \leq \kappa_1$ and $0 < T < T_0$. Note that $\mathrm{div} \cdot (D_{\boldsymbol{A}} S_{\mathrm{CB}}(\mathbf{0})) = \mathbf{0}$ in the explicit expressions in Propositions 4.1 and 4.2. This implies that $\boldsymbol{z}(\mathbf{0}, \mathbf{0}, T) = \mathbf{0}$. By implicit function theorem, there exist positive constants κ_2 and κ_3 such that for $\|\boldsymbol{f}\|_{W^{m,p}} \leq \kappa_2$ there is a unique solution $\boldsymbol{v}(\boldsymbol{f}) \in X$ that

$$\boldsymbol{z}(\boldsymbol{v}(\boldsymbol{f}), \boldsymbol{f}, T) = \mathbf{0}, \quad \|\boldsymbol{v}(\boldsymbol{f})\|_{W^{m+2,p}} \leq \kappa_3, \tag{5.10}$$

and $\boldsymbol{v}(\mathbf{0}) = \mathbf{0}$. Now we fix f with $\|\boldsymbol{f}\|_{W^{m,p}} \leq \kappa_2$. Denote $\boldsymbol{u}_{\mathrm{CB}} = \boldsymbol{v}(\boldsymbol{f})$. Thus, we have $\boldsymbol{u}_{\mathrm{CB}}$ solves (2.14) and $\|\boldsymbol{u}_{\mathrm{CB}} - \boldsymbol{x} \cdot \boldsymbol{B}\|_{W^{m+2,p}} \leq \kappa_3$.

Finally, we show that $\boldsymbol{u}_{\mathrm{CB}}$ is a $W^{1,\infty}$ local minimizer of (2.10). For any $\boldsymbol{v}$ with $\boldsymbol{v} - \boldsymbol{x} \cdot \boldsymbol{B} \in X$, the Taylor expansion leads to

$$\mathcal{I}[\boldsymbol{v}] - \mathcal{I}[\boldsymbol{u}_{\mathrm{CB}}] = \int_\Omega \nabla(\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}) : \left(\int_0^1 (1-t) D_{\boldsymbol{A}}^2 W_{\mathrm{CB}}(\nabla \boldsymbol{w}(t))\,\mathrm{d}t \right) : \nabla(\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}})\,\mathrm{d}\boldsymbol{x}. \tag{5.11}$$

where $\boldsymbol{w}(t) = t\boldsymbol{v} + (1-t)\boldsymbol{u}_{\mathrm{CB}}$. It is easy to see that $\boldsymbol{w}(t) - \boldsymbol{x} \cdot \boldsymbol{B} \in X$ for $t \in [0,1]$. There exists a positive constant δ such that if $\|\boldsymbol{f}\|_{W^{m,p}} \leq \kappa_2$ and $\|\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}\|_{W^{1,\infty}} \leq \delta$, then

$$\int_\Omega \nabla(\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}) : D_{\boldsymbol{A}}^2 W_{\mathrm{CB}}(\nabla \boldsymbol{w}(t)) : \nabla(\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}})\,\mathrm{d}\boldsymbol{x} \geq (C_1/4) \|\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}\|_{H^1}^2 \tag{5.12}$$

for any $t \in [0,1]$. Thus

$$\mathcal{I}[\boldsymbol{v}] - \mathcal{I}[\boldsymbol{u}_{\mathrm{CB}}] \geq (C_1/4) \|\boldsymbol{v} - \boldsymbol{u}_{\mathrm{CB}}\|_{H^1}^2 \tag{5.13}$$

and $\boldsymbol{u}_{\mathrm{CB}}$ is a $W^{1,\infty}$ local minimizer of (2.10). ∎

REMARK 5.1. The method of perturbation used in this proof provides us an estimate on the critical temperature T_c at which some instability of the crystalline solid may occur. More precisely, at the undeformed lattice structure, i.e., $\boldsymbol{B}=\boldsymbol{0}$ with $\kappa_1=0$, we have the lower bound $T_c \geq \frac{C_1}{M_2(0)}$ from (5.9) in the proof of Theorem 3.1. Optimal $C_1=\frac{\pi^2}{\pi^2+d}\Lambda$ is achieved by taking product of Λ from the Legendre–Hadamand condition and the Poincaré constant from the Poincaré inequality $\|\boldsymbol{u}\|_{L^2(\Omega)} \leq \frac{\sqrt{d}}{\pi}\|\nabla \boldsymbol{u}\|_{L^2(\Omega)}$ where $\sqrt{d}$ is the diameter of a unit cube in $\mathbb{R}^d$. Moreover, the constant $M_2(0)$ is now equal to $\|D^2_{\boldsymbol{A}} S_{\mathrm{CB}}(\boldsymbol{0})\|_\infty = \max_{\alpha,\beta,\gamma,\delta}\left|\frac{\partial^2 S_{\mathrm{CB}}(\boldsymbol{0})}{\partial A_{\alpha\beta}\partial A_{\gamma\delta}}\right|$. Therefore, we have an explicit estimate

$$T_c \geq \frac{\pi^2}{\pi^2+d}\frac{\Lambda}{\|D^2_{\boldsymbol{A}} S_{\mathrm{CB}}(\boldsymbol{0})\|_\infty}. \tag{5.14}$$

This estimate holds as long as the harmonic approximation is valid (see more details in the Appendix for the harmonic approximation). Here the critical temperature T_c may not be T^* in Theorem 3.1. In general, T_c is greater than T^* whenever the harmonic approximation is valid. Similar estimate works for the Frobenius norm of the critical macroscopic strain $\boldsymbol{B}_c$. More precisely, setting $T=0$, we obtain the following estimate

$$\|\boldsymbol{B}_c\|_{\mathrm{F}} \geq \frac{\pi^2}{\pi^2+d}\frac{\Lambda}{M_1(\kappa_1)}, \tag{5.15}$$

where $M_1(\kappa_1)=\sup_{\|\boldsymbol{A}\|_{\mathrm{F}}\leq\kappa_1}\|D^3_{\boldsymbol{A}} U_{\mathrm{CB}}(\boldsymbol{A})\|_2$ and $\|\boldsymbol{B}_c\|_{\mathrm{F}} \leq \kappa_1$ for some $\kappa_1 \geq 0$. Thanks to the monotonicity of $M_1(\cdot)$, we have

$$\|\boldsymbol{B}_c\|_{\mathrm{F}} \geq \kappa_c, \tag{5.16}$$

where κ_c is the unique solution to the following nonlinear algebraic equation $\kappa_c M_1(\kappa_c) = \frac{\pi^2\Lambda}{\pi^2+d}$.

REMARK 5.2. The constants C in Theorem 3.2 may increase with the temperature T^*. Although we have a lower bound for the critical temperature T_c (see (5.14)), a more quantitative form of the dependence $C=C(T^*)$ in Theorem 3.2 is hard to achieve since we have used the implicit function theorem in the proof.

Besides these possible instabilities, it is even more important to show the stability for the undeformed crystalline solid at low but finite temperature. To do this, we prove the following lemma which has a similar statement as Lemma 6.7 in [8]. However, they are not exactly the same because the Hessian matrix in our setting has an extra temperature-related term. More precisely, the Hessian matrix at zero temperature $\boldsymbol{H}^{0,\kappa\kappa'}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}')$ is used in Lemma 6.7 of [8], while we use the Hessian matrix

$$\begin{aligned}\boldsymbol{H}^{T,\kappa\kappa'}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}') &:= \varepsilon^{2-d}\frac{\partial^2 \mathcal{F}_\varepsilon[\boldsymbol{y}]}{\partial \boldsymbol{y}^\kappa(\boldsymbol{x})\partial \boldsymbol{y}^{\kappa'}(\boldsymbol{x}')}\\ &= \varepsilon^{2-d}\frac{\partial^2 \mathcal{U}_\varepsilon[\boldsymbol{y}]}{\partial \boldsymbol{y}^\kappa(\boldsymbol{x})\partial \boldsymbol{y}^{\kappa'}(\boldsymbol{x}')} - T\varepsilon^{2-d}\frac{\partial^2 \mathcal{S}_\varepsilon[\boldsymbol{y}]}{\partial \boldsymbol{y}^\kappa(\boldsymbol{x})\partial \boldsymbol{y}^{\kappa'}(\boldsymbol{x}')}\\ &= \boldsymbol{H}^{0,\kappa\kappa'}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}') - T\boldsymbol{G}^{\kappa\kappa'}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}'),\end{aligned} \tag{5.17}$$

where $\boldsymbol{G}^{\kappa\kappa'}_\varepsilon[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}') := \varepsilon^{2-d}\frac{\partial^2 \mathcal{S}_\varepsilon[\boldsymbol{y}]}{\partial \boldsymbol{y}^\kappa(\boldsymbol{x})\partial \boldsymbol{y}^{\kappa'}(\boldsymbol{x}')}$.

LEMMA 5.2 (stability condition with perturbation in T and $\boldsymbol{y}$). *If there exists a positive constant κ_1 such that*

$$\varepsilon^d \boldsymbol{z}\cdot\boldsymbol{H}_\varepsilon^{T_1}[\boldsymbol{y}_1]\boldsymbol{z}\geq\kappa_1\|\boldsymbol{z}\|_{\mathrm{d}}^2 \tag{5.18}$$

for all $\boldsymbol{z}=(\boldsymbol{z}^A,\boldsymbol{z}^B)$ on Ω_ε, then there exist positive constants δ and ε_0 such that for any $\boldsymbol{y}_2$ with $|\boldsymbol{y}_1-\boldsymbol{y}_2|_{W_\varepsilon^{1,\infty}}\leq\delta$, $|T_1-T_2|\leq\delta$, and $0<\varepsilon<\varepsilon_0$, we have

$$\varepsilon^d \boldsymbol{z}\cdot\boldsymbol{H}_\varepsilon^{T_2}[\boldsymbol{y}_2]\boldsymbol{z}\geq\frac{\kappa_1}{2}\|\boldsymbol{z}\|_{\mathrm{d}}^2 \tag{5.19}$$

for all $\boldsymbol{z}=(\boldsymbol{z}^A,\boldsymbol{z}^B)$ on Ω_ε.

Proof. Using the translation invariance, we have for any $T>0$, $\boldsymbol{y}=(vy^A,\boldsymbol{y}^B)$ defined on Ω_ε, $\boldsymbol{x}\in\Omega_\varepsilon$, and $\kappa=A,B$,

$$\sum_{\boldsymbol{x}',\kappa'}\boldsymbol{H}_\varepsilon^{T,\kappa\kappa'}[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}')=\boldsymbol{0}.$$

This implies that

$$\boldsymbol{z}\cdot\boldsymbol{H}_\varepsilon^{T}[\boldsymbol{y}]\boldsymbol{z}=-\frac{1}{2}\sum_{\boldsymbol{x},\boldsymbol{x}',\kappa,\kappa'}(\boldsymbol{z}^\kappa(\boldsymbol{x})-\boldsymbol{z}^{\kappa'}(\boldsymbol{x}'))\cdot\boldsymbol{H}_\varepsilon^{T,\kappa\kappa'}[\boldsymbol{y}](\boldsymbol{x},\boldsymbol{x}')(\boldsymbol{z}^\kappa(\boldsymbol{x})-\boldsymbol{z}^{\kappa'}(\boldsymbol{x}')).$$

By the smoothness and finite range of potential V, we have

$$\begin{aligned}
&\left\|\boldsymbol{H}_\varepsilon^{T_1,\kappa\kappa'}[\boldsymbol{y}_1]-\boldsymbol{H}_\varepsilon^{T_2,\kappa\kappa'}[\boldsymbol{y}_2]\right\|_{L_\varepsilon^\infty}\\
\leq&\left\|\boldsymbol{H}_\varepsilon^{T_1,\kappa\kappa'}[\boldsymbol{y}_1]-\boldsymbol{H}_\varepsilon^{T_1,\kappa\kappa'}[\boldsymbol{y}_2]\right\|_{L_\varepsilon^\infty}+\left\|\boldsymbol{H}_\varepsilon^{T_1,\kappa\kappa'}[\boldsymbol{y}_2]-\boldsymbol{H}_\varepsilon^{T_2,\kappa\kappa'}[\boldsymbol{y}_2]\right\|_{L_\varepsilon^\infty}\\
=&\left\|\boldsymbol{H}_\varepsilon^{T_1,\kappa\kappa'}[\boldsymbol{y}_1]-\boldsymbol{H}_\varepsilon^{T_1,\kappa\kappa'}[\boldsymbol{y}_2]\right\|_{L_\varepsilon^\infty}+|T_1-T_2|\|\boldsymbol{G}_\varepsilon^{\kappa\kappa'}[\boldsymbol{y}_2]\|_{L_\varepsilon^\infty}\\
\leq&C|\boldsymbol{y}_1-\boldsymbol{y}_2|_{W_\varepsilon^{1,\infty}}+C|T_1-T_2|\leq C\delta.
\end{aligned}$$

Note that

$$\|\boldsymbol{z}^A(\boldsymbol{x})-\boldsymbol{z}^B(\boldsymbol{x}')\|^2\leq 2\|\boldsymbol{z}^A(\boldsymbol{x})-\boldsymbol{z}^B(\boldsymbol{x})\|^2+2\|\boldsymbol{z}^B(\boldsymbol{x})-\boldsymbol{z}^B(\boldsymbol{x}')\|^2.$$

Using the above inequalities and the fact that potential V is finite-ranged again, we have

$$\begin{aligned}
&\left|\varepsilon^d\boldsymbol{z}\cdot\left(\boldsymbol{H}_\varepsilon^{T_1}[\boldsymbol{y}_1]-\boldsymbol{H}_\varepsilon^{T_2}[\boldsymbol{y}_2]\right)\boldsymbol{z}\right|\\
=&\frac{\varepsilon^d}{2}\left|\sum_{\boldsymbol{x},\boldsymbol{x}',\kappa,\kappa'}(\boldsymbol{z}^\kappa(\boldsymbol{x})-\boldsymbol{z}^{\kappa'}(\boldsymbol{x}'))\cdot\left(\boldsymbol{H}_\varepsilon^{T_1,\kappa\kappa'}[\boldsymbol{y}_1](\boldsymbol{x},\boldsymbol{x}')-\boldsymbol{H}_\varepsilon^{T_2,\kappa\kappa'}[\boldsymbol{y}_2](\boldsymbol{x},\boldsymbol{x}')\right)(\boldsymbol{z}^\kappa(\boldsymbol{x})-\boldsymbol{z}^{\kappa'}(\boldsymbol{x}'))\right|\\
\leq&C\left\|\boldsymbol{H}_\varepsilon^{T_1,\kappa\kappa'}[\boldsymbol{y}_1]-\boldsymbol{H}_\varepsilon^{T_2,\kappa\kappa'}[\boldsymbol{y}_2]\right\|_{L_\varepsilon^\infty}\varepsilon^d\sum_{\boldsymbol{x}}\sum_{\|\boldsymbol{x}-\boldsymbol{x}'\|=\varepsilon}\left(\|\boldsymbol{z}^A(\boldsymbol{x})-\boldsymbol{z}^A(\boldsymbol{x}')\|^2+\|\boldsymbol{z}^B(\boldsymbol{x})-\boldsymbol{z}^B(\boldsymbol{x}')\|^2\right)\\
&+C\left\|\boldsymbol{H}_\varepsilon^{T_1,\kappa\kappa'}[\boldsymbol{y}_1]-\boldsymbol{H}_\varepsilon^{T_2,\kappa\kappa'}[\boldsymbol{y}_2]\right\|_{L_\varepsilon^\infty}\varepsilon^d\sum_{\boldsymbol{x}}\|\boldsymbol{z}^A(\boldsymbol{x})-\boldsymbol{z}^B(\boldsymbol{x})\|^2\leq C\delta\|\boldsymbol{z}\|_{\mathrm{d}}^2,
\end{aligned}$$

where, in the last inequality we use the following inequality which is essentially obtained in Lemma 6.4 of [8]:

$$\varepsilon^d\sum_{\boldsymbol{x}}\sum_{\|\boldsymbol{x}-\boldsymbol{x}'\|=\varepsilon}\left(\|\boldsymbol{z}^A(\boldsymbol{x})-\boldsymbol{z}^A(\boldsymbol{x}')\|^2+\|\boldsymbol{z}^B(\boldsymbol{x})-\boldsymbol{z}^B(\boldsymbol{x}')\|^2\right)+\varepsilon^d\sum_{\boldsymbol{x}}\|\boldsymbol{z}^A(\boldsymbol{x})-\boldsymbol{z}^B(\boldsymbol{x})\|^2\leq C\|\boldsymbol{z}\|_{\mathrm{d}}^2.$$

Setting $\delta = \kappa_1/2C$, we obtain the desired lower bound:

$$\begin{aligned}\varepsilon^d \boldsymbol{z}\cdot\boldsymbol{H}_\varepsilon^{T_2}[\boldsymbol{y}_2]\boldsymbol{z} &= \varepsilon^d \boldsymbol{z}\cdot\boldsymbol{H}_\varepsilon^{T_1}[\boldsymbol{y}_2]\boldsymbol{z} + \varepsilon^d \boldsymbol{z}\cdot\Big(\boldsymbol{H}_\varepsilon^{T_2}[\boldsymbol{y}_2]-\boldsymbol{H}_\varepsilon^{T_1}[\boldsymbol{y}_1]\Big)\boldsymbol{z}\\ &\ge \kappa_1\|\boldsymbol{z}\|_{\mathrm{d}}^2 - C\delta\|\boldsymbol{z}\|_{\mathrm{d}}^2\\ &\ge \frac{\kappa_1}{2}\|\boldsymbol{z}\|_{\mathrm{d}}^2.\end{aligned}$$

∎

This lemma leads to the stability of crystalline solid at finite temperature stated in Theorem 3.3. Now we give its proof.

Proof. **(Proof of Theorem 3.3.)** The condition $\|\boldsymbol{y}-\boldsymbol{x}-\boldsymbol{x}\cdot\boldsymbol{B}\|_{W_\varepsilon^{1,\infty}} \le \delta$ implies that $\|\boldsymbol{y}-\boldsymbol{x}\|_{W_\varepsilon^{1,\infty}} \le \delta/2$ for sufficiently small $\|\boldsymbol{B}\|_{\mathrm{F}}$. By definition, we have $\varepsilon^d \boldsymbol{z}\cdot\boldsymbol{H}_\varepsilon^0[\boldsymbol{x}]\boldsymbol{z} = \|\boldsymbol{z}\|_{\mathrm{d}}^2$. Set $T_1 = 0$ and $T_2 = T$. Then Lemma 5.2 implies the stability result $\boldsymbol{z}\cdot\boldsymbol{H}_\varepsilon^T[\boldsymbol{y}]\boldsymbol{z} \ge C\|\boldsymbol{z}\|_{\mathrm{d}}^2$. ∎

6. Local minimizer for atomistic model; consistency and convergence

In this section, we first show the consistency of continuum model with delicate asymptotic analysis. Then this, with the stability result, established in the last section, leads to the convergence of the continuum model.

6.1. Consistency for simple lattice. To achieve the consistency with an appropriate order of truncation error, we construct an approximate solution by using the first few terms in the asymptotic expansion of $\boldsymbol{u} = \boldsymbol{u}_0 + \varepsilon\boldsymbol{u}_1 + \varepsilon^2\boldsymbol{u}_2 + \cdots$. Each $\boldsymbol{u}_i$ can be obtained by operators in the asymptotic expansion for $\mathcal{L}_\varepsilon = \mathcal{L}_0 + \varepsilon\mathcal{L}_1 + \varepsilon^2\mathcal{L}_2 + \cdots$. More precisely, we have the following propositions.

PROPOSITION 6.1 (asymptotic expansion of $\mathcal{L}_\varepsilon$, simple lattice). *If we take the asymptotic expansion for the operator*

$$\mathcal{L}_\varepsilon = \mathcal{L}_0 + \varepsilon\mathcal{L}_1 + \varepsilon^2\mathcal{L}_2 + \cdots, \tag{6.1}$$

then we have $\mathcal{L}_0 = \mathcal{L}_{\mathrm{CB}}$, $\mathcal{L}_1 = 0$, *and* $\mathcal{L}_k$ *is an operator in divergence form for* $k \ge 2$.

Proof. Recall the expressions for $\mathcal{S}_\varepsilon[\boldsymbol{y}]$ and $\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}]$. For any test function $\boldsymbol{\varphi} \in C^\infty(\Omega;\mathbb{R}^d)$, we have

$$\begin{aligned}\left\langle \frac{\delta\mathcal{S}_\varepsilon}{\delta\boldsymbol{y}}[\boldsymbol{y}],\boldsymbol{\varphi}\right\rangle_\varepsilon &= \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}_\varepsilon[\boldsymbol{y}+t\boldsymbol{\varphi}] = -\varepsilon^d\sum_{\boldsymbol{x}}\frac{1}{2}k_{\mathrm{B}}D_{\boldsymbol{M}}K(\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}]) : \frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}+t\boldsymbol{\varphi}])\\ &= -\varepsilon^d\sum_{\boldsymbol{x}}\frac{1}{2}k_{\mathrm{B}}D_{\boldsymbol{M}}K(\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}]) : \sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\Big[(\partial_1+\partial_2)^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}]\cdot\mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{\varphi}\\ &\quad + \sum_{j=1}^{2}\partial_j^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]\cdot\mathcal{D}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}\Big]\\ &= -\varepsilon^d\sum_{\boldsymbol{x}}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{4}\Big[k_{\mathrm{B}}D_{\boldsymbol{M}}K(\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}]) : (\partial_1+\partial_2)^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}]\Big]\cdot\mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{\varphi}\\ &\quad -\varepsilon^d\sum_{\boldsymbol{x}}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{4}\Big[k_{\mathrm{B}}D_{\boldsymbol{M}}K(\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}]) : \sum_{j=1}^{2}\partial_j^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]\Big]\cdot\mathcal{D}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}.\end{aligned}$$

Therefore, the Euler–Lagrange equation of atomistic model has the following explicit expression

$$\begin{aligned}\langle \mathcal{L}_\varepsilon[\boldsymbol{y}],\boldsymbol{\varphi}\rangle_\varepsilon &= \varepsilon^d \sum_{\boldsymbol{x}}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}\cdot \mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{\varphi} - T\left\langle \frac{\delta \mathcal{S}_\varepsilon}{\delta \boldsymbol{y}}[\boldsymbol{y}],\boldsymbol{\varphi}\right\rangle_\varepsilon \\ &= \varepsilon^d \sum_{\boldsymbol{x}}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\Big[\frac{1}{2}\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2} + \frac{1}{4}k_{\mathrm{B}}TD_M K(\boldsymbol{H}^0_\varepsilon[\boldsymbol{y}]):(\partial_1+\partial_2)^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}]\Big]\cdot \mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{\varphi} \\ &\quad + \varepsilon^d \sum_{\boldsymbol{x}}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{4}\Big[k_{\mathrm{B}}TD_M K(\boldsymbol{H}^0_\varepsilon[\boldsymbol{y}]):\sum_{j=1}^{2}\partial_j^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]\Big]\cdot \mathcal{D}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}.\end{aligned}$$

Let $\mathcal{L}_\varepsilon = \sum_{k=0}^{\infty}\varepsilon^k\mathcal{L}_k$. Thus for any test function $\boldsymbol{\varphi}\in C^\infty(\Omega;\mathbb{R}^d)$, we have

$$\langle \mathcal{L}_\varepsilon[\boldsymbol{y}],\boldsymbol{\varphi}\rangle_\varepsilon = \sum_{k=0}^{\infty}\varepsilon^k\langle \mathcal{L}_k[\boldsymbol{u}],\boldsymbol{\varphi}\rangle_\varepsilon. \tag{6.2}$$

For $(\boldsymbol{s}_1,\boldsymbol{s}_2)\in S_{\mathrm{int}}$ and $i=1,2$, we define $\nabla^k_{\boldsymbol{s}_i}\boldsymbol{\varphi} = \frac{1}{k!}(\boldsymbol{s}_i\cdot\nabla)^k\boldsymbol{\varphi}$, $k\in\mathbb{N}$ for function $\boldsymbol{\varphi}\in H^k(\Omega;\mathbb{R}^d)$. Then by the Taylor expansion of $\boldsymbol{\varphi}$ and $\boldsymbol{y}$, we have

$$\begin{aligned}\mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{\varphi} &= \nabla^1_{\boldsymbol{s}_i}\boldsymbol{\varphi} + \varepsilon\nabla^2_{\boldsymbol{s}_i}\boldsymbol{\varphi} + \varepsilon^2\nabla^3_{\boldsymbol{s}_i}\boldsymbol{\varphi} + O(\varepsilon^3),\\ \mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{y} &= \boldsymbol{s}_i + \nabla^1_{\boldsymbol{s}_i}\boldsymbol{u} + \varepsilon\boldsymbol{a}_i + \varepsilon^2\boldsymbol{b}_i + O(\varepsilon^3),\end{aligned}$$

where $\boldsymbol{a}_i := \nabla^2_{\boldsymbol{s}_i}\boldsymbol{u}$ and $\boldsymbol{b}_i := \nabla^3_{\boldsymbol{s}_i}\boldsymbol{u}$. We also have

$$\begin{aligned}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi} &= \boldsymbol{\varphi} - \varepsilon\nabla^1_{\boldsymbol{s}_j}\boldsymbol{\varphi} + \varepsilon^2\nabla^2_{\boldsymbol{s}_j}\boldsymbol{\varphi} + O(\varepsilon^3),\\ \mathcal{D}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi} &= \nabla^1_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi} + \varepsilon\nabla^2_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi} + \varepsilon^2\nabla^3_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi} + O(\varepsilon^3)\\ &= \nabla^1_{\boldsymbol{s}_i}\boldsymbol{\varphi} - \varepsilon\nabla^1_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\varphi} + \varepsilon^2\nabla^2_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\varphi} + \varepsilon\nabla^2_{\boldsymbol{s}_i}\boldsymbol{\varphi} - \varepsilon^2\nabla^1_{\boldsymbol{s}_j}\nabla^2_{\boldsymbol{s}_i}\boldsymbol{\varphi} + \varepsilon^2\nabla^3_{\boldsymbol{s}_i}\boldsymbol{\varphi} + O(\varepsilon^3)\\ &= \nabla^1_{\boldsymbol{s}_i}\boldsymbol{\varphi} + \varepsilon(\nabla^2_{\boldsymbol{s}_i} - \nabla^1_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i})\boldsymbol{\varphi} + \varepsilon^2(\nabla^3_{\boldsymbol{s}_i} - \nabla^1_{\boldsymbol{s}_j}\nabla^2_{\boldsymbol{s}_i} + \nabla^2_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i})\boldsymbol{\varphi} + O(\varepsilon^3),\\ \mathcal{D}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y} &= \boldsymbol{s}_i + \nabla^1_{\boldsymbol{s}_i}\boldsymbol{u} + \varepsilon\tilde{\boldsymbol{a}}_{ij} + \varepsilon^2\tilde{\boldsymbol{b}}_{ij} + O(\varepsilon^3),\end{aligned}$$

where $\tilde{\boldsymbol{a}}_{ij} = (\nabla^2_{\boldsymbol{s}_i} - \nabla^1_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i})\boldsymbol{u}$ and $\tilde{\boldsymbol{b}}_{ij} = (\nabla^3_{\boldsymbol{s}_i} - \nabla^1_{\boldsymbol{s}_j}\nabla^2_{\boldsymbol{s}_i} + \nabla^2_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i})\boldsymbol{u}$. Recall the notations in (4.4) and (4.5) with $\boldsymbol{A} = \nabla\boldsymbol{u}$. By the Taylor expansion again, we have

$$\begin{aligned}\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2} &= \partial_i V + \left(\sum_{k=1}^{2}(\varepsilon\boldsymbol{a}_k + \varepsilon^2\boldsymbol{b}_k)\cdot\partial_k\right)\partial_i V + \frac{1}{2}\left(\sum_{k=1}^{2}(\varepsilon\boldsymbol{a}_k + \varepsilon^2\boldsymbol{b}_k)\cdot\partial_k\right)^2\partial_i V + O(\varepsilon^3)\\ &= \left\{1 + \varepsilon\sum_{k=1}^{2}(\boldsymbol{a}_k\cdot\partial_k) + \varepsilon^2\sum_{k=1}^{2}\left(\boldsymbol{b}_k\cdot\partial_k + \frac{1}{2}(\boldsymbol{a}_k\cdot\partial_k)^2\right)\right\}\partial_i V + O(\varepsilon^3),\end{aligned}$$

$$\begin{aligned}&\partial_j^2 V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]\\ =&\partial_j^2 V + \left(\sum_{k=1}^{2}(\varepsilon\tilde{\boldsymbol{a}}_{kj} + \varepsilon^2\tilde{\boldsymbol{b}}_{kj})\cdot\partial_k\right)\partial_j^2 V + \frac{1}{2}\left(\sum_{k=1}^{2}(\varepsilon\tilde{\boldsymbol{a}}_{kj} + \varepsilon^2\tilde{\boldsymbol{b}}_{kj})\cdot\partial_k\right)^2\partial_j^2 V + O(\varepsilon^3)\\ =&\left\{1 + \varepsilon\sum_{k=1}^{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k) + \varepsilon^2\sum_{k=1}^{2}\left(\tilde{\boldsymbol{b}}_{kj}\cdot\partial_k + \frac{1}{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k)^2\right)\right\}\partial_j^2 V + O(\varepsilon^3).\end{aligned}$$

Similar expressions hold for $(\partial_1+\partial_2)^2 V_{\boldsymbol{s}_1,\boldsymbol{s}_2}$, $(\partial_1+\partial_2)^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}$, and $\partial_j^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]$. Recall Equation (4.6). This, with the Taylor expansion leads to

$$\begin{aligned}\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}] &= \sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}\left\{1+\varepsilon\sum_{k=1}^{2}(\boldsymbol{a}_k\cdot\partial_k)+\varepsilon^2\sum_{k=1}^{2}\left(\boldsymbol{b}_k\cdot\partial_k+\frac{1}{2}(\boldsymbol{a}_k\cdot\partial_k)^2\right)\right\}(\partial_1+\partial_2)^2 V\\ &\quad+\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{j=1}^{2}\frac{1}{2}\left\{1+\varepsilon\sum_{k=1}^{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k)+\varepsilon^2\sum_{k=1}^{2}\left(\tilde{\boldsymbol{b}}_{kj}\cdot\partial_k+\frac{1}{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k)^2\right)\right\}\partial_j^2 V+O(\varepsilon^3)\\ &= \boldsymbol{H}_{\mathrm{CB}}^0+\varepsilon\boldsymbol{Q}_1+\varepsilon^2\boldsymbol{Q}_2+O(\varepsilon^3),\end{aligned}\tag{6.3}$$

where

$$\begin{aligned}\boldsymbol{Q}_1 &= \sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}\left\{\sum_{k=1}^{2}(\boldsymbol{a}_k\cdot\partial_k)(\partial_1+\partial_2)^2 V+\sum_{j=1}^{2}\sum_{k=1}^{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k)\partial_j^2 V\right\},\\ \boldsymbol{Q}_2 &= \sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}\left\{\sum_{k=1}^{2}\left(\boldsymbol{b}_k\cdot\partial_k+\frac{1}{2}(\boldsymbol{a}_k\cdot\partial_k)^2\right)(\partial_1+\partial_2)^2 V+\sum_{j=1}^{2}\sum_{k=1}^{2}\left(\tilde{\boldsymbol{b}}_{kj}\cdot\partial_k+\frac{1}{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k)^2\right)\partial_j^2 V\right\}.\end{aligned}$$

In particular, the $O(1)$ term in Equation (6.3) equals $\boldsymbol{H}_{\mathrm{CB}}^0=\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}(\partial_1^2+\frac{1}{2}\partial_1\partial_2+\frac{1}{2}\partial_2\partial_1+\partial_2^2)V$, according to Lemma 4.1. Then

$$D_{\boldsymbol{M}}K(\boldsymbol{H}_\varepsilon^0[\boldsymbol{y}])=D_{\boldsymbol{M}}K+\varepsilon D_{\boldsymbol{M}}^2K:\boldsymbol{Q}_1+\varepsilon^2\left[D_{\boldsymbol{M}}^2K:\boldsymbol{Q}_2+\frac{1}{2}(D_{\boldsymbol{M}}^3K:\boldsymbol{Q}_1):\boldsymbol{Q}_1\right]+O(\varepsilon^3).$$

Comparing the coefficients of each order, we obtain the following expressions for $\mathcal{L}_k$, $k=0,1,2,\ldots$,

$$\langle\mathcal{L}_0[\boldsymbol{u}],\boldsymbol{\varphi}\rangle_\varepsilon=\varepsilon^d\sum_{\boldsymbol{x}}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\left[\partial_i V+k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\left(\partial_1^2+\frac{1}{2}\partial_1\partial_2+\frac{1}{2}\partial_2\partial_1+\partial_2^2\right)\partial_i V\right]\cdot\nabla_{\boldsymbol{s}_i}^1\boldsymbol{\varphi},\tag{6.4}$$

$$\begin{aligned}\langle\mathcal{L}_1[\boldsymbol{u}],\boldsymbol{\varphi}\rangle_\varepsilon=\varepsilon^d\sum_{\boldsymbol{x}}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\Bigg\{&\left[\frac{1}{2}\sum_{k=1}^{2}(\boldsymbol{a}_k\cdot\partial_k)\partial_i V+\frac{1}{4}k_BT\left(D_{\boldsymbol{M}}^2K:\boldsymbol{Q}_1\right):(\partial_1+\partial_2)^2\partial_i V\right.\\ &\left.+\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\sum_{k=1}^{2}(\boldsymbol{a}_k\cdot\partial_k)(\partial_1+\partial_2)^2\partial_i V\right]\cdot\nabla_{\boldsymbol{s}_i}^1\boldsymbol{\varphi}\\ &+\sum_{j=1}^{2}\left[\frac{1}{4}k_{\mathrm{B}}T\left(D_{\boldsymbol{M}}^2K:\boldsymbol{Q}_1\right):\partial_j^2\partial_i V+\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\sum_{k=1}^{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k)\partial_j^2\partial_i V\right]\cdot\nabla_{\boldsymbol{s}_i}^1\boldsymbol{\varphi}\\ &+\left[\frac{1}{2}\partial_i V+\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:(\partial_1+\partial_2)^2\partial_i V\right]\cdot\nabla_{\boldsymbol{s}_i}^2\boldsymbol{\varphi}\\ &+\sum_{j=1}^{2}\left[\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\partial_j^2\partial_i V\right]\cdot\left(\nabla_{\boldsymbol{s}_j}^2-\nabla_{\boldsymbol{s}_j}^1\nabla_{\boldsymbol{s}_i}^1\right)\boldsymbol{\varphi}\Bigg\},\end{aligned}\tag{6.5}$$

and

$$\begin{aligned}\langle\mathcal{L}_2[\boldsymbol{u}],\boldsymbol{\varphi}\rangle_\varepsilon=\varepsilon^d\sum_{\boldsymbol{x}}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\Bigg\{&\left[\frac{1}{2}\sum_{k=1}^{2}\left(\boldsymbol{b}_k\cdot\partial_k+\frac{1}{2}(\boldsymbol{a}_k\cdot\partial_k)^2\right)\partial_i V\right.\\ &\left.+\frac{1}{4}k_{\mathrm{B}}T\left(D_{\boldsymbol{M}}^2K:\boldsymbol{Q}_2+\frac{1}{2}(D_{\boldsymbol{M}}^3K:\boldsymbol{Q}_1):\boldsymbol{Q}_1\right):(\partial_1+\partial_2)^2\partial_i V\right.\end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{4}k_{\mathrm{B}}T\Big(D^2_{\boldsymbol{M}}K:\boldsymbol{Q}_1\Big):\sum_{k=1}^{2}(\boldsymbol{a}_k\cdot\partial_k)(\partial_1+\partial_2)^2\partial_i V\\
&+\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\sum_{k=1}^{2}\Big(\boldsymbol{b}_k\cdot\partial_k+\frac{1}{2}(\boldsymbol{a}_k\cdot\partial_k)^2\Big)(\partial_1+\partial_2)^2\partial_i V\Bigg]\cdot\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\varphi}\\
&+\sum_{j=1}^{2}\Bigg[\frac{1}{4}k_{\mathrm{B}}T\Big(D^2_{\boldsymbol{M}}K:\boldsymbol{Q}_2+\frac{1}{2}(D^3_{\boldsymbol{M}}K:\boldsymbol{Q}_1):\boldsymbol{Q}_1\Big):\partial_j^2\partial_i V\\
&+\frac{1}{4}k_{\mathrm{B}}T\Big(D^2_{\boldsymbol{M}}K:\boldsymbol{Q}_1\Big):\sum_{k=1}^{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k)\partial_j^2\partial_i V\\
&+\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\sum_{k=1}^{2}\Big(\tilde{\boldsymbol{b}}_{kj}\cdot\partial_k+\frac{1}{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k)^2\Big)\partial_j^2\partial_i V\Bigg]\cdot\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\varphi}\\
&+\Bigg[\frac{1}{2}\sum_{k=1}^{2}(\boldsymbol{a}_k\cdot\partial_k)\partial_i V+\frac{1}{4}k_B T\Big(D^2_{\boldsymbol{M}}K:\boldsymbol{Q}_1\Big):(\partial_1+\partial_2)^2\partial_i V\\
&+\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\sum_{k=1}^{2}(\boldsymbol{a}_k\cdot\partial_k)(\partial_1+\partial_2)^2\partial_i V\Bigg]\cdot\nabla^2_{\boldsymbol{s}_i}\boldsymbol{\varphi}\\
&+\sum_{j=1}^{2}\Bigg[\frac{1}{4}k_B T\Big(D^2_{\boldsymbol{M}}K:\boldsymbol{Q}_1\Big):\partial_j^2\partial_i V\\
&+\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\sum_{k=1}^{2}(\tilde{\boldsymbol{a}}_{kj}\cdot\partial_k)\partial_j^2\partial_i V\Bigg]\cdot\Big(\nabla^2_{\boldsymbol{s}_j}-\nabla^1_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i}\Big)\boldsymbol{\varphi}\\
&+\Bigg[\frac{1}{2}\partial_i V+\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:(\partial_1+\partial_2)^2\partial_i V\Bigg]\cdot\nabla^3_{\boldsymbol{s}_i}\boldsymbol{\varphi}\\
&+\sum_{j=1}^{2}\Bigg[\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\partial_j^2\partial_i V\Bigg]\cdot\Big(\nabla^3_{\boldsymbol{s}_i}-\nabla^1_{\boldsymbol{s}_j}\nabla^2_{\boldsymbol{s}_i}+\nabla^2_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i}\Big)\boldsymbol{\varphi}\Bigg\}. \qquad (6.6)
\end{aligned}
$$

First of all, we note that $\mathcal{L}_1[\boldsymbol{u}]=\boldsymbol{0}$ because for any $\boldsymbol{x}$ the summand in Equation (6.5) is odd in both $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$. Secondly, passing to the limit $\varepsilon\to 0$, we have

$$
\begin{aligned}
&\int_\Omega \mathcal{L}_0[\boldsymbol{u}]\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}=\lim_{\varepsilon\to 0}\langle\mathcal{L}_0[\boldsymbol{u}],\boldsymbol{\varphi}\rangle_\varepsilon\\
&=\int_\Omega\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\Bigg[\partial_i V+k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\Big(\partial_1^2+\frac{1}{2}\partial_1\partial_2+\frac{1}{2}\partial_2\partial_1+\partial_2^2\Big)\partial_i V\Bigg]\cdot\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}\\
&=\int_\Omega -\mathrm{div}\cdot\Bigg\{\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\Bigg[\partial_i V+k_{\mathrm{B}}TD_{\boldsymbol{M}}K:\Big(\partial_1^2+\frac{1}{2}\partial_1\partial_2+\frac{1}{2}\partial_2\partial_1+\partial_2^2\Big)\partial_i V\Bigg]\otimes\boldsymbol{s}_i\Bigg\}\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}\\
&=\int_\Omega\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}]\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}.
\end{aligned}
$$

We use the integration by parts and Proposition 4.1 in the last two equalities. Finally, taking limit $\varepsilon\to 0$ and applying integration by parts to Equation (6.6), we obtain that $\mathcal{L}_2[\boldsymbol{u}]$ is in a divergence form. For higher order $\mathcal{L}_k[\boldsymbol{u}]$, $k>2$, the explicit expression can be derived similarly. In particular, $\mathcal{L}_k[\boldsymbol{u}]$, $k>2$, is in a divergence form. ∎

PROPOSITION 6.2 (asymptotic expansion of u, simple lattice). *If we take the asymptotic expansion for the solution*

$$\boldsymbol{u} = \sum_{k=0}^{\infty} \varepsilon^k \boldsymbol{u}_k, \tag{6.7}$$

then $\boldsymbol{u}_0 = \boldsymbol{u}_{\mathrm{CB}}$, $\boldsymbol{u}_1 = \boldsymbol{0}$, *and there exists a function* $\boldsymbol{u}_2 \in X$ *satisfying* $\frac{\delta \mathcal{L}_{\mathrm{CB}}}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_2 = -\mathcal{L}_2[\boldsymbol{u}_0]$.

Proof. Taking the asymptotic expansion, we obtain

$$\begin{aligned}\mathcal{L}_\varepsilon[\boldsymbol{y}] = \mathcal{L}_0[\boldsymbol{u}_0] + \varepsilon \left\{ \tfrac{\delta \mathcal{L}_0}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_1 + \mathcal{L}_1[\boldsymbol{u}_0] \right\} \\ + \varepsilon^2 \left\{ \tfrac{\delta \mathcal{L}_0}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_2 + \tfrac{1}{2} \left(\tfrac{\delta^2 \mathcal{L}_0}{\delta \boldsymbol{u}^2}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_1 \right) \cdot \boldsymbol{u}_1 + \tfrac{\delta \mathcal{L}_1}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_1 + \mathcal{L}_2[\boldsymbol{u}_0] \right\} + O(\varepsilon^3).\end{aligned}$$

Recall that the Euler–Lagrange equation is $\mathcal{L}_\varepsilon[\boldsymbol{y}] = \boldsymbol{f}$. For the leading order, we have $\boldsymbol{u}_0 = \boldsymbol{u}_{\mathrm{CB}}$ which follows from $\mathcal{L}_0 = \mathcal{L}_{\mathrm{CB}}$ with the same periodic boundary condition.

For order $O(\varepsilon)$, we have $\frac{\delta \mathcal{L}_0}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_1 = -\mathcal{L}_1[\boldsymbol{u}_0] = \boldsymbol{0}$. The stability assumption implies that the linear operator $\frac{\delta \mathcal{L}_0}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] = \frac{\delta \mathcal{L}_{\mathrm{CB}}}{\delta \boldsymbol{u}}[\boldsymbol{u}_{\mathrm{CB}}]$ is invertible at the solution $\boldsymbol{u}_{\mathrm{CB}} = \boldsymbol{u}_0$. Thus $\boldsymbol{u}_1 = \boldsymbol{0}$.

For order $O(\varepsilon^2)$, we have

$$\tfrac{\delta \mathcal{L}_0}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_2 = -\tfrac{1}{2} \left(\tfrac{\delta^2 \mathcal{L}_0}{\delta \boldsymbol{u}^2}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_1 \right) \cdot \boldsymbol{u}_1 - \tfrac{\delta \mathcal{L}_1}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_1 - \mathcal{L}_2[\boldsymbol{u}_0] = -\mathcal{L}_2[\boldsymbol{u}_0].$$

Note that $\int_\Omega \mathcal{L}_2[\boldsymbol{u}_0] \mathrm{d}\boldsymbol{x} = \boldsymbol{0}$ because $\mathcal{L}_2$ is of divergence form. Thus $\frac{\delta \mathcal{L}_{\mathrm{CB}}}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_2 = -\mathcal{L}_2[\boldsymbol{u}_0]$ is solvable for $\boldsymbol{u}_2$. ∎

PROPOSITION 6.3 (construction of approximate solution $\tilde{y}$, simple lattice). *Define*

$$\tilde{\boldsymbol{y}} = \boldsymbol{x} + \boldsymbol{u}_0(\boldsymbol{x}) + \varepsilon^2 \boldsymbol{u}_2(\boldsymbol{x}). \tag{6.8}$$

There exist positive constants κ_1, κ_2, T^*, ε_0, *and* C *such that for any* $\boldsymbol{B} \in \mathbb{R}^{d \times d}$ *with* $\|\boldsymbol{B}\|_{\mathrm{F}} \le \kappa_1$, $f \in W^{m,p}(\Omega) \cap W^{1,p}_{\#}(\Omega)$ *with* $\|\boldsymbol{f}\|_{W^{m,p}} \le \kappa_2$, $0 < T < T^*$, *and* $0 < \varepsilon < \varepsilon_0$, *we have*

$$\|\mathcal{L}_\varepsilon[\tilde{\boldsymbol{y}}] - \boldsymbol{f}\|_{L^\infty_\varepsilon} \le C\varepsilon^3. \tag{6.9}$$

We remark that C may depend on the norm $\|\boldsymbol{u}_0\|_{W^{m+2,p}}$ and hence the norm $\|\boldsymbol{f}\|_{W^{m,p}}$.

Proof. This can be checked directly

$$\begin{aligned}\|\mathcal{L}_\varepsilon[\tilde{\boldsymbol{y}}] - \boldsymbol{f}\|_{L^\infty_\varepsilon} &\le \left\| \mathcal{L}_\varepsilon[\tilde{\boldsymbol{y}}] - \mathcal{L}_0[\boldsymbol{u}_0 + \varepsilon^2 \boldsymbol{u}_2] - \varepsilon^2 \mathcal{L}_2[\boldsymbol{u}_0 + \varepsilon^2 \boldsymbol{u}_2] \right\|_{L^\infty_\varepsilon} \\ &\quad + \left\| \mathcal{L}_0[\boldsymbol{u}_0 + \varepsilon^2 \boldsymbol{u}_2] + \varepsilon^2 \mathcal{L}_2[\boldsymbol{u}_0 + \varepsilon^2 \boldsymbol{u}_2] - \boldsymbol{f} \right\|_{L^\infty_\varepsilon} \\ &\le C\varepsilon^3 + \left\| \mathcal{L}_0[\boldsymbol{u}_0 + \varepsilon^2 \boldsymbol{u}_2] - \varepsilon^2 \tfrac{\delta \mathcal{L}_0}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_2 - \mathcal{L}_0[\boldsymbol{u}_0] \right\|_{L^\infty_\varepsilon} \\ &\le C\varepsilon^3 + C\varepsilon^4 \le C\varepsilon^3.\end{aligned}$$

In the inequality, we use $\mathcal{L}_0[\boldsymbol{u}_0] = \boldsymbol{f}$ and $\frac{\delta \mathcal{L}_0}{\delta \boldsymbol{u}}[\boldsymbol{u}_0] \cdot \boldsymbol{u}_2 = -\mathcal{L}_2[\boldsymbol{u}_0]$ in Proposition 6.2. ∎

6.2. Consistency for complex lattice.

PROPOSITION 6.4 (existence of shift p). *There exists a positive constant κ_1 such that given $\boldsymbol{A}\in\mathbb{R}^{d\times d}$ and $\|\boldsymbol{A}\|_{\mathrm{F}}\le\kappa_1$ the minimization problem $\min_{\boldsymbol{p}\in\Omega}W(\boldsymbol{A},\boldsymbol{p})$ is solvable.*

Proof. Since $\boldsymbol{p}^0=\arg\min_{\boldsymbol{p}\in\Omega}W(\boldsymbol{0},\boldsymbol{p})$, we have $\partial_{\boldsymbol{p}}W(\boldsymbol{0},\boldsymbol{p}^0)=\boldsymbol{0}$. By the implicit function theorem, there is a $\kappa_1>0$ such that for $\|\boldsymbol{A}\|_{\mathrm{F}}\le\kappa_1$, $\partial_{\boldsymbol{p}}W(\boldsymbol{A},\boldsymbol{p})=\boldsymbol{0}$ has a unique solution which is denoted as $\boldsymbol{p}(\boldsymbol{A})$. By Assumption 3.1, $\boldsymbol{p}(\boldsymbol{A})$ is the unique minimizer of $W(\boldsymbol{A},\boldsymbol{p})$. ∎

The asymptotic analysis has the same spirit as the simple lattice case, though it is more complicated.

PROPOSITION 6.5 (construction of approximate solution $\tilde{y}$, complex lattice). *There exist positive constants κ_1, κ_2, T^*, ε_0, and C such that for any $\boldsymbol{B}\in\mathbb{R}^{d\times d}$ with $\|\boldsymbol{B}\|_{\mathrm{F}}\le\kappa_1$, $\boldsymbol{f}\in W^{m,p}(\Omega)\cap W^{1,p}_{\#}(\Omega)$ with $\|\boldsymbol{f}\|_{W^{m,p}}\le\kappa_2$, $0<T<T^*$, and $0<\varepsilon<\varepsilon_0$, we can find functions $\{\boldsymbol{u}_k\}_{k=0}^2$ and $\{\boldsymbol{v}_k\}_{k=1}^4$ such that*

$$\|\mathcal{L}_\varepsilon^\kappa[\tilde{\boldsymbol{y}}]-\boldsymbol{f}^\kappa\|_{L^\infty_\varepsilon}\le C\varepsilon^3,\quad \kappa=A,B. \tag{6.10}$$

where the approximate solution $\tilde{\boldsymbol{y}}=(\tilde{\boldsymbol{y}}^A,\tilde{\boldsymbol{y}}^B)$ is defined as follows:

$$\tilde{\boldsymbol{y}}^A=\boldsymbol{x}+\boldsymbol{u}_0(\boldsymbol{x})+\varepsilon\boldsymbol{u}_1(\boldsymbol{x})+\varepsilon^2\boldsymbol{u}_2(\boldsymbol{x}), \tag{6.11}$$

$$\tilde{\boldsymbol{y}}^B=\tilde{\boldsymbol{y}}^A+\varepsilon\boldsymbol{v}_1(\boldsymbol{x})+\varepsilon^2\boldsymbol{v}_2(\boldsymbol{x})+\varepsilon^3\boldsymbol{v}_3(\boldsymbol{x})+\varepsilon^4\boldsymbol{v}_4(\boldsymbol{x}). \tag{6.12}$$

Proof. We define

$$\boldsymbol{y}^A=\boldsymbol{x}+\boldsymbol{u},\quad \boldsymbol{u}=\sum_{k=0}^{\infty}\varepsilon^k\boldsymbol{u}_k, \tag{6.13}$$

$$\boldsymbol{y}^B=\boldsymbol{y}^A+\sum_{k=1}^{\infty}\varepsilon^k\boldsymbol{v}_k. \tag{6.14}$$

The proof is long and divided into five steps.

(i) Basic asymptotic expansions. Recall the expressions for $\mathcal{S}_\varepsilon[\boldsymbol{y}]$ and $\boldsymbol{H}^{0,\kappa}_\varepsilon[\boldsymbol{y}]$. For any test functions $\boldsymbol{\varphi}^A,\boldsymbol{\varphi}^B\in C^\infty(\Omega;\mathbb{R}^d)$, we have

$$\begin{aligned}
&\sum_\kappa\left\langle\frac{\delta\mathcal{S}_\varepsilon}{\delta\boldsymbol{y}^\kappa}[\boldsymbol{y}],\boldsymbol{\varphi}^\kappa\right\rangle_\varepsilon\\
&=\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}_\varepsilon[\boldsymbol{y}+t\boldsymbol{\varphi}]=-\varepsilon^d\sum_{\boldsymbol{x},\kappa}\frac{1}{2}k_{\mathrm{B}}D_{\boldsymbol{M}}K(\boldsymbol{H}^{0,\kappa}_\varepsilon[\boldsymbol{y}]):\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{H}^{0,\kappa}_\varepsilon[\boldsymbol{y}+t\boldsymbol{\varphi}])\\
&=-\varepsilon^d\sum_{\boldsymbol{x},\kappa,\kappa'}\frac{1}{2}k_{\mathrm{B}}D_{\boldsymbol{M}}K(\boldsymbol{H}^{0,\kappa}_\varepsilon[\boldsymbol{y}]):\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\Big[(\partial_1+\partial_2)^2\partial_iV^{\kappa'\kappa}_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}]\cdot\mathcal{D}^{\kappa'\kappa}_{\boldsymbol{s}_i}\boldsymbol{\varphi}\\
&\quad+\sum_{j=1}^{2}\partial_j^2\partial_iV^{\kappa\kappa'}_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]\cdot\mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}\Big]\\
&=-\varepsilon^d\sum_{\boldsymbol{x},\kappa,\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\left\{\frac{1}{4}\Big[k_{\mathrm{B}}D_{\boldsymbol{M}}K(\boldsymbol{H}^{0,\kappa}_\varepsilon[\boldsymbol{y}]):(\partial_1+\partial_2)^2\partial_iV^{\kappa'\kappa}_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\boldsymbol{y}]\Big]\cdot\mathcal{D}^{\kappa'\kappa}_{\boldsymbol{s}_i}\boldsymbol{\varphi}\right.\\
&\quad\left.+\frac{1}{4}\Big[k_{\mathrm{B}}D_{\boldsymbol{M}}K(\boldsymbol{H}^{0,\kappa}_\varepsilon[\boldsymbol{y}]):\sum_{j=1}^{2}\partial_j^2\partial_iV^{\kappa\kappa'}_{\boldsymbol{s}_1,\boldsymbol{s}_2}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]\Big]\cdot\mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}\right\}.
\end{aligned}$$

Therefore, the Euler–Lagrange equation of atomistic model has the following explicit expression

$$\begin{aligned}\sum_{\kappa}\langle\mathcal{L}_\varepsilon^\kappa[\boldsymbol{y}],\boldsymbol{\varphi}^\kappa\rangle_\varepsilon &= \varepsilon^d\sum_{\boldsymbol{x},\kappa,\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\frac{1}{2}\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}^{\kappa\kappa'}[\boldsymbol{y}]\cdot\mathcal{D}_{\boldsymbol{s}_i}^{\kappa\kappa'}\boldsymbol{\varphi}-\sum_{\kappa}T\left\langle\frac{\delta\mathcal{S}_\varepsilon}{\delta\boldsymbol{y}^\kappa}[\boldsymbol{y}],\boldsymbol{\varphi}^\kappa\right\rangle_\varepsilon\\ &=\varepsilon^d\sum_{\boldsymbol{x},\kappa,\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\Bigg\{\frac{1}{2}\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}^{\kappa'\kappa}[\boldsymbol{y}]\cdot\mathcal{D}_{\boldsymbol{s}_i}^{\kappa'\kappa}\boldsymbol{\varphi}\\ &\quad+\frac{1}{4}\left[k_{\mathrm{B}}TD_{\boldsymbol{M}}K(\boldsymbol{H}_\varepsilon^{0,\kappa}[\boldsymbol{y}]):(\partial_1+\partial_2)^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}^{\kappa'\kappa}[\boldsymbol{y}]\right]\cdot\mathcal{D}_{\boldsymbol{s}_i}^{\kappa'\kappa}\boldsymbol{\varphi}\\ &\quad+\frac{1}{4}\left[k_{\mathrm{B}}TD_{\boldsymbol{M}}K(\boldsymbol{H}_\varepsilon^{0,\kappa}[\boldsymbol{y}]):\sum_{j=1}^{2}\partial_j^2\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}^{\kappa\kappa'}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]\right]\cdot\mathcal{D}_{\boldsymbol{s}_i}^{\kappa\kappa'}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}\Bigg\}.\end{aligned}\tag{6.15}$$

For $\boldsymbol{s}=(\boldsymbol{s}_1,\boldsymbol{s}_2)\in S_{\mathrm{int}}$ and $i=1,2$, we define $\nabla_{\boldsymbol{s}_i}^k\boldsymbol{\varphi}=\frac{1}{k!}(\boldsymbol{s}_i\cdot\nabla)^k\boldsymbol{\varphi}$, $k\in\mathbb{N}$ for function $\boldsymbol{\varphi}\in H^k(\Omega,\mathbb{R}^d)$. The key here is to split finite difference operators into two parts: the inter-spicies one and the intra-spicies one, that is, $\mathcal{D}_{\boldsymbol{s}_i}^{BA}=\mathcal{D}_{\boldsymbol{s}_i}^{BB}+\mathcal{D}_{\boldsymbol{0}}^{BA}$ and $\mathcal{D}_{\boldsymbol{s}_i}^{AB}=\mathcal{D}_{\boldsymbol{s}_i}^{AA}-\mathcal{D}_{\boldsymbol{0}}^{BA}$. By the Taylor series of $\boldsymbol{\varphi}$ and $\boldsymbol{y}$, we obtain

$$\begin{aligned}&\mathcal{D}_{\boldsymbol{s}_i}^{\kappa\kappa}\boldsymbol{\varphi}=\mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{\varphi}^\kappa=\nabla_{\boldsymbol{s}_i}^1\boldsymbol{\varphi}^\kappa+\varepsilon\nabla_{\boldsymbol{s}_i}^2\boldsymbol{\varphi}^\kappa+\varepsilon^2\nabla_{\boldsymbol{s}_i}^3\boldsymbol{\varphi}^\kappa+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{0}}^{BA}\boldsymbol{y}=\varepsilon^{-1}(\boldsymbol{y}^B-\boldsymbol{y}^A)=\boldsymbol{v}_1+\varepsilon\boldsymbol{v}_2+\varepsilon^2\boldsymbol{v}_3+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{s}_i}^{AA}\boldsymbol{y}=\mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{y}^A=\boldsymbol{s}_i+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{u}+\varepsilon\boldsymbol{a}_i^{AA}+\varepsilon^2\boldsymbol{b}_i^{AA}+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{s}_i}^{BB}\boldsymbol{y}=\mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{y}^A+\varepsilon\mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{v}_1+\varepsilon^2\mathcal{D}_{\boldsymbol{s}_i}\boldsymbol{v}_2+O(\varepsilon^3)=\boldsymbol{s}_i+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{u}+\varepsilon\boldsymbol{a}_i^{BB}+\varepsilon^2\boldsymbol{b}_i^{BB}+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{s}_i}^{BA}\boldsymbol{y}=\mathcal{D}_{\boldsymbol{s}_i}^{BB}\boldsymbol{y}+\mathcal{D}_{\boldsymbol{0}}^{BA}\boldsymbol{y}=\boldsymbol{s}_i+(\nabla_{\boldsymbol{s}_i}^1\boldsymbol{u}+\boldsymbol{v}_1)+\varepsilon\boldsymbol{a}_i^{BA}+\varepsilon^2\boldsymbol{b}_i^{BA}+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{s}_i}^{AB}\boldsymbol{y}=\mathcal{D}_{\boldsymbol{s}_i}^{AA}\boldsymbol{y}-\mathcal{D}_{\boldsymbol{0}}^{BA}\boldsymbol{y}=\boldsymbol{s}_i+(\nabla_{\boldsymbol{s}_i}^1\boldsymbol{u}-\boldsymbol{v}_1)+\varepsilon\boldsymbol{a}_i^{AB}+\varepsilon^2\boldsymbol{b}_i^{AB}+O(\varepsilon^3),\end{aligned}$$

where

$$\boldsymbol{a}_i^{AA}=\nabla_{\boldsymbol{s}_i}^2\boldsymbol{u},\quad \boldsymbol{b}_i^{AA}=\nabla_{\boldsymbol{s}_i}^3\boldsymbol{u},\tag{6.16}$$

$$\boldsymbol{a}_i^{BB}=\nabla_{\boldsymbol{s}_i}^2\boldsymbol{u}+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{v}_1,\quad \boldsymbol{b}_i^{BB}=\nabla_{\boldsymbol{s}_i}^3\boldsymbol{u}+\nabla_{\boldsymbol{s}_i}^2\boldsymbol{v}_1+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{v}_2,\tag{6.17}$$

$$\boldsymbol{a}_i^{BA}=\nabla_{\boldsymbol{s}_i}^2\boldsymbol{u}+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{v}_1+\boldsymbol{v}_2,\quad \boldsymbol{b}_i^{BA}=\nabla_{\boldsymbol{s}_i}^3\boldsymbol{u}+\nabla_{\boldsymbol{s}_i}^2\boldsymbol{v}_1+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{v}_2+\boldsymbol{v}_3,\tag{6.18}$$

$$\boldsymbol{a}_i^{AB}=\nabla_{\boldsymbol{s}_i}^2\boldsymbol{u}-\boldsymbol{v}_2,\quad \boldsymbol{b}_i^{AB}=\nabla_{\boldsymbol{s}_i}^3\boldsymbol{u}-\boldsymbol{v}_3.\tag{6.19}$$

By the Taylor series of the translation $\mathcal{T}_{-\boldsymbol{s}_j}$ of $\boldsymbol{\varphi}$ and $\boldsymbol{y}$, we have

$$\begin{aligned}&\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}=\boldsymbol{\varphi}-\varepsilon\nabla_{\boldsymbol{s}_j}^1\boldsymbol{\varphi}+\varepsilon^2\nabla_{\boldsymbol{s}_j}^2\boldsymbol{\varphi}+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{s}_i}^{\kappa\kappa}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}=\nabla_{\boldsymbol{s}_i}^1\boldsymbol{\varphi}^\kappa+\varepsilon(\nabla_{\boldsymbol{s}_i}^2-\nabla_{\boldsymbol{s}_j}^1\nabla_{\boldsymbol{s}_i}^1)\boldsymbol{\varphi}^\kappa+\varepsilon^2(\nabla_{\boldsymbol{s}_i}^3-\nabla_{\boldsymbol{s}_j}^1\nabla_{\boldsymbol{s}_i}^2+\nabla_{\boldsymbol{s}_j}^2\nabla_{\boldsymbol{s}_i}^1)\boldsymbol{\varphi}^\kappa+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{0}}^{BA}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}=\mathcal{T}_{-\boldsymbol{s}_j}\mathcal{D}_{\boldsymbol{0}}^{BA}\boldsymbol{y}=\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{v}_1+\varepsilon\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{v}_2+\varepsilon^2\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{v}_3+O(\varepsilon^3)\\ &\qquad=\boldsymbol{v}_1+\varepsilon(-\nabla_{\boldsymbol{s}_j}^1\boldsymbol{v}_1+\boldsymbol{v}_2)+\varepsilon^2(\nabla_{\boldsymbol{s}_j}^2\boldsymbol{v}_1-\nabla_{\boldsymbol{s}_j}^1\boldsymbol{v}_2+\boldsymbol{v}_3)+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{s}_i}^{AA}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}=\mathcal{D}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}^A=\boldsymbol{s}_i+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{u}+\varepsilon\tilde{\boldsymbol{a}}_{ij}^{AA}+\varepsilon^2\tilde{\boldsymbol{b}}_{ij}^{AA}+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{s}_i}^{BB}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}=\mathcal{D}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}^A+\varepsilon\mathcal{D}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{v}_1+\varepsilon^2\mathcal{D}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{v}_2+O(\varepsilon^3)\\ &\qquad=\boldsymbol{s}_i+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{u}+\varepsilon\tilde{\boldsymbol{a}}_i^{BB}+\varepsilon^2\tilde{\boldsymbol{b}}_i^{BB}+O(\varepsilon^3),\\ &\mathcal{D}_{\boldsymbol{s}_i}^{BA}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}=\mathcal{D}_{\boldsymbol{s}_i}^{BB}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}+\mathcal{D}_{\boldsymbol{0}}^{BA}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}=\boldsymbol{s}_i+(\nabla_{\boldsymbol{s}_i}^1\boldsymbol{u}+\boldsymbol{v}_1)+\varepsilon\tilde{\boldsymbol{a}}_i^{BA}+\varepsilon^2\tilde{\boldsymbol{b}}_i^{BA}+O(\varepsilon^3),\end{aligned}$$

$$\mathcal{D}_{\boldsymbol{s}_i}^{AB}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}=\mathcal{D}_{\boldsymbol{s}_i}^{AA}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}-\mathcal{D}_{\boldsymbol{0}}^{BA}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}=\boldsymbol{s}_i+(\nabla_{\boldsymbol{s}_i}^1\boldsymbol{u}-\boldsymbol{v}_1)+\varepsilon\tilde{\boldsymbol{a}}_i^{AB}+\varepsilon^2\tilde{\boldsymbol{b}}_i^{AB}+O(\varepsilon^3),$$

where

$$\tilde{\boldsymbol{a}}_{ij}^{AA}=(\nabla_{\boldsymbol{s}_i}^2-\nabla_{\boldsymbol{s}_j}^1\nabla_{\boldsymbol{s}_i}^1)\boldsymbol{u},\qquad \tilde{\boldsymbol{b}}_{ij}^{AA}=(\nabla_{\boldsymbol{s}_i}^3-\nabla_{\boldsymbol{s}_j}^1\nabla_{\boldsymbol{s}_i}^2+\nabla_{\boldsymbol{s}_j}^2\nabla_{\boldsymbol{s}_i}^1)\boldsymbol{u}, \tag{6.20}$$

$$\tilde{\boldsymbol{a}}_{ij}^{BB}=\tilde{\boldsymbol{a}}_{ij}^{AA}+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{v}_1,\qquad \tilde{\boldsymbol{b}}_{ij}^{BB}=\tilde{\boldsymbol{b}}_{ij}^{AA}+(\nabla_{\boldsymbol{s}_i}^2-\nabla_{\boldsymbol{s}_j}^1\nabla_{\boldsymbol{s}_i}^1)\boldsymbol{v}_1+\nabla_{\boldsymbol{s}_i}^1\boldsymbol{v}_2, \tag{6.21}$$

$$\tilde{\boldsymbol{a}}_{ij}^{BA}=\tilde{\boldsymbol{a}}_{ij}^{BB}-\nabla_{\boldsymbol{s}_j}^1\boldsymbol{v}_1+\boldsymbol{v}_2,\qquad \tilde{\boldsymbol{b}}_{ij}^{BA}=\tilde{\boldsymbol{b}}_{ij}^{BB}+\nabla_{\boldsymbol{s}_j}^2\boldsymbol{v}_1-\nabla_{\boldsymbol{s}_j}^1\boldsymbol{v}_2+\boldsymbol{v}_3, \tag{6.22}$$

$$\tilde{\boldsymbol{a}}_{ij}^{AB}=\tilde{\boldsymbol{a}}_{ij}^{AA}+\nabla_{\boldsymbol{s}_j}^1\boldsymbol{v}_1-\boldsymbol{v}_2,\qquad \tilde{\boldsymbol{b}}_{ij}^{AB}=\tilde{\boldsymbol{b}}_{ij}^{AA}-\nabla_{\boldsymbol{s}_j}^2\boldsymbol{v}_1+\nabla_{\boldsymbol{s}_j}^1\boldsymbol{v}_2-\boldsymbol{v}_3. \tag{6.23}$$

Now we recall notations in (4.11), (4.12), (4.13), and (4.14) with $\boldsymbol{A}=\nabla\boldsymbol{u}$ and $\boldsymbol{p}=\boldsymbol{v}_1$. By the Taylor series again, with notations defined in (6.16)–(6.23), we have for $\kappa,\kappa'=A,B$,

$$\partial_i V_{\boldsymbol{s}_1,\boldsymbol{s}_2}^{\kappa\kappa'}[\boldsymbol{y}]=\left\{1+\varepsilon\sum_{k=1}^{2}(\boldsymbol{a}_k^{\kappa\kappa'}\cdot\partial_k)+\varepsilon^2\sum_{k=1}^{2}\left(\boldsymbol{b}_k^{\kappa\kappa'}\cdot\partial_k+\frac{1}{2}(\boldsymbol{a}_k^{\kappa\kappa'}\cdot\partial_k)^2\right)\right\}\partial_i V^{\kappa\kappa'}+O(\varepsilon^3),$$

$$\partial_j^2 V_{\boldsymbol{s}_1,\boldsymbol{s}_2}^{\kappa\kappa'}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]=\left\{1+\varepsilon\sum_{k=1}^{2}(\tilde{\boldsymbol{a}}_{kj}^{\kappa\kappa'}\cdot\partial_k)+\varepsilon^2\sum_{k=1}^{2}\left(\tilde{\boldsymbol{b}}_{kj}^{\kappa\kappa'}\cdot\partial_k+\frac{1}{2}(\tilde{\boldsymbol{a}}_{kj}^{\kappa\kappa'}\cdot\partial_k)^2\right)\right\}\partial_j^2 V^{\kappa\kappa'}+O(\varepsilon^3).$$

Other derivatives of $V_{\boldsymbol{s}_1,\boldsymbol{s}_2}^{\kappa\kappa'}[\boldsymbol{y}]$ and $V_{\boldsymbol{s}_1,\boldsymbol{s}_2}^{\kappa\kappa'}[\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{y}]$ can be obtained similarly. Thus we have the expansions for $\boldsymbol{H}_\varepsilon^{0,\kappa}[\boldsymbol{y}]$.

$$\begin{aligned}\boldsymbol{H}_\varepsilon^{0,\kappa}[\boldsymbol{y}]=&\sum_{\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}\left\{1+\varepsilon\sum_{k=1}^{2}(\boldsymbol{a}_k^{\kappa\kappa'}\cdot\partial_k)+\varepsilon^2\sum_{k=1}^{2}\left(\boldsymbol{b}_k^{\kappa\kappa'}\cdot\partial_k+\frac{1}{2}(\boldsymbol{a}_k^{\kappa\kappa'}\cdot\partial_k)^2\right)\right\}(\partial_1+\partial_2)^2V^{\kappa'\kappa}\\&+\sum_{\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{j=1}^{2}\frac{1}{2}\left\{1+\varepsilon\sum_{k=1}^{2}(\tilde{\boldsymbol{a}}_{kj}^{\kappa\kappa'}\cdot\partial_k)+\varepsilon^2\sum_{k=1}^{2}\left(\tilde{\boldsymbol{b}}_{kj}^{\kappa\kappa'}\cdot\partial_k+\frac{1}{2}(\tilde{\boldsymbol{a}}_{kj}^{\kappa\kappa'}\cdot\partial_k)^2\right)\right\}\partial_j^2V^{\kappa\kappa'}\\&+O(\varepsilon^3)\\=&\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}+\varepsilon\boldsymbol{Q}_1^\kappa+\varepsilon^2\boldsymbol{Q}_2^\kappa+O(\varepsilon^3),\end{aligned} \tag{6.24}$$

where

$$\boldsymbol{Q}_1^\kappa=\sum_{\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}\left\{\sum_{k=1}^{2}(\boldsymbol{a}_k^{\kappa\kappa'}\cdot\partial_k)(\partial_1+\partial_2)^2V^{\kappa'\kappa}+\sum_{j=1}^{2}\sum_{k=1}^{2}(\tilde{\boldsymbol{a}}_{kj}^{\kappa\kappa'}\cdot\partial_k)\partial_j^2V^{\kappa\kappa'}\right\},$$

$$\begin{aligned}\boldsymbol{Q}_2^\kappa=&\sum_{\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\frac{1}{2}\left\{\sum_{k=1}^{2}\left(\boldsymbol{b}_k^{\kappa\kappa'}\cdot\partial_k+\frac{1}{2}(\boldsymbol{a}_k^{\kappa\kappa'}\cdot\partial_k)^2\right)(\partial_1+\partial_2)^2V^{\kappa'\kappa}\right.\\&\left.+\sum_{j=1}^{2}\sum_{k=1}^{2}\left(\tilde{\boldsymbol{b}}_{kj}^{\kappa\kappa'}\cdot\partial_k+\frac{1}{2}(\tilde{\boldsymbol{a}}_{kj}^{\kappa\kappa'}\cdot\partial_k)^2\right)\partial_j^2V^{\kappa\kappa'}\right\}.\end{aligned}$$

In particular, the $O(1)$ term in Equation (6.24) equals $\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}$, according to Lemma 4.2. Then

$$\begin{aligned}D_{\boldsymbol{M}}K(\boldsymbol{H}_\varepsilon^{0,\kappa}[\boldsymbol{y}])=&D_{\boldsymbol{M}}K(\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa})+\varepsilon D_{\boldsymbol{M}}^2K(\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}):\boldsymbol{Q}_1^\kappa+\varepsilon^2\left[D_{\boldsymbol{M}}^2K(\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}):\boldsymbol{Q}_2^\kappa\right.\\&\left.+\frac{1}{2}\left(D_{\boldsymbol{M}}^3K(\boldsymbol{H}_{\mathrm{CB}}^{0,\kappa}):\boldsymbol{Q}_1^\kappa\right):\boldsymbol{Q}_1^\kappa\right]+O(\varepsilon^3).\end{aligned}$$

(ii) Finding $\mathcal{L}_0$. If $\boldsymbol{\varphi}^A=\boldsymbol{\varphi}^B=\boldsymbol{\psi}\in C^\infty(\Omega;\mathbb{R}^d)$, then

$$\mathcal{D}^{\kappa\kappa'}_{\boldsymbol{s}_i}\boldsymbol{\varphi}=\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\psi}+\varepsilon\nabla^2_{\boldsymbol{s}_i}\boldsymbol{\psi}+\varepsilon^2\nabla^3_{\boldsymbol{s}_i}\boldsymbol{\psi}+O(\varepsilon^3). \tag{6.25}$$

The leading order in (6.15) with $\boldsymbol{\varphi}^A=-\boldsymbol{\varphi}^B=\boldsymbol{\psi}$ is $O(1)$. We set $\mathcal{L}^A_\varepsilon+\mathcal{L}^B_\varepsilon=\sum_{k=0}^\infty\varepsilon^k\mathcal{L}_k$, that is,

$$\langle\mathcal{L}^A_\varepsilon[\boldsymbol{y}],\boldsymbol{\psi}\rangle_\varepsilon+\langle\mathcal{L}^B_\varepsilon[\boldsymbol{y}],\boldsymbol{\psi}\rangle_\varepsilon=\sum_{k=0}^\infty\varepsilon^k\langle\mathcal{L}_k[\boldsymbol{u},\{\boldsymbol{v}_j\}_{j=1}^\infty],\boldsymbol{\psi}\rangle_\varepsilon. \tag{6.26}$$

By (6.15), the leading order operator only depends on $\boldsymbol{u}$ and $\boldsymbol{v}_1$ (since the evaluation of V^{AB} (and V^{BA}) depends on $\nabla\boldsymbol{u}$ and $\boldsymbol{v}_1$):

$$\begin{aligned}\langle\mathcal{L}_0[\boldsymbol{u},\boldsymbol{v}_1],\boldsymbol{\psi}\rangle_\varepsilon=\varepsilon^d\sum_{\boldsymbol{x},\kappa,\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^2\Bigg\{&\frac{1}{2}\partial_iV^{\kappa'\kappa}+\frac{1}{4}k_{\mathrm{B}}TD_{\boldsymbol{M}}K(\boldsymbol{H}^{0,\kappa}_{\mathrm{CB}})\\&:\left[(\partial_1+\partial_2)^2\partial_iV^{\kappa'\kappa}+\sum_{j=1}^2\partial_j^2\partial_iV^{\kappa\kappa'}\right]\Bigg\}\cdot\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\psi}.\end{aligned} \tag{6.27}$$

Passing to the limit $\varepsilon\to0$, we have

$$\begin{aligned}\int_\Omega\mathcal{L}_0[\boldsymbol{u},\boldsymbol{v}_1]\cdot\boldsymbol{\psi}\,\mathrm{d}\boldsymbol{x}&=\int_\Omega\sum_{\kappa,\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^2\frac{1}{2}\Bigg\{\partial_iV^{\kappa'\kappa}+\frac{1}{2}k_{\mathrm{B}}TD_{\boldsymbol{M}}K(\boldsymbol{H}^{0,\kappa}_{\mathrm{CB}})\\&\qquad:\left[(\partial_1+\partial_2)^2\partial_iV^{\kappa'\kappa}+(\partial_1^2+\partial_2^2)\partial_iV^{\kappa\kappa'}\right]\Bigg\}\cdot\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\psi}\,\mathrm{d}\boldsymbol{x}\\&=\int_\Omega-\mathrm{div}\cdot\Bigg\{\sum_{\kappa,\kappa'}\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^2\frac{1}{2}\Bigg[\partial_iV^{\kappa'\kappa}+\frac{1}{2}k_{\mathrm{B}}TD_{\boldsymbol{M}}K(\boldsymbol{H}^{0,\kappa}_{\mathrm{CB}})\\&\qquad:\left((\partial_1+\partial_2)^2\partial_iV^{\kappa'\kappa}+(\partial_1^2+\partial_2^2)\partial_iV^{\kappa\kappa'}\right)\Bigg]\otimes\boldsymbol{s}_i\Bigg\}\cdot\boldsymbol{\psi}\,\mathrm{d}\boldsymbol{x},\end{aligned} \tag{6.28}$$

where we have used the integration by parts in the last equality. Higher order terms can be obtained similarly. In particular, higher order differential operators $\mathcal{L}_k$ ($k\ge1$) are in divergence form and depend on $\boldsymbol{u},\boldsymbol{v}_1,\dots,\boldsymbol{v}_{k+1}$, that is, $\mathcal{L}_k=\mathcal{L}_k[\boldsymbol{u},\{\boldsymbol{v}_j\}_{j=1}^{k+1}]$. From (6.28) we can only conclude that $\mathcal{L}_0=\mathcal{L}_0[\boldsymbol{u},\boldsymbol{v}_1]$ which does not imply $\mathcal{L}_0=2\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}]$. (Note that this factor 2 is due to our definition.) This gap will be filled up according to the rest of the proof. In particular, we should study with the test functions $\boldsymbol{\varphi}^A=-\boldsymbol{\varphi}^B=\boldsymbol{\psi}$.

(iii) Solving $\boldsymbol{v}_k$, $k\ge1$. If $\boldsymbol{\varphi}^A=-\boldsymbol{\varphi}^B=\boldsymbol{\psi}$, then

$$\mathcal{D}^{AA}_{\boldsymbol{s}_i}\boldsymbol{\varphi}=-\mathcal{D}^{BB}_{\boldsymbol{s}_i}\boldsymbol{\varphi}=\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\psi}+\varepsilon\nabla^2_{\boldsymbol{s}_i}\boldsymbol{\psi}+\varepsilon^2\nabla^3_{\boldsymbol{s}_i}\boldsymbol{\psi}+O(\varepsilon^3), \tag{6.29}$$

$$\mathcal{D}^{AB}_{\boldsymbol{s}_i}\boldsymbol{\varphi}=-\mathcal{D}^{BA}_{\boldsymbol{s}_i}\boldsymbol{\varphi}=2\varepsilon^{-1}\boldsymbol{\psi}+\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\psi}+\varepsilon\nabla^2_{\boldsymbol{s}_i}\boldsymbol{\psi}+\varepsilon^2\nabla^3_{\boldsymbol{s}_i}\boldsymbol{\psi}+O(\varepsilon^3). \tag{6.30}$$

This, with the translation operator leads to the following expressions:

$$\mathcal{D}^{BA}_{\boldsymbol{0}}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}=-2\varepsilon^{-1}\boldsymbol{\psi}+2\nabla^1_{\boldsymbol{s}_j}\boldsymbol{\psi}-2\varepsilon\nabla^2_{\boldsymbol{s}_j}\boldsymbol{\psi}+2\varepsilon^2\nabla^3_{\boldsymbol{s}_j}\boldsymbol{\psi}+O(\varepsilon^3), \tag{6.31}$$

$$\begin{aligned}\mathcal{D}^{AA}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}&=-\mathcal{D}^{BB}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}=\nabla^1_{\boldsymbol{s}_i}\boldsymbol{\psi}+\varepsilon(\nabla^2_{\boldsymbol{s}_i}-\nabla^1_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i})\boldsymbol{\psi}\\&\quad+\varepsilon^2(\nabla^3_{\boldsymbol{s}_i}-\nabla^1_{\boldsymbol{s}_j}\nabla^2_{\boldsymbol{s}_i}+\nabla^2_{\boldsymbol{s}_j}\nabla^1_{\boldsymbol{s}_i})\boldsymbol{\psi}+O(\varepsilon^3),\end{aligned} \tag{6.32}$$

$$\mathcal{D}^{AB}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}=-\mathcal{D}^{BA}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}=\mathcal{D}^{AA}_{\boldsymbol{s}_i}\mathcal{T}_{-\boldsymbol{s}_j}\boldsymbol{\varphi}$$
$$+2\varepsilon^{-1}\boldsymbol{\psi}-2\nabla^1_{\boldsymbol{s}_j}\boldsymbol{\psi}+2\varepsilon\nabla^2_{\boldsymbol{s}_j}\boldsymbol{\psi}-2\varepsilon^2\nabla^3_{\boldsymbol{s}_j}\boldsymbol{\psi}+O(\varepsilon^3). \tag{6.33}$$

The leading order in (6.15) with $\boldsymbol{\varphi}^A=-\boldsymbol{\varphi}^B=\boldsymbol{\psi}$ is $O(\varepsilon^{-1})$. We set $\mathcal{L}^A_\varepsilon-\mathcal{L}^B_\varepsilon=\sum_{k=-1}^{\infty}\varepsilon^k\mathcal{N}_k$, that is,

$$\langle\mathcal{L}^A_\varepsilon[\boldsymbol{y}],\boldsymbol{\psi}\rangle_\varepsilon-\langle\mathcal{L}^B_\varepsilon[\boldsymbol{y}],\boldsymbol{\psi}\rangle_\varepsilon=\sum_{k=-1}^{\infty}\varepsilon^k\langle\mathcal{N}_k[\boldsymbol{u},\{\boldsymbol{v}_j\}_{j=1}^{\infty}],\boldsymbol{\psi}\rangle_\varepsilon. \tag{6.34}$$

On the other hand, we have

$$\langle\mathcal{L}^A_\varepsilon[\boldsymbol{y}],\boldsymbol{\psi}\rangle_\varepsilon-\langle\mathcal{L}^B_\varepsilon[\boldsymbol{y}],\boldsymbol{\psi}\rangle_\varepsilon=\varepsilon^d\sum_{\boldsymbol{x}}(\boldsymbol{f}(\boldsymbol{x})-\boldsymbol{f}(\boldsymbol{x}+\varepsilon\boldsymbol{p}^0))\cdot\boldsymbol{\psi}(\boldsymbol{x})=\sum_{k=1}^{\infty}\varepsilon^k\langle-\nabla^k_{\boldsymbol{p}^0}\boldsymbol{f},\boldsymbol{\psi}\rangle_\varepsilon, \tag{6.35}$$

where $\nabla^k_{\boldsymbol{p}^0}\boldsymbol{f}=\frac{1}{k!}(\boldsymbol{p}_0\cdot\nabla)^k\boldsymbol{f}$. Thus $\mathcal{N}_{-1}=\boldsymbol{0}$, $\mathcal{N}_0=\boldsymbol{0}$, and $\mathcal{N}_k=-\nabla^k_{\boldsymbol{p}^0}\boldsymbol{f}$, $k\geq1$. Moreover, from the above detailed expansions, we conclude that the dependence is $\mathcal{N}_k=\mathcal{N}_k[\boldsymbol{u},\{\boldsymbol{v}_j\}_{j=1}^{k+2}]$, $k\geq-1$. By (6.15), the leading order $O(\varepsilon^{-1})$ depends only on $\boldsymbol{u}$ and $\boldsymbol{v}_1$, that is, $\boldsymbol{0}=\mathcal{N}_{-1}=\mathcal{N}_{-1}[\boldsymbol{u},\boldsymbol{v}_1]$. More precisely, we have

$$\begin{aligned}\boldsymbol{0}=\sum_{\boldsymbol{s}_1,\boldsymbol{s}_2}\sum_{i=1}^{2}\Big\{&\partial_iV^{AB}-\partial_iV^{BA}+\frac{1}{2}k_{\mathrm{B}}TD_{\boldsymbol{M}}K(\boldsymbol{H}^{0,B}_{\mathrm{CB}}):(\partial_1+\partial_2)^2\partial_iV^{AB}\\&-\frac{1}{2}k_{\mathrm{B}}TD_{\boldsymbol{M}}K(\boldsymbol{H}^{0,A}_{\mathrm{CB}}):(\partial_1+\partial_2)^2\partial_iV^{BA}+\frac{1}{2}k_{\mathrm{B}}TD_{\boldsymbol{M}}K(\boldsymbol{H}^{0,B}_{\mathrm{CB}}):(\partial_1^2+\partial_2^2)\partial_iV^{AB}\\&-\frac{1}{2}k_{\mathrm{B}}TD_{\boldsymbol{M}}K(\boldsymbol{H}^{0,A}_{\mathrm{CB}}):(\partial_1^2+\partial_2^2)\partial_iV^{BA}\Big\}.\end{aligned} \tag{6.36}$$

Note that this right-hand side equals $D_{\boldsymbol{p}}W(\boldsymbol{A},\boldsymbol{p})$ with $\boldsymbol{A}=\nabla\boldsymbol{u}(\boldsymbol{x})$ and $\boldsymbol{p}=\boldsymbol{v}_1(\boldsymbol{x})$, $\boldsymbol{x}\in\Omega_\varepsilon$. Recall that $W(\boldsymbol{A},\boldsymbol{p})=U(\boldsymbol{A},\boldsymbol{p})-TS(\boldsymbol{A},\boldsymbol{p})$ and that $D^2_{\boldsymbol{p}}U(\boldsymbol{0},\boldsymbol{p}^0)$ is positive definite (See Lemma 5.1). Therefore, $D^2_{\boldsymbol{p}}W(\boldsymbol{A},\boldsymbol{p})$ is invertible for small T and $\|\boldsymbol{A}\|_{\mathrm{F}}$. By implicit function theorem, $\boldsymbol{p}=\boldsymbol{p}(\boldsymbol{A})$ is solvable. In other words, we have $\boldsymbol{v}_1=\boldsymbol{v}_1(\nabla\boldsymbol{u})$. Thus (6.28) implies that $\mathcal{L}_0[\boldsymbol{u},\boldsymbol{p}(\nabla\boldsymbol{u})]=2\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}]$.

Next we find that $\boldsymbol{v}_2$ can be solved from $\mathcal{N}_0=\boldsymbol{0}$. In fact, $\boldsymbol{v}_2$ comes from $\boldsymbol{a}_k^{\kappa\kappa'}$ and $\tilde{\boldsymbol{a}}_{kj}^{\kappa\kappa'}$. By (6.16)–(6.23), these terms are linear in $\boldsymbol{v}_2$. It can be checked that the coefficient of $\boldsymbol{v}_2$ in $\mathcal{N}_0=\boldsymbol{0}$ is $D^2_{\boldsymbol{p}}W(\boldsymbol{A},\boldsymbol{p})$ which is invertible at $\boldsymbol{A}=\nabla\boldsymbol{u}(\boldsymbol{x})$ and $\boldsymbol{p}=\boldsymbol{v}_1(\boldsymbol{x})$. Hence $\boldsymbol{v}_2$ is solvable $\boldsymbol{v}_2=\boldsymbol{v}_2(\boldsymbol{u},\boldsymbol{v}_1)$. Similarly, $\boldsymbol{v}_k=\boldsymbol{v}_k(\boldsymbol{u},\{\boldsymbol{v}_j\}_{j=1}^{k-1})$ can be solved algebraically from $\mathcal{N}_{k-2}[\boldsymbol{u},\{\boldsymbol{v}_j\}_{j=1}^{k}]=-\nabla^k_{\boldsymbol{p}^0}\boldsymbol{f}$ for $k\geq3$.

(iv) Solving $\boldsymbol{u}_k$, $k\geq0$. Taking the asymptotic expansion for $\mathcal{L}^A_\varepsilon+\mathcal{L}^B_\varepsilon$, we obtain

$$\begin{aligned}\mathcal{L}^A_\varepsilon[\boldsymbol{y}]+\mathcal{L}^B_\varepsilon[\boldsymbol{y}]&=\sum_{k=0}^{\infty}\varepsilon^k\mathcal{L}_k[\boldsymbol{u},\{\boldsymbol{v}_j\}_{j=1}^{k+1}]\\&=\mathcal{L}_0[\boldsymbol{u}_0,\boldsymbol{v}_1]+\varepsilon\Big\{\tfrac{\delta\mathcal{L}_0}{\delta\boldsymbol{u}}[\boldsymbol{u}_0,\boldsymbol{v}_1]\cdot\boldsymbol{u}_1+\mathcal{L}_1[\boldsymbol{u}_0,\boldsymbol{v}_1,\boldsymbol{v}_2]\Big\}+\varepsilon^2\Big\{\tfrac{\delta\mathcal{L}_0}{\delta\boldsymbol{u}}[\boldsymbol{u}_0,\boldsymbol{v}_1]\cdot\boldsymbol{u}_2\\&\quad+\tfrac{1}{2}\Big(\tfrac{\delta^2\mathcal{L}_0}{\delta\boldsymbol{u}^2}[\boldsymbol{u}_0,\boldsymbol{v}_1]\cdot\boldsymbol{u}_1\Big)\cdot\boldsymbol{u}_1+\tfrac{\delta\mathcal{L}_1}{\delta\boldsymbol{u}}[\boldsymbol{u}_0,\boldsymbol{v}_1,\boldsymbol{v}_2]\cdot\boldsymbol{u}_1+\mathcal{L}_2[\boldsymbol{u}_0,\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3]\Big\}+O(\varepsilon^3).\end{aligned} \tag{6.37}$$

Recall that the Euler–Lagrange equation is

$$\mathcal{L}^A_\varepsilon[\boldsymbol{y}]+\mathcal{L}^B_\varepsilon[\boldsymbol{y}]=\boldsymbol{f}^A+\boldsymbol{f}^B=2\boldsymbol{f}+\sum_{k=1}^{\infty}\varepsilon^k\nabla^k_{p_0}\boldsymbol{f}. \tag{6.38}$$

We compare each order $O(\varepsilon^k)$ in (6.37) and (6.38). Since $\boldsymbol{v}_1=\boldsymbol{v}_1(\nabla\boldsymbol{u})$ and $\mathcal{L}_0[\boldsymbol{u},\boldsymbol{p}(\nabla\boldsymbol{u})]=2\mathcal{L}_{\mathrm{CB}}[\boldsymbol{u}]$, we have $\boldsymbol{u}_0=\boldsymbol{u}_{\mathrm{CB}}$ which is the solution to $\mathcal{L}_0[\boldsymbol{u}_0,\boldsymbol{v}_1]=2\boldsymbol{f}$.

For order $O(\varepsilon)$, we have $\frac{\delta\mathcal{L}_0}{\delta\boldsymbol{u}}[\boldsymbol{u}_0,\boldsymbol{v}_1]\cdot\boldsymbol{u}_1=-\mathcal{L}_1[\boldsymbol{u}_0,\boldsymbol{v}_1,\boldsymbol{v}_2]+\nabla^1_{\boldsymbol{p}_0}\boldsymbol{f}$. The stability assumption implies that the linear operator $\frac{\delta\mathcal{L}_0}{\delta\boldsymbol{u}}[\boldsymbol{u}_0,\boldsymbol{v}_1]=\frac{\delta\mathcal{L}_{\mathrm{CB}}}{\delta\boldsymbol{u}}[\boldsymbol{u}_{\mathrm{CB}}]$ is invertible at the solution $\boldsymbol{u}_{\mathrm{CB}}=\boldsymbol{u}_0$ and $\boldsymbol{v}_1=\boldsymbol{v}_1(\nabla\boldsymbol{u}_0)$. Also note that $\mathcal{L}_1$ is in the divergence form. Thus $\boldsymbol{u}_1$ is solvable. Similarly, for order $O(\varepsilon^2)$, we have

$$\frac{\delta\mathcal{L}_0}{\delta\boldsymbol{u}}[\boldsymbol{u}_0,\boldsymbol{v}_1]\cdot\boldsymbol{u}_2=-\frac{1}{2}\left(\frac{\delta^2\mathcal{L}_0}{\delta\boldsymbol{u}^2}[\boldsymbol{u}_0,\boldsymbol{v}_1]\cdot\boldsymbol{u}_1\right)\cdot\boldsymbol{u}_1-\frac{\delta\mathcal{L}_1}{\delta\boldsymbol{u}}[\boldsymbol{u}_0,\boldsymbol{v}_1,\boldsymbol{v}_2]\cdot\boldsymbol{u}_1-\mathcal{L}_2[\boldsymbol{u}_0,\boldsymbol{v}_1,\boldsymbol{v}_2,\boldsymbol{v}_3]+\nabla^2_{\boldsymbol{p}_0}\boldsymbol{f}.$$

Note that this right-hand side is in the divergence form. Thus $\boldsymbol{u}_2$ is also solvable. For higher order terms, $\boldsymbol{u}_k$, $k\geq 3$ can be solved in a similar way although we will not use them to construct the approximate solution.

(v) Constructing $\tilde{\boldsymbol{y}}$. Based on the solutions $\{\boldsymbol{u}_k\}_{k=0}^2$ and $\{\boldsymbol{v}_k\}_{k=1}^4$, we construct the approximate solution $\tilde{\boldsymbol{y}}^A$ and $\tilde{\boldsymbol{y}}^B$ by (6.11) and (6.12). From the above derivation for $\{\boldsymbol{u}_k\}_{k=0}^2$ and $\{\boldsymbol{v}_k\}_{k=1}^4$, we have used the conditions $\mathcal{L}_0-2\boldsymbol{f}=\boldsymbol{0}$, $\mathcal{L}_k-\nabla^k_{\boldsymbol{p}_0}\boldsymbol{f}=\boldsymbol{0}$, $k=1,2$, and $\mathcal{N}_{-1}=\boldsymbol{0}$, $\mathcal{N}_0=\boldsymbol{0}$, $\mathcal{N}_k+\nabla^k_{\boldsymbol{p}_0}\boldsymbol{f}=\boldsymbol{0}$, $k=1,2$. This implies that $|\mathcal{L}^A_\varepsilon[\tilde{\boldsymbol{y}}]+\mathcal{L}^B_\varepsilon[\tilde{\boldsymbol{y}}]-\boldsymbol{f}^A-\boldsymbol{f}^B|\leq C\varepsilon^3$ and $|\mathcal{L}^A_\varepsilon[\tilde{\boldsymbol{y}}]-\mathcal{L}^B_\varepsilon[\tilde{\boldsymbol{y}}]-\boldsymbol{f}^A+\boldsymbol{f}^B|\leq C\varepsilon^3$. Hence $|\mathcal{L}^\kappa_\varepsilon[\tilde{\boldsymbol{y}}]-\boldsymbol{f}^\kappa|\leq C\varepsilon^3$, $\kappa=A,B$. ∎

6.3. Convergence. The framework established in [8] shows that the consistency, stability, and a fixed-point argument imply the convergence. We use this strategy.

Proof. **(Proof of Theorem 3.2.)** Recall that we have the approximate solution $\tilde{\boldsymbol{y}}$ by Propositions 6.3 and 6.5. In particular, it provides the same accuracy $O(\varepsilon^3)$. Then the proofs of Theorems 2.2 and 2.3 in [8] can be applied with a minor revision here. The difference is that we need to replace Lemma 6.7 in [8] by Lemma 5.2 in this paper. ∎

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Compliance with ethical standards. Conflict of interest. The authors declare that they have no conflict of interest.

Appendix. Harmonic approximation and the stress. In this appendix, we explain the relation of the finite temperature Cauchy–Born rule proposed in [28] and a Helmholtz free energy model similar to the one used in this paper. The difference between the Helmholtz free energy discussed below and the one used in our paper is as follows: the dynamical matrix in (A.2) is Fourier-transformed while we consider its spatial version in (2.6).

Consider a molecular system consisting of N atoms of which the atom positions are $\boldsymbol{Y}=\{\boldsymbol{y}_i\}_{i=1}^N$ with the reference perfect lattice $\boldsymbol{X}=\{\boldsymbol{x}_i\}_{i=1}^N$. Let $U=U(\{\boldsymbol{y}_i\}_{i=1}^N)$ be the potential energy. Suppose that there is no external force $f(\boldsymbol{x})$. Given a macroscopic deformation $\boldsymbol{A}$, we have that $U=U(\boldsymbol{A})=U(\{\boldsymbol{x}_i+\boldsymbol{x}_i\cdot\boldsymbol{A}\}_{i=1}^N)$ is the internal energy at the local minimizer $\{\boldsymbol{x}_i+\boldsymbol{x}_i\cdot\boldsymbol{A}\}_{i=1}^N$ with zero temperature.

As mentioned in [11,18], using quantum theory of harmonic approximation [2], the Helmholtz free energy at temperature T under deformation A can be written as:

$$F(\boldsymbol{A};T)=U(\boldsymbol{A})+k_{\mathrm{B}}T\sum_{i=1}^{N}\sum_{\beta=1}^{d}\log\left[2\sinh\left(\frac{h\omega_{\beta i}}{4\pi k_{\mathrm{B}}T}\right)\right], \tag{A.1}$$

where $\omega_{\beta i}$ are the frequencies of the dN normal modes. A further local harmonic approximation (treat each atom as independent oscillator) with classical limit ($h\to 0$), we can approximate (A.1) as

$$F(\boldsymbol{A};T)=U(\boldsymbol{A})+k_{\mathrm{B}}T\sum_{i=1}^{N}\log\left[\frac{\hbar\det(\boldsymbol{D}_{ii}(\boldsymbol{A}))^{1/2}}{k_{\mathrm{B}}T}\right], \tag{A.2}$$

where $\det(\boldsymbol{D}_{ii}(\boldsymbol{A}))=\prod_{\beta=1}^{d}\omega_{\beta i}$ is the determinant of the (Fourier-transformed) local dynamics matrix of atom i, the reduced Planck constant $\hbar=\frac{h}{2\pi}$, and we have used the first order Taylor expansion to approximate the hyperbolic sine function $\sinh(x)$. This is exactly the energy we used in (2.3).

Now if we take a derivative of $F(\boldsymbol{A};T)$ with respect to the deformation $\boldsymbol{A}$, we can gain the first Piola–Kirchhoff stress:

$$\begin{aligned}\boldsymbol{P}&=\frac{\partial F(\boldsymbol{A};T)}{\partial \boldsymbol{A}}\\&=\frac{\partial U}{\partial \boldsymbol{A}}+\sum_{i=1}^{N}\frac{1}{2}k_{\mathrm{B}}T\det(\boldsymbol{D}_{ii}(\boldsymbol{A}))^{-1}\frac{\partial\det(\boldsymbol{D}_{ii}(\boldsymbol{A}))}{\partial \boldsymbol{A}}\\&=\frac{\partial U}{\partial \boldsymbol{A}}+\sum_{i=1}^{N}\frac{1}{2}k_{\mathrm{B}}T\det(\boldsymbol{D}_{ii}(\boldsymbol{A}))^{-1}\frac{\partial\det(\boldsymbol{D}_{ii}(\boldsymbol{A}))}{\partial \boldsymbol{D}_{ii}(\boldsymbol{A})}:\frac{\partial \boldsymbol{D}_{ii}(\boldsymbol{A})}{\partial \boldsymbol{A}}\\&=\frac{\partial U}{\partial \boldsymbol{A}}+\sum_{i=1}^{N}\frac{1}{2}k_{\mathrm{B}}T\boldsymbol{D}_{ii}^{-1}(\boldsymbol{A}):\frac{\partial \boldsymbol{D}_{ii}(\boldsymbol{A})}{\partial \boldsymbol{A}}.\end{aligned} \tag{A.3}$$

where in the last equality we have used the formula $\frac{\partial\det(\boldsymbol{C})}{\partial \boldsymbol{C}}=\det(\boldsymbol{C})\boldsymbol{C}^{-\mathrm{T}}$ for a matrix $\boldsymbol{C}$ and the fact that $\boldsymbol{D}_{ii}$ is symmetric. Furthermore, the above formula (A.3) can also be extended to the complex lattice case if we replace $\boldsymbol{D}_{ii}(\boldsymbol{A})$ with $\boldsymbol{D}_{ii}(\boldsymbol{A},\boldsymbol{p}(\boldsymbol{A}))$.

This stress formulation is essentially the same as that in [28]. The difference is that in the above derivation we use quantum harmonic approximation to simplify the free energy, while in [28], classical harmonic approximation method is used. This difference, however, appears only as an additive constant ($\log\frac{\hbar}{k_{\mathrm{B}}T}$) in the free energy, which will not affect the expression of the stress since it will vanish when derivative is taken. Furthermore, we use (spatial) local harmonic approximation in this paper to approximate the force constants, while [28] utilizes Fourier transform to block diagonalize the force constants.

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