The Continuum Limit of the Thomas-Fermi-Dirac-von Weizsäcker Model

by

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Dissertation submitted in partial fulfillment of the requirements for the degree of
Doctor of Philosophy in the Department of Mathematics
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Abstract

This work studies the atomistic Thomas-Fermi-Dirac-von Weiszacker model on a Bravais lattice, and establishes its relationship with the continuum elasticity model, thus provides it a solid microscopic foundation at the atomistic level. More specifically, we derive the stored energy density from the atomistic TFDW functional by homogenization. In addition, by assuming a reasonable stability condition, the discrete deformation function we get from the atomistic model converges to the Cauchy-Born solution from solving the continuum model with a quadratic rate due to underlying inversion symmetry of the lattice. In our analysis, we use the two-scale ansatz to construct approximate solutions, the discrete Fourier analysis in the consistence estimate, and the perturbation technique as well as the decaying property to analyze the Hessian in the stability analysis.

Contents

List of Abbreviations and Symbols

Abbreviations

at	atomistic model.
CB	Cauchy-Born.
exa	exact solution.
TFDW	Thomas-Fermi-Dirac-von Weizsäcker.
per	periodic solution.
undeform	undeformed lattice.

Symbols

$\mathbb{L}$	A simple Bravais lattice.
Ω	The unit domain of a Bravais lattice.
Ω^*	The reciprocal of Ω.
$\epsilon\mathbb{L}$	An ϵ-scaled simple Bravais lattice.
Ω_ϵ	$\Omega \cap \epsilon\mathbb{L}$.
Ω_ϵ^*	The reciprocal of Ω_ϵ.
X_i	An undeformed atom position in Ω_ϵ.
ξ	A wave character in Ω_ϵ^*.
Y	The discrete deformation function defined on Ω_ϵ.
u	The continuous deformation.
τ	The Fourier interpolation of Y, sometimes denoted as τ_Y.

τ_ϵ	The ϵ-scaled version of τ.
u_{CB}	The solution of the continuum elasticity model, derived from Cauchy-born rule.
Y_{CB}	The discrete version of u_{CB}.
m_a	A locally compact background charge function for one atom, which also has the inversion symmetry.
ρ_b	The background charge function defined on a Bravais lattice $\mathbb{L}$.
ρ_ϵ	The ϵ-scaled background charge function.
$\mathcal{V}$	A shorthand for a general pair of electron density function and the potential (ν, V).
$(\nu_{\text{per}}, V_{\text{per}})$	A pair of undeformed periodic solutions of (ν, V).
$\mathcal{V}_{\text{per}}$	A shorthand for $(\nu_{\text{per}}, V_{\text{per}})$.
$(\nu_{\text{CB}}, V_{\text{CB}})$	A pair of Cauchy-Born solutions of (ν, V).
$\mathcal{V}_{\text{CB}}$	A shorthand for $(\nu_{\text{CB}}, V_{\text{CB}})$.
(ν^0, V^0)	A pair of two-scale ansatz approximation of (ν, V).
$\mathcal{V}^0$	A shorthand for (ν^0, V^0).
$(\nu_{\text{exa}}, V_{\text{exa}})$	A pair of exact solutions of (ν, V).
$\mathcal{V}_{\text{exa}}$	A shorthand for $(\nu_{\text{exa}}, V_{\text{exa}})$.
$(\nu^\epsilon, V^\epsilon)$	A pair of general ϵ-scaled solutions of (ν, V).
$\mathcal{F}_{\text{TFDW}}$	The system of Euler-Lagrange equations of the Thomas-Fermi-Dirac-von Weizsäcker model.
$\mathcal{F}_{\text{CB}}$	The Euler-Lagrange equation of the continuum elasticity model derived from the Cauchy-Born rule.
W_{CB}	The stored energy density function of the continuum elasticity model derived from the Cauchy-Born rule.
$\mathcal{L}_{(\mathcal{V},\tau)}$	The linearized operator of the atomistic TFDW functional evaluated at $(\mathcal{V}, \tau)$.
$\mathcal{H}_{\text{at}}[Y]$	The Hessian of the atomistic TFDW functional evaluated at Y.

$\mathcal{H}_{\text{at}}[\text{Id}]$	The Hessian of the atomistic TFDW functional evaluated at $Y = \text{Id}$.
$\mathcal{D}^{Y}_{\text{at}}[\xi]$	The dynamical matrix of $\mathcal{H}_{\text{at}}[Y]$ evaluated at $\xi \in \Omega^*_\epsilon$.
$\mathcal{D}^{\text{Id}}_{\text{at}}[\xi]$	The dynamical matrix of $\mathcal{H}_{\text{at}}[\text{Id}]$ evaluated at $\xi \in \Omega^*_\epsilon$.
$w^{Y}_{j}[\xi]$	The eigenvalues of $\mathcal{D}^{Y}_{\text{at}}$ evaluated at $\xi \in \Omega^*_\epsilon$.
$w^{\text{Id}}_{j}[\xi]$	The eigenvalues of $\mathcal{D}^{\text{Id}}_{\text{at}}$ evaluated at $\xi \in \Omega^*_\epsilon$.

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1

Introduction

One interesting problem in studying solid materials is to connect the macroscopic and the microscopic models. At the macroscopic level, one of the models we use to study the mechanical property of the material is the continuum theory. While at the microscopic level, we use quantum mechanics to study the atomistic and electronic properties of the material. So it is natural to ask what the relationship between these two kinds of theories is.

This idea of connecting macro and microscopic models of solids dates back to Cauchy as in Cauchy (1828a), Cauchy (1828b). Cauchy studies solids with the assumption that the atoms interact via a pairwise central potential, with which he derived expressions for the elastic moduli of cubic crystals. Later armed with the principles of quantum mechanics, Born extended Cauchy's work to initiate a systematic study of the microscopic foundation of macroscopic properties of solids. A central object formulated by him that we will discuss is the so-called Cauchy-Born rule. The classic reference is the book "Dynamical Theories of Crystal Lattice", Born and Huang (1968), and more description about the classical Cauchy-Born rule can be found in Ball and James (1992), Ericksen (2005). In addition, more recent application of Cauchy-Born rule can be found in E and Ming (2007a), E and Ming (2007b), E and Lu (2007), E and Lu (2011), E and Lu (2012).

Specifically, the purpose of this work is to provide a microscopic foundation of one macroscopic model for the simple crystal lattices as stated in E and Lu (2014). More specifically, we are going to study the relationship between the continuum model and the atomistic-electronic model of the deformation of a simple crystal lattice called the Bravais lattice. Macroscopically, we use a continuum elasticity model to describe the deformation in which the corresponding functional involves a stored energy density function of the gradient of the deformation. So this model can be regarded as a first-order description of the elasticity problem. Meanwhile, crystal lattices can also be studied on the atomistic level, and in this work we use the Thomas-Fermi-Dirac-von Weizsacker model which uses an electron density function to describe the system. We will derive the stored energy density from this atomistic TFDW model by the Cauchy-Born rule. With this connection between the two models, we show quadratic convergence of the deformations derived from the models in a limiting process.

A similar work connecting microscopic and macroscopic models is done in E and Ming (2007a) using the classical potential function instead of the TFDW model we will use. Blanc et al. (2002) studies the TFDW model for smoothly deformed crystals and shows the convergence of the total energy of the system to a limiting value given by the Cauchy-Born rule in the continuum limit. A similar analysis of the electronic TFDW model with spin-polarization is given in E and Lu (2012). Another useful reference using the classical potential is Lu and Ming (2013) in which a force-based hybrid method is used to combine discrete and continuum models. A more general discussion on the Thomas-Fermi type models is provided in Lieb (1981). Friesecke and Theil (2002) studied a lattice-spring model and showed minimizers may not satisfy the Cauchy-Born rule. Parallel to the Thomas-Fermi type of models, or more generally, orbital-free models, there is another type of quantum mecahnics models among which the Kohn-Sham density functional model is an important one. **?**, Kohn and Sham (1965) provide more details on this type of model. Finally, a thorough overview is given in the survey E and Lu (2014).

One recent related work is Nazar and Ortner (2015) which establishes a pointwise stability estimate for the Thomas-Fermi-von Weizs$\ddot{a}$cker (TFW) model and demonstrates that a local perturbation of a nuclear arrangement results in a local response in the electron density and electrostatic potential. This locality property will also play an important role in this work. For the numerical algorithm application of the locality property, please consult Benzi et al. (2013), **?**, Ismail-Beigi and Arias (1999), Prodan and Kohn (2005) for Kohn-Sham type models.

This work makes improvement by studying the Thomas-Fermi-Dirac-von Weizsacker model at the atomistic level involving the discrete deformation function of the lattice. More specifically, following this line of analysis, derivation of the stored energy density, the consistence estimate and the concept of stability are established at the atomistic level, which extends analysis of the classic electronic TFDW model.

In this work, we will use the Cauchy-Born rule in several contexts. The Cauchy-Born rule is the principle that we use to connect microscopic and macroscopic models. The rule states that the stored energy density W_{CB} in the macroscopic continuum elasticity model can be obtained from the energy density of a uniformly deformed lattice as given below

$$W_{\text{CB}}(A) = \lim_{n\to\infty} \frac{1}{|n\Omega|} \mathcal{I}_{\text{TFDW}}(\mathcal{V}_{\text{CB}}(A); \rho_{b,0}(A)) \tag{1.1}$$

where $\mathcal{I}_{\text{TFDW}}$ is the total energy functional, Ω is the unit cell, A is a constant matrix representing the uniform deformation. So $\frac{1}{|n\Omega|}\mathcal{I}_{\text{TFDW}}$ represents the energy density. As we will show in this work, because of periodicity, we can nicely remove the limit and thus get an explicit expression of W_{CB}.

Besides its use to derive the stored energy density, we also apply the principle of the Cauchy-Born rule in our analysis of the electronic TFDW model with a fixed deformation to construct the leading-order approximate solution $\mathcal{V}_{\text{CB}}$ of the electron density and the potential. In this context, we combine the Cauchy-Born rule and the two-scale ansatz so that locally around each atom, we approximate the electron density ν and the potential V with a uniform deformation as illustrated below

$$\nu_{\text{CB}}(x) := \nu_{\text{CB}}(\frac{x}{\epsilon}; \nabla u(x)), \quad V_{\text{CB}}(x) := V_{\text{CB}}(\frac{x}{\epsilon}; \nabla u(x)). \tag{1.2}$$

Now let us describe the problem in more detail. The underlying object we study in this work is the deformation of a crystal lattice. So let us introduce the definition of a Bravais lattice which contains only one kind of atom. A Bravais lattice $\mathbb{L}$ is a discrete set of points in $\mathbb{R}^3$:

$$\mathbb{L} = \{X \in \mathbb{R}^3 | X = \sum_{j=1}^{3} n_j a_j, n_j \in \mathbb{Z}\}. \tag{1.3}$$

where $\{a_1, a_2, a_3\}$ are the basis vectors of $\mathbb{L}$.

The unit cell or unit domain Ω of $\mathbb{L}$ is

$$\Omega = \{x \in \mathbb{R}^3 | x = \sum_{j=1}^{3} c_j a_j, 0 \leqslant c_j < 1\}. \tag{1.4}$$

The deformation u of the lattice is a function defined on the unit domain

$$u : \Omega \to \mathbb{R}^3. \tag{1.5}$$

Our macroscopic model is described by the following continuum elasticity functional

$$\mathcal{I}_{\text{ct}}(v) = \int_{\Omega} W_{\text{CB}}(\nabla v(x)) - f(x) \cdot v(x) dx, \tag{1.6}$$

where f is an external force. We want to find a local minimizer u such that

$$\mathcal{I}_{\mathrm{ct}}(u) = \min_{v - B\cdot x \in X} \mathcal{I}_{\mathrm{ct}}(v), \quad u - B\cdot x \in X, \tag{1.7}$$

where

$$X = \{v \in W_1^{m+2,p} | \int_{\Omega} v = 0\}, \tag{1.8}$$

in which $B \in M_{3\times 3}$ is a constant matrix, and $W_1^{m+2,p}$ represents the space of periodic $W^{m+2,p}$ functions from Ω to $\mathbb{R}^3$.

For this purpose, we will study the corresponding Euler-Lagrange equation

$$\begin{cases} -\mathrm{div} D_A W_{\mathrm{CB}}(\nabla v) = f & \text{in } \Omega \\ v - B\cdot x \quad \text{periodic on } \partial\Omega. \end{cases} \tag{1.9}$$

On the microscopic level, we use the Thomas-Fermi-Dirac-von Weizsäcker model, in which the total energy functional is

$$\mathcal{I}_{\mathrm{TFDW}} = \int_{\mathbb{R}^3} \rho^{\frac{5}{3}}(y) + |\nabla\sqrt{\rho(y)}|^2 - \rho^{\frac{4}{3}}(y)dy + \frac{1}{2}D(\rho - \rho_b, \rho - \rho_b), \tag{1.10}$$

where $\rho : \mathbb{R}^3 \to \mathbb{R}$ is the electronic density in Eulerian coordinates with the constraints $\int_{\mathbb{R}^3} \rho(y)dy = \int_{\mathbb{R}^3} \rho_b(y)dy$ and $\rho > 0$, where ρ_b is the background charge density. The shorthand notation $D(\cdot,\cdot)$ is defined as

$$D(f,g) = \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{f(y_1)g(y_2)}{|y_1 - y_2|} dy_1 dy_2 \tag{1.11}$$

Thus

$$D(\rho - \rho_b, \rho - \rho_b) = \int_{\mathbb{R}^3} V(y)(\rho - \rho_b)(y)dy, \tag{1.12}$$

where V is the potential

$$V(y) = \int_{\mathbb{R}^3} \frac{\rho(y') - \rho_b(y')}{|y - y'|} dy'. \tag{1.13}$$

In our context, we will use a periodic version of the TFDW functional

$$\mathcal{I}_{\text{TFDW}} = \int_{\Omega} \rho^{\frac{5}{3}}(y) + |\nabla\sqrt{\rho(y)}|^2 - \rho^{\frac{4}{3}}(y)dy + \frac{1}{2}D_{\Omega}(\rho - \rho_b, \rho - \rho_b), \tag{1.14}$$

Next, in order to describe the limiting process, we consider scaling of the system. We introduce a scaling parameter $\epsilon = \frac{1}{n}$ to scale the lattice, and thus the whole problem. As $n \to \infty$ or $\epsilon \to 0$, the lattice in the fixed unit domain will become a macroscopic piece of solid, thus this liming process provides the connection which we need between our macroscopic and microscopic models.

For a fixed scaling parameter $\epsilon = \frac{1}{n}$, where n is a positive integer, the scaled lattice is

$$\mathbb{L}_{\epsilon} = \{\epsilon X | X \in \mathbb{L}\}. \tag{1.15}$$

Define Ω_{ϵ} as

$$\Omega_{\epsilon} = \Omega \cap \mathbb{L}_{\epsilon} = \{X \in \mathbb{R}^3 | X = \sum_{j=1}^{3} c_j a_j, c_j \in \epsilon\mathbb{Z} \cap [0,1)\} \tag{1.16}$$

which contains all the scaled atom positions in the unit domain.

We then define the discrete deformation function Y on Ω_{ϵ} which is simply the restriction of the deformation u to the discrete atom positions in Ω. Otherwise, we can also define Y, and interpret the deformation u as an interpolation of Y.

The above scaling is called ϵ-scaling. Sometimes it is easier to analyze the system with a unit scaling which assume that the consecutive atom positions have a unit scale. For example, with ϵ-scaling, The system of Euler-Lagrange equations for $(\nu_{\epsilon} = \sqrt{\rho(\frac{\cdot}{\epsilon})}, V_{\epsilon} = V(\frac{\cdot}{\epsilon}))$ in Eulerian coordinates is

$$\begin{cases} -\epsilon^2 \Delta \nu_{\epsilon} + \frac{5}{3}\nu_{\epsilon}^{\frac{7}{3}} - \frac{4}{3}\nu_{\epsilon}^{\frac{5}{3}} + V_{\epsilon}\nu_{\epsilon} = 0, \quad y \in \Omega \\ -\epsilon^2 \Delta V_{\epsilon} = 4\pi(\nu_{\epsilon}^2 - \rho_b^{\epsilon}), \quad y \in \Omega, \end{cases} \tag{1.17}$$

While with unit scaling, the corresponding system of Euler-Lagrange equations of $(\nu = \sqrt{\rho}, V)$ in Eulerian coordinates with a fixed Y^ϵ which is the scaled version of Y is

$$\begin{cases} -\Delta\nu + \frac{5}{3}\nu^{\frac{7}{3}} - \frac{4}{3}\nu^{\frac{5}{3}} + V\nu = 0, \quad y \in n\Omega \\ -\Delta V = 4\pi(\nu^2 - \rho_b), \quad y \in n\Omega. \end{cases} \tag{1.18}$$

Next, we introduce the stored energy density function. The connection between the continuum elasticity model and the TFDW model is the derivation of the stored energy density from the TFDW functional by the Cauchy-Born rule. More specifically, the stored energy density in the macroscopic continuum elasticity model can be obtained from the energy density of a uniformly deformed lattice. So explicitly with a fixed deformation $\tau = id + u$ which extends Y to Ω, we construct the Cauchy-Born solutions

$$\nu_{\mathrm{CB}}(x) := \nu_{\mathrm{CB}}(\frac{x}{\epsilon}; \nabla u(x)), \quad V_{\mathrm{CB}}(x) := V_{\mathrm{CB}}(\frac{x}{\epsilon}; \nabla u(x)), \tag{1.19}$$

and the corresponding TFDW functional is

$$\mathcal{I}_{\mathrm{TFDW}}(\nu_{\mathrm{CB}}, V_{\mathrm{CB}}, \rho_{b,0}) \tag{1.20}$$

$$= \int_\Omega \nu_{\mathrm{CB}}^{\frac{10}{3}} + |\nabla\nu_{\mathrm{CB}}|^2 - \nu_{\mathrm{CB}}^{\frac{8}{3}} + \frac{1}{2}V_{\mathrm{CB}}(\nu_{\mathrm{CB}}^2 - \rho_{b,0})dy - \epsilon^3|\Omega| \sum_{X\in\Omega_\epsilon} f(X)(Y(X) - X) \tag{1.21}$$

$$= \int_\Omega F_{\mathrm{CB}}(\frac{x}{\epsilon}, x)dx - \epsilon^3|\Omega| \sum_{X\in\Omega_\epsilon} f(X)(Y(X) - X) \tag{1.22}$$

where $\rho_{b,0}$ is the first-order approximation of ρ_b.

Now we assume the deformation is uniform, i.e. $u(x) = Ax$ for any $x \in \Omega$, where A is a constant matrix. Then the stored energy density is defined as

$$W_{\mathrm{CB}}(A) = \lim_{n\to\infty} \frac{1}{|n\Omega|}\mathcal{I}_{\mathrm{TFDW}}(\nu_{\mathrm{CB}}, V_{\mathrm{CB}}, \rho_{b,0}) \tag{1.23}$$

In order to assure that the Cauchy-Born rule gives a stable approximation, we need certain stability conditions at various levels. In order to give the stability conditions, we need to analyze the linearization of the system of Euler-Lagrange equations. When there is no deformation, denote the electron density and the potential as $(\nu_{\text{per}}, V_{\text{per}})$ which are periodic, then the linearization of the system of the Euler-Lagrange equations without deformation is

$$\mathcal{L}_{\text{per}} \begin{pmatrix} \omega \\ W \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{1,\text{per}} & \nu_{\text{per}} \\ \nu_{\text{per}} & \frac{1}{8\pi}\Delta \end{pmatrix} \begin{pmatrix} \omega \\ W \end{pmatrix} \tag{1.24}$$

in which

$$\mathcal{L}_{1,\text{per}} = -\Delta + \frac{35}{9}\nu_{\text{per}}^{\frac{4}{3}} - \frac{20}{9}\nu_{\text{per}}^{\frac{2}{3}} + V_{\text{per}}. \tag{1.25}$$

The **Stability Condition A** states that

$$\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((L_n^2)^2)} \leqslant M_{\text{per}} \tag{1.26}$$

for any arbitrary positive integer $n = \frac{1}{\epsilon}$, where M_{per} is a positive constant independent of n.

Once we solve the electronic TFDW model and get the local minimizer $(\nu_{\text{exa}}, V_{\text{exa}})$, we define the the atomistic TFDW functional $\mathcal{I}_{\text{at}}(Y) = \mathcal{I}_{\text{TFDW}}(\nu_{\text{exa}}(Y), V_{\text{exa}}(Y), Y)$ as a functional of the discrete deformation function Y. Denote the Hessian of the functional as $\mathcal{H}_{\text{at}}[\text{Id}]$ in the undeformed case. Then **Stability Condition B** states that the eigenvalues $w_k^{\text{Id}}[\xi]$ of the dynamical matrix $\mathcal{D}_{\text{at}}^{\text{Id}}[\xi]$ of the Hessian $\mathcal{H}_{\text{at}}[\text{Id}]$ satisfy

$$|w_k^{\text{Id}}[\xi]| \geqslant \Lambda|\xi|^2, \tag{1.27}$$

for $k = 1, 2, 3$, any $\xi \in \Omega_\epsilon^*$ and some constant $\Lambda > 0$, where Ω_ϵ^* is the reciprocal space of Ω_ϵ. Finally **Stability Conditions A** and **B** imply the following **Stability Condition C** for the continuum elasticity model

$$D_A^2 W_{\text{CB}}(0)(\xi \otimes \eta, \xi \otimes \eta) \geqslant \Lambda|\xi|^2|\eta|^2 \tag{1.28}$$

for any $\xi, \eta \in \mathbb{R}^3$.

With the above brief description of the setup, we now give the main theorem

Theorem 1.0.1. *Under* **Stability Conditions A, B** *(then* **Stability Condition C** *holds), there exists a positive constant M so that if $m_a \in C_0^\infty(R^3)$ (used in defining ρ_b), and $\|f\|_{W^{27,p}(\Omega)} \leqslant \delta_f$ for some constant $\delta_f > 0$ and $p > 1$, we have*

$$\|Y_{at} - Y_{CB}\|_{\epsilon,7} \leqslant M\epsilon^2. \tag{1.29}$$

where Y_{at} is a $W_\epsilon^{1,\infty}$ local minimizer of the atomistic TFDW functional

$$\mathcal{I}_{at}(Y) = \mathcal{I}_{TFDW}(\nu_{exa}(Y), V_{exa}(Y), Y),$$

and Y_{CB} is the restriction of $\tau_{CB} = id + u_{CB}$ which is a $W_1^{1,\infty}$ local minimizer of the continuum elasticity functional

$$\mathcal{I}_{ct}(v) = \int_\Omega W_{CB}(\nabla v(x)) - f(x) \cdot v(x) dx.$$

The reason we can achieve quadratic rate of convergence though the Cauchy-Born rule only provides a first-order approximation is that the underlying lattice has inversion symmetry which leads to the cancelation of the first-order terms.

Finally, we introduce the methods used to prove the main theorem. We first study the system of the Euler-Lagrange equations in (ν, V) with a fixed deformation u under **Stability Condition A** to get the solution $(\nu_{\text{exa}}, V_{\text{exa}})$. Then we study the atomistic TFDW functional $\mathcal{I}_{\text{at}}(Y) = \mathcal{I}_{\text{TFDW}}(\nu_{\text{exa}}(Y), V_{\text{exa}}(Y), Y)$ under **Stability Condition B** to construct Y_{at}. In the process of constructing Y_{at}, we use Y_{CB} which we get from the continuum elasticity model $\mathcal{I}_{\text{ct}}$ which by homogenization is the leading-order approximation of $\mathcal{I}_{\text{at}}(Y)$ under **Stability Condition C** as the first-order approximation. Then explicit computation shows that the first-order approximation vanishes due to the inversion symmetry of the underlying lattice, thus we can achieve quadratic rate of convergence.

In our analysis of the TFDW model with a fixed deformation, we are going to find a local minimizer of the functional by solving the system of Euler-Lagrange equations in (ν, V). We start with the undeformed case, and get $(\nu_{\text{per}}, V_{\text{per}})$ from a system of Poisson equations. Then we analyze the equations with a small uniform deformation $u(x) = Bx$. By using the implicit function theorem in normed spaces and the Cauchy-Born rule, we get the Cauchy-Born solutions $(\nu_{\text{CB}}, V_{\text{CB}})$. Then in order to achieve higher-order approximation, we use the two-scale ansatz to decompose the equations, and get $\nu^0 = \nu_{\text{CB}} + \epsilon\nu_1 + \epsilon^2\nu_2$, $V^0 = V_{\text{CB}} + \epsilon V_1 + \epsilon^2 V_2$. Finally we are able to use Newton-Raphson iteration to get the exact solutions $(\nu_{\text{exa}}, V_{\text{exa}})$. These exact solutions preserve the decaying property which originally holds for the background charge ρ_b:

$$\|\frac{\partial}{\partial Y_i}\nu_{\text{exa}}(x, Y)\| \leqslant \frac{C}{\epsilon} e^{-\gamma|x + \frac{-X_i + r_{i,\epsilon x}}{\epsilon}|} \tag{1.30}$$

$$\|\frac{\partial}{\partial Y_i}V_{\text{exa}}(x, Y)\| \leqslant \frac{C}{\epsilon} e^{-\gamma|x + \frac{-X_i + r_{i,\epsilon x}}{\epsilon}|}, \tag{1.31}$$

Furthermore, we study the perturbation of the exact solutions with respect to the deformation which will be used for our analysis of the perturbation of the Hessian $\mathcal{H}_{\text{at}}[\text{Id}]$:

$$\|\frac{\partial}{\partial Y_j}\mathcal{V}_{\text{exa}}(x, Y_2) - \frac{\partial}{\partial Y_j}\mathcal{V}_{\text{exa}}(x, Y_1)\| \leqslant C\epsilon^{-2} e^{-\gamma|x - \frac{X_j + r_{j,\epsilon,x}}{\epsilon}|}\|Y_2 - Y_1\|_{W_\epsilon^{3,\infty}}$$

where $\mathcal{V}_{\text{exa}} = (\nu_{\text{exa}}, V_{\text{exa}})$.

Besides the stability conditions, we also need the following consistence estimate in the proof of the main theorem

$$\|\mathcal{F}_{\text{at}}[Y_{\text{CB}}]\|_{\epsilon,5} \leqslant C(\|u_{\text{CB}}\|_{H_1^{29}})\epsilon^2. \tag{1.32}$$

where $\mathcal{F}_{\text{at}}[Y]$ denotes the Euler-Lagrange equation in Y of the atomistic TDFW functional $\mathcal{I}_{\text{at}}(Y)$. Notice that our final quadratic rate of convergence comes from the ϵ^2 factor in the consistence estimate. In the derivation of the estimate, we first expand $\mathcal{F}_{\text{at}}[Y_{\text{CB}}]$ according to orders of ϵ. Then the leading-order terms form the Euler-Lagrange equation of the continuum elasticity model in which u_{CB} is the solution, so these terms vanish. The ϵ-order terms are all canceled due to the inversion symmetry of the underlying lattice. Therefore we can achieve ϵ^2-order estimate on the right hand side.

The other component we will need is the following stability result which we prove in the final part of this work:

Given **Stability Condition B**, i.e. the eigenvalues of the dynamical matrix $\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi]$ without deformation satisfy

$$|w_j^{\mathrm{Id}}[\xi]|^2 \geqslant \Lambda|\xi|^2, \quad j = 1, 2, 3 \tag{1.33}$$

for every $\xi \in \Omega_\epsilon^*$, then the eigenvalues of the dynamical matrix $\mathcal{D}_{\mathrm{at}}^{Y^t}[\xi]$ at Y^t satisfy

$$|w_j^{Y^t}[\xi]|^2 \geqslant C_t\Lambda|\xi|^2, \quad j = 1, 2, 3 \tag{1.34}$$

for every $\xi \in \Omega_\epsilon^*$. Here $Y^t = tY + (1-t)Y_{\mathrm{CB}}$ for $0 < t < 1$, and Y is close to Y_{CB}.

This result comes from the analysis of the perturbation of the Hessian with respect to the deformation:

$$\|\mathcal{H}_{\mathrm{at}}[Y_2](i,j) - \mathcal{H}_{\mathrm{at}}[Y_1](i,j)\| \leqslant C_{\mathcal{H}}\epsilon^{-2}e^{-\frac{\gamma}{\epsilon}|X_i - X_j|}\|Y_2 - Y_1\|_{W_\epsilon^{1,\infty}} \tag{1.35}$$

whose proof needs our previous estimate on the decaying property of the potential and the perturbation of the linearized operator:

$$\begin{aligned}
&\|\mathcal{L}_{(\mathcal{V}_1,\tau_1)} - \mathcal{L}_{(\mathcal{V}_2,\tau_2)}\|_{\mathcal{L}((H_n^{k+2})^2,(H_n^k)^2)} \\
\leqslant& C_{\mathcal{L}}\max(\|\mathcal{V}_1 - \mathcal{V}_2\|_{(W^{k,\infty}(n\Omega))^2}, \|\tau_1 - \tau_2\|_{W_1^{k+3,\infty}}) \\
\leqslant& C_{\mathcal{L}}\max(\|\mathcal{V}_1 - \mathcal{V}_2\|_{(H^{k+2}(n\Omega))^2}, \|\tau_1 - \tau_2\|_{W_1^{k+3,\infty}})
\end{aligned}$$

With these estimates in hand, it is then straightforward to apply the fixed point theorem to prove the main theorem.

2

Basic Setup

In this chapter, we introduce the necessary objects and tools for this work.

2.1 Lattice, Domain and Scaling

We consider Bravais lattices which are simple lattices. They take the form:

$$\mathbb{L} = \{X \in \mathbb{R}^3 | X = \sum_{j=1}^{3} n_j a_j, n_j \in \mathbb{Z}\}. \tag{2.1}$$

where $\{a_1, a_2, a_3\}$ are the basis vectors of $\mathbb{L}$. Define the reciprocal basis vectors $\{b_1, b_2, b_3\}$ that satisfies $a_i \cdot b_j = 2\pi\delta_{ij}$, where δ_{ij} is the Kronecker delta. Then the corresponding reciprocal lattice is defined as

$$\mathbb{L}^* = \{\xi \in \mathbb{R}^3 | \xi = \sum_{j=1}^{3} n_j b_j, n_j \in \mathbb{Z}\}, \tag{2.2}$$

Notice that both $\mathbb{L}$ and $\mathbb{L}^*$ have the translational symmetry.

The unit cell or unit domain Ω of $\mathbb{L}$ is

$$\Omega = \{x \in \mathbb{R}^3 | x = \sum_{j=1}^{3} c_j a_j, 0 \leqslant c_j < 1\}. \tag{2.3}$$

Similarly the unit domain of the reciprocal lattice is

$$\Omega^* = \{\xi \in \mathbb{R}^3 | \xi = \sum_{j=1}^{3} c_j b_j, -\frac{1}{2} \leqslant c_j < \frac{1}{2}\}. \tag{2.4}$$

For a fixed scaling parameter $\epsilon = \frac{1}{n}$, where n is a positive integer, the scaled lattice is

$$\mathbb{L}_\epsilon = \{\epsilon X | X \in \mathbb{L}\}. \tag{2.5}$$

Define Ω_ϵ as

$$\Omega_\epsilon = \Omega \cap \mathbb{L}_\epsilon = \{X \in \mathbb{R}^3 | X = \sum_{j=1}^{3} c_j a_j, c_j \in \epsilon\mathbb{Z} \cap [0, 1)\} \tag{2.6}$$

which contains all the scaled atom positions in the unit domain.

The corresponding reciprocal space Ω_ϵ^* is

$$\Omega_\epsilon^* = \{\xi \in \mathbb{R}^3 | \xi = \sum_{j=1}^{3} c_j b_j, c_j \in \mathbb{Z} \cap [-\frac{1}{2\epsilon}, \frac{1}{2\epsilon})\}. \tag{2.7}$$

Notice that $\xi = O(\frac{1}{\epsilon})$, and

$$e^{\imath X \cdot \xi} = 1, \quad \forall X \in \mathbb{L}, \forall \xi \in \Omega_\epsilon^*. \tag{2.8}$$

Furthermore, the cardinality is

$$\mathrm{card}(\Omega_\epsilon) = \mathrm{card}(\Omega_\epsilon^*) = n^3 = \epsilon^{-3}. \tag{2.9}$$

The space $n\Omega$ is call the supercell which is more convenient to use in some context, and define its discrete version Ω_n as

$$\Omega_n = n\Omega_\epsilon. \tag{2.10}$$

Next consider the basic wave functions defined on Ω_ϵ: $\{e^{\imath X \cdot \xi}\}_{X \in \Omega_\epsilon}$ for each fixed $\xi \in \Omega_\epsilon^*$. If $X = \sum_{j=1}^{3} X^j a_j, \xi = \sum_{k=1}^{3} \xi^k b_k$, then $X \cdot \xi = \sum_{j,k=1}^{3} X^j \xi^k a_j b_k = 2\pi \sum_{j,k=1}^{3} X_j \xi^k \delta_{jk} = 2\pi \sum_{j=1}^{3} X^j \xi^j$. We have the following orthonormality

Lemma 2.1.1.

$$\epsilon^3 \sum_{\xi\in\Omega_\epsilon^*} e^{\imath(X_i-X_j)\cdot\xi} = \delta_{ij}, \quad \forall X_i, X_j \in \Omega_\epsilon. \tag{2.11}$$

Proof. If $X_i = X_j$, then $\epsilon^3 \sum_{\xi\in\Omega_\epsilon^*} 1 = \epsilon^3 n^3 = 1$.

If $X_i \neq X_j$, without loss of generality, assume $X_i^1 \neq X_j^1$, then

$$\begin{aligned}
&\sum_{\xi\in\Omega_\epsilon^*} e^{\imath(X_i-X_j)\cdot\xi} \\
&= \sum_{\xi\in\Omega_\epsilon^*} e^{2\pi\imath\sum_{k=1}^3 (X_i^k - X_j^k)\xi^k} \\
&= \sum_{\xi^2,\xi^3\in\mathbb{Z}\cap[-\frac{n}{2},\frac{n}{2})} e^{2\pi\imath\sum_{k=2}^3 (X_i^k - X_j^k)\xi^k} \sum_{\xi^1\in\mathbb{Z}\cap[-\frac{n}{2},\frac{n}{2})} e^{2\pi\imath(X_i^1 - X_j^1)\xi^1} \\
&= \sum_{\xi^2,\xi^3\in\mathbb{Z}\cap[-\frac{n}{2},\frac{n}{2})} e^{2\pi\imath\sum_{k=2}^3 (X_i^k - X_j^k)\xi^k} \frac{e^{2\pi\imath(X_i^1-X_j^1)\lceil -\frac{n}{2}\rceil}\left(1 - e^{2\pi\imath(X_i^1-X_j^1)n}\right)}{1 - e^{2\pi\imath(X_i^1-X_j^1)}} \\
&= 0.
\end{aligned}$$

Notice $X_i^1, X_j^1 \in \epsilon(\mathbb{Z}\cap[0,\frac{1}{\epsilon}))$ and $\mathbb{Z}\cap[-\frac{n}{2},\frac{n}{2})$ contains n integers, so $(X_i^1 - X_j^1)n \in \mathbb{Z}$ which implies $e^{2\pi\imath(X_i^1-X_j^1)n} = 1$. □

Similarly, for each fixed $X \in \Omega_\epsilon$, we have a basic wave function defined the reciprocal space Ω_ϵ^*: $\{e^{\imath X\cdot\xi}\}_{\xi\in\Omega_\epsilon^*}$ which satisfy the orthonormality condition

Lemma 2.1.2.

$$\epsilon^3 \sum_{X\in\Omega_\epsilon} e^{\imath X\cdot(\xi_i-\xi_j)} = \delta_{ij}, \quad \forall \xi_i, \xi_j \in \Omega_\epsilon^*. \tag{2.12}$$

The proof is similar to that of the previous lemma.

2.2 Periodic Function Spaces

We will need to study various functions defined on spaces related to the lattice. Since the lattice has the translational symmetry, we consider periodic functions. We first define function spaces on the unit domain Ω, and then define their discrete counterpart on Ω_ϵ.

2.2.1 Functions on the continuous domains

For a given $n = \frac{1}{\epsilon} \in \mathbb{N}$, define

$$L^p_n = \{f \in \mathscr{S}'(\mathbb{R}^3) | \tau_R f = f, \forall R \in n\mathbb{L}, \int_{n\Omega} |f|^p dx < \infty\}, \tag{2.13}$$

with the norm

$$\|f\|_{L^p_n} = (n^{-3} \int_{n\Omega} |f|^p dx)^{\frac{1}{p}} \quad 1 \leqslant p < \infty. \tag{2.14}$$

Similarly define

$$L^\infty_n = \{f \in \mathscr{S}'(\mathbb{R}^3) | \tau_R f = f, \forall R \in n\mathbb{L}, \inf\{a \in \mathbb{R} : \mu(f^{-1}(a, \infty)) = 0\} < \infty\}, \tag{2.15}$$

with the norm

$$\|f\|_{L^\infty_n} = \inf\{a \in \mathbb{R} : \mu(f^{-1}(a, \infty)) = 0\}. \tag{2.16}$$

In the above definitions, τ_R is the translational operator on $n\mathbb{L}$ with translation vector R, $(\tau_R f)(x) = f(x - R)$.

Similarly we define the periodic Sobolev space

$$H^k_n = \{f \in \mathscr{S}'(\mathbb{R}^3) | \tau_R f = f, \forall R \in n\mathbb{L}, f \in H^k(n\Omega)\}, \tag{2.17}$$

with norm

$$\|f\|_{H^k_n} = \sum_{|\alpha| \leqslant k} \|\partial^\alpha f\|_{L^2_n} \quad k \in \mathbb{Z}_+. \tag{2.18}$$

Similarly,

$$W^{k,\infty}_n = \{f \in \mathscr{S}'(\mathbb{R}^3) | \tau_R f = f, \forall R \in n\mathbb{L}; f \in W^{k,\infty}(n\Omega)\}, \tag{2.19}$$

with norm

$$\|f\|_{W^{k,\infty}_n} = \sum_{|\alpha| \leqslant k} \|\partial^\alpha f\|_{L^\infty_n} \quad k \in \mathbb{Z}_+. \tag{2.20}$$

2.2.2 Sobolev Inequalities

We will use the following Sobolev inequality: if $\frac{k-r-\alpha}{n} = \frac{1}{p}$ with $\alpha \in (0,1)$, then $W^{k,p}(\mathbb{R}^n) \subset C^{r,\alpha}(\mathbb{R}^n)$.

Pick $n = 3, p = 2, \alpha = \frac{1}{2}$, then $r = k - 2$, so we get

$$H^k(\mathbb{R}^3) \subset C^{k-2,\frac{1}{2}}(\mathbb{R}^3) \subset W^{k-2,\infty}(\mathbb{R}^3) \subset H^k(\mathbb{R}^3).$$

Then on the torus, we have

$$H^k(n\Omega) \subset W^{k-2,\infty}(n\Omega) \subset H^k(n\Omega). \tag{2.21}$$

2.2.3 Lattice Functions

After introducing periodic functions on Ω_n, we now define periodic discrete functions on Ω_ϵ.

A lattice function $u : \mathbb{L}_\epsilon \to \mathbb{R}^3$ is called Ω_ϵ-*periodic* if

$$u(X) = u(X') \quad \forall X, X' \in \mathbb{L}_\epsilon, X - X' = a_j \text{ for some } j = 1, 2, 3,$$

where $\{a_1, a_2, a_3\}$ is the basis of the lattice $\mathbb{L}$. Therefore it is sufficient to specify its restriction on Ω_ϵ.

Define the translation operator T_ϵ^μ with $\mu \in \mathbb{Z}^3$

$$(T_\epsilon^\mu u)(X) = u(X + \epsilon \sum_{j=1}^{3} \mu_j a_j), \quad X \in \mathbb{R}^3, \tag{2.22}$$

for $u : \Omega_\epsilon \to \mathbb{R}^3$.

Define the forward and backward discrete gradient operators

$$D_{\epsilon,s}^+ = \epsilon^{-1}(T_\epsilon^\mu - I), \quad D_{\epsilon,s}^- = \epsilon^{-1}(I - T_\epsilon^{-\mu}), \tag{2.23}$$

where $s = \sum_{j=1}^{3} \mu_j a_j$, I is the identity operator. Notice $D_{\epsilon,-s}^+ = -D_{\epsilon,s}^-$.

Given a multi-index $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, with $\alpha_j \geqslant 0, j = 1, 2, 3$, $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$, define the difference operator

$$D_\epsilon^\alpha = \prod_{j=1}^{3} (D_{\epsilon,a_j}^+)^{\alpha_j}. \tag{2.24}$$

For a lattice function $u : \Omega_\epsilon \to \mathbb{R}^3$, a nonnegative integer k, define the difference norm

$$\|u\|_{\epsilon,k}^2 = \sum_{0 \leqslant |\alpha| \leqslant k} \epsilon^3 \sum_{X \in \Omega_\epsilon} |(D_\epsilon^\alpha u)(X)|^2. \tag{2.25}$$

Denote the corresponding spaces as H_ϵ^k and L_ϵ^2 when $k = 0$. Similarly define the uniform norms on Ω_ϵ

$$\|u\|_{L_\epsilon^\infty} = \max_{X \in \Omega_\epsilon} |u(X)|, \tag{2.26}$$

$$\|u\|_{W_\epsilon^{k,\infty}} = \sum_{0 \leqslant |\alpha| \leqslant k} \max_{X \in \Omega_\epsilon} |(D_\epsilon^\alpha u)(X)|. \tag{2.27}$$

2.3 Fourier Transform And Fourier Interpolation

2.3.1 Discrete Fourier Transformation

The discrete Fourier transform of a lattice function $f : \Omega_\epsilon \to \mathbb{R}^3$ is

$$\hat{f}(\xi) = \epsilon^3 \sum_{X \in \Omega_\epsilon} e^{-\imath X \cdot \xi} f(X), \xi \in \Omega_\epsilon^*. \tag{2.28}$$

The corresponding inversion is

$$f(X) = \sum_{\xi \in \Omega_\epsilon^*} e^{\imath X \cdot \xi} \hat{f}(\xi), X \in \Omega_\epsilon. \tag{2.29}$$

The Plancherel-type formula holds

$$\|f\|_{\epsilon,0}^2 = \sum_{\xi \in \Omega_\epsilon^*} |\hat{f}(\xi)|^2. \tag{2.30}$$

Moreover, the discrete Sobolev norm has a simple equivalent representation

$$c\|f\|_{\epsilon,k}^2 \leqslant \sum_{\xi\in\Omega_\epsilon^*} \Lambda_\epsilon^{2k}(\xi)|\hat{f}(\xi)|^2 \leqslant C\|f\|_{\epsilon,k}^2, \tag{2.31}$$

with positive constants c, C depending on k and the basis $\{a_j\}$. Let

$$\Lambda_{j,\epsilon}(\xi) = \frac{1}{\epsilon}|e^{\imath\epsilon\xi_j} - 1|, \quad j = 1, 2, 3,$$

then $\Lambda_\epsilon^2(\xi)$ is defined as

$$\Lambda_\epsilon^2(\xi) = 1 + \sum_{j=1}^{3} \Lambda_{j,\epsilon}^2(\xi) = 1 + \sum_{j=1}^{3} \frac{4}{\epsilon^2}\sin^2\left(\frac{\epsilon\xi_j}{2}\right). \tag{2.32}$$

We will consider functions with $\hat{f}(0) = 0$, so we need to estimate nonzero ξ:

Lemma 2.3.1. *For any nonzero $\xi \in \Omega_\epsilon^*$, then*

$$c\Lambda_\epsilon^2(\xi) \leqslant |\xi|^2 \leqslant C\Lambda_\epsilon^2(\xi) \tag{2.33}$$

for some positive constants c, C.

Proof. It is easy to see $1+|\xi|^2 \geqslant \Lambda_\epsilon^2(\xi)$. For any $\xi \in \Omega_\epsilon^*\backslash 0$, we have $|\xi| \geqslant \min_{j=1,2,3}|b_j| = b > 0$, then

$$|\xi|^2 = \frac{1}{2}(|\xi|^2 + |\xi|^2) \geqslant \frac{1}{2}(b^2 + |\xi|^2) \geqslant \frac{1}{2}\min(b^2, 1)(1 + |\xi|^2) = c_b(1 + |\xi|^2) \geqslant c_b\Lambda_\epsilon^2(\xi).$$

On the other hand, from $c\Lambda^2(\xi) \leqslant \Lambda_\epsilon^2(\xi)$, where $\Lambda^2(\xi) = 1 + |\xi|^2$, we get $|\xi|^2 \leqslant C\Lambda_\epsilon^2(\xi)$. □

2.3.2 Fourier Interpolation

Given a function $\varphi : \Omega \to \mathbb{R}^3$ which can be extended periodically to $\mathbb{R}^3$

$$\varphi(x + r) = \varphi(x), \quad \forall x \in \Omega, r \in \mathbb{L}.$$

The Fourier coefficients are

$$\hat{\varphi}(\xi) = \frac{1}{|\Omega|}\int_{\Omega} e^{-\imath x\cdot\xi}\varphi(x)dx, \quad \forall \xi \in \mathbb{L}^*. \tag{2.34}$$

Then we have the **plane-wave expansion**

$$\varphi(x) = \sum_{\xi\in\mathbb{L}^*} \hat{\varphi}(\xi)e^{\imath x\cdot\xi}, \quad \forall x \in \Omega. \tag{2.35}$$

Notice $\Omega_\epsilon \subset \Omega$ and consider the finite set of values or equivalently a lattice function $\{\varphi(X)|X \in \Omega_\epsilon\}$ which contains $\epsilon^{-3} = n^3$ values. Take the discrete Fourier transform

$$\hat{\varphi}_d(\xi) = \epsilon^3 \sum_{X\in\Omega_\epsilon} e^{-\imath X\cdot\xi}\varphi(X), \quad \forall \xi \in \Omega_\epsilon^*. \tag{2.36}$$

Then

$$\varphi(X) = \sum_{\xi\in\Omega_\epsilon^*} \hat{\varphi}_d(\xi)e^{\imath X\cdot\xi}. \tag{2.37}$$

Now we can define the **Fourier interpolation** of the lattice function $\{\varphi(X)|X \in \Omega_\epsilon\}$

$$\begin{aligned}\varphi_\epsilon(x) &= \sum_{\xi\in\Omega_\epsilon^*} \hat{\varphi}_d(\xi)e^{\imath x\cdot\xi} \\ &= \sum_{\xi\in\mathbb{L}^*} \hat{\varphi}_d(\xi)e^{\imath x\cdot\xi},\end{aligned} \tag{2.38}$$

where we define $\hat{\varphi}_d(\xi) = 0$ for $\xi \in \mathbb{L}^*\backslash\Omega_\epsilon^*$.

Denote the lattice function $\{\varphi(X)|X \in \Omega_\epsilon\}$ as φ_d, then we have the following lemma

Lemma 2.3.2. *For $k \geqslant 0$, there exists constants $c_k, C_k > 0$ such that for any φ_d,*

$$c_k\|\varphi_d\|_{\epsilon,k} \leqslant \|\varphi_\epsilon\|_{H^k(\Omega)} \leqslant C_k\|\varphi_d\|_{\epsilon,k}. \tag{2.39}$$

Proof. This is easily deduced from the inequalities

$$c(1 + |\xi|^2) \leqslant \Lambda_\epsilon^2(\xi) \leqslant 1 + |\xi|^2, \quad \forall \xi \in \Omega_\epsilon^*. \tag{2.40}$$

□

Moreover, the following **Poisson summation formula** holds

Lemma 2.3.3.

$$\hat{\varphi}_d(\xi) = \sum_{\eta \in \epsilon^{-1}\mathbb{L}^*} \hat{\varphi}(\xi + \eta), \quad \forall \xi \in \Omega_\epsilon^* \tag{2.41}$$

Proof. By the DFT formula, it suffices to show

$$\varphi(X) = \sum_{\xi \in \Omega_\epsilon^*} \Big(\sum_{\eta \in \epsilon^{-1}\mathbb{L}^*} \hat{\varphi}(\xi + \eta) \Big) e^{\imath X \cdot \xi}, \quad \forall X \in \Omega_\epsilon.$$

The computation is straightforward

$$\begin{aligned}
&\sum_{\xi \in \Omega_\epsilon^*} \Big(\sum_{\eta \in \epsilon^{-1}\mathbb{L}^*} \hat{\varphi}(\xi + \eta) \Big) e^{\imath X \cdot \xi} \\
=& \sum_{\eta \in \epsilon^{-1}\mathbb{L}^*} \sum_{\xi \in \Omega_\epsilon^*} \hat{\varphi}(\xi + \eta) e^{\imath X \cdot \xi} \\
=& \sum_{\eta \in \epsilon^{-1}\mathbb{L}^*} \sum_{\xi \in \Omega_\epsilon^* + \eta} \hat{\varphi}(\xi) e^{\imath X \cdot (\xi - \eta)} \\
=& \sum_{\xi \in \Omega_\epsilon^* + \eta, \eta \in \epsilon^{-1}\mathbb{L}^*} \hat{\varphi}(\xi) e^{\imath X \cdot \xi} \\
=& \sum_{\xi \in \mathbb{L}^*} \hat{\varphi}(\xi) e^{\imath X \cdot \xi} \\
=& \varphi(X).
\end{aligned}$$

Notice that $X \cdot \eta = 2\pi \sum_{k=1}^3 X^k \eta^k$, where $X^k \in \epsilon\mathbb{Z}$ and $\eta^k \in \epsilon^{-1}\mathbb{Z}$, so $e^{-\imath X \cdot \eta} = 1$. ☐

We will also need the following interpolation error between φ and φ_ϵ

Theorem 2.3.4. *For the periodic function $\varphi : \Omega \to \mathbb{R}^3$, if $\varphi \in C^p, p \geqslant 3 + |\alpha|$, then*

$$|D^\alpha \varphi(x) - D^\alpha \varphi_\epsilon(x)| \leqslant C\epsilon^{p-3-|\alpha|}, \quad \forall x \in \Omega. \tag{2.42}$$

Proof. From the discrete Fourier transform, we know

$$D^\alpha \varphi(x) = \imath^{|\alpha|} \sum_{\xi \in \mathbb{L}_*} \hat{\varphi}(\xi) \xi^\alpha e^{\imath x \cdot \xi}.$$

If $\varphi \in C^p$, then $|\hat{\varphi}(\xi)| \leqslant C|\xi|^{-p}$.

Let $b_{\min} = \text{argmin}_{b_1,b_2,b_3}\{|b_1|, |b_2|, |b_3|\}$, for any $\xi \in \Omega_\epsilon^*$, $p \geqslant 3 + |\alpha| > 2$, from the Poisson summation formula, we have

$$\begin{aligned}
|\hat{\varphi}_d(\xi) - \hat{\varphi}(\xi)| =& |\sum_{\eta \in \epsilon^{-1}\mathbb{L}^*, \eta \neq 0} \hat{\varphi}(\xi + \eta)| \\
\leqslant& C \sum_{\eta \in \epsilon^{-1}\mathbb{L}^*, \eta \neq 0} |\xi + \eta|^{-p} \\
\leqslant& C \sum_{m \in \mathbb{Z}^3, m \neq 0} \epsilon^p \big(\frac{|b_{\min}|}{2} \min_m\{|m_1|, |m_2|, |m_3|\}\big)^{-p} \\
\leqslant& C\epsilon^p \sum_{m_1,m_2,m_3 \in \mathbb{Z}^3} \big(\frac{|b_{\min}|}{2}|m_1||m_2||m_3|\big)^{-p} \\
=& C'\epsilon^p.
\end{aligned}$$

Therefore

$$|\hat{\varphi}_d(\xi) - \hat{\varphi}(\xi)| \leqslant C'\epsilon^p, \quad \forall \xi \in \Omega_\epsilon^*$$

Now we can estimate the pointwise difference of the derivatives

$$\begin{aligned}
&|D^\alpha \varphi(x) - D^\alpha \varphi_\epsilon(x)| \\
\leqslant& \sum_{\xi \in \mathbb{L}^*} |\xi|^{|\alpha|} |\hat{\varphi}(\xi) - \hat{\varphi}_d(\xi)| \\
=& \sum_{\xi \in \Omega_\epsilon^*} |\xi|^{|\alpha|} |\hat{\varphi}(\xi) - \hat{\varphi}_d(\xi)| + \sum_{\xi \in \mathbb{L}^* \backslash \Omega_\epsilon^*} |\xi|^{|\alpha|} |\hat{\varphi}(\xi)| \\
=& I + II,
\end{aligned}$$

in which

$$\begin{aligned}
I \leqslant& C\epsilon^p \sum_{\xi \in \Omega_\epsilon^*} |\xi|^{|\alpha|} \\
\leqslant& C'\epsilon^p \iiint_{[-\frac{n}{2}, \frac{n}{2})^3} |\xi|^{|\alpha|} d\xi
\end{aligned}$$

$$
\begin{aligned}
&\leqslant C''\epsilon^p \iiint\limits_{B_{\frac{n}{2}}(0)} |\xi|^{|\alpha|} d\xi \\
&= C''\epsilon^p \int_0^\pi \int_0^{2\pi} \int_0^{\frac{n}{2}} r^{|\alpha|+2} \sin\theta dr d\theta d\varphi \\
&= C'''\epsilon^{p-3-|\alpha|}
\end{aligned}
$$

and

$$
\begin{aligned}
II \leqslant & C \sum_{\xi \in \mathbb{L}^* \setminus \Omega_\epsilon^*} |\xi|^{|\alpha|-p} \\
\leqslant & C' \iiint\limits_{\mathbb{R}^3 \setminus [-\frac{n}{2}, \frac{n}{2})^3} |\xi|^{|\alpha|-p} d\xi \\
\leqslant & C'' \iiint\limits_{\mathbb{R}^3 \setminus B_{\frac{n}{2}}(0)} |\xi|^{|\alpha|-p} d\xi \\
= & C'' \int_0^\pi \int_0^{2\pi} \int_{\frac{n}{2}}^\infty r^{|\alpha|-p+2} \sin\theta dr d\theta d\varphi \\
= & C'''\epsilon^{p-3-|\alpha|}.
\end{aligned}
$$

Therefore

$$
|D^\alpha \varphi(x) - D^\alpha \varphi_\epsilon(x)| \leqslant C\epsilon^{p-3-|\alpha|}.
$$

□

2.4 Deformation Of The Lattice

The deformation of the crystal lattice is described either by the discrete deformed atom positions or the continuous deformation function. The connection between these two functions is simulated by the Fourier interpolation.

2.4.1 The Deformed Atom Positions

the deformed atom positions can be described by a discrete vector function defined on Ω_ϵ:

$$Y : \Omega_\epsilon \to \mathbb{R}^3,$$

and it is extended periodically to $\mathbb{L}_\epsilon$,

$$Y : \mathbb{L}_\epsilon \to \mathbb{R}^3.$$

by

$$Y(X + r) = Y(X) - r$$

for any $X \in \Omega_\epsilon, r \in \mathbb{L}$.

2.4.2 The Deformation

Fix a deformed atom position function $Y : \Omega_\epsilon \to \mathbb{R}^3$, define τ as the Fourier interpolation of Y

$$\begin{aligned}\tau(x) =& \sum_{\xi \in \Omega_\epsilon^*} e^{\imath x \cdot \xi} \hat{Y}(X) \\ =& \epsilon^3 \sum_{\xi \in \Omega_\epsilon^*} \sum_{X \in \Omega_\epsilon} e^{\imath \xi \cdot (x - X)} Y(X).\end{aligned} \tag{2.43}$$

Let $\tau(x) = x + u(x)$, then u is the deformation corresponding to Y. From Lemma 2.3.2 we have

$$c_k \|Y\|_{\epsilon,k} \leqslant \|u\|_{H^k(\Omega)} \leqslant C_k \|Y\|_{\epsilon,k}, \tag{2.44}$$

for $k \in \mathbb{N}_+$ and constants $c_k, C_k > 0$.

Furthermore, since the crystal does not collapse, it is reasonable to assume a nondegeneracy condition on the deformation function: $\inf_{x \in \Omega} |\nabla \tau(x)| \geqslant \delta_\tau > 0$ for $\tau \in W_1^{1,\infty}$.

2.5 Background Charge

2.5.1 Definition

Assume $m_a \in C_0^\infty(\mathbb{R}^3)$ is a compactly supported smooth function which represents the background charge contribution from each nucleus. Then the total charge contribution from the nuclei on an undeformed lattice $\mathbb{L}$ is

$$\rho_b(x) = \sum_{X \in \mathbb{L}} m_a(x - X), \quad x \in \mathbb{R}^3. \tag{2.45}$$

Now assume the lattice is scaled by a constant $\epsilon = \frac{1}{n}$, and is deformed by the periodic atom position function $Y : \Omega_\epsilon \to \mathbb{R}^3$, then define the corresponding background charge as

$$\rho_b^\epsilon(y, Y) = \sum_{X \in \mathbb{L}_\epsilon} m_a(\frac{y - Y(X)}{\epsilon}), \quad y \in \mathbb{R}^3. \tag{2.46}$$

Let $\tau : \Omega \to \mathbb{R}^3$ be the Fourier interpolation of $Y : \Omega_\epsilon \to \mathbb{R}^3$, then we can represent the background charge function in Lagrangian coordinates:

$$\rho_b^\epsilon(x, Y) = J(x) \sum_{X \in \mathbb{L}_\epsilon} m_a(\frac{\tau(x) - \tau(X)}{\epsilon}), \quad x \in \mathbb{R}^3 \tag{2.47}$$

We assume the normalization constraint on the electron density

$$\int_{n\Omega} \rho_b(x) dx = \epsilon^{-3} \mathcal{Z} \tag{2.48}$$

which is equivalent to

$$\int_{\Omega} \rho_b^\epsilon(x) dx = \mathcal{Z} \tag{2.49}$$

2.5.2 Periodicity

The background charge inherits the periodicity of Y

$$\rho_b^\epsilon(x, Y) = \rho_b^\epsilon(x + r, Y), \quad \forall r \in \mathbb{L}. \tag{2.50}$$

Because of this periodicity, we restrict the domain to Ω.

2.5.3 Two-Scale Ansatz

In order to study the system by approximation, we will use a two-scale ansatz of the background charge on a deformed lattice $\mathbb{L}_\epsilon$ with Y,

$$\rho_b^\epsilon(x) = \rho_{b,0}(\frac{x}{\epsilon}, x) + \epsilon\rho_{b,1}(\frac{x}{\epsilon}, x) + \epsilon^2\rho_{b,2}(\frac{x}{\epsilon}, x) + O(\epsilon^3), \quad x \in \Omega, \tag{2.51}$$

in which

$$\rho_{b,0}(z,x) = \sum_{X\in\mathbb{L}} m_a(\nabla\tau(x)(z-X)) \tag{2.52a}$$

$$\rho_{b,1}(z,x) = -\sum_{X\in\mathbb{L}} m_a'\big(\nabla\tau(x)(z-X)\big)\sum_{|\beta|=2}\frac{1}{\beta!}\frac{\partial^\beta\tau(x)}{\partial x^\beta}(X-z)^\beta \tag{2.52b}$$

$$\begin{aligned}\rho_{b,2}(z,x) =& \frac{1}{2}\sum_{X\in\mathbb{L}} m_a''\big(\nabla\tau(x)(z-X)\big)\Big(\sum_{|\beta|=2}\frac{1}{\beta!}\frac{\partial^\beta\tau(x)}{\partial x^\beta}(X-z)^\beta\Big)^2 \\ &-\sum_{X\in\mathbb{L}} m_a'\big(\nabla\tau(x)(z-X)\big)\sum_{|\beta|=3}\frac{1}{\beta!}\frac{\partial^\beta\tau(x)}{\partial x^\beta}(X-z)^\beta,\end{aligned} \tag{2.52c}$$

for $x \in \Omega, z \in n\Omega$. Notice that $\rho_{b,0}, \rho_{b,1}, \rho_{b,2}$ are periodic in $z \in \Omega$.

Lemma 2.5.1. *If $m_a \in C^k$, then $\rho_{b,0}$ is C^k in $\nabla\tau$; $\rho_{b,1}$ is C^{k-1} in $\nabla\tau$, C^∞ in $\nabla^2\tau$; and $\rho_{b,2}$ is C^{k-2} in $\nabla\tau$, C^∞ in $\nabla^2\tau, \nabla^3\tau$.*

In order to study the consistency of the Cauchy-Born rule, we will derive even higher-order expansion of ρ_b^ϵ in Chapter 6.

2.5.4 Inversion Symmetry

It is reasonable to assume the function m_a has inversion symmetry $m_a(x) = m_a(-x)$, for any $x \in \mathbb{R}^3$, then so is the background charge on undeformed lattice with or without scaling:

$$\rho_b(x) = \rho_b(-x), \quad \rho_b^\epsilon = \rho_b^\epsilon(-x), \quad x \in \mathbb{R}^3. \tag{2.53}$$

This is because the undeformed lattices $\mathbb{L}$ and $\mathbb{L}_\epsilon$ have the inversion symmetry. We will see that this inversion symmetry plays a vital role in our analysis, and it improves the rate of convergence.

Moreover, from the two-scale ansatz expansion, it is straightforward to see that

$$\rho_{b,0}(z,x) = \rho_{b,0}(-z,x)$$

$$\rho_{b,1}(z,x) = -\rho_{b,1}(-z,x)$$

$$\rho_{b,2}(z,x) = \rho_{b,2}(-z,x)$$

2.5.5 Localization and Decaying Property

Lemma 2.5.2. *Assume m_a has compact support such that $m_a(x) = 0$ for any $|x| \geqslant M_a$, M_a is a given positive constant. Then m_a satisfies the pointwise decaying property:*

$$|m_a(x)| \leqslant C_0 e^{-\gamma|x|}$$

where $C_0 = e\|m_a\|_{L^\infty}$, $0 < \gamma \leqslant \frac{1}{M_a}$. More generally,

$$|\nabla^k m_a(x)| \leqslant C_k e^{-\gamma|x|},$$

where k is any positive integer, $C_k = e\|m_a\|_{W^{k,\infty}}$, $0 < \gamma \leqslant \frac{1}{M_a}$.

Proof. From $m_a(x) = 0$ for any $|x| \geqslant M_a$, it is easy to see that in order for

$$\|m_a\|_{L^\infty} \leqslant C_0 e^{-\gamma M_a}$$

to hold, we need

$$\gamma \leqslant \frac{1}{M_a} \ln \frac{C_0}{\|m_a\|_{L^\infty}}$$

So we can pick $C_0 = e\|m_a\|_{L^\infty}, 0 < \gamma \leqslant \frac{1}{M_a}$. The same analysis applies to prove the second inequality. □

Define a set

$$S = \{0, \pm a_1, \pm a_2, \pm a_3, \pm a_1 \pm a_2, \pm a_1 \pm a_3, \pm a_2 \pm a_3, \pm a_1 \pm a_2 \pm a_3\} \tag{2.54}$$

Then $S + \Omega$ are all the translations of Ω that intersect Ω.

Lemma 2.5.3. *Assume* $\tau \in W_1^{1,\infty}$ *has the nondegeneracy property* $\inf_{x\in\Omega} |\nabla\tau| \geqslant \delta_\tau > 0$*, then* $\rho_b^\epsilon(x, Y)$ *has the following expression*

$$\rho_b^\epsilon(x, Y) = \sum_{X\in\Omega_\epsilon} \sum_{r\in S} m_a\left(\frac{\tau(x) - \tau(X) + r}{\epsilon}\right) \tag{2.55}$$

Proof. If $|x + r - X| > \frac{\epsilon M_a}{\delta_\tau}$, then

$$|\tau(x + r) - \tau(X)| \geqslant (\inf |\nabla\tau|)|x + r - X| \geqslant \delta_\tau|x + r - X| \geqslant \epsilon M_a,$$

then $|\frac{\tau(x+r)-\tau(X)}{\epsilon}| > M_a$, so $m_a(\frac{\tau(x+r)-\tau(X)}{\epsilon}) = 0$. Therefore for any $x \in \Omega, X \in \Omega_\epsilon$, we only consider those $r \in \mathbb{L}$ such that $|x + r - X| \leqslant \frac{\epsilon M_a}{\delta_\tau}$. By choosing ϵ small enough, it is sufficient to only consider $r \in S$. Thus

$$\begin{aligned}
\rho_b^\epsilon(x, Y) &= \sum_{X\in\mathbb{L}_\epsilon} m_a\left(\frac{\tau(x) - \tau(X)}{\epsilon}\right) \\
&= \sum_{X\in\Omega_\epsilon} \sum_{r\in\mathbb{L}} m_a\left(\frac{\tau(x) - \tau(X) + r}{\epsilon}\right) \\
&= \sum_{X\in\Omega_\epsilon} \sum_{r\in S} m_a\left(\frac{\tau(x) - \tau(X) + r}{\epsilon}\right)
\end{aligned}$$

□

Proposition 2.5.4. *Assume* $\inf_{x\in\Omega} |\nabla\tau(x)| \geqslant \delta_\tau > 0$*, then for* ϵ *small enough, the following pointwise estimates hold*

$$\left\|\frac{\partial}{\partial Y_i}\rho_b^\epsilon(x, Y)\right\| \leqslant \frac{C}{\epsilon} e^{-\frac{\gamma}{\epsilon}|x - X_i + r_{i,x}|} \tag{2.56}$$

$$\left\|\frac{\partial^2}{\partial Y_i \partial Y_j}\rho_b^\epsilon(x, Y)\right\| \leqslant \frac{C}{\epsilon^2} e^{-\frac{\gamma}{\epsilon}|x - X_i + r_{i,x}|} e^{-\frac{\gamma}{\epsilon}|x - X_j + r_{j,x}|} \tag{2.57}$$

for all small positive constant $\gamma > 0$*. Moreover* $x \in \Omega$*,* $Y_i = Y(X_i), Y_j = Y(X_j)$ *with* $X_i, X_j \in \Omega_\epsilon$*.* $r_{i,x}, r_{j,x} \in S$*, and their choices depend on* x, X_i *or* x, X_j*.*

Proof. By choosing ϵ small enough, for any $x \in \Omega, X_i \in \Omega_\epsilon$, there is at most one $r_{i,x} \in S$, such that $|x + r_{i,x} - X_i| \leqslant \frac{\epsilon M_a}{\delta_\tau}$. If no such $r_{i,x}$ exists, then the inequalities are trivially true. Moreover, $r_{i,x}$ is smooth in x a.e..

The first inequality is easily derived from the above expression of $\rho_b^\epsilon(x, Y)$ and $|\tau(x+r_{i,x}) - \tau(X_i)| \geqslant \delta_\tau |x + r_{i,k} - X_i|$, so $C = e\|m_a\|_{1,\infty}, 0 < \gamma \leqslant \frac{\delta_\tau}{M_a}$. For the second inequality, notice that $\frac{\partial^2}{\partial Y_i \partial Y_j}\rho_b^\epsilon(x, Y) = 0$ if $i \neq j$. Then the case $i = j$ is obvious and $C = e\|m_a\|_{2,\infty}, 0 < \gamma \leqslant \frac{\delta_\tau}{2M_a}$.

□

By a change of variable, with the same notations in the previous proposition, it is straightforward to get

Proposition 2.5.5.

$$\|\frac{\partial}{\partial Y_i}\rho_b(x, Y)\| \leqslant \frac{C}{\epsilon} e^{-\gamma|x + \frac{-X_i + r_{i,\epsilon x}}{\epsilon}|} \tag{2.58}$$

$$\|\frac{\partial^2}{\partial Y_i \partial Y_j}\rho_b(x, Y)\| \leqslant \frac{C}{\epsilon^2} e^{-\gamma|x + \frac{-X_i + r_{i,\epsilon x}}{\epsilon}|} e^{-\gamma|x + \frac{-X_j + r_{j,\epsilon x}}{\epsilon}|} \tag{2.59}$$

for $x \in n\Omega$.

2.5.6 Perturbation

Lemma 2.5.6. *Given a deformed atom position function Y_1, which satisfies the nondegeneracy condition $inf_{x\in\Omega}|\nabla \tau_1(x)| \geqslant \delta_\tau$ for some $\delta_\tau > 0$. Assume there is another Y_2 close to Y_1 such that $\|\tau_2 - \tau_1\|_{1,\infty} < \frac{\delta_\tau}{2}$, we have the following estimate for the difference between the corresponding background charge functions*

$$\|\rho_b(Y_2) - \rho_b(Y_1)\|_{L^\infty(n\Omega)} = \|\rho_b^\epsilon(Y_2) - \rho_b^\epsilon(Y_1)\|_{L^\infty(\Omega)} \leqslant C_b\|m_a\|_{1,\infty}\|Y_2 - Y_1\|_{W_\epsilon^{1,\infty}} \tag{2.60}$$

or equivalently

$$\|\rho_b(\tau_2) - \rho_b(\tau_1)\|_{L^\infty(n\Omega)} = \|\rho_b^\epsilon(\tau_2) - \rho_b^\epsilon(\tau_1)\|_{L^\infty(\Omega)} \leqslant C_b\|m_a\|_{1,\infty}\|\tau_2 - \tau_1\|_{1,\infty} \tag{2.61}$$

Proof. By our condition on τ_1, τ_2, we have $\inf_{x\in\Omega}|\nabla\tau_1(x)|, \inf_{x\in\Omega}|\nabla\tau_2(x)| \geqslant \frac{\delta_\tau}{2}$.

$$
\begin{aligned}
&|\rho_b^\epsilon(x,\tau_2) - \rho_b^\epsilon(x,\tau_1)| \\
\leqslant &\sum_{X\in\Omega, r\in\mathbb{L}} |m_a(\frac{\tau_2(x)-\tau_2(X)+r}{\epsilon}) - m_a(\frac{\tau_1(x)-\tau_1(X)+r}{\epsilon})| \\
\leqslant &\sum_{r\in S}\sum_{X\in\Omega_\epsilon:|(x+r)-X|\leqslant 2\epsilon M_a/\delta_\tau} |m_a(\frac{\tau_2(x+r)-\tau_2(X)}{\epsilon}) - m_a(\frac{\tau_1(x+r)-\tau_1(X)}{\epsilon})| \\
\leqslant &\sum_{r\in S}\sum_{X\in\Omega_\epsilon:|(x+r)-X|\leqslant 2\epsilon M_a/\delta_\tau} \|m_a\|_{1,\infty}\frac{1}{\epsilon}|(\tau_2-\tau_1)(x+r)-(\tau_2-\tau_1)(X)|
\end{aligned}
$$

As in previous context, we assume ϵ is small enough so that only $r \in S$ come into play. The second inequality holds because, if $|x+r-X| \geqslant \frac{2\epsilon M_a}{\delta_\tau}$, then $|\tau_i(x+r) - \tau_i(X)| \geqslant (\inf|\nabla\tau_i|)|x+r-X| \geqslant \epsilon M_a$, so $m_a(\frac{\tau_i(x+r)-\tau_i(X)}{\epsilon}) = 0$ for $i = 1, 2$.

Pick consecutive atom positions $\{X = X_{n_1}, X_{n_2}, \cdots, X_{n_l}\}$ so that $x + r \in \Omega_{n_l} = X_{n_l} + \epsilon\Omega$, which means $|X_{n_{i+1}} - X_{n_i}| = \epsilon a_k$ for some $k = 1, 2, 3$ and any $i = 1, \ldots, l-1$. Then $l \sim O(1)$ since $|(x+r) - X| \leqslant 2\epsilon M_a/\delta_\tau = O(\epsilon)$. Therefore

$$
\begin{aligned}
&|\rho_b^\epsilon(x,\tau_2) - \rho_b^\epsilon(x,\tau_1)| \\
\leqslant &\sum_{r\in S}\sum_{X\in\Omega_\epsilon:|(x+r)-X|\leqslant 2\epsilon M_a/\delta_\tau} \|m_a\|_{1,\infty}\Big(\sum_{i=1}^{l-1}\frac{1}{\epsilon}|(\tau_2-\tau_1)(X_{n_i})-(\tau_2-\tau_1)(X_{n_{i+1}})| \\
&+ \frac{1}{\epsilon}|(\tau_2-\tau_1)(X_{n_l})-(\tau_2-\tau_1)(x+r)|\Big) \\
\leqslant &\sum_{r\in S}\sum_{X\in\Omega_\epsilon:|(x+r)-X|\leqslant 2\epsilon M_a/\delta_\tau} \|m_a\|_{1,\infty}\Big(\sum_{i=1}^{l-1}|D^+_{\epsilon,a_{k_i}}(\tau_2-\tau_1)(X_{n_i^*})| + \|\tau_2-\tau_1\|_{1,\infty}\Big) \\
\leqslant &C\|Y_2 - Y_1\|_{W^{1,\infty}_\epsilon} + \|\tau_2-\tau_1\|_{1,\infty} \\
\leqslant &C'\|Y_2 - Y_1\|_{W^{1,\infty}_\epsilon} \\
\leqslant &C''\|\tau_2-\tau_1\|_{1,\infty},
\end{aligned}
$$

$a_{k_i} \in \{a_1, a_2, a_3\}$, $X_{n_i^*} \in \{X_{n_i}, X_{n_{i+1}}\}$, and notice that $\#\{X \in \Omega_\epsilon : |(x+r) - X| \leqslant \epsilon M_a/\delta_\tau\} = O(1)$.

$\square$

From the equivalence of $\|\tau\|_{1,\infty}$ and $\|Y\|_{W_\epsilon^{1,\infty}}$, it is easy to see

$$|J_\epsilon(x, \tau_{Y_2}) - J_\epsilon(x, \tau_{Y_1})| = |J(\epsilon x, \tau_{Y_2}) - J(\epsilon x, \tau_{Y_1})| \leqslant C_J \|Y_2 - Y_1\|_{W_\epsilon^{1,\infty}}, \quad x \in n\Omega,$$

so

$$\|J_\epsilon(x, \tau_{Y_2}) - J_\epsilon(x, \tau_{Y_1})\|_{L^\infty(n\Omega)} \leqslant C_J \|Y_2 - Y_1\|_{W_\epsilon^{1,\infty}}.$$

Furthermore we have

Lemma 2.5.7. *Denote $Y_i = Y(X_i), Y_j = Y(X_j)$, for $X_i, X_j \in \Omega_\epsilon$, and $\partial_i = \frac{\partial}{\partial Y_i}, \partial_j = \frac{\partial}{\partial Y_j}$, assume $inf_{x\in\Omega}|\nabla\tau_1(x)| \geqslant \delta_\tau$ for some $\delta_\tau > 0$ and $\|\tau_2 - \tau_1\|_{1,\infty} < \frac{\delta_\tau}{2}$, then*

$$|\partial_j \rho_b^\epsilon(x, Y_2) - \partial_j \rho_b^\epsilon(x, Y_1)| \leqslant C_b \epsilon^{-1} e^{-\frac{\gamma}{\epsilon}|x - X_j + r_{j,x}|} \|Y_2 - Y_1\|_{W_\epsilon^{1,\infty}} \tag{2.62}$$

$$|\partial_i\partial_j \rho_b^\epsilon(x, Y_2) - \partial_i\partial_j \rho_b^\epsilon(x, Y_1)| \leqslant C_b \epsilon^{-2} e^{-\frac{\gamma}{\epsilon}|x - X_i + r_{i,x}|} e^{-\frac{\gamma}{\epsilon}|x - X_j + r_{j,x}|} \|Y_2 - Y_1\|_{W_\epsilon^{1,\infty}} \tag{2.63}$$

for all small positive constant $\gamma > 0$.

Proof. First we compute

$$\begin{aligned} &\partial_j \rho_b^\epsilon(x, Y) \\ =&\sum_{r\in\mathbb{L}} -\frac{1}{\epsilon}\nabla m_a\left(\frac{\tau(x) - \tau(X_j) + r}{\epsilon}\right) \\ =&-\frac{1}{\epsilon}\sum_{k=0}^{6}\nabla m_a\left(\frac{\tau(x + r_k) - \tau(X_j)}{\epsilon}\right) \end{aligned}$$

if we assume ϵ is small enough. Then

$$\begin{aligned} &|\partial_j \rho_b^\epsilon(x, Y_2) - \partial_j \rho_b^\epsilon(x, Y_1)| \\ \leqslant&\frac{1}{\epsilon}\left|\nabla m_a\left(\frac{\tau_2(x + r_{j,x}) - \tau_2(X_j)}{\epsilon}\right) - \nabla m_a\left(\frac{\tau_1(x + r_k) - \tau_1(X_j)}{\epsilon}\right)\right| \end{aligned}$$

$$\leqslant \frac{1}{\epsilon}|\nabla^2 m_a(\frac{\tau_t(x+r_{j,x})-\tau_t(X_j)}{\epsilon})|\frac{1}{\epsilon}|(\tau_2-\tau_1)(x+r_{j,x})-(\tau_2-\tau_1)(X_j)|$$

where $\tau_t = (1-t)\tau_1 + t\tau_2$ for some $0 < t < 1$. For any $x \in \mathbb{R}^3$,

$$\begin{aligned}|\nabla\tau_t(x)| =&|(1-t)\nabla\tau_1(x) + t\nabla\tau_2(x)|\\ =&|\nabla\tau_1(x) + t(\nabla\tau_2(x) - \nabla\tau_1(x))|\\ \geqslant&|\nabla\tau_1(x)| - t|\nabla\tau_2(x) - \nabla\tau_1(x)|\\ \geqslant&|\nabla\tau_1(x)| - |\nabla\tau_2(x) - \nabla\tau_1(x)|\\ \geqslant&\delta_\tau - \frac{\delta_\tau}{2} = \frac{\delta_\tau}{2}.\end{aligned}$$

So $\inf_{x\in\Omega} = \inf_{x\in\mathbb{R}^3} |\nabla\tau_t(x)| \geqslant \frac{\delta_\tau}{2}$ because $\nabla\tau_t$ is periodic on Ω. Thus

$$\begin{aligned}&|\nabla^2 m_a(\frac{\tau_t(x+r_k)-\tau_t(X_j)}{\epsilon})|\\ \leqslant&C_2 e^{-\frac{\gamma}{\epsilon}|\tau_t(x+r_k)-\tau_t(X_j)|}\\ \leqslant&C_2 e^{-\frac{\gamma}{\epsilon}\inf|\nabla\tau_t||x+r_k-X_j|}\\ \leqslant&C_2 e^{-\frac{\gamma}{\epsilon}\frac{\delta_\tau}{2}|x+r_k-X_j|}\\ \leqslant&C_2 e^{-\frac{\gamma''}{\epsilon}|x+r_k-X_j|},\end{aligned}$$

where $0 < \gamma'' = \frac{\delta_\tau}{2}\gamma \leqslant \frac{\delta_\tau}{2M_a}$.

We can use the same technique as in the previous lemma to analyze $\frac{1}{\epsilon}|(\tau_2-\tau_1)(x+r_{j,x})-(\tau_2-\tau_1)(X_j)|$, then we can conclude

$$|\partial_j\rho_b^\epsilon(x,Y_2) - \partial_j\rho_b^\epsilon(x,Y_1)| \leqslant C_b\epsilon^{-1}e^{-\frac{\gamma}{\epsilon}|x-X_j+r_{j,x}|}\|Y_2-Y_1\|_{W_\epsilon^{1,\infty}}. \tag{2.64}$$

Next notice that when $i \neq j$, $\partial_i\partial_j\rho_b^\epsilon(x,Y) = 0$, then it is easy to use the same method to show

$$|\partial_i\partial_j\rho_b^\epsilon(x,Y_2)-\partial_i\partial_j\rho_b^\epsilon(x,Y_1)| \leqslant C_b\epsilon^{-2}e^{-\frac{\gamma}{\epsilon}|x-X_i+r_{i,x}|}e^{-\frac{\gamma}{\epsilon}|x-X_j+r_{j,x}|}\|Y_2-Y_1\|_{W_\epsilon^{1,\infty}}, \tag{2.65}$$

for some positive constant C_b and all small enough positive constant γ. □

By a change of variable, we have

Proposition 2.5.8.

$$|\partial_j \rho_b(x, Y_2) - \partial_j \rho_b(x, Y_1)| \leqslant C_b \epsilon^{-1} e^{-\gamma|x + \frac{-X_j + r_{j,\epsilon x}}{\epsilon}|} \|Y_2 - Y_1\|_{W_\epsilon^{1,\infty}} \tag{2.66}$$

$$|\partial_i \partial_j \rho_b(x, Y_2) - \partial_i \partial_j \rho_b(x, Y_1)| \leqslant C_b \epsilon^{-2} e^{-\gamma|x + \frac{-X_i + r_{i,\epsilon x}}{\epsilon}|} e^{-\gamma|x + \frac{-X_j + r_{j,\epsilon x}}{\epsilon}|} \|Y_2 - Y_1\|_{W_\epsilon^{1,\infty}} \tag{2.67}$$

for $x \in n\Omega$.

3

Formulation Of The Problem

In this chapter, we decompose the main problem into three subproblems. We first solve the electronic TFDW model assuming a fixed deformation, then once we have $\mathcal{V}_{\text{exa}}$, we proceed to study the atomistic TFDW model in which we interpret the discrete deformation function Y as varied. Meanwhile, we also study the Cauchy-Boron continuum elasticity model. Finally, we combine results from these models together to give the statement of the main result.

3.1 The electronic TFDW model

Assume a deformation represented by a discrete atom position function $Y : \Omega_\epsilon \to \mathbb{R}^3$ is given and fixed, the electronic TFDW functional is

$$I(\nu, V; \rho_b) = \int_{n\Omega} \nu^{\frac{10}{3}} + |\nabla \nu|^2 - \nu^{\frac{8}{3}} + \frac{1}{2} V(\nu^2 - \rho_b) dy \tag{3.1}$$

where the background charge ρ_b is given

$$\rho_b(y, Y) = \sum_{X \in \mathbb{L}} m_a(y - Y(X)). \tag{3.2}$$

The electronic TFDW problem with a fixed deformation is formulated as follows: Given a deformation $Y \in H^7_\epsilon$ or equivalently $u \in H^7_1$, find $(\nu, V) \in (W^{1,\infty}_n)^2$ such that

$$(\nu_{\text{exa}}, V_{\text{exa}}) = \text{argmin}_{(\nu,V)\in(W^{1,\infty}_n)^2} I(\nu, V; \rho_b) \tag{3.3}$$

The system of Euler-Lagrange equations $\mathcal{F}_{\text{TFDW}}(\nu, V) = 0$ in $n\Omega$ is

$$\begin{cases} -\Delta\nu + \frac{5}{3}\nu^{\frac{7}{3}} - \frac{4}{3}\nu^{\frac{5}{3}} + V\nu = 0 \\ -\Delta V = 4\pi(\nu^2 - \rho_b). \end{cases} \tag{3.4}$$

Theorem 3.1.1. *Under Stability Condition A, i.e., the linearized operator of the the above equations at undeformed solutions satisfies* $\|\mathcal{L}^{-1}_{per}\|_{\mathcal{L}((L^2_n)2)} \leqslant M_{per}$ *for any* n*, and* M_{per} *is a positive constant independent of* $\epsilon = \frac{1}{n}$*, then there exist positive constants* h_0, ϵ_0, δ *such that for any* $\|u\|_{W^{7,\infty}_1} \leqslant h_0, \epsilon \leqslant \epsilon_0$*, there exists a unique solution* $\mathcal{V}_{exa} = (\nu_{exa}, V_{exa}) \in (H^2_n)^2$ *with the properties*

1. (ν_{exa}, V_{exa}) *satisfies the system of Euler-Lagrange equations*

$$\mathcal{F}_{TFDW}(\nu_{exa}, V_{exa}) = 0$$

2. (ν_{exa}, V_{exa}) *is close to the approximation given by the Cauchy-Born rule*

$$\|(\nu_{exa}, V_{exa}) - (\nu_{CB}(x; \nabla u(\epsilon x)), V_{CB}(x; \nabla u(\epsilon x)))\|_{(H^2_n)^2} \leqslant \delta\epsilon. \tag{3.5}$$

3. (ν_{exa}, V_{exa}) *is a* $(H^1_n)^2$ *local minimizer of the electronic TFDW functional* $I(\nu, V; \rho_b)$.

3.2 The atomistic TFDW model

The above solution $(\nu_{\text{exa}}, V_{\text{exa}})$ and the background charge ρ_b depend on the deformation u which is constructed as the Fourier interpolation of the discrete atom position function Y:

$$\tau_Y(x) = x + u_Y(x) = \epsilon^3 \sum_{X\in\Omega_\epsilon, \xi\in\Omega^*_\epsilon} e^{\imath(x-X)\cdot\xi} Y(X). \tag{3.6}$$

Now consider the following atomistic TFDW functional

$$I_{\mathrm{at}}(Y) = I(\nu_{\mathrm{exa}}(\tau_Y), V_{\mathrm{exa}}(\tau_Y), \rho_b^\epsilon(\tau_Y, Y)) \tag{3.7}$$

where we assume $\|u_Y\|_{W_1^{7,\infty}} \leqslant h_0$, so that $(\nu_{\mathrm{exa}}, V_{\mathrm{exa}})$ is well-defined.

Define the space of the discrete deformation function Y as

$$X_\epsilon = \big\{Y : \epsilon\mathbb{L} \to \mathbb{R}^3 | Y(X) = X + u(X), u \text{ is } \Omega_\epsilon\text{-periodic}, \sum_{X \in \Omega_\epsilon} u(X) = 0\big\}. \tag{3.8}$$

The atomistic TFDW problem is formulated as follows: Given an external force $f_\epsilon : \Omega_\epsilon \to \mathbb{R}^3$, find $Y \in X_\epsilon$ such that

$$Y = \mathrm{argmin}_{z \in X_\epsilon} I_{\mathrm{at}}(z). \tag{3.9}$$

The Euler-Lagrange equation for the atomistic problem is

$$\mathcal{F}_{\mathrm{at}}[Y](X) = f_\epsilon(X), \quad X \in \Omega_\epsilon, \tag{3.10}$$

where

$$\mathcal{F}_{\mathrm{at}}[Y](X_i) = -\int_{n\Omega} V_{\mathrm{exa}} \frac{\partial \rho_b}{\partial Y_i} dy \tag{3.11}$$

and

$$\sum_{X \in \Omega_\epsilon} f_\epsilon(X) = 0. \tag{3.12}$$

Theorem 3.2.1. *Under Stability Condition B, i.e., the dynamical matrix $\mathcal{D}_{at}^{Id}[\xi]$ of the Hessian $\mathcal{H}_{at}[Id]$ of the above Euler-Lagrange equation in the undeformed state, i.e., $Y = Id$ or $u = 0$, satisfies*

$$\det \mathcal{D}_{at}^{Id}[\xi] \geqslant a_{at} \Lambda_{0,\epsilon}^6(\xi), \quad \xi \in \Omega_\epsilon^*, \tag{3.13}$$

further assume $m_a \in C_0^\infty(\mathbb{R}^3), f_\epsilon \in W_\epsilon^{27,\infty}$ with $\|f_\epsilon\|_{W_\epsilon^{27,\infty}} \leqslant h_f$ for some constant $h_f > 0$, then there exists a unique $Y_{at} \in H_\epsilon^7 \cap X_\epsilon$ with the properties

1. Y_{at} *satisfies the Euler-Lagrange equation*

$$\mathcal{F}_{at}[Y_{at}](X) = f_\epsilon(X), \quad X \in \Omega_\epsilon \tag{3.14}$$

2. *The consistency estimate of the Cauchy-Born rule holds*

$$\|\mathcal{F}_{at}[Y_{CB}]\|_{\epsilon,5} \leqslant C(\|u_{at}\|_{W_1^{29,\infty}})\epsilon^2 \tag{3.15}$$

3. Y_{at} *is a discrete* $W_\epsilon^{1,\infty}$ *local minimizer of the atomistic TFDW functional* $I_{at}(Y)$.

3.3 The Cauchy-Born continuum elasticity model

Assume the above f_ϵ is constructed from a function f defined on Ω with zero mean,

$$f_\epsilon(X) = \epsilon^{-3}\int_{X+\epsilon\Omega} f(z)dz. \tag{3.16}$$

Define

$$X = \left\{v : \Omega \to \mathbb{R}^3 | v \in W_1^{m+2,p}, \int_\Omega v = 0\right\} \tag{3.17}$$

for $m \geqslant 0, p > 3$.

The Cauchy-Born continuum elasticity problem is formulated as follows: find a deformation function $u \in X$ such that

$$u = \mathrm{argmin}_{v\in X} I_{\mathrm{CB}}(v) \tag{3.18}$$

where

$$I_{\mathrm{CB}}(v) = \int_\Omega W_{\mathrm{CB}}(\nabla v(x)) - f(x)(v(x) - x)dx, \tag{3.19}$$

in which the Cauchy-Born stored energy density W_{CB} is

$$\begin{aligned} W_{\mathrm{CB}}(A) =& \frac{1}{|\Omega|}\int_\Omega J^{-\frac{2}{3}}(A)\nu_{\mathrm{CB}}^{\frac{10}{3}}(A) - \nu_{\mathrm{CB}}a^{ij}(A)\partial_{z_i}\partial_{z_j}\nu_{\mathrm{CB}}(A) \\ &- J^{-\frac{1}{3}}(A)\nu_{\mathrm{CB}}^{\frac{8}{3}}(A) + \frac{1}{2}V_{\mathrm{CB}}(A)(\nu_{\mathrm{CB}}^2(A) - J(A)\rho_{b,0}(A))dz \end{aligned}$$

The corresponding Euler-Lagrange equation is

$$\mathcal{F}_{\mathrm{CB}}(u(x)) = f(x), \quad x \in \Omega \tag{3.20}$$

where

$$\mathcal{F}_{\mathrm{CB}}(u(x)) = -\nabla \cdot (D_A W_{\mathrm{CB}}(\nabla u(x))). \tag{3.21}$$

Theorem 3.3.1. *If Stability Condition C holds*

$$D_A^2 W_{CB}(0)(\xi \otimes \eta, \xi \otimes \eta) \geqslant \Lambda |\xi|^2 |\eta|^2, \tag{3.22}$$

and $p > 3, m \geqslant 0$, then there exist constants $\delta, \kappa_1, \kappa_2$, such that for any $B \in \mathbb{R}_+^{3\times3}$ with $\|B\| \leqslant \kappa_1$ and $\|f\|_{W^{m,p}(\Omega)} \leqslant \kappa_2$, there exists a unique solution $u_{CB} \in X$ such that the following properties hold

1. *u_{CB} satisfies the Euler-Lagrange equation*

$$\mathcal{F}_{CB}(u_{CB}(x)) = f(x), \quad x \in \Omega; \tag{3.23}$$

2. *u_{CB} is a $W_1^{1,\infty}$ local minimizer of the Cauchy-Born continuum elasticity functional $I_{CB}(v)$.*

3. *$\|u_{CB} - B \cdot x\|_{W^{m+2,p}} \leqslant \delta$, for any $x \in \Omega$.*

3.4 the Main Theorem

Theorem 3.4.1. *With the assumptions in the above theorems, further assume $m \geqslant 27$, denote Y_{CB} as the discrete deformation function associated with u_{CB}, then there exists a positive constant C independent of ϵ such that*

$$\|Y_{at} - Y_{CB}\|_{\epsilon,7} \leqslant C\epsilon^2. \tag{3.24}$$

4

TFDW Functional

4.1 Setup of the TFDW Functional

4.1.1 Original TFDW functional

The original deformed unscaled TFDW functional is

$$I(\rho, \rho_b) = \int_{\mathbb{R}^3} \rho^{\frac{5}{3}}(y) + |\nabla\sqrt{\rho(y)}|^2 - \rho^{\frac{4}{3}}(y)dy + \frac{1}{2}D(\rho - \rho_b, \rho - \rho_b), \tag{4.1}$$

where $\rho : \mathbb{R}^3 \to \mathbb{R}$ is the electron density in Eulerian coordinates with the constraints $\int_{\mathbb{R}^3} \rho dy = \int_{\mathbb{R}^3} \rho_b dy$ and $\rho \geqslant C > 0$. The shorthand notation $D(\cdot, \cdot)$ is defined as

$$D(f, g) = \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(y_1)g(y_2)}{|y_1 - y_2|} dy_1 dy_2 \tag{4.2}$$

Thus

$$D(\rho - \rho_b, \rho - \rho_b) = \int_{\mathbb{R}^3} V(\rho - \rho_b)dy, \tag{4.3}$$

where V is the potential

$$V(y) = \int_{\mathbb{R}^3} \frac{\rho(y') - \rho_b(y')}{|y - y'|} dy'. \tag{4.4}$$

Moreover, ρ_b is the background charge density

$$\rho_b(y, Y) = \sum_{X_i \in \mathbb{L}} m_a(y - Y(X_i))$$

where $Y : \mathbb{L} \to \mathbb{R}^3$ is a discrete deformation function. In the use of $m_a(y - Y(X_i))$, we assume the charge contribution of each nucleus does not change under the deformation. We also denote $Y(X_i)$ as Y_i.

4.1.2 Periodicity and scaling

Now assume we have a periodic discrete deformation function $Y : \Omega_\epsilon \to \mathbb{R}^3$, define the rescaled version of it $Y^\epsilon : \Omega_n \to \mathbb{R}^3$

$$Y^\epsilon(X) := \frac{1}{\epsilon} Y(\epsilon X), \quad \forall X \in \Omega_n \tag{4.5}$$

then Y^ϵ is periodic in Ω_n.

Next we define the periodic TFDW functional with unit scaling as

$$I(\rho, \rho_b) = \int_{n\Omega} \rho^{\frac{5}{3}} + |\nabla \sqrt{\rho}|^2 - \rho^{\frac{4}{3}} dy + \frac{1}{2} D_{n\Omega}(\rho - \rho_b(Y^\epsilon), \rho - \rho_b(Y^\epsilon)), \tag{4.6}$$

with the constraints $\int_{n\Omega} \rho dy = \int_{n\Omega} \rho_b(Y^\epsilon) dy = \mathcal{Z}$ and $\rho \geqslant C > 0$ for a constant C and

$$D_{n\Omega}(\rho - \rho_b(Y^\epsilon), \rho - \rho_b(Y^\epsilon)) = \int_{n\Omega} V(\rho - \rho_b(Y^\epsilon)) dy, \tag{4.7}$$

where V satisfies

$$\begin{cases} -\Delta V = 4\pi(\rho - \rho_b(Y^\epsilon)) & \text{in } n\Omega \\ V \text{ is periodic on } \partial(n\Omega). \end{cases} \tag{4.8}$$

Introduce $\nu = \sqrt{\rho}$. We can rescale the system by the ϵ-scaling with $\epsilon = \frac{1}{n}$. Let us change the variables correspondingly for $y \in \Omega$:

$$\rho_b^\epsilon(y, Y) := \rho_b(\frac{y}{\epsilon}, Y^\epsilon)$$

$$
\begin{aligned}
&= \sum_{X \in \mathbb{L}} m_a(\frac{y}{\epsilon} - Y^\epsilon(X)) \\
&= \sum_{X \in \mathbb{L}_\epsilon} m_a(\frac{y - Y(X)}{\epsilon}) \\
&= \sum_{X_i \in \Omega_\epsilon} \sum_{r \in \mathbb{L}} m_a(\frac{y + r - Y_i}{\epsilon})
\end{aligned}
$$

$$
\begin{aligned}
\nu_\epsilon(y) :=& \nu(\frac{y}{\epsilon}) = \sqrt{\rho(\frac{y}{\epsilon})} \\
V_\epsilon(y) :=& V(\frac{y}{\epsilon}).
\end{aligned}
$$

Then we have

$$
\int_\Omega \nu_\epsilon^2 dy = \int_\Omega \rho_b^\epsilon(Y) dy = \mathcal{Z}.
$$

The following formula gives the connection between the unit scaling and the ϵ-scaling for the TFDW functional:

$$
\begin{aligned}
I =& \int_{n\Omega} \nu^{\frac{10}{3}} + |\nabla \nu|^2 - \nu^{\frac{8}{3}} + \frac{1}{2} V(\nu^2 - \rho_b(Y^\epsilon)) dy \\
=& \epsilon^{-3} \int_\Omega \nu_\epsilon^{\frac{10}{3}} + \epsilon^2 |\nabla \nu_\epsilon|^2 - \nu_\epsilon^{\frac{8}{3}} + \frac{1}{2} V_\epsilon(\nu_\epsilon^2 - \rho_b^\epsilon(Y)) dy.
\end{aligned} \tag{4.9}
$$

4.1.3 The Lagrangian coordinates

Given the periodic discrete deformation function $Y : \Omega_\epsilon \to \mathbb{R}^3$, the corresponding deformation function u or $\tau = \mathrm{id} + u : \Omega \to \mathbb{R}^3$ is given as the Fourier interpolation of Y. We also use τ_Y or u_Y to explicitly indicate its dependence on Y. Let $J(x) = \det \nabla \tau(x)$, and also define the scaled version of the deformation: $\tau_\epsilon(x) := \frac{1}{\epsilon}\tau(\epsilon x)$ for $x \in n\Omega$. Denote $J_\epsilon(x) = \det \nabla \tau_\epsilon(x)$ for $x \in n\Omega$, then $J_\epsilon(x) = J(\epsilon x)$.

Define

$$
\nu(x) = J_\epsilon^{\frac{1}{2}}(x) \nu(\tau_\epsilon(x)), V(x) = V(\tau_\epsilon(x)), \rho_b(x) = J_\epsilon(x) \rho_b(\tau_\epsilon(x), Y^\epsilon), x \in n\Omega
$$

$$\nu_\epsilon(x) = J^{\frac{1}{2}}(x)\nu_\epsilon(\tau(x)), V_\epsilon(x) = V_\epsilon(\tau(x)), \rho_b^\epsilon(x) = \rho_b^\epsilon(\tau(x), Y), x \in \Omega$$

then the TFDW functional in Lagrangian coordinates is

$$I = \int_{n\Omega} J_\epsilon^{-\frac{2}{3}}\nu^{\frac{10}{3}} + J_\epsilon|\nabla\tau_\epsilon^{-T}\nabla(J_\epsilon^{-\frac{1}{2}}\nu)|^2 - J_\epsilon^{-\frac{1}{3}}\nu^{\frac{8}{3}} + \frac{1}{2}V(\nu^2 - J_\epsilon\rho_b(Y^\epsilon))dx \tag{4.10}$$

$$= \epsilon^{-3}\int_\Omega J^{-\frac{2}{3}}\nu_\epsilon^{\frac{10}{3}} + \epsilon^2 J|\nabla\tau^{-T}\nabla(J^{-\frac{1}{2}}\nu_\epsilon)|^2 - J^{-\frac{1}{3}}\nu_\epsilon^{\frac{8}{3}} + \frac{1}{2}V_\epsilon(\nu_\epsilon^2 - J\rho_b^\epsilon(Y))dx. \tag{4.11}$$

4.2 Euler-Lagrange Equations

4.2.1 ϵ-scaling

The ϵ-scaled TFDW functional with an external force $f : \Omega_\epsilon \to \mathbb{R}^3$ is

$$\begin{aligned} &I(\nu_\epsilon, V_\epsilon, \rho_b^\epsilon) - |\Omega| \sum_{X\in\Omega_\epsilon} f(X)Y(X) \\ =&\epsilon^{-3}\int_\Omega \nu_\epsilon^{\frac{10}{3}} + \epsilon^2|\nabla\nu_\epsilon|^2 - \nu_\epsilon^{\frac{8}{3}} + \frac{1}{2}V_\epsilon(\nu_\epsilon^2 - \rho_b^\epsilon)dy - |\Omega| \sum_{X\in\Omega_\epsilon} f(X)Y(X) \end{aligned} \tag{4.12}$$

Assume Y is fixed, then the system of Euler-Lagrange equations of ν_ϵ, V_ϵ in Eulerian coordinates is

$$\begin{cases} -\epsilon^2\Delta\nu_\epsilon + \frac{5}{3}\nu_\epsilon^{\frac{7}{3}} - \frac{4}{3}\nu_\epsilon^{\frac{5}{3}} + V_\epsilon\nu_\epsilon = 0, \\ -\epsilon^2\Delta V_\epsilon = 4\pi(\nu_\epsilon^2 - \rho_b^\epsilon), \quad y \in \Omega, \end{cases} \tag{4.13}$$

The system of Euler-Lagrange equations of ν^ϵ, V^ϵ in Lagrangian coordinates is

$$\begin{cases} -\epsilon^2 D_1\nu_\epsilon + \frac{5}{3}J^{-\frac{2}{3}}\nu_\epsilon^{\frac{7}{3}} - \frac{4}{3}J^{-\frac{1}{3}}\nu_\epsilon^{\frac{5}{3}} + V_\epsilon\nu_\epsilon = 0 \\ -\epsilon^2 JD_2V_\epsilon = 4\pi(\nu_\epsilon^2 - J\rho_b^\epsilon), \quad x \in \Omega, \end{cases} \tag{4.14}$$

where $D_1 = \sum_{ij} a_{ij}\partial_i\partial_j + \sum_j b_j\partial_j + c$ in which

$$\begin{cases} a_{ij} = (\nabla\tau^{-1}\nabla\tau^{-T})_{ij} \\ b_j = \sum_{ik}\nabla\tau_{ik}^{-1}\partial_i\nabla\tau_{kj}^{-T} - 2J^{\frac{1}{2}}\sum_i a_{ij}\partial_i J^{-\frac{1}{2}} \\ c = J^{\frac{1}{2}}\sum_{ijk}\nabla\tau_{ik}^{-1}\partial_i\nabla\tau_{kj}^{-T}\partial_j J^{-\frac{1}{2}} + J^{\frac{1}{2}}\sum_{ij} a_{ij}\partial_i\partial_j J^{-\frac{1}{2}} \end{cases} \tag{4.15}$$

and $D_2 = \sum_{ij} a_{ij}\partial_i\partial_j + \sum_j d_j\partial_j$ in which

$$\begin{cases} a_{ij} = (\nabla\tau^{-1}\nabla\tau^{-T})_{ij} \\ d_j = \sum_{ik} \nabla\tau^{-1}_{ik}\partial_i\nabla\tau^{-T}_{kj} \end{cases} \tag{4.16}$$

4.2.2 Unit scaling

The TFDW functional under unit scaling with the external force $f : \Omega_\epsilon \to \mathbb{R}^3$ is

$$\begin{aligned} & I(\nu, V, \rho_b) - \sum_{X\in\Omega_n} \epsilon|\Omega|f(\epsilon X)Y^\epsilon(X) \\ = & \int_{n\Omega} \nu^{\frac{10}{3}} + |\nabla\nu|^2 - \nu^{\frac{8}{3}} + \frac{1}{2}V(\nu^2 - \rho_b)dy - \sum_{X\in\Omega_n} \epsilon|\Omega|f(\epsilon X)Y^\epsilon(X), \end{aligned} \tag{4.17}$$

the system of Euler-Lagrange equations of ν, V with fixed Y^ϵ in Eulerian coordinates is

$$\begin{cases} -\Delta\nu + \frac{5}{3}\nu^{\frac{7}{3}} - \frac{4}{3}\nu^{\frac{5}{3}} + V\nu = 0, \\ -\Delta V = 4\pi(\nu^2 - \rho_b), \quad y \in n\Omega, \end{cases} \tag{4.18}$$

the system of Euler-Lagrange equations of ν, V in Lagrangian coordinates is

$$\begin{cases} -D_1^\epsilon\nu + \frac{5}{3}J_\epsilon^{-\frac{2}{3}}\nu^{\frac{7}{3}} - \frac{4}{3}J_\epsilon^{-\frac{1}{3}}\nu^{\frac{5}{3}} + V\nu = 0 \\ -J_\epsilon D_2^\epsilon V = 4\pi(\nu^2 - J_\epsilon\rho_b), \quad x \in n\Omega, \end{cases} \tag{4.19}$$

where $D_1^\epsilon = \sum_{ij} a_{ij}^\epsilon\partial_i\partial_j + \sum_j b_j^\epsilon\partial_j + c^\epsilon$ in which

$$\begin{cases} a_{ij}^\epsilon(x) = a_{ij}(\epsilon x) \\ b_j^\epsilon(x) = b_j(\epsilon x) \\ c^\epsilon(x) = c(\epsilon x) \end{cases} \tag{4.20}$$

and $D_2^\epsilon = \sum_{ij} a_{ij}^\epsilon\partial_i\partial_j + \sum_j d_j^\epsilon\partial_j$ in which

$$\begin{cases} a_{ij}^\epsilon(x) = a_{ij}(\epsilon x) \\ d_j^\epsilon(x) = d_j(\epsilon x) \end{cases} \tag{4.21}$$

4.3 Linearization of the System of Euler-Lagrange Equations

Denote $\mathcal{V}_\epsilon = (\nu_\epsilon, V_\epsilon)$, the linearized operator $\mathcal{L}_{\mathcal{V}_\epsilon}$ of the system of Euler-Lagrange equations of $(\nu_\epsilon, V_\epsilon)$ in Eulerian coordinates is given by

$$\mathcal{L}_{\mathcal{V}_\epsilon}\begin{pmatrix}\omega\\ W\end{pmatrix} = \begin{pmatrix}(-\epsilon^2\Delta + \frac{35}{9}\nu_\epsilon^{\frac{4}{3}} - \frac{20}{9}\nu_\epsilon^{\frac{2}{3}} + V_\epsilon)\omega + \nu W\\ \nu_\epsilon\omega + \frac{\epsilon^2}{8\pi}\Delta W\end{pmatrix} \tag{4.22}$$

where $\omega, W \in L^2(\Omega, \mathbb{R})$.

Similarly, with unit scaling, denote $\mathcal{V} = (\nu, V)$, the linearized operator $\mathcal{L}_\mathcal{V}$ of the system of Euler-Lagrange equations of (ν, V) in Eulerian coordinates is given by

$$\mathcal{L}_{\mathcal{V}}\begin{pmatrix}\omega\\ W\end{pmatrix} = \begin{pmatrix}(-\Delta + \frac{35}{9}\nu^{\frac{4}{3}} - \frac{20}{9}\nu^{\frac{2}{3}} + V)\omega + \nu W\\ \nu\omega + \frac{1}{8\pi}\Delta W\end{pmatrix} \tag{4.23}$$

where $\omega, W \in L^2(n\Omega, \mathbb{R})$.

Moreover, the above linearized operator $\mathcal{L}_\mathcal{V}$ in Lagrangian coordinates is given by

$$\mathcal{L}_{\mathcal{V}}\begin{pmatrix}\omega\\ W\end{pmatrix} = \begin{pmatrix}\mathcal{L}_{\mathcal{V},1} & \nu\\ \nu & \frac{1}{8\pi}D_2^\epsilon\end{pmatrix}\begin{pmatrix}\omega\\ W\end{pmatrix} \tag{4.24}$$

where

$$\mathcal{L}_{\mathcal{V},1} = -D_1^\epsilon + \frac{35}{9}J_\epsilon^{-\frac{2}{3}}\nu^{\frac{4}{3}} - \frac{20}{9}J_\epsilon^{-\frac{1}{3}}\nu^{\frac{2}{3}} + V. \tag{4.25}$$

4.4 Solutions In Undeformed Crystals

Assume there is no deformation $u = 0$, so $Y(X) = X, X \in \Omega_\epsilon$. Then the background charge becomes $\rho_{b,\mathrm{per}}(x) = \sum_{X\in\mathbb{L}} m_a(x - X)$ which is periodic in Ω. So ν, V shall also be periodic in Ω. Denote them as $\nu_{\mathrm{per}}, V_{\mathrm{per}}$, and we solve the corresponding Euler-Lagrange equations

$$\begin{cases}-\Delta\nu_{\mathrm{per}} + \frac{5}{3}\nu_{\mathrm{per}}^{\frac{7}{3}} - \frac{4}{3}\nu_{\mathrm{per}}^{\frac{5}{3}} + V_{\mathrm{per}}\nu_{\mathrm{per}} = 0, & x \in \Omega\\ -\Delta V_{\mathrm{per}} = 4\pi(\nu_{\mathrm{per}}^2 - \rho_{b,\mathrm{per}}), & x \in \Omega\end{cases} \tag{4.26}$$

with the constraints $\int_\Omega \nu_{\text{per}}^2 dx = \int_\Omega \rho_{b,\text{per}} dx$ and $\nu_{\text{per}} \geqslant C > 0$ for some positive constant C.

Given $m_a \in C_0^\infty(\mathbb{R}^3) \cap W^{k,\infty}$, we have $\nu_{\text{per}}, V_{\text{per}} \in W_1^{k,\infty}$, and can be extended periodically to $\nu_{\text{per}}, V_{\text{per}} \in W_n^{k,\infty}$.

4.5 The Stability Condition

The undeformed solutions $\nu_{\text{per}}, V_{\text{per}} \in W_n^{k,\infty}$ satisfy the Euler-Lagrange equations

$$\begin{cases} -\Delta\nu_{\text{per}} + \frac{5}{3}\nu_{\text{per}}^{\frac{7}{3}} - \frac{4}{3}\nu_{\text{per}}^{\frac{5}{3}} + V_{\text{per}}\nu_{\text{per}} = 0, & x \in n\Omega \\ -\Delta V_{\text{per}} = 4\pi(\nu_{\text{per}}^2 - \rho_b), & x \in n\Omega \end{cases} \tag{4.27}$$

for any n. The linearization in $n\Omega$ becomes

$$\mathcal{L}_{\text{per}} \begin{pmatrix} \omega \\ W \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{1,\text{per}} & \nu_{\text{per}} \\ \nu_{\text{per}} & \frac{1}{8\pi}\Delta \end{pmatrix} \begin{pmatrix} \omega \\ W \end{pmatrix} \tag{4.28}$$

where

$$\mathcal{L}_{1,\text{per}} = -\Delta + \frac{35}{9}\nu_{\text{per}}^{\frac{4}{3}} - \frac{20}{9}\nu_{\text{per}}^{\frac{2}{3}} + V_{\text{per}}. \tag{4.29}$$

We introduce the electronic stability condition which we call **Stability Condition A**:

$$\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((L_n^2)^2)} \leqslant M \tag{4.30}$$

for arbitrary n, where M is a positive constant independent of n.

4.6 The Cauchy-Born Solution With Fixed Deformation

In order to construct the exact solutions ν, V on $n\Omega$, we first construct approximate solutions by the two-scale ansatz of $\nu_\epsilon, V_\epsilon, \rho_b^\epsilon$, in which the first step is to construct the Cauchy-Born solution of the leading-order equation. We give the construction of the Cauchy-Born solution in this section.

4.6.1 Two-Scale Ansatz

We assume the following approximation for $x \in \Omega$,

$$\begin{cases} \nu_\epsilon(x) = \nu_0(\frac{x}{\epsilon}, x) + \epsilon\nu_1(\frac{x}{\epsilon}, x) + \epsilon^2\nu_2(\frac{x}{\epsilon}, x), \\ V_\epsilon(x) = V_0(\frac{x}{\epsilon}, x) + \epsilon V_1(\frac{x}{\epsilon}, x) + \epsilon^2 V_2(\frac{x}{\epsilon}, x), \\ \rho_b^\epsilon(x) = \rho_{b,0}(\frac{x}{\epsilon}, x) + \epsilon\rho_{b,1}(\frac{x}{\epsilon}, x) + \epsilon^2\rho_{b,2}(\frac{x}{\epsilon}, x). \end{cases} \tag{4.31}$$

Recall that $\rho_{b,0}, \rho_{b,1}, \rho_{b,2}$ are periodic in $z = \frac{x}{\epsilon}$ in Ω, so we assume the same periodic property for ν_0, ν_1, ν_2 and V_0, V_1, V_2.

Plug the ansatz into the system of Euler-Lagrange equations of $(\nu_\epsilon, V_\epsilon)$ (4.14), combine terms of the same orders of ϵ, we get the leading-order ϵ^0 system of equations:

$$\begin{cases} -\sum_{ij} a_{ij}\partial_{z_i}\partial_{z_j}\nu_0 + \frac{5}{3}J^{-\frac{2}{3}}\nu_0^{\frac{7}{3}} - \frac{4}{3}J^{-\frac{1}{3}}\nu_0^{\frac{5}{3}} + V_0\nu_0 = 0 \\ -J\sum_{ij} a_{ij}\partial_{z_i}\partial_{z_j}V_0 = 4\pi(\nu_0^2 - J\rho_{b,0}). \end{cases} \tag{4.32}$$

In addition, the system of equations of order ϵ^1 is

$$\begin{cases} -\sum_{ij} a_{ij}\partial_{z_i}\partial_{z_j}\nu_1 + \frac{35}{9}J^{-\frac{2}{3}}\nu_0^{\frac{4}{3}}\nu_1 - \frac{20}{9}J^{-\frac{1}{3}}\nu_0^{\frac{2}{3}}\nu_1 + V_0\nu_1 \\ -\sum_{ij} a_{ij}(\partial_{x_j}\partial_{z_i}\nu_0 + \partial_{x_i}\partial_{z_j}\nu_0) - \sum_j b_j\partial_{z_j}\nu_0 + V_1\nu_0 = 0 \\ \\ -J\sum_{ij} a_{ij}\partial_{z_i}\partial_{z_j}V_1 - 8\pi\nu_0\nu_1 + 4\pi J\rho_{b,1} \\ -J\sum_{ij} a_{ij}(\partial_{x_j}\partial_{z_i}V_0 + \partial_{x_i}\partial_{z_j}V_0) - J\sum_j d_j\partial_{z_j}V_0 = 0, \end{cases} \tag{4.33}$$

and equations of order ϵ^2 are

$$\begin{cases} -\sum_{ij} a_{ij}\partial_{z_i}\partial_{z_j}\nu_2 + \frac{35}{9}J^{-\frac{2}{3}}\nu_0^{\frac{4}{3}}\nu_2 - \frac{20}{9}J^{-\frac{1}{3}}\nu_0^{\frac{2}{3}}\nu_2 + V_0\nu_2 \\ -\sum_{ij} a_{ij}(\partial_{x_j}\partial_{z_i}\nu_1 + \partial_{x_i}\partial_{z_j}\nu_1) - \sum_{ij} b_j\partial_{z_j}\nu_1 + \frac{70}{27}J^{-\frac{2}{3}}\nu_0^{\frac{1}{3}}\nu_1^2 - \frac{20}{27}J^{-\frac{1}{3}}\nu_0^{-\frac{1}{3}}\nu_1^2 + V_1\nu_1 \\ -\sum_{ij} a_{ij}\partial_{x_i}\partial_{x_j}\nu_0 - \sum_j b_j\partial_{x_j}\nu_0 - c\nu_0 + V_2\nu_0 = 0 \\ \\ -J\sum_{ij} a_{ij}\partial_{z_i}\partial_{z_j}V_2 - 8\pi\nu_0\nu_2 + 4\pi J\rho_{b,2} \\ -J\sum_{ij} a_{ij}(\partial_{x_j}\partial_{z_i}V_1 + \partial_{x_i}\partial_{z_j}V_1) - J\sum_j d_j\partial_{z_j}V_1 - 4\pi\nu_1^2 \\ -J\sum_{ij} a_{ij}\partial_{x_i}\partial_{x_j}V_0 - J\sum_j d_j\partial_{x_j}V_0 = 0. \end{cases} \tag{4.34}$$

4.6.2 Regularity of the linearized operator

In order to achieve higher regularity of the solutions, we need the following lemma

Lemma 4.6.1. *Assume* **Stability Condition A** *holds, that is* $\|\mathcal{L}_{per}^{-1}\|_{\mathcal{L}((L_n^2)^2)} \leqslant M$ *for a positive constant* M *and all nonnegative integer* n*, then we have*

$$\|\mathcal{L}_{per}^{-1}\|_{\mathcal{L}((H_n^k)^2,(H_n^{k+2})^2)} \leqslant C(k)M, \tag{4.35}$$

where $C(k)$ *is constant for each nonnegative integer* k *provided* $\nu_{per}, V_{per} \in W_n^{k,\infty}$*. Specifically, when* $n = 1$*, we have*

$$\|\mathcal{L}_{per}^{-1}\|_{\mathcal{L}((H_1^k)^2,(H_1^{k+2})^2)} \leqslant C(k)M. \tag{4.36}$$

Proof. We use induction to prove the lemma. For $k = 0$, we want $\mathcal{L}_{\text{per}}^{-1} : (L_n^2)^2 \to (H_n^2)^2$ to be bounded. This is to say given $(\omega, W) \in (L_n^2)^2$, we want to show

$$\|\mathcal{L}_{\text{per}}^{-1}\begin{pmatrix}\omega\\W\end{pmatrix}\|_{(H_n^2)^2} \leqslant C(0)M\|\begin{pmatrix}\omega\\W\end{pmatrix}\|_{(L_n^2)^2}.$$

It suffices to prove

$$\|A\mathcal{L}_{\text{per}}^{-1}\begin{pmatrix}\omega\\W\end{pmatrix}\|_{(L_n^2)^2} \lesssim M\|\begin{pmatrix}\omega\\W\end{pmatrix}\|_{(L_n^2)^2},$$

where $A = \begin{pmatrix}-\Delta & 0\\ 0 & \frac{1}{8\pi}\Delta\end{pmatrix}$.

Since

$$\begin{pmatrix}\omega\\W\end{pmatrix} = \mathcal{L}_{\text{per}}\mathcal{L}_{\text{per}}^{-1}\begin{pmatrix}\omega\\W\end{pmatrix} = [A + \begin{pmatrix}F & \nu_{\text{per}}\\ \nu_{\text{per}} & 0\end{pmatrix}]\mathcal{L}_{\text{per}}^{-1}\begin{pmatrix}\omega\\W\end{pmatrix}$$

where $F = \frac{35}{9}\nu_{\text{per}}^{\frac{4}{3}} - \frac{20}{9}\nu_{\text{per}}^{\frac{2}{3}} + V_{\text{per}}$, we get

$$A\mathcal{L}_{\text{per}}^{-1}\begin{pmatrix}\omega\\W\end{pmatrix} = \begin{pmatrix}\omega\\W\end{pmatrix} - \begin{pmatrix}F & \nu_{\text{per}}\\ \nu_{\text{per}} & 0\end{pmatrix}\mathcal{L}_{\text{per}}^{-1}\begin{pmatrix}\omega\\W\end{pmatrix}.$$

Therefore

$$
\begin{aligned}
&\|A\mathcal{L}_{\text{per}}^{-1}\begin{pmatrix}\omega\\ W\end{pmatrix}\|_{(L_n^2)^2}\\
\leqslant&\|\begin{pmatrix}\omega\\ W\end{pmatrix}\|_{(L_n^2)^2}+\max(\|F\|_{L_n^\infty},\|\nu_{\text{per}}\|_{L_n^\infty})\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((L_n^2)^2)}\|\begin{pmatrix}\omega\\ W\end{pmatrix}\|_{(L_n^2)^2}\\
\lesssim&M\|\begin{pmatrix}\omega\\ W\end{pmatrix}\|_{(L_n^2)^2}.
\end{aligned}
$$

Next, assume

$$
\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^k)^2,(H_n^{k+2})^2)}\leqslant C(k)M
$$

for $k\leqslant k_0$. Then for $k=k_0+1$, it suffices to prove

$$
\|\nabla\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^k)^2,(H_n^{k+1})^2)}\lesssim M
$$

Notice

$$
\begin{aligned}
\nabla\mathcal{L}_{\text{per}}^{-1}&=\mathcal{L}_{\text{per}}^{-1}\nabla+[\nabla,\mathcal{L}_{\text{per}}^{-1}]\\
&=\mathcal{L}_{\text{per}}^{-1}\nabla-\mathcal{L}_{\text{per}}^{-1}[\nabla,\mathcal{L}_{\text{per}}]\mathcal{L}_{\text{per}}^{-1},
\end{aligned}
$$

so it suffices to prove

$$
\|\mathcal{L}_{\text{per}}^{-1}[\nabla,\mathcal{L}_{\text{per}}]\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^k)^2,(H_n^{k+1})^2)}\lesssim M.
$$

Direct calculation yields

$$
\begin{aligned}
&[\nabla,\mathcal{L}_{\text{per}}]=\nabla\mathcal{L}_{\text{per}}-\mathcal{L}_{\text{per}}\nabla\\
=&\begin{pmatrix}\nabla & \\ & \nabla\end{pmatrix}\begin{pmatrix}-\Delta+F & \nu_{\text{per}}\\ \nu_{\text{per}} & \frac{1}{8\pi}\Delta\end{pmatrix}-\begin{pmatrix}-\Delta+F & \nu_{\text{per}}\\ \nu_{\text{per}} & \frac{1}{8\pi}\Delta\end{pmatrix}\begin{pmatrix}\nabla & \\ & \nabla\end{pmatrix}\\
=&\begin{pmatrix}-\nabla\Delta+\nabla F & \nabla\nu_{\text{per}}\\ \nabla\nu_{\text{per}} & \frac{1}{8\pi}\nabla\Delta\end{pmatrix}-\begin{pmatrix}-\Delta\nabla+F\nabla & \nu_{\text{per}}\nabla\\ \nu_{\text{per}}\nabla & \frac{1}{8\pi}\Delta\nabla\end{pmatrix}\\
=&\begin{pmatrix}\nabla F-F\nabla & \nabla\nu_{\text{per}}-\nu_{\text{per}}\nabla\\ \nabla\nu_{\text{per}}-\nu_{\text{per}}\nabla & 0\end{pmatrix}.
\end{aligned}
$$

Notice $\nabla F, \nabla \nu_{\text{per}} \in W_n^{k-1,\infty}$ since $\nu_{\text{per}}, V_{\text{per}} \in W_n^{k,\infty}$ and so $F \in W_n^{k,\infty}$. Hence we get the bound

$$\|[\nabla, \mathcal{L}_{\text{per}}]\|_{\mathcal{L}((H_n^{k+1})^2,(H_n^{k-1})^2)} \lesssim M.$$

Thus

$$\begin{aligned} &\|\mathcal{L}_{\text{per}}^{-1}[\nabla, \mathcal{L}_{\text{per}}]\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^{k})^2,(H_n^{k+1})^2)} \\ \leqslant &\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^{k-1})^2,(H_n^{k+1})^2)}\|[\nabla, \mathcal{L}_{\text{per}}]\|_{\mathcal{L}((H_n^{k+1})^2,(H_n^{k-1})^2)}\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^{k-1})^2,(H_n^{k+1})^2)} \\ \leqslant &C(k)M. \end{aligned}$$

□

4.6.3 Cauchy-Born Rule

Now we apply the Cauchy-Born rule to analyze the system of leading order ϵ^0 equations $\mathcal{F}_0(\mathcal{V}_0, \nabla u(x)) = 0$,

$$\begin{cases} -\sum_{ij} a_{ij}(x)\partial_{z_i}\partial_{z_j}\nu_0(x,z) + \frac{5}{3}J^{-\frac{2}{3}}(x)\nu_0^{\frac{7}{3}}(x,z) - \frac{4}{3}J^{-\frac{1}{3}}(x)\nu_0^{\frac{5}{3}}(x,z) + V_0(x,z)\nu_0(x,z) \\ = 0, \\ -J(x)\sum_{ij} a_{ij}(x)\partial_{z_i}\partial_{z_j}V_0(x,z) = 4\pi(\nu_0^2(x,z) - J(x)\rho_{b,0}(x,z)), \end{cases} \tag{4.37}$$

where we assume $x \in \Omega$ is fixed thus the deformation is homogeneously linear, and $z \in \Omega$ is the variable.

We will use the implicit function theorem in the functional form to find the solution. So first recall the undeformed base case in which $u \equiv 0$. Then $\tau(x) = x, J(x) = 1$ and $\mathcal{F}_0(\mathcal{V}_0, \nabla u(x)) = 0$ becomes

$$\begin{cases} -\Delta\nu_0(z) + \frac{5}{3}\nu_0^{\frac{7}{3}}(z) - \frac{4}{3}\nu_0^{\frac{5}{3}}(z) + V_0(z)\nu_0(z) = 0 \\ -\Delta V_0(z) = 4\pi(\nu_0^2(z) - \rho_{b,\text{per}}(z)), \end{cases} \tag{4.38}$$

where $\rho_{b,\text{per}}(z) = \sum_{X_i \in \mathbb{L}} m_a(z - X_i)$ is periodic in $z \in \Omega$.

Lemma 4.6.2. *If $m_a \in H^{k+2}$, then there exist periodic solutions $\mathcal{V}_{per} = (\nu_{per}, V_{per}) \in (W_1^{k,\infty})^2$ and $\nu_{per} \geqslant C_\nu > 0$ in Ω for some constant $C_\nu > 0$.*

Recall the linearized operator at the undeformed solutions $\mathcal{V}_{\text{per}}$ is

$$\mathcal{L}_{\text{per}} = \begin{pmatrix} \mathcal{L}_{1,\text{per}} & \nu_{\text{per}} \\ \nu_{\text{per}} & \frac{1}{8\pi}\Delta \end{pmatrix}, \tag{4.39}$$

where $\mathcal{L}_{1,\text{per}}\omega = -\Delta\omega + \frac{35}{9}\nu_{\text{per}}^{\frac{4}{3}}\omega - \frac{20}{9}\nu_{\text{per}}^{\frac{2}{3}}\omega + V_{\text{per}}\omega$, and according to **Stability Condition A**, it satisfies $\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((L_n^2)^2)} \leqslant M$.

Based on our construction of the undeformed periodic solution $\mathcal{V}_{\text{per}}$, we next construct solutions with a small homogeneously linear deformation.

Lemma 4.6.3. *If the deformation is homogeneously linear in the sense that $u(x) = Ax$ for some 3×3 matrix A. Then under* **Stability Condition A** *and $\mathcal{V}_{per} \in W_1^{k,\infty}$, there exist positive constants h and δ, and a unique smooth map from $B_{h,M_{3\times 3}}$ to $(H_1^k)^2$: $A \mapsto \mathcal{V}(\cdot;A) = (\nu(\cdot;A), V(\cdot;A))$ such that $\|\mathcal{V}(\cdot;A) - \mathcal{V}_{per}\|_{(H_1^k)^2} \leqslant \delta$ and $\mathcal{F}_0(\mathcal{V}(\cdot;A), A) = 0$. Here $B_{h,M_{3\times 3}} = \{A \in M_{3\times 3} | \|A\|_F < h\}$.*

Proof. When $u(x) = Ax$, we have $\nabla\tau(x) = \mathcal{I} + A$, then

$$\begin{aligned} a_{ij}(x) &= [(\nabla\tau(x))^{-1}(\nabla\tau(x))^{-T}]_{ij} = [(\mathcal{I}+A)^{-1}(\mathcal{I}+A)^{-T}]_{ij} \\ J(x) &= \det\nabla\tau(x) = \det(\mathcal{I}+A). \end{aligned}$$

So $\mathcal{F}_0(\mathcal{V}_0, \nabla u(x)) = 0$ becomes

$$\begin{cases} -\sum_{ij}[(\mathcal{I}+A)^{-1}(\mathcal{I}+A)^{-T}]_{ij}\partial_{z_i}\partial_{z_j}\nu_0(z;A) + \frac{5}{3}\det(\mathcal{I}+A)^{-\frac{2}{3}}\nu_0^{\frac{7}{3}}(z;A) \\ -\frac{4}{3}\det(\mathcal{I}+A)^{-\frac{1}{3}}\nu_0^{\frac{5}{3}}(z;A) + V_0(z;A)\nu_0(z;A) = 0 \\ -\det(\mathcal{I}+A)\sum_{ij}[(\mathcal{I}+A)^{-1}(\mathcal{I}+A)^{-T}]_{ij}\partial_{z_i}\partial_{z_j}V_0(z;A) \\ = 4\pi(\nu_0^2(z;A) - \det(\mathcal{I}+A)\rho_{b,0}(z;A)), \end{cases}$$

where $\rho_{b,0}(z;A) = \sum_{X_i\in\mathbb{L}} m_a((\mathcal{I}+A)(z-X_i))$.

The functional $\mathcal{F}_0 : (H_1^k)^2 \times M_{3\times 3} \to (H_1^{k-2})^2$ satisfies the following conditions:

1. When $u(x) = Ax \equiv 0$, $\mathcal{F}_0(\mathcal{V}_{\text{per}}, \mathbf{0}) = 0$ for $\mathcal{V}_{\text{per}} \in (W_1^{k,\infty})^2 \subset (H_1^k)^2$,

2. $\mathcal{F}_0$ is C^∞ in $\mathcal{V}_0 = (\nu_0, V_0)$ and A,

3. $$\frac{\delta \mathcal{F}_0(\mathcal{V}_0, A)}{\delta \mathcal{V}_0}|_{(\mathcal{V}_{\text{per}}, \mathbf{0})} = \mathcal{L}_{\text{per}} : (H_1^k)^2 \to (H_1^{k-2})^2$$

   satisfies

   $$\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_1^{k-2})^2, (H_1^k)^2)} \leqslant C(k-2)M$$

   by Lemma 4.6.1 since $\mathcal{V}_{\text{per}} \in (W_1^{k,\infty})^2 \subset (W_1^{k-2,\infty})^2$.

So we can apply the implicit function theorem for Banach spaces. There exist a neighborhood of $A = \mathbf{0}$: $B_{h,M_{3\times3}} = \{A \in M_{3\times3} | \|A\|_F < h\}$ and a neighborhood of $\mathcal{V}_{\text{per}}$: $D_\delta = \{\mathcal{V} | \|\mathcal{V} - \mathcal{V}_{\text{per}}\|_{(H_1^k)^2} \leqslant \delta\}$ such that there exists a unique C^∞ map from $B_{h,M_{3\times3}}$ to D_δ : $A \mapsto \mathcal{V}(\cdot; A)$ which satisfies $\mathcal{F}_0(\mathcal{V}(\cdot; A), A) = 0$.

Notice that by Sobolev inequality, $\|\nu - \nu_{\text{per}}\|_{L_1^\infty} \leqslant \|\nu - \nu_{\text{per}}\|_{H_1^2} \leqslant \delta$, so if we let $\|\nu - \nu_{\text{per}}\|_{L_1^\infty} \leqslant C_\nu/2$, then $\nu \geqslant C_\nu/2 > 0$. □

Finally we can construct the Cauchy-Born solution:

Theorem 4.6.4. *For the system of ϵ^0 order equations $\mathcal{F}_0(\mathcal{V}_0, \nabla u(x)) = 0$, under* **Stability Condition A**, *i.e. $\|\mathcal{L}_{per}^{-1}\|_{\mathcal{L}((L_1^2)^2)} \leqslant M$ and $m_a \in H_1^{k+2}$ so that $\mathcal{V}_{per} \in (W_1^{k,\infty})^2$, there exist positive constants h and δ such that for any deformation u satisfying $\|u\|_{H_1^m} \leqslant h$ for any positive integer m, there exists a unique solution $\mathcal{V}_0(z, x) \in H^{m-1}(\Omega, (H_1^k)^2)^2$ so that $\mathcal{F}_0(\mathcal{V}_0(\frac{x}{\epsilon}, x), \nabla u(x)) = 0$ for any $x \in \Omega$ and $\|\mathcal{V}_0(\cdot, x) - \mathcal{V}_{per}(\cdot)\|_{(H_1^k)^2} \leqslant \delta$.*

Proof. For each fixed $x \in \Omega$, $u(x) = Ax$ for some matrix $A \in B_{h,M_{3\times3}}$ which depends on x. From the previous lemma, there exists a unique solution $\mathcal{V}_0(z; A)$ satisfying $\mathcal{F}_0(\mathcal{V}_0(z; A), A) = 0$ at each fixed $x \in \Omega$. Define $\mathcal{V}_0(z, x) = \mathcal{V}_0(z; A) =$

$\mathcal{V}_0(z;\nabla u(x))$, then $\mathcal{V}_0(\cdot,x)\in(H_1^k)^2$. Since $u\in H_1^m$ and $\mathcal{V}_0(z;\nabla u(x))$ is C^∞ in $\nabla u(x)$, $\mathcal{V}_0(z,\cdot)\in(H_1^{m-1})^2$. Extend $\mathcal{V}_0(\cdot,x)$ periodically from Ω to $n\Omega$, so that finally we have $\mathcal{F}_0(\mathcal{V}_0(\frac{x}{\epsilon},x),\nabla u(x))=0$ for any $x\in\Omega$. □

We call $\mathcal{V}_0(\frac{x}{\epsilon},x)$ the Cauchy-Born solution, and denote it as $\mathcal{V}_{\mathrm{CB}}=(\nu_{\mathrm{CB}},V_{\mathrm{CB}})$ so that $\mathcal{V}_{\mathrm{CB}}(x)=(\nu_{\mathrm{CB}}(x),V_{\mathrm{CB}}(x))=(\nu_0(\frac{x}{\epsilon},x),V_0(\frac{x}{\epsilon},x))$.

4.7 The Exact Solution With Fixed Deformation

Theorem 4.7.1. *Under Stability Assumption A, $\|\mathcal{L}_{per}^{-1}\|_{\mathcal{L}((L_n^2)^2)}\leqslant M$, there exist positive constants h, ϵ_0 and δ, such that for any deformation $\|u\|_{W_1^{5,\infty}(\Omega)}\leqslant h$, and any $\epsilon\leqslant\epsilon_0$, there exists a unique solution $\mathcal{V}_{exa}=(\nu_{exa},V_{exa})\in(H_n^2)^2$ that satisfy*

1. *$\mathcal{F}(\mathcal{V}_{exa})=0$*
2. *$\|\mathcal{V}_{exa}-\mathcal{V}_{CB}\|_{(H_n^2)^2}\leqslant\delta\epsilon^3$,*

where $\mathcal{V}_{CB}$ is the Cauchy-Born solution and $\mathcal{F}(\mathcal{V})=0$ is given by

$$\begin{cases}-D_1\nu+\frac{5}{3}J^{-\frac{2}{3}}\nu^{\frac{7}{3}}-\frac{4}{3}J^{-\frac{1}{3}}\nu^{\frac{5}{3}}+V\nu=0\\ -JD_2V=4\pi(\nu^2-\rho_b).\end{cases}\tag{4.40}$$

4.8 Minimizing the TFDW Functional

In the above analysis of the TFDW functional, we assumed the deformation Y or u is fixed. In order to study $\inf_{\nu_\epsilon,V_\epsilon,Y}I(\nu_\epsilon,V_\epsilon,\rho_b^\epsilon(Y))$, we use the Hellmann-Feymann theorem which states that if

$$(\nu_{\mathrm{exa}}(Y),V_{\mathrm{exa}}(Y))=\mathrm{arginf}_{\nu_\epsilon,V_\epsilon}I(\nu_\epsilon,V_\epsilon,\rho_b^\epsilon(Y)),\tag{4.41}$$

then

$$\inf_{\nu_\epsilon,V_\epsilon,Y}I(\nu_\epsilon,V_\epsilon,\rho_b^\epsilon(Y))=\inf_Y I(\nu_{\mathrm{exa}}(Y),V_{\mathrm{exa}}(Y),\rho_b^\epsilon(Y)).\tag{4.42}$$

Recall $I_{\text{at}}(Y) = I(\nu_{\text{exa}}(Y), V_{\text{exa}}(Y), \rho_b^\epsilon(Y))$ is the atomistic TFDW functional which we will study in the later chapters. The Hellmann-Feymann theorem tells us that the minimizer Y_{at} of $I_{\text{at}}(Y)$ together with $\mathcal{V}_{\text{exa}}(Y_{\text{at}}) = (\nu_{\text{exa}}(Y_{\text{at}}), V_{\text{exa}}(Y_{\text{at}}))$ form the minimizer of $I(\nu^\epsilon, V^\epsilon, \rho_b^\epsilon(Y))$.

5

The Fixed Deformation Case

5.1 Introduction

In this chapter, we are going to solve the system of Euler-Lagrange equations of (ν, V) in Lagrangian coordinates on $n\Omega$. The system of the equations is

$$\begin{cases} -D_1^\epsilon \nu + \frac{5}{3} J_\epsilon^{-\frac{2}{3}} \nu^{\frac{7}{3}} - \frac{4}{3} J_\epsilon^{-\frac{1}{3}} \nu^{\frac{5}{3}} + V\nu = 0 \\ -J_\epsilon D_2^\epsilon V = 4\pi(\nu^2 - J_\epsilon \rho_b), \quad x \in n\Omega, \end{cases} \tag{5.1}$$

where $D_1^\epsilon = \sum_{ij} a_{ij}^\epsilon \partial_i \partial_j + \sum_j b_j^\epsilon \partial_j + c^\epsilon$ in which

$$\begin{cases} a_{ij}^\epsilon(x) = a_{ij}(\epsilon x) \\ b_j^\epsilon(x) = b_j(\epsilon x) \\ c^\epsilon(x) = c(\epsilon x) \end{cases} \tag{5.2}$$

and $D_2^\epsilon = \sum_{ij} a_{ij}^\epsilon \partial_i \partial_j + \sum_j d_j^\epsilon \partial_j$ in which

$$\begin{cases} a_{ij}^\epsilon(x) = a_{ij}(\epsilon x) \\ d_j^\epsilon(x) = d_j(\epsilon x) \end{cases} \tag{5.3}$$

In the previous chapter, we constructed the undeformed solution $(\nu_{\text{per}}, V_{\text{per}})$, based on which we applied the Cauchy-Born rule to get the first-order approximate solution

$(\nu_{\text{CB}}, V_{\text{CB}})$. In this chapter we will use the two-scale ansatz technique to construct an approximate solution (ν^0, V^0) with higher accuracy so that we can use the Newton-Raphson iteration to find the exact solution $(\nu_{\text{exa}}, V_{\text{exa}}) \in (H_n^2)^2$.

After we derive the exact solution, we will prove that the exact solution preserves the decaying property

$$\|\partial_i \nu_{\text{exa}}(x, Y)\| \leqslant \frac{C}{\epsilon} e^{-\gamma|x + \frac{-X_i + r_{i,\epsilon x}}{\epsilon}|} \tag{5.4}$$

$$\|\partial_i V_{\text{exa}}(x, Y)\| \leqslant \frac{C}{\epsilon} e^{-\gamma|x + \frac{-X_i + r_{i,\epsilon x}}{\epsilon}|}, \tag{5.5}$$

for any $x \in n\Omega$ and $\gamma > 0$ small enough but independent of ϵ, which holds for the background charge ρ_b.

For further analysis in later chapters, we need to study the perturbation of the exact solution and combine it with the decaying property to derive the following estimate for the potential V_{exa}

$$\|\partial_j \mathcal{V}_{\text{exa}}(x, Y_2) - \partial_j \mathcal{V}_{\text{exa}}(x, Y_1)\| \leqslant C\epsilon^{-2} e^{-\gamma|x - \frac{X_j + r_{j,\epsilon,x}}{\epsilon}|} \|Y_2 - Y_1\|_{W_\epsilon^{3,\infty}}$$

The essential tool we use for these estimates is the perturbation of the linearized operator. Since this perturbation is used in various places and in various forms, we now prove a general proposition of it.

5.2 Perturbation Of The Linearized Operator

Proposition 5.2.1. *Given two sets of functions $\mathcal{V}_1 = (\nu_1, V_1), \mathcal{V}_2 = (\nu_2, V_2)$ satisfying $\|\mathcal{V}_{1,2}\|_{(W^{k,\infty}(n\Omega))^2} \leqslant h_{\mathcal{V}}, \nu_{1,2} \geqslant C_\nu > 0$ and two deformations τ_1, τ_2 satisfying $\|\tau_{1,2}\|_{W_1^{k+3,\infty}} \leqslant h_\tau, |\nabla \tau_{1,2}| \geqslant \delta_\tau > 0$, we have the following estimate for the perturbation of the linearized operator*

$$\begin{aligned}&\|\mathcal{L}_{(\mathcal{V}_1,\tau_1)} - \mathcal{L}_{(\mathcal{V}_2,\tau_2)}\|_{\mathcal{L}((H_n^{k+2})^2,(H_n^k)^2)}\\ \leqslant &C \max(\|\mathcal{V}_1 - \mathcal{V}_2\|_{(W^{k,\infty}(n\Omega))^2}, \|\tau_1 - \tau_2\|_{W_1^{k+3,\infty}})\end{aligned}$$

$$\leqslant C \max(\|\mathcal{V}_1 - \mathcal{V}_2\|_{(H^{k+2}(n\Omega))^2}, \|\tau_1 - \tau_2\|_{W_1^{k+3,\infty}})$$

where $C = C(h_{\mathcal{V}}, h_\tau, C_\nu, \delta_\tau) > 0$*.*

Proof. Recall the linearized operator $\mathcal{L}_{(\mathcal{V},\tau)}$ in Lagrangian coordinates is given by

$$\mathcal{L}_{\mathcal{V}} \begin{pmatrix} \omega \\ W \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{\mathcal{V},1} & \nu \\ \nu & \frac{1}{8\pi} D_2^\epsilon \end{pmatrix} \begin{pmatrix} \omega \\ W \end{pmatrix} \tag{5.6}$$

where $(\omega, W) \in (H^2(n\Omega))^2$ and

$$\mathcal{L}_{\mathcal{V},1} = -D_1^\epsilon + \frac{35}{9} J_\epsilon^{-\frac{2}{3}} \nu^{\frac{4}{3}} - \frac{20}{9} J_\epsilon^{-\frac{1}{3}} \nu^{\frac{2}{3}} + V. \tag{5.7}$$

Notice that by using the notation $\mathcal{L}_{(\mathcal{V},\tau)}$ instead of $\mathcal{L}_{\mathcal{V}}$, we do not assume the deformation τ is fixed.

Denote $\mathcal{W} = (\omega, W)$, we consider $\mathcal{L}_{(\mathcal{V},\tau)}$ acting on $\mathcal{W} \in (H_n^{k+2})^2$, we have

$$\begin{aligned} \|\mathcal{L}_{(\mathcal{V},\tau)}\mathcal{W}\|_{(H_n^k)^2} =& n^{-\frac{3}{2}} \|\mathcal{L}_{(\mathcal{V},\tau)}\mathcal{W}\|_{(H^k(n\Omega))^2} \\ \leqslant& n^{-\frac{3}{2}} \|\mathcal{L}_{(\mathcal{V},\tau)}\|_{\mathcal{L}((H^{k+2}(n\Omega))^2,(H^k(n\Omega))^2)} \|\mathcal{W}\|_{(H^{k+2}(n\Omega))^2} \\ =& \|\mathcal{L}_{(\mathcal{V},\tau)}\|_{\mathcal{L}((H^{k+2}(n\Omega))^2,(H^k(n\Omega))^2)} \|\mathcal{W}\|_{(H_n^{k+2})^2}, \end{aligned}$$

then

$$\|\mathcal{L}\|_{\mathcal{L}((H_n^{k+2})^2,(H_n^k)^2)} \leqslant \|\mathcal{L}_{(\mathcal{V},\tau)}\|_{\mathcal{L}((H^{k+2}(n\Omega))^2,(H^k(n\Omega))^2)}.$$

So we analyze $\|\mathcal{L}_{(\mathcal{V}_1,\tau_1)} - \mathcal{L}_{(\mathcal{V}_2,\tau_2)}\|_{\mathcal{L}((H^{k+2}(n\Omega))^2,(H^k(n\Omega))^2)}$.

We have

$$\mathcal{L}_{(\mathcal{V}_1,\tau_1)} - \mathcal{L}_{(\mathcal{V}_2,\tau_2)} = \begin{pmatrix} \mathcal{L}_{(\mathcal{V}_1,\tau_1),1} - \mathcal{L}_{(\mathcal{V}_2,\tau_2),1} & \nu_1 - \nu_2 \\ \nu_1 - \nu_2 & \frac{1}{8\pi}(D_2^\epsilon(\tau_1) - D_2^\epsilon(\tau_2)) \end{pmatrix}$$

where

$$\begin{aligned} &\mathcal{L}_{(\mathcal{V}_1,\tau_1),1} - \mathcal{L}_{(\mathcal{V}_2,\tau_2),1} \\ =& -(D_1^\epsilon(\tau_1) - D_1^\epsilon(\tau_2)) + \frac{35}{9}\left[J_\epsilon^{-\frac{2}{3}}(\tau_1)\nu_1^{\frac{4}{3}} - J_\epsilon^{-\frac{2}{3}}(\tau_2)\nu_2^{\frac{4}{3}}\right] \end{aligned}$$

$$-\frac{20}{9}\big[J_\epsilon^{-\frac{1}{3}}(\tau_1)\nu_1^{\frac{2}{3}} - J_\epsilon^{-\frac{1}{3}}(\tau_2)\nu_2^{\frac{2}{3}}\big] + (V_1 - V_2)$$

It is straightforward to analyze the two $\nu_1 - \nu_2$ terms:

$$\|(\nu_1-\nu_2)W\|_{H^k(n\Omega)} \leqslant \|\nu_1-\nu_2\|_{W^{k,\infty}(n\Omega)}\|W\|_{H^k(n\Omega)} \leqslant \|\nu_1-\nu_2\|_{W^{k,\infty}(n\Omega)}\|W\|_{H^{k+2}(n\Omega)}.$$

so

$$\|\nu_1-\nu_2\|_{\mathcal{L}(H^{k+2}(n\Omega),H^k(n\Omega))} \leqslant \|\nu_1-\nu_2\|_{W^{k,\infty}(n\Omega)}.$$

and similarly

$$\|V_1-V_2\|_{\mathcal{L}(H^{k+2}(n\Omega),H^k(n\Omega))} \leqslant \|V_1-V_2\|_{W^{k,\infty}(n\Omega)}.$$

Next we analyze

$$\begin{aligned}
&\|J_\epsilon^{-\frac{2}{3}}(\tau_1)\nu_1^{\frac{4}{3}} - J_\epsilon^{-\frac{2}{3}}(\tau_2)\nu_2^{\frac{4}{3}}\|_{\mathcal{L}(H^{k+2}(n\Omega),H^k(n\Omega))}\\
\leqslant&\|J_\epsilon^{-\frac{2}{3}}(\tau_1)\nu_1^{\frac{4}{3}} - J_\epsilon^{-\frac{2}{3}}(\tau_2)\nu_2^{\frac{4}{3}}\|_{W^{k,\infty}(n\Omega)}\\
\leqslant&\|J_\epsilon^{-\frac{2}{3}}(\tau_1) - J_\epsilon^{-\frac{2}{3}}(\tau_2)\|_{W^{k,\infty}(n\Omega)}\|\nu_1^{\frac{4}{3}}\|_{W^{k,\infty}(n\Omega)} + \|J_\epsilon^{-\frac{2}{3}}(\tau_2)\|_{W^{k,\infty}(n\Omega)}\|\nu_1^{\frac{4}{3}} - \nu_2^{\frac{4}{3}}\|_{W^{k,\infty}(n\Omega)}
\end{aligned}$$

By the mean value theorem, we get

$$\begin{aligned}
&\|\nu_1^{\frac{4}{3}} - \nu_2^{\frac{4}{3}}\|_{W^{k,\infty}(n\Omega)}\\
\leqslant&\frac{4}{3}\|(t\nu_1+(1-t)\nu_2)^{\frac{1}{3}}\|_{W^{k,\infty}(n\Omega)}\|\nu_1-\nu_2\|_{W^{k,\infty}(n\Omega)}\\
\leqslant&C(h_{\mathcal{V}},C_\nu)\|\nu_1-\nu_2\|_{W^{k,\infty}(n\Omega)}\\
&\|J_\epsilon^{-\frac{2}{3}}(\tau_1) - J_\epsilon^{-\frac{2}{3}}(\tau_2)\|_{W^{k,\infty}(n\Omega)}\\
\leqslant&\frac{1}{3}\|(sJ_\epsilon(\tau_1)+(1-s)J_\epsilon(\tau_2))^{-\frac{5}{3}}\|_{W^{k,\infty}(n\Omega)}\|J_\epsilon(\tau_1)-J_\epsilon(\tau_2)\|_{W^{k,\infty}(n\Omega)}\\
\leqslant&C(h_\tau,\delta_\tau)\|\tau_1-\tau_2\|_{W_1^{k+1,\infty}},
\end{aligned}$$

for some $0 < s, t < 1$. So

$$\|J_\epsilon^{-\frac{2}{3}}(\tau_1)\nu_1^{\frac{4}{3}} - J_\epsilon^{-\frac{2}{3}}(\tau_2)\nu_2^{\frac{4}{3}}\|_{\mathcal{L}(H_n^{k+2},H_n^k)}$$

$$\leqslant C \max(\|\mathcal{V}_1 - \mathcal{V}_2\|_{(W^{k,\infty}(n\Omega))^2}, \|\tau_1 - \tau_2\|_{W_1^{k+1,\infty}})$$

$$\leqslant C \max(\|\mathcal{V}_1 - \mathcal{V}_2\|_{(H^{k+2}(n\Omega))^2}, \|\tau_1 - \tau_2\|_{W_1^{k+1,\infty}}),$$

and similarly

$$\|J_\epsilon^{-\frac{1}{3}}(\tau_1)\nu_1^{\frac{2}{3}} - J_\epsilon^{-\frac{1}{3}}(\tau_2)\nu_2^{\frac{2}{3}}\|_{\mathcal{L}(H_n^{k+2}, H_n^k)}$$

$$\leqslant C \max(\|\mathcal{V}_1 - \mathcal{V}_2\|_{(H^{k+2}(n\Omega))^2}, \|\tau_1 - \tau_2\|_{W_1^{k+1,\infty}}),$$

where $C = C(h_\mathcal{V}, h_\tau, C_\nu, \delta_\tau) > 0$.

Next we analyze $D_1^\epsilon(\tau_1) - D_1^\epsilon(\tau_2)$ and $D_2^\epsilon(\tau_1) - D_2^\epsilon(\tau_2)$. Recall $D_1^\epsilon = \sum_{ij} a_{ij}^\epsilon \partial_i \partial_j + \sum_j b_j^\epsilon \partial_j + c^\epsilon$ in which

$$\begin{cases} a_{ij}^\epsilon(x) = a_{ij}(\epsilon x) \\ b_j^\epsilon(x) = b_j(\epsilon x) \\ c^\epsilon(x) = c(\epsilon x) \end{cases} \tag{5.8}$$

and $D_2^\epsilon = \sum_{ij} a_{ij}^\epsilon \partial_i \partial_j + \sum_j d_j^\epsilon \partial_j$ in which

$$\begin{cases} a_{ij}^\epsilon(x) = a_{ij}(\epsilon x) \\ d_j^\epsilon(x) = d_j(\epsilon x) \end{cases} \tag{5.9}$$

Further recall

$$\begin{cases} a_{ij} = (\nabla\tau^{-1}\nabla\tau^{-T})_{ij} \\ b_j = \sum_{ik} \nabla\tau_{ik}^{-1}\partial_i\nabla\tau_{kj}^{-T} - 2J^{\frac{1}{2}}\sum_i a_{ij}\partial_i J^{-\frac{1}{2}} \\ c = J^{\frac{1}{2}}\sum_{ijk}\nabla\tau_{ik}^{-1}\partial_i\nabla\tau_{kj}^{-T}\partial_j J^{-\frac{1}{2}} + J^{\frac{1}{2}}\sum_{ij} a_{ij}\partial_i\partial_j J^{-\frac{1}{2}} \end{cases} \tag{5.10}$$

and

$$\begin{cases} a_{ij} = (\nabla\tau^{-1}\nabla\tau^{-T})_{ij} \\ d_j = \sum_{ik} \nabla\tau_{ik}^{-1}\partial_i\nabla\tau_{kj}^{-T} \end{cases} \tag{5.11}$$

So

$$\|D_1^\epsilon(\tau_1) - D_1^\epsilon(\tau_2)\|_{\mathcal{L}(H^{k+2}(n\Omega), H^k(n\Omega))}$$

$$\leqslant \| \sum_{ij} (a_{ij}^{\epsilon}(\tau_1) - a_{ij}^{\epsilon}(\tau_2)) \partial_i \partial_j \|_{\mathcal{L}(H^{k+2}(n\Omega), H^k(n\Omega))} + \| \sum_j (b_j^{\epsilon}(\tau_1) - b_j^{\epsilon}(\tau_2)) \partial_j \|_{\mathcal{L}(H^{k+2}(n\Omega), H^k(n\Omega))}$$

$$+ \| c^{\epsilon}(\tau_1) - c^{\epsilon}(\tau_2) \|_{\mathcal{L}(H^{k+2}(n\Omega), H^k(n\Omega))}$$

$$\leqslant \sum_{ij} \| a_{ij}^{\epsilon}(\tau_1) - a_{ij}^{\epsilon}(\tau_2) \|_{W^{k,\infty}(n\Omega)} + \sum_j \| b_j^{\epsilon}(\tau_1) - b_j^{\epsilon}(\tau_2) \|_{W^{k,\infty}(n\Omega)} + \| c^{\epsilon}(\tau_1) - c^{\epsilon}(\tau_2) \|_{W^{k,\infty}(n\Omega)}$$

$$\leqslant C(h_\tau, \delta_\tau) \| \tau_1 - \tau_2 \|_{W_1^{k+3,\infty}}.$$

Similarly,

$$\| D_2^{\epsilon}(\tau_1) - D_2^{\epsilon}(\tau_2) \|_{\mathcal{L}(H^{k+2}(n\Omega), H^k(n\Omega))} \leqslant C(h_\tau, \delta_\tau) \| \tau_1 - \tau_2 \|_{W_1^{k+3,\infty}}.$$

Therefore we can combine these estimates to get the proof of the proposition.

□

5.3 Approximate Solution From Two-Scale Ansatz

Recall the systems of equations of orders ϵ^1 and ϵ^2: For ϵ^1:

$$\begin{cases} -\sum_{ij} a_{ij} \partial_{z_i} \partial_{z_j} \nu_1 + \frac{35}{9} J^{-\frac{2}{3}} \nu_0^{\frac{4}{3}} \nu_1 - \frac{20}{9} J^{-\frac{1}{3}} \nu_0^{\frac{2}{3}} \nu_1 + V_0 \nu_1 \\ -\sum_{ij} a_{ij} (\partial_{x_j} \partial_{z_i} \nu_0 + \partial_{x_i} \partial_{z_j} \nu_0) - \sum_j b_j \partial_{z_j} \nu_0 + V_1 \nu_0 = 0 \\ \\ -J \sum_{ij} a_{ij} \partial_{z_i} \partial_{z_j} V_1 - 8\pi \nu_0 \nu_1 + 4\pi J \rho_{b,1} \\ -J \sum_{ij} a_{ij} (\partial_{x_j} \partial_{z_i} V_0 + \partial_{x_i} \partial_{z_j} V_0) - J \sum_j d_j \partial_{z_j} V_0 = 0, \end{cases} \tag{5.12}$$

For ϵ^2:

$$\begin{cases} -\sum_{ij} a_{ij} \partial_{z_i} \partial_{z_j} \nu_2 + \frac{35}{9} J^{-\frac{2}{3}} \nu_0^{\frac{4}{3}} \nu_2 - \frac{20}{9} J^{-\frac{1}{3}} \nu_0^{\frac{2}{3}} \nu_2 + V_0 \nu_2 \\ -\sum_{ij} a_{ij} (\partial_{x_j} \partial_{z_i} \nu_1 + \partial_{x_i} \partial_{z_j} \nu_1) - \sum_{ij} b_j \partial_{z_j} \nu_1 + \frac{70}{27} J^{-\frac{2}{3}} \nu_0^{\frac{1}{3}} \nu_1^2 - \frac{20}{27} J^{-\frac{1}{3}} \nu_0^{-\frac{1}{3}} \nu_1^2 + V_1 \nu_1 \\ -\sum_{ij} a_{ij} \partial_{x_i} \partial_{x_j} \nu_0 - \sum_j b_j \partial_{x_j} \nu_0 - c\nu_0 + V_2 \nu_0 = 0 \\ \\ -J \sum_{ij} a_{ij} \partial_{z_i} \partial_{z_j} V_2 - 8\pi \nu_0 \nu_2 + 4\pi J \rho_{b,2} \\ -J \sum_{ij} a_{ij} (\partial_{x_j} \partial_{z_i} V_1 + \partial_{x_i} \partial_{z_j} V_1) - J \sum_j d_j \partial_{z_j} V_1 - 4\pi \nu_1^2 \\ -J \sum_{ij} a_{ij} \partial_{x_i} \partial_{x_j} V_0 - J \sum_j d_j \partial_{x_j} V_0 = 0. \end{cases} \tag{5.13}$$

Rewrite the equations as

$$\mathcal{L}_{\mathcal{V}_{\rm CB}}\mathcal{V}_1 = \begin{pmatrix} f_1 \\ g_1 \end{pmatrix}, \quad \mathcal{L}_{\mathcal{V}_{\rm CB}}\mathcal{V}_2 = \begin{pmatrix} f_2 \\ g_2 \end{pmatrix},$$

where $\mathcal{L}_{\mathcal{V}_{\rm CB}} = \begin{pmatrix} \mathcal{L}_{\mathcal{V}_{\rm CB},1} & \nu_{\rm CB} \\ \nu_{\rm CB} & \frac{J}{8\pi}D_3 \end{pmatrix}$, $D_3 = \sum_{ij} a_{ij}\partial_{z_i}\partial_{z_j}$, and

$$\mathcal{L}_{\mathcal{V}_{\rm CB},1} = -D_3 + \frac{35}{9}J^{-\frac{2}{3}}\nu_{\rm CB}^{\frac{4}{3}} - \frac{20}{9}J^{-\frac{1}{3}}\nu_{\rm CB}^{\frac{2}{3}} + V_{\rm CB}$$

$$\begin{cases} f_1 = \sum_{ij} a_{ij}(\partial_{x_j}\partial_{z_i}\nu_{\rm CB} + \partial_{x_i}\partial_{z_j}\nu_{\rm CB}) + \sum_j b_j\partial_{z_j}\nu_{\rm CB} \\ g_1 = -\frac{J}{8\pi}\sum_{ij} a_{ij}(\partial_{x_j}\partial_{z_i}V_{\rm CB} + \partial_{x_i}\partial_{z_j}V_{\rm CB}) - \frac{J}{8\pi}\sum_j b_j\partial_{z_j}V_{\rm CB} + \frac{1}{2}J\rho_{b,1} \end{cases}$$

$$\begin{cases} f_2 = & \sum_{ij} a_{ij}(\partial_{x_j}\partial_{z_i}\nu_1 + \partial_{x_i}\partial_{z_j}\nu_1) + \sum_j b_j\partial_{z_j}\nu_1 - \frac{70}{27}J^{-\frac{2}{3}}\nu_{\rm CB}^{\frac{1}{3}}\nu_1^2 + \frac{20}{27}J^{-\frac{1}{3}}\nu_{\rm CB}^{-\frac{1}{3}}\nu_1^2 \\ & -V_1\nu_1 + \sum_{ij} a_{ij}\partial_{x_i}\partial_{x_j}\nu_{\rm CB} + \sum_j b_j\partial_{x_j}\nu_{\rm CB} + c\nu_{\rm CB} - V_2\nu_{\rm CB} \\ g_2 = & \frac{1}{2}J\rho_{b,2} - \frac{J}{8\pi}\sum_{ij} a_{ij}(\partial_{x_j}\partial_{z_i}V_1 + \partial_{x_i}\partial_{z_j}V_1) - \frac{J}{8\pi}\sum_j d_j\partial_{z_j}V_1 - \frac{1}{2}\nu_1^2 \\ & -\frac{J}{8\pi}\sum_{ij} a_{ij}\partial_{x_i}\partial_{x_j}V_{\rm CB} - \frac{J}{8\pi}\sum_j d_j\partial_{x_j}V_{\rm CB}. \end{cases}$$

Let us establish the regularity of $\mathcal{L}_{\mathcal{V}_{\rm CB}}$:

Proposition 5.3.1. *For sufficiently small $h > 0, \delta > 0$ such that $\|u\|_{W_1^{k+3,\infty}} \leqslant h, \|\mathcal{V}_{CB} - \mathcal{V}_{per}\|_{(H_1^{k+2})^2} \leqslant \delta$, $\mathcal{L}_{\mathcal{V}_{CB}} : (H_1^{k+2})^2 \to (H_1^k)^2$ is invertible, and*

$$\|\mathcal{L}_{\mathcal{V}_{CB}}^{-1}\|_{\mathcal{L}((H_1^k)^2,(H_1^{k+2})^2)} \leqslant C(k)M.$$

Proof. Fix $x \in \Omega$, consider $\|\mathcal{L}_{\mathcal{V}_{\rm CB}}^{-1} - \mathcal{L}_{\mathcal{V}_{\rm per}}^{-1}\|_{\mathcal{L}((H_1^k)^2,(H_1^{k+2})^2)}$, from

$$\mathcal{L}_{\mathcal{V}_{\rm CB}}^{-1} - \mathcal{L}_{\mathcal{V}_{\rm per}}^{-1} = \mathcal{L}_{\mathcal{V}_{\rm per}}^{-1}\sum_{n=1}^{\infty}(-1)^n[(\mathcal{L}_{\mathcal{V}_{\rm CB}} - \mathcal{L}_{\mathcal{V}_{\rm per}})\mathcal{L}_{\mathcal{V}_{\rm per}}^{-1}]^n$$

we have

$$\|\mathcal{L}_{\mathcal{V}_{\rm CB}}^{-1} - \mathcal{L}_{\mathcal{V}_{\rm per}}^{-1}\|_{\mathcal{L}((H_1^k)^2,(H_1^{k+2})^2)} \leqslant C(k)M\sum_{n=1}^{\infty}[C(k)M\|\mathcal{L}_{\mathcal{V}_{\rm CB}} - \mathcal{L}_{\mathcal{V}_{\rm per}}\|_{\mathcal{L}((H_1^{k+2})^2,(H_1^k)^2)}]^n.$$

It is sufficient to show $\|\mathcal{L}_{\mathcal{V}_{\text{CB}}} - \mathcal{L}_{\mathcal{V}_{\text{per}}}\|_{\mathcal{L}((H_1^{k+2})^2,(H_1^k)^2)} < \frac{1}{C(k)M}$, which is a special case of **Proposition** 5.2.1 by choosing $n = 1, \tau_1 = \text{id} + u, \tau_2 = \text{id}, \mathcal{V}_1 = \mathcal{V}_{\text{CB}}, \mathcal{V}_2 = \mathcal{V}_{\text{per}}$.

□

Theorem 5.3.2. *If $\|u\|_{H_1^m} \leqslant h_u, \|m_a\|_{H^{k+2}} \leqslant h_a$ for sufficiently small $h_u, h_a > 0$, we have*

$$\mathcal{V}_{CB}(z,x) \in H^{m-1}(\Omega, (H_1^k)^2)^2$$

$$\mathcal{V}_1(z,x) \in H^{m-2}(\Omega, (H_1^k)^2)^2$$

$$\mathcal{V}_2(z,x) \in H^{m-3}(\Omega, (H_1^k)^2)^2.$$

Proof. From previous construction we have $\mathcal{V}_{\text{CB}} \in H^{m-1}(\Omega, (H_1^k)^2)^2$. This implies $f_1, g_1 \in H^{m-2}(\Omega, (H_1^{k-1})^2)$. So by the proposition just proved, we have

$$\|\mathcal{L}^{-1}_{\mathcal{V}_{\text{CB}}}\|_{\mathcal{L}((H_1^{k-2})^2,(H_1^k)^2)} \leqslant C(k-2)M.$$

Then it follows that $\mathcal{V}_1 \in H^{m-2}(\Omega, (H_1^k)^2)$. By the same argument and the fact that $\nu_0 \geqslant C_\nu > 0$ so $\nu_0^{-\frac{1}{3}}$ is bounded above, we have $f_2, g_2 \in H^{m-3}(\Omega, (H_1^{k-1})^2)$, and thus $\mathcal{V}_2 \in H^{m-3}(\Omega, (H_1^k)^2)$.

□

5.4 General approximate solution

With the spirit of the previous section, we can construct approximate solutions up to higher orders of ϵ. More generally, we consider

$$\nu_\epsilon(x) = \nu_{\text{CB}}(\frac{x}{\epsilon}, x) + \sum_{k=1}^{l} \epsilon^k \nu_k(\frac{x}{\epsilon}, x) \tag{5.14}$$

$$V_\epsilon(x) = V_{\text{CB}}(\frac{x}{\epsilon}, x) + \sum_{k=1}^{l} \epsilon^k V_k(\frac{x}{\epsilon}, x) \tag{5.15}$$

$$\rho_b^\epsilon(x) = \rho_{b,0}(\frac{x}{\epsilon}, x) + \sum_{k=1}^{l} \epsilon^k \rho_{b,k}(\frac{x}{\epsilon}, x). \tag{5.16}$$

Plug the above $\nu_\epsilon, V_\epsilon, \rho_b^\epsilon$ into the Euler-Lagrange equations

$$\begin{cases} -\epsilon^2 D_1 \nu^\epsilon + \frac{5}{3} J^{-\frac{2}{3}} (\nu^\epsilon)^{\frac{7}{3}} - \frac{4}{3} J^{-\frac{1}{3}} (\nu^\epsilon)^{\frac{5}{3}} + V^\epsilon \nu^\epsilon = 0 \\ -\epsilon^2 J D_2 V^\epsilon = 4\pi((\nu^\epsilon)^2 - J\rho_b^\epsilon) \end{cases} \tag{5.17}$$

then we have

$$\begin{cases} -\sum_{ij} a_{ij} \partial_{z_i} \partial_{z_j} \nu_{\text{CB}} + \frac{5}{3} J^{-\frac{2}{3}} \nu_{\text{CB}}^{\frac{7}{3}} - \frac{4}{3} J^{-\frac{1}{3}} \nu_{\text{CB}}^{\frac{5}{3}} + V_{\text{CB}} \nu_{\text{CB}} = 0 \\ -J \sum_{ij} a_{ij} \partial_{z_i} \partial_{z_j} V_{\text{CB}} = 4\pi(\nu_{\text{CB}}^2 - J\rho_{b,0}) \end{cases} \tag{5.18}$$

and

$$\mathcal{L}_{\mathcal{V}_{\text{CB}}} \begin{pmatrix} \nu_k \\ V_k \end{pmatrix} = \begin{pmatrix} f_k \\ g_k \end{pmatrix}, \quad k = 1, \ldots, l, \tag{5.19}$$

where

$$f_k = f_k(\nabla^\alpha \tau, \partial_x^{\beta_1} \partial_z^{\beta_2} \mathcal{V}_q; \alpha = 1, 2, 3, q = 0, \ldots, k-1, |\beta_1| + q \leqslant k, |\beta_2| = 0, 1)$$

$$g_k = g_k(\nabla^\alpha \tau, \partial_x^{\beta_1} \partial_z^{\beta_2} \mathcal{V}_q, \rho_{b,k}; \alpha = 1, 2, 3, q = 0, \ldots, k-1, |\beta_1| + q \leqslant k, |\beta_2| = 0, 1)$$

Theorem 5.4.1. *Given $u \in H_1^m, m_a \in H^{k+2}$, we have*

$$\mathcal{V}_k \in H^{m-k-1}(\Omega, (H_1^k)^2), \quad k = 1, \ldots, l. \tag{5.20}$$

Proof. The result holds for $k = 1, 2$ from previous section. Generally, $f_k, g_k \in H^{m-k-1}(\Omega, (H_1^{k-1})^2)$ implies $\mathcal{V}_k \in H^{m-k-1}(\Omega, (H_1^k)^2)$, which further implies $f_{k+1}, g_{k+1} \in H^{m-k-2}(\Omega, (H_1^{k-1})^2)$. So the theorem holds by induction. □

5.5 Analysis of the Cauchy-Born approximate solution

For the purpose to achieve $\mathcal{V}_{\text{exa}} \in (H_n^2)^2$ for the exact solution $\mathcal{V}_{\text{exa}} = (\nu_{\text{exa}}, V_{\text{exa}})$ on $n\Omega$.

We give three lemmas for $\mathcal{V}^0 = (\nu^0, V^0)$ that will be used in the construction of the exact solution by Newton-Raphson iteration, where

$$\nu^0(x) = \nu_{\text{CB}}(x, \epsilon x) + \epsilon \nu_1(x, \epsilon x) + \epsilon^2 \nu_2(x, \epsilon x)$$

$$V^0(x) = V_{\text{CB}}(x, \epsilon x) + \epsilon V_1(x, \epsilon x) + \epsilon^2 V_2(x, \epsilon x),$$

in which we rescale the functions so that $x \in n\Omega$ and $\epsilon = \frac{1}{n}$. In Theorem 5.3.2 if we assume $m \geqslant 5, k \geqslant 2$, then $\mathcal{V}^0 \in (H_n^2)^2$.

Lemma 5.5.1. *With the above assumption, we have*

$$\|\mathcal{F}(\mathcal{V}^0)\|_{(L_n^2)^2} \lesssim \epsilon^3.$$

Proof. Recall the expression of $\mathcal{F}(\mathcal{V}^0)$:

$$\begin{cases} -D_1^\epsilon \nu^0 + \frac{5}{3} J_\epsilon^{-\frac{2}{3}} (\nu^0)^{\frac{7}{3}} - \frac{4}{3} J_\epsilon^{-\frac{1}{3}} (\nu^0)^{\frac{5}{3}} + V^0 \nu^0 = f \\ -J_\epsilon D_2^\epsilon V^0 - 4\pi((\nu^0)^2 - J_\epsilon \rho_b) = g \end{cases}$$

Plug in the expression of the two-scale ansatz approximate solution $\mathcal{V}^0$ and remove equations for $\nu_0, \nu_1, \nu_2, V_0, V_1, V_2$ from f, g, so only ϵ^3 or higher order terms are left. More specifically,

$$f = f_1 + f_2 + f_3 + f_4,$$

where

$$\begin{aligned} f_1 =& -\epsilon^3 \sum_{ij} a_{ij}^\epsilon \partial_{x_i} \partial_{x_j} \nu_1 - \epsilon^3 \sum_j b_j^\epsilon \partial_{x_j} \nu_1 - \epsilon^3 c^\epsilon \nu_1 \\ & -\epsilon^4 \sum_{ij} a_{ij}^\epsilon \partial_{x_i} \partial_{x_j} \nu_2 - 2\epsilon^3 \sum_{ij} a_{ij}^\epsilon \partial_{x_j} \partial_{z_i} \nu_2 - \epsilon^3 \sum_j b_j^\epsilon \partial_{z_j} \nu_2 - \epsilon^4 \sum_j b_j^\epsilon \partial_{x_j} \nu_2 - \epsilon^4 c^\epsilon \nu_2 \\ f_2 =& \frac{5}{3} J_\epsilon^{-\frac{2}{3}} (\nu_{\text{CB}} + \epsilon \nu_1 + \epsilon^2 \nu_2)^{\frac{7}{3}} - \frac{5}{3} J_\epsilon^{-\frac{2}{3}} \nu_{\text{CB}}^{\frac{7}{3}} - \frac{35}{9} \epsilon J_\epsilon^{-\frac{2}{3}} \nu_{\text{CB}}^{\frac{4}{3}} \nu_1 \\ & -\frac{35}{9} \epsilon^2 J_\epsilon^{-\frac{2}{3}} \nu_{\text{CB}}^{\frac{4}{3}} \nu_2 - \frac{70}{27} \epsilon^2 J_\epsilon^{-\frac{2}{3}} \nu_{\text{CB}}^{\frac{1}{3}} \nu_1^2 \\ f_3 =& -\frac{4}{3} J_\epsilon^{-\frac{1}{3}} (\nu_{\text{CB}} + \epsilon \nu_1 + \epsilon^2 \nu_2)^{\frac{5}{3}} + \frac{4}{3} J_\epsilon^{-\frac{1}{3}} \nu_{\text{CB}}^{\frac{5}{3}} + \frac{20}{9} \epsilon J_\epsilon^{-\frac{1}{3}} \nu_{\text{CB}}^{\frac{2}{3}} \nu_1 \\ & +\frac{20}{9} \epsilon^2 J_\epsilon^{-\frac{1}{3}} \nu_{\text{CB}}^{\frac{2}{3}} \nu_2 + \frac{20}{27} \epsilon^2 J_\epsilon^{-\frac{1}{3}} \nu_{\text{CB}}^{-\frac{1}{3}} \nu_1^2 \\ f_4 =& \epsilon^3 V_1 \nu_2 + \epsilon^3 V_2 \nu_1 + \epsilon^4 V_2 \nu_2. \end{aligned}$$

Similarly,

$$g = g_1 + g_2,$$

where

$$\begin{aligned} g_1 =& - \epsilon^3 J_\epsilon \sum_{ij} a^\epsilon_{ij} \partial_{x_i} \partial_{x_j} V_1 - \epsilon^3 J_\epsilon \sum_j d^\epsilon_j \partial_{x_j} V_1 - \epsilon^4 J_\epsilon \sum_{ij} a^\epsilon_{ij} \partial_{x_i} \partial_{x_j} V_2 \\ & - 2\epsilon^3 J_\epsilon \sum_{ij} a^\epsilon_{ij} \partial_{x_j} \partial_{z_i} V_2 - \epsilon^4 J_\epsilon \sum_j d^\epsilon_j \partial_{x_j} V_2 - \epsilon^3 J_\epsilon \sum_j d^\epsilon_j \partial_{z_j} V_2 \\ g_2 =& - 8\pi\epsilon^3 \nu_1 \nu_2 - 4\pi \epsilon^4 \nu_2^2. \end{aligned}$$

Recall

$$\begin{cases} a^\epsilon_{ij}(x) = a_{ij}(\epsilon x) \\ b^\epsilon_j(x) = b_j(\epsilon x) \\ c^\epsilon(x) = c(\epsilon x) \\ J_\epsilon(x) = J(\epsilon x) = \nabla\tau(\epsilon x) \end{cases}$$

and

$$\begin{cases} a_{ij} = (\nabla\tau^{-1}\nabla\tau^{-T})_{ij} \\ b_j = \sum_{ik} \nabla\tau^{-1}_{ik} \partial_i \nabla\tau^{-T}_{kj} - 2J^{\frac{1}{2}} \sum_i a_{ij} \partial_i J^{-\frac{1}{2}} \\ c = J^{\frac{1}{2}} \sum_{ijk} \nabla\tau^{-1}_{ik} \partial_i \nabla\tau^{-T}_{kj} \partial_j J^{-\frac{1}{2}} + J^{\frac{1}{2}} \sum_{ij} a_{ij} \partial_i \partial_j J^{-\frac{1}{2}} \end{cases}$$

Thus if $\|u\|_{W_1^{m,\infty}} \leqslant h_u, \mathcal{V}^0 \in (H^2_n)^2$, then we have

$$\|\mathcal{F}(\mathcal{V}^0)\|_{(L^2_n)^2} = \|(f, g)\|_{(L^2_n)^2} \lesssim \epsilon^3.$$

$\square$

Lemma 5.5.2. *There exist positive constants h_u and ϵ_0 such that for all $0 < \epsilon \leqslant \epsilon_0$ and $\|u\|_{W_1^{5,\infty}} \leqslant h_u$, we have*

$$\|\mathcal{L}^{-1}_{\mathcal{V}^0}\|_{\mathcal{L}((L^2_n)^2,(H^2_n)^2)} \lesssim 1.$$

Proof. Notice $\mathcal{L}_{\mathcal{V}^0} = \mathcal{L}_{\mathcal{V}_{\text{per}}} + (\mathcal{L}_{\mathcal{V}^0} - \mathcal{L}_{\mathcal{V}_{\text{per}}})$, so $\mathcal{L}^{-1}_{\mathcal{V}^0} = \mathcal{L}^{-1}_{\mathcal{V}_{\text{per}}}(\mathcal{I} + (\mathcal{L}_{\mathcal{V}^0} - \mathcal{L}_{\mathcal{V}_{\text{per}}})\mathcal{L}^{-1}_{\mathcal{V}_{\text{per}}})^{-1}$. Therefore it suffices to impose $\|\mathcal{L}_{\mathcal{V}^0} - \mathcal{L}_{\mathcal{V}_{\text{per}}}\|_{\mathcal{L}((H^2_n)^2,(L^2_n)^2)}$ to be small enough so that the series expansion of $(\mathcal{I}+(\mathcal{L}_{\mathcal{V}^0}-\mathcal{L}_{\mathcal{V}_{\text{per}}})\mathcal{L}_{\mathcal{V}_{\text{per}}}^{-1})^{-1}$ can be finite. This is a simple case of **Proposition** 5.2.1 by choosing $\tau_1=\tau_2=\text{id}+u, \mathcal{V}_1=\mathcal{V}^0, \mathcal{V}_2=\mathcal{V}_{\text{per}}$ so that

$$\|\mathcal{L}_{\mathcal{V}^0}-\mathcal{L}_{\mathcal{V}_{\text{per}}}\|_{\mathcal{L}((H_n^2)^2,(L_n^2)^2)} \leqslant C\|\mathcal{V}^0-\mathcal{V}_{\text{per}}\|_{W^{k,\infty}(n\Omega)}$$

where

$$\|\mathcal{V}^0-\mathcal{V}_{\text{per}}\|_{W^{k,\infty}(n\Omega)} \leqslant \|\mathcal{V}^0-\mathcal{V}_{\text{CB}}\|_{W^{k,\infty}(n\Omega)}+\|\mathcal{V}_{\text{CB}}-\mathcal{V}_{\text{per}}\|_{W^{k,\infty}(n\Omega)} \lesssim \epsilon+\delta.$$

□

Lemma 5.5.3. *If* $\|\mathcal{V}^k-\mathcal{V}^0\|_{(H_n^2)^2} \leqslant C_1\epsilon^3$ *and* $\|\mathcal{V}^{k-1}-\mathcal{V}^0\|_{(H_n^2)^2} \leqslant C_1\epsilon^3$*, then*

$$\|\mathcal{L}_{\mathcal{V}^0}^{-1}(\mathcal{F}(\mathcal{V}^k)-\mathcal{F}(\mathcal{V}^{k-1})-\mathcal{L}_{\mathcal{V}^0}(\mathcal{V}^k-\mathcal{V}^{k-1}))\|_{(H_n^2)^2} \leqslant C(C_1)\epsilon^{\frac{3}{2}}\|\mathcal{V}^k-\mathcal{V}^{k-1}\|_{(H_n^2)^2}.$$

Proof. Recall $\frac{\delta\mathcal{F}}{\delta\mathcal{V}}=\mathcal{L}_{\mathcal{V}}$, so

$$\begin{aligned}&\mathcal{F}(\mathcal{V}^k)-\mathcal{F}(\mathcal{V}^{k-1})-\mathcal{L}_{\mathcal{V}^0}(\mathcal{V}^k-\mathcal{V}^{k-1})\\ &=\int_0^1(\mathcal{L}_{\mathcal{V}^t}-\mathcal{L}_{\mathcal{V}^0})(\mathcal{V}^k-\mathcal{V}^{k-1})dt\end{aligned}$$

where $\mathcal{V}^t=t\mathcal{V}^k+(1-t)\mathcal{V}^{k-1}$. So it suffices to prove

$$\|\mathcal{L}_{\mathcal{V}^t}-\mathcal{L}_{\mathcal{V}^0}\|_{\mathcal{L}((H_n^2)^2),(L_n^2)^2} \leqslant C(C_1)\epsilon^{-\frac{3}{2}}\|\mathcal{V}^t-\mathcal{V}^0\|_{(H_n^2)^2},$$

which is the consequence of **Proposition** 5.2.1 with $\tau_1=\tau_2=\tau$ and notice that $\|\mathcal{V}^t-\mathcal{V}^0\|_{(H^2(n\Omega))^2}=\epsilon^{-\frac{3}{2}}\|\mathcal{V}^t-\mathcal{V}^0\|_{(H_n^2)^2}$.

□

5.6 Newton-Raphson Iteration

Recall our main theorem on the electronic TFDW model

Assume $m_a \in H^4$ and **Stability Condition A**, i.e. $\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((L_n^2)^2)} \leqslant M$, there exists positive constants h_0, ϵ_0, δ, such that for any deformation u satisfying $\|u\|_{W_1^{5,\infty}} \leqslant h_0$, and any $0<\epsilon\leqslant\epsilon_0$, there exists a unique solution $\mathcal{V}_{\text{exa}}=(\nu_{\text{exa}}, V_{\text{exa}}) \in (H_n^2)^2$ that satisfy

1. $\mathcal{F}(\mathcal{V}_{\text{exa}}) = 0$ on $n\Omega$,

2. $\|\mathcal{V}_{\text{exa}} - \mathcal{V}^0\|_{(H_n^2)^2} \leqslant \delta\epsilon^3$.

Recall $\mathcal{V}^0$ is the two-scale ansatz approximate solution $\mathcal{V}^0 = \mathcal{V}_{\text{CB}} + \epsilon\mathcal{V}_1 + \epsilon^2\mathcal{V}^2$.

Proof. We use Newton-Raphson iteration to define

$$\mathcal{V}^{k+1} := \mathcal{V}^k - \mathcal{L}_{\mathcal{V}^0}^{-1}\mathcal{F}(\mathcal{V}^k),$$

for integer $k \geqslant 0$.

When $k = 0$,

$$\begin{aligned}\|\mathcal{V}^1 - \mathcal{V}^0\|_{(H_n^2)^2} =& \|\mathcal{L}_{\mathcal{V}^0}^{-1}\mathcal{F}(\mathcal{V}^0)\|_{(H_n^2)^2} \\ \leqslant& \|\mathcal{L}_{\mathcal{V}^0}^{-1}\|_{\mathcal{L}((L_n^2)^2,(H_n^2)^2)}\|\mathcal{F}(\mathcal{V}^0)\|_{(L_n^2)^2} \\ \leqslant& C_1\epsilon^{\frac{3}{2}}.\end{aligned}$$

Now suppose for any $k \leqslant k_0$, we have $\|\mathcal{V}^k - \mathcal{V}^0\|_{(H_n^2)^2} \leqslant C_1\epsilon^3$, then for any $k \leqslant k_0$,

$$\mathcal{V}^{k+1} - \mathcal{V}^k = -\mathcal{L}_{\mathcal{V}^0}^{-1}(\mathcal{F}(\mathcal{V}^k) - \mathcal{F}(\mathcal{V}^{k-1}) - \mathcal{L}_{\mathcal{V}^0}(\mathcal{V}^k - \mathcal{V}^{k-1}))$$

so

$$\|\mathcal{V}^{k+1} - \mathcal{V}^k\|_{(H_n^2)^2} \leqslant C(C_1)\epsilon^{\frac{3}{2}}\|\mathcal{V}^k - \mathcal{V}^{k-1}\|_{(H_n^2)^2}$$

Assume $C(C_1)\epsilon^{\frac{3}{2}} < \frac{1}{2}$, then

$$\|\mathcal{V}^{k+1} - \mathcal{V}^k\|_{(H_n^2)^2} \leqslant (\frac{1}{2})^k\|\mathcal{V}^1 - \mathcal{V}^0\|_{(H_n^2)^2}$$

then

$$\begin{aligned}&\|\mathcal{V}^{k_0+1} - \mathcal{V}^0\|_{(H_n^2)^2} \\ \leqslant& \sum_{k=0}^{k_0}\|\mathcal{V}^{k+1} - \mathcal{V}^k\|_{(H_n^2)^2}\end{aligned}$$

$$\leqslant 2\|\mathcal{V}^1 - \mathcal{V}^0\|_{(H_n^2)^2}$$
$$\leqslant C_1\epsilon^3.$$

Therefore for any integer $k \geqslant 0$, we have

$$\|\mathcal{V}^k - \mathcal{V}^0\|_{(H_n^2)^2} \leqslant C_1\epsilon^3$$

and

$$\|\mathcal{V}^{k+1} - \mathcal{V}^k\|_{(H_n^2)^2} \leqslant \frac{1}{2}\|\mathcal{V}^k - \mathcal{V}^{k-1}\|_{(H_n^2)^2}$$

then $\{\mathcal{V}^n\}$ is Cauchy. Suppose the unique limit is $\mathcal{V}^* = (\nu^*, V^*)$, then it is easy to see

$$\|\mathcal{V}^* - \mathcal{V}^0\|_{(H_n^2)^2} \leqslant C_1\epsilon^3$$

and since $\mathcal{F}(\mathcal{V}^k)$ is C^∞ in $\mathcal{V}^k$,

$$\|\mathcal{F}(\mathcal{V}^*)\|$$
$$= \lim_{k\to\infty} \|\mathcal{F}(\mathcal{V}^k)\|$$
$$\leqslant \lim_{k\to\infty} \|\mathcal{L}_{\mathcal{V}^0}\|\|\mathcal{V}^{k+1} - \mathcal{V}^k\|$$
$$=0.$$

Thus this unique limit $\mathcal{V}^*$ is the exact solution $\mathcal{V}_{\text{exa}} \in (H_n^2)^2$.

□

5.7 Properties of the approximate solution and the exact solution

5.7.1 Preservation of the Decaying Property

Let us first establish the invertability of the linearized operator $\mathcal{L}_{\mathcal{V}_{\text{exa}}}$ at the exact solution $\mathcal{V}_{\text{exa}}$:

Proposition 5.7.1. *The linearized operator $\mathcal{L}_{\mathcal{V}_{exa}}$ satisfies*

$$\|\mathcal{L}_{\mathcal{V}_{exa}}^{-1}\|_{\mathcal{L}((L_n^2)^2, (H_n^2)^2)} \leqslant C,$$

for some constant $C > 0$ independent of $\epsilon = \frac{1}{n}$.

Proof. Recall

$$\|\mathcal{V}_{\text{exa}} - \mathcal{V}^0\|_{(H_n^2)^2} \leqslant \delta\epsilon^3$$

So by **Proposition** 5.2.1, we have

$$\begin{aligned}&\|\mathcal{L}_{\mathcal{V}_{\text{exa}}} - \mathcal{L}_{\mathcal{V}^0}\|_{\mathcal{L}((H_n^2)^2,(L_n^2)^2)}\\ \leqslant& C\|\mathcal{V}_{\text{exa}} - \mathcal{V}^0\|_{(H^2(n\Omega))^2}\\ \leqslant& Cn^{\frac{3}{2}}\|\mathcal{V}_{\text{exa}} - \mathcal{V}^0\|_{(H_n^2)^2}\\ \leqslant& C\delta\epsilon^{\frac{3}{2}}.\end{aligned}$$

Combined with the previous estimate on $\mathcal{L}_{\mathcal{V}^0}^{-1}$

$$\|\mathcal{L}_{\mathcal{V}^0}^{-1}\|_{\mathcal{L}((L_n^2)^2,(H_n^2)^2)} \leqslant C,$$

and the formula

$$\mathcal{L}_{\mathcal{V}_{\text{exa}}}^{-1} - \mathcal{L}_{\mathcal{V}^0}^{-1} = \mathcal{L}_{\mathcal{V}^0}^{-1}\sum_{n=1}^{\infty}(-1)^n[(\mathcal{L}_{\mathcal{V}_{\text{exa}}} - \mathcal{L}_{\mathcal{V}^0})\mathcal{L}_{\mathcal{V}^0}^{-1}]^n$$

it is straightforward to finally prove the result.

□

Proposition 5.7.2. *Recall that the background charge function has the decaying property*

$$\|\partial_i\rho_b(x, Y)\| \leqslant \frac{C}{\epsilon}e^{-\gamma|x+\frac{-X_i+r_{i,\epsilon x}}{\epsilon}|}, \quad x \in n\Omega, \tag{5.21}$$

for any $0 < \gamma \leqslant \frac{\delta_\tau}{M}$. This implies the same decaying property for ν_{exa}, V_{exa}:

$$\|\partial_i\nu_{exa}(x, Y)\| \leqslant \frac{C}{\epsilon}e^{-\gamma|x+\frac{-X_i+r_{i,\epsilon x}}{\epsilon}|} \tag{5.22}$$

$$\|\partial_i V_{exa}(x, Y)\| \leqslant \frac{C}{\epsilon}e^{-\gamma|x+\frac{-X_i+r_{i,\epsilon x}}{\epsilon}|}, \tag{5.23}$$

for any $x \in n\Omega$ and $\gamma > 0$ small enough but independent of ϵ.

Proof. By taking linearization of the system of Euler-Lagrange equations, the following formula holds

$$\mathcal{L}_{\mathcal{V}_{\text{exa}}}\begin{pmatrix}\epsilon\partial_i\nu_{\text{exa}}\\ \epsilon\partial_i V_{\text{exa}}\end{pmatrix}=\begin{pmatrix}0\\ \frac{\epsilon}{2}\partial_i\rho_b\end{pmatrix}.$$

Denote $\eta(x)=|x-\frac{X_i+r_{i,x}}{\epsilon}|$, then $\|\eta\|_{W^{2,\infty}(n\Omega)}\leqslant C$, where $C>0$ is independent of ϵ.

Given an exponential function $e^{s\eta}$, define the perturbed operator

$$\mathcal{L}_{s,\mathcal{V}_{\text{exa}}}(\mathcal{W})=e^{s\eta}\mathcal{L}_{\mathcal{V}_{\text{exa}}}(e^{-s\eta}\mathcal{W}).$$

So given a system of linear elliptic equations

$$\mathcal{L}_{\mathcal{V}_{\text{exa}}}\mathcal{W}=f$$

we have

$$\mathcal{L}_{s,\mathcal{V}_{\text{exa}}}(e^{s\eta}\mathcal{W})=e^{s\eta}f.$$

Notice $e^{s\eta}f\in(L^2(n\Omega))^2\subset(L^\infty(n\Omega))^2$ means $|f(x)|\leqslant C_f e^{-s\eta(x)}$ for any $x\in n\Omega$ and some constant $C_f>0$. So we say $\mathcal{L}_{\mathcal{V}_{\text{exa}}}$ preserves the decaying property if $e^{s\eta}f\in(L^2(n\Omega))^2$ implies $e^{s\eta}\mathcal{W}\in(H^2(n\Omega))^2$. Then it is sufficient to show

$$||\mathcal{L}^{-1}_{s,\mathcal{V}_{\text{exa}}}||_{\mathcal{L}((L^2(n\Omega))^2,(H^2(n\Omega))^2)}\leqslant M'$$

for some constants $s>0$ and $M'>0$ provided

$$||\mathcal{L}^{-1}_{\mathcal{V}_{\text{exa}}}||_{\mathcal{L}((L^2(n\Omega))^2,(H^2(n\Omega))^2)}\leqslant M,$$

for some constant $M>0$.

Then

$$\begin{aligned}\|e^{s\eta}\mathcal{W}\|_{(L^\infty(n\Omega))^2}\leqslant&C\|e^{s\eta}\mathcal{W}\|_{(H^2(n\Omega))^2}\\ &\leqslant||\mathcal{L}^{-1}_{\mathcal{V}_{\text{exa}}}||_{\mathcal{L}((L^2(n\Omega))^2,(H^2(n\Omega))^2)}\|e^{s\eta}f\|_{(L^2(n\Omega))^2}\leqslant CM'C_f\end{aligned}$$

which means $|\mathcal{W}(x)| \leqslant CM'C_f e^{-s\eta(x)}$.

Now let us establish

$$\|\mathcal{L}_{s,\mathcal{V}_{\text{exa}}} - \mathcal{L}_{\mathcal{V}_{\text{exa}}}\|_{\mathcal{L}((L^2(n\Omega))^2,(H^2(n\Omega))^2)} \leqslant C|s|.$$

Recall

$$\mathcal{L}_{\mathcal{V}_{\text{exa}}} \begin{pmatrix} \omega \\ W \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{\mathcal{V}_{\text{exa}},1} & \nu_{\text{exa}} \\ \nu_{\text{exa}} & \frac{1}{8\pi} D_2^\epsilon \end{pmatrix} \begin{pmatrix} \omega \\ W \end{pmatrix}$$

where

$$\mathcal{L}_{\mathcal{V}_{\text{exa}},1} = -D_1^\epsilon + \frac{35}{9} J_\epsilon^{-\frac{2}{3}} \nu_{\text{exa}}^{\frac{4}{3}} - \frac{20}{9} J_\epsilon^{-\frac{1}{3}} \nu_{\text{exa}}^{\frac{2}{3}} + V_{\text{exa}},$$

and $D_1^\epsilon = \sum_{ij} a_\epsilon^{ij} \partial_i \partial_j + \sum_j b_\epsilon^j \partial_j + c_\epsilon$, $D_2^\epsilon = \sum_{ij} a_\epsilon^{ij} \partial_i \partial_j + \sum_j d_\epsilon^j \partial_j$.

So

$$\begin{aligned} &(\mathcal{L}_{s,\mathcal{V}_{\text{exa}}} - \mathcal{L}_{\mathcal{V}_{\text{exa}}}) \begin{pmatrix} \omega \\ W \end{pmatrix} \\ =&(e^{s\eta} \mathcal{L}_{\mathcal{V}_{\text{exa}}} e^{-s\eta} - \mathcal{L}_{\mathcal{V}_{\text{exa}}}) \begin{pmatrix} \omega \\ W \end{pmatrix} \\ =& \begin{pmatrix} (e^{s\eta} \mathcal{L}_{\mathcal{V}_{\text{exa}},1} e^{-s\eta} - \mathcal{L}_{\mathcal{V}_{\text{exa}},1})\omega \\ \frac{1}{8\pi}(e^{s\eta} D_2^\epsilon e^{-s\eta} - D_2^\epsilon) W \end{pmatrix} \\ =& \begin{pmatrix} -(e^{s\eta} D_1^\epsilon e^{-s\eta} - D_1^\epsilon)\omega \\ \frac{1}{8\pi}(e^{s\eta} D_2^\epsilon e^{-s\eta} - D_2^\epsilon) W \end{pmatrix} \end{aligned}$$

Compute

$$\begin{aligned} e^{s\eta}\partial_j(e^{-s\eta}w) - \partial_j w =& -s\partial_j \eta w \\ e^{s\eta}\partial_i\partial_j(e^{-s\eta}w) - \partial_i\partial_j w =& -s(\partial_i\eta\partial_j w + \partial_j\eta\partial_i w + \partial_i\partial_j\eta w) + s^2 \partial_i\partial_j \eta w \end{aligned}$$

Thus

$$\|(\mathcal{L}_{s,\mathcal{V}_{\text{exa}}} - \mathcal{L}_{\mathcal{V}_{\text{exa}}}) \begin{pmatrix} \omega \\ W \end{pmatrix}\|_{(L^2(n\Omega))^2} \leqslant C|s| \| \begin{pmatrix} \omega \\ W \end{pmatrix} \|_{(H^1(n\Omega))^2} \leqslant C|s| \| \begin{pmatrix} \omega \\ W \end{pmatrix} \|_{(H^2(n\Omega))^2}$$

Therefore

$$\|\mathcal{L}_{s,\nu_{\text{exa}}} - \mathcal{L}_{\nu_{\text{exa}}}\|_{\mathcal{L}((L^2(n\Omega))^2,(H^2(n\Omega))^2)} \leqslant C|s|.$$

$$
\begin{aligned}
\mathcal{L}^{-1}_{s,\mathcal{V}_{\text{exa}}} &= (\mathcal{L}_{s,\mathcal{V}_{\text{exa}}} - \mathcal{L}_{\mathcal{V}_{\text{exa}}} + \mathcal{L}_{\mathcal{V}_{\text{exa}}})^{-1} \\
&= \left(\mathcal{I} + \mathcal{L}^{-1}_{\mathcal{V}_{\text{exa}}}(\mathcal{L}_{s,\mathcal{V}_{\text{exa}}} - \mathcal{L}_{\mathcal{V}_{\text{exa}}})\right)^{-1}\mathcal{L}^{-1}_{\mathcal{V}_{\text{exa}}} \\
&= \left(\mathcal{I} + \sum_{k=1}^{\infty}[-\mathcal{L}^{-1}_{\mathcal{V}_{\text{exa}}}(\mathcal{L}_{s,\mathcal{V}_{\text{exa}}} - \mathcal{L}_{\mathcal{V}_{\text{exa}}})]^k\right)\mathcal{L}^{-1}_{\mathcal{V}_{\text{exa}}}
\end{aligned}
$$

Pick s so that $|s| < \frac{1}{MC}$, then

$$
\|\mathcal{L}^{-1}_{\mathcal{V}_{\text{exa}}}(\mathcal{L}_{s,\mathcal{V}_{\text{exa}}} - \mathcal{L}_{\mathcal{V}_{\text{exa}}})\|_{\mathcal{L}((L^2(n\Omega))^2,(H^2(n\Omega))^2)} \leqslant MC|s| < 1.
$$

Therefore from the above expansion of $\mathcal{L}^{-1}_{s,\mathcal{V}_{\text{exa}}}$, we get the proof.

□

5.7.2 Perturbation of the exact solution

Lemma 5.7.3. *Assume $\|\tau_{Y_1}\|_{W_1^{5,\infty}} \leqslant h, \|\tau_{Y_2}\|_{W_1^{5,\infty}} \leqslant h$. Let $\mathcal{V}^t = t\mathcal{V}_{exa}(Y_2) + (1-t)\mathcal{V}_{exa}(Y_1), \tau^t = t\tau_{Y_2} + (1-t)\tau_{Y_1}, 0 < t < 1$, then $\|\mathcal{L}^{-1}_{(\mathcal{V}^t,\tau^t)}\|_{\mathcal{L}((L_n^2)^2,(H_n^2)^2)} \leqslant M$.*

Proof. By the assumptions $\|\tau_{Y_1}\|_{W_1^{5,\infty}} \leqslant h, \|\tau_{Y_2}\|_{W_1^{5,\infty}} \leqslant h$, we have

$$
\|\mathcal{V}_{\text{exa}}(Y_1) - \mathcal{V}_{\text{per}}\|_{(H^2(n\Omega))^2} \leqslant \max(C\epsilon, \delta_h)
$$
$$
\|\mathcal{V}_{\text{exa}}(Y_2) - \mathcal{V}_{\text{per}}\|_{(H^2(n\Omega))^2} \leqslant \max(C\epsilon, \delta_h),
$$

then

$$
\begin{aligned}
&\|\mathcal{V}^t - \mathcal{V}_{\text{per}}\|_{(H^2(n\Omega))^2} \\
=&\|(1-t)\mathcal{V}_{\text{exa}}(Y_1) + t\mathcal{V}_{\text{exa}}(Y_2) - \mathcal{V}_{\text{per}}\|_{(H^2(n\Omega))^2} \\
\leqslant&(1-t)\|\mathcal{V}_{\text{exa}}(Y_1) - \mathcal{V}_{\text{per}}\|_{(H^2(n\Omega))^2} + t\|\mathcal{V}_{\text{exa}}(Y_2) - \mathcal{V}_{\text{per}}\|_{(H^2(n\Omega))^2} \\
\leqslant&\max(C\epsilon, \delta_h).
\end{aligned}
$$

Then by **Proposition** 5.2.1, we have

$$
\|\mathcal{L}_{(\mathcal{V}^t,\tau^t)} - \mathcal{L}_{\text{per}}\|_{\mathcal{L}((H_n^2)^2,(L_n^2)^2)}
$$

$$\leqslant C\max(\|\mathcal{V}^t - \mathcal{V}_{\text{per}}\|_{(H^2(n\Omega))^2}, \|\tau^t - \tau_{Y_1}\|_{W_1^{3,\infty}}) \leqslant C\max(\epsilon, \delta_h, h)$$

which could be made as small as desired if we pick ϵ and h small enough. So again from the expansion formula

$$\mathcal{L}^{-1}_{(\mathcal{V}^t,\tau^t)} - \mathcal{L}^{-1}_{\text{per}} = \mathcal{L}^{-1}_{\text{per}} \sum_{n=1}^{\infty} (-1)^n [(\mathcal{L}_{(\mathcal{V}^t,\tau^t)} - \mathcal{L}_{\text{per}})\mathcal{L}^{-1}_{\text{per}}]^n$$

it is straightforward to finally prove the result similar to the proof in previous proposition.

□

Lemma 5.7.4.

$$\|V_{exa}(Y_2) - V_{exa}(Y_1)\|_{L^\infty(n\Omega)} \leqslant C\|Y_2 - Y_1\|_{W_\epsilon^{1,\infty}} \tag{5.24}$$

Proof. The exact solution $\mathcal{V}_{\text{exa}} = (\nu_{\text{exa}}, \mathcal{V}_{\text{exa}})$ satisfies the system of Euler-Lagrange equations

$$\begin{cases} -D_1^\epsilon \nu_{\text{exa}} + \frac{5}{3} J_\epsilon^{-\frac{2}{3}} \nu_{\text{exa}}^{\frac{7}{3}} - \frac{4}{3} J_\epsilon^{-\frac{1}{3}} \nu_{\text{exa}}^{\frac{5}{3}} + V_{\text{exa}}\nu_{\text{exa}} = 0 \\ -J_\epsilon D_2^\epsilon V_{\text{exa}} = 4\pi(\nu_{\text{exa}}^2 - \rho_b) \end{cases} \tag{5.25}$$

Denote

$$\mathcal{F}(\mathcal{V}_{\text{exa}}) = \begin{pmatrix} -D_1^\epsilon \nu + \frac{5}{3} J_\epsilon^{-\frac{2}{3}} \nu^{\frac{7}{3}} - \frac{4}{3} J_\epsilon^{-\frac{1}{3}} \nu^{\frac{5}{3}} + V\nu = 0 \\ \frac{1}{8\pi} J_\epsilon D_2^\epsilon V + \frac{1}{2}\nu_{\text{exa}}^2 \end{pmatrix} \tag{5.26}$$

Then

$$\mathcal{F}(\mathcal{V}_{\text{exa}}(Y_1)) = \begin{pmatrix} 0 \\ \frac{1}{2}\rho_b(Y_1) \end{pmatrix} =: \frac{1}{2}\rho_b(Y_1). \tag{5.27}$$

Then from $\mathcal{F}(\mathcal{V}_{\text{exa}}(Y_2)) = \frac{1}{2}\rho_b(Y_2)$, we get

$$\mathcal{F}(\mathcal{V}_{\text{exa}}(Y_2) - \mathcal{V}_{\text{exa}}(Y_1) + \mathcal{V}_{\text{exa}}(Y_1)) = \frac{1}{2}\rho_b(Y_2) - \frac{1}{2}\rho_b(Y_1) + \frac{1}{2}\rho_b(Y_1) \tag{5.28}$$

Expand it to the first order, we get

$$\mathcal{F}(\mathcal{V}_{\text{exa}}(Y_1)) + \mathcal{L}_{(\mathcal{V}^t,\tau^t)}(\mathcal{V}_{\text{exa}}(Y_2) - \mathcal{V}_{\text{exa}}(Y_1)) = \frac{1}{2}\rho_b(Y_1) + \frac{1}{2}\rho_b(Y_2) - \frac{1}{2}\rho_b(Y_1), \tag{5.29}$$

Which simplifies to

$$\mathcal{L}_{(\mathcal{V}^t,\tau^t)}\big(\mathcal{V}_{\text{exa}}(Y_2)-\mathcal{V}_{\text{exa}}(Y_1)\big)=\frac{1}{2}\rho_b(Y_2)-\frac{1}{2}\rho_b(Y_1) \tag{5.30}$$

where $\mathcal{V}^t=t\mathcal{V}_{\text{exa}}(Y_2)+(1-t)\mathcal{V}_{\text{exa}}(Y_1), \tau^t=t\tau_2+(1-t)\tau_1$, for some $0<t<1$.

Therefore

$$\begin{aligned}
&\|V_{\text{exa}}(Y_2)-V_{\text{exa}}(Y_1)\|_{(L^\infty(n\Omega))^2}\\
\leqslant& C\|V_{\text{exa}}(Y_2)-V_{\text{exa}}(Y_1)\|_{(H^2(n\Omega))^2}\\
=& Cn^{\frac{3}{2}}\|V_{\text{exa}}(Y_2)-V_{\text{exa}}(Y_1)\|_{(H^2_n)^2}\\
\leqslant& \frac{1}{2}Cn^{\frac{3}{2}}\|\mathcal{L}^{-1}_{(\mathcal{V}^t,\tau^t)}\|_{\mathcal{L}((L^2_n)^2,(H^2_n)^2)}\|\rho_b(Y_2)-\rho_b(Y_1)\|_{(L^2_n)^2}\\
\leqslant& C'\|\rho_b(Y_2)-\rho_b(Y_1)\|_{L^2(n\Omega)}\\
\leqslant& C'\|\rho_b(Y_2)-\rho_b(Y_1)\|_{L^\infty(n\Omega)}\\
\leqslant& C'\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}.
\end{aligned}$$

□

Proposition 5.7.5.

$$\|\partial_j\mathcal{V}_{exa}(x,Y_2)-\partial_j\mathcal{V}_{exa}(x,Y_1)\|\leqslant C\epsilon^{-2}e^{-\gamma|x-\frac{X_j+r_{j,\epsilon,x}}{\epsilon}|}\|Y_2-Y_1\|_{W^{3,\infty}_\epsilon}$$

Proof. Given

$$\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_1)}(\partial_j\mathcal{V}_{\text{exa}}(Y_1))=\partial_j\rho_b(Y_1)$$
$$\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_2)}(\partial_j\mathcal{V}_{\text{exa}}(Y_2))=\partial_j\rho_b(Y_2)$$

we have

$$\begin{aligned}
&\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_1)}(\partial_j\mathcal{V}_{\text{exa}}(Y_2)-\partial_j\mathcal{V}_{\text{exa}}(Y_1))\\
=&(\partial_j\rho_b(Y_2)-\partial_j\rho_b(Y_1))+(\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_1)}-\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_2)})(\partial_j\mathcal{V}_{\text{exa}}(Y_2))
\end{aligned}$$

Then it suffices to show

$$\|e^{s\eta}(\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_1)} - \mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_2)})(\partial_j \mathcal{V}_{\text{exa}}(Y_2))\|_{(L^\infty(n\Omega)^2} \leqslant C\epsilon^{-1}\|Y_2 - Y_1\|_{W_\epsilon^{3,\infty}}.$$

We proceed as follows

$$\begin{aligned}
&\|e^{s\eta}(\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_1)} - \mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_2)})(\partial_j \mathcal{V}_{\text{exa}}(Y_2))\|_{(L^\infty(n\Omega))^2} \\
\leqslant& C\|e^{s\eta}(\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_1)} - \mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_2)})(\partial_j \mathcal{V}_{\text{exa}}(Y_2))\|_{(H^2(n\Omega))^2} \\
\leqslant& C\|e^{s\eta}(\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_1)} - \mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_2)})\|_{\mathcal{L}((L^2(n\Omega))^2,(H^2(n\Omega))^2)}\|\partial_j \mathcal{V}_{\text{exa}}(Y_2))\|_{(L^2(n\Omega))^2} \\
\leqslant& C'\epsilon^{-1}\|e^{s\eta}\|_{W^{2,\infty}(n\Omega)}\|\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_1)} - \mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_2)}\|_{\mathcal{L}((L^2(n\Omega))^2,(H^2(n\Omega))^2)} \\
\leqslant& C''\epsilon^{-1}\|\mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_1)} - \mathcal{L}_{\mathcal{V}_{\text{exa}}(Y_2)}\|_{\mathcal{L}((L^2(n\Omega))^2,(H^2(n\Omega))^2)} \\
\leqslant& C'''\epsilon^{-1}\max(\|\mathcal{V}_{\text{exa}}(Y_1) - \mathcal{V}_{\text{exa}}(Y_2)\|_{(L^\infty(n\Omega))^2}, \|\tau_1 - \tau_2\|_{W_1^{3,\infty}}) \\
\leqslant& C'''\epsilon^{-1}\|Y_1 - Y_2\|_{W_\epsilon^{3,\infty}}.
\end{aligned}$$

□

6

Consistency Of Cauchy-Born Rule

6.1 The Consistency Estimate

In this chapter, we are going to prove the following estimate of the consistency of the Cauchy-Born rule. This estimate will be used in the last chapter to derive the quadratic rate convergence in the main theorem.

Theorem 6.1.1. *Given a deformation, $Y_{CB} = id_{\Omega_\epsilon} + u_{CB}$, where u_{CB} solves the Euler-Lagrange equation of the continuum elasticity model, we have*

$$\|\mathcal{F}_{at}[Y_{CB}]\|_{\epsilon,5} \leqslant C(\|u_{CB}\|_{H^{29}(\Omega)})\epsilon^2. \tag{6.1}$$

In the above estimate, we can achieve ϵ^2 control instead of the typical ϵ control because we can exploit the inversion symmetry of the underlying Bravais lattice.

Now recall the atomistic TFDW functional is

$$I_{\text{at}}(Y) = \int_{n\Omega} \nu_{\text{exa}}^{\frac{10}{3}} + |\nabla_y \nu_{\text{exa}}|^2 - \nu_{\text{exa}}^{\frac{8}{3}} + \frac{1}{2}V_{\text{exa}}(\nu_{\text{exa}}^2 - \rho_b)dy - \sum_{X\in\Omega_\epsilon} f(X)Y(X)$$

So

$$\mathcal{F}_{\text{at}}[Y](X_i) = \frac{\partial}{\partial Y_i} I_{\text{at}}(Y)$$

$$= \int_{n\Omega} [\frac{10}{3}\nu_{\text{exa}}^{\frac{7}{3}} - 2\Delta_y \nu_{\text{exa}} - \frac{8}{3}\nu_{\text{exa}}^{\frac{5}{3}} + V_{\text{exa}}\nu_{\text{exa}}]\partial_{Y_i}\nu_{\text{exa}} dy$$

$$- \int_{n\Omega} V_{\text{exa}}\partial_{Y_i}\rho_b dy - f(X_i)$$

$$= - \int_{n\Omega} J_\epsilon V_{\text{exa}}\partial_{Y_i}\rho_b dx - f(X_i)$$

There the explicit form of the corresponding Euler-Lagrange equation is

$$- \int_{n\Omega} J_\epsilon V_{\text{exa}}\partial_{Y_i}\rho_b dx = f(X_i).$$

6.2 Derivation Of The Stored Energy Density

Next we derive the stored energy density W_{CB} we will use in the continuum elasticity model from the above atomistic TFDW functional. Recall with a fixed deformation $\tau = \text{Id} + u$ which interpolates Y on Ω, we constructed the Cauchy-Born solutions

$$\nu_{\text{CB}}(x) = \nu_{\text{CB}}(\frac{x}{\epsilon}; \nabla u(x)), \quad V_{\text{CB}}(x) = V_{\text{CB}}(\frac{x}{\epsilon}; \nabla u(x)), x \in \Omega. \tag{6.2}$$

The corresponding atomistic TFDW functional in Eulerian coordinates is

$$I_{\text{TFDW}}(\nu_{\text{CB}}, V_{\text{CB}}) = \epsilon^{-3} \int_{\Omega} \nu_{\text{CB}}^{\frac{10}{3}} + |\nabla \nu_{\text{CB}}|^2 - \nu_{\text{CB}}^{\frac{8}{3}} + \frac{1}{2} V_{\text{CB}}(\nu_{\text{CB}}^2 - \rho_{b,0}) dy \tag{6.3}$$

The Cauchy-Born continuum elasticity functional is given as

$$I_{\text{CB}}(v) = \int_{\Omega} W_{\text{CB}}(\nabla v(x)) - f(x)v(x) dx \tag{6.4}$$

where the Cauchy-Born stored energy density $W_{\text{CB}}(A)$ is defined as

$$W_{\text{CB}}(A)$$

$$= \lim_{n\to\infty} \frac{1}{|n\Omega|} I_{\text{TFDW}}(\mathcal{V}_{\text{CB}}(A); \rho_{b,0}(A))$$

$$= \lim_{n\to\infty} \frac{\epsilon^{-3}}{|n\Omega|} \int_{\Omega} \nu_{\text{CB}}^{\frac{10}{3}}(y;A) + \epsilon^2 |\nabla_y \nu_{\text{CB}}(y;A)|^2 - \nu_{\text{CB}}^{\frac{8}{3}}(y;A) + \frac{1}{2} V_{\text{CB}}(y;A)\big(\nu_{\text{CB}}^2(y;A)$$

$$- \rho_{b,0}(y;A)\big) dy$$

$$= \frac{1}{|\Omega|} \int_{\Omega} \nu_{\text{CB}}^{\frac{10}{3}}(y;A) + \epsilon^2 |\nabla_y \nu_{\text{CB}}(y;A)|^2 - \nu_{\text{CB}}^{\frac{8}{3}}(y;A) + \frac{1}{2} V_{\text{CB}}(y;A)\big(\nu_{\text{CB}}^2(y;A)$$

$$- \rho_{b,0}(y;A)\big) dy$$

With the explicit expression of W_{CB}, we now derive the Euler-Lagrange equation for the Cauchy-Born continuum elasticity model. First compute $D_A W_{\text{CB}}(A)$

$$\begin{aligned} & D_A W_{\text{CB}}(A) \\ =& \frac{1}{|\Omega|} \int_{\Omega} 2\big(\frac{5}{3}\nu_{\text{CB}}^{\frac{7}{3}} - \epsilon^2 \Delta_y \nu_{\text{CB}} - \frac{4}{3}\nu_{\text{CB}}^{\frac{5}{3}} + V_{\text{CB}}\nu_{\text{CB}}\big) D_A \nu_{\text{CB}} dy \\ & - \frac{1}{|\Omega|} \int_{\Omega} V_{\text{CB}} D_A \rho_{b,0} dy \\ =& - \frac{1}{|\Omega|} \int_{\Omega} J(A) V_{\text{CB}}(z;A) D_A \rho_{b,0}(z;A) dz \end{aligned}$$

where

$$\rho_{b,0}(z;A) = \sum_{X\in\Omega_\epsilon, r\in\mathbb{L}} m_a\Big(\frac{z-(I+A)X+r}{\epsilon}\Big).$$

Then the Euler-Lagrange equation

$$-\text{div}_x D_A W_{\text{CB}}(\nabla u(x)) = f(x)$$

is

$$\frac{1}{|\Omega|} \int_{\Omega} \text{div}_x [J(\nabla u(x)) V_{\text{CB}}(z;\nabla u(x)) D_A \rho_{b,0}(z;\nabla u(x))] dz = f(x)$$

The above Euler-Lagrange equation will appear in $\mathcal{F}_{\text{at}}[Y_{\text{CB}}]$ valued at each $X \in \Omega_\epsilon$ as the leading-order approximation which vanishes. As we will see, the next order terms also vanish due to the inversion symmetry of the lattice. Thus we can achieve ϵ^2 estimate.

6.3 Homogenization

We will need the following homogenization-type estimate in our analyze of $\mathcal{F}_{\rm at}[Y_{\rm CB}]$:

Theorem 6.3.1. *Given a function $\varphi(z,x)$ periodic and H^2 in $z \in \Omega$, while periodic and H^{12+k} in $x \in \Omega$, we have the following estimate:*

$$\|\epsilon^{-3}\int_\Omega \varphi(\frac{x}{\epsilon},x)\partial_{Y_i}\nabla\tau(x)dx + \int_\Omega div_x\varphi(z,X_i)dz\|_{\epsilon,5} \lesssim \epsilon^k.$$

Proof.

$$\begin{aligned}
&\epsilon^{-3}\int_\Omega \varphi(\frac{x}{\epsilon},x)\partial_{Y_i}\nabla\tau(x)dx\\
=&\epsilon^{-3}\int_\Omega \varphi(\frac{x}{\epsilon},x)\epsilon^3\sum_{\xi\in\Omega_\epsilon^*} e^{\imath\xi\cdot(x-X_i)}\imath\xi dx\\
=&\epsilon^{-3}\int_\Omega \frac{1}{|\Omega|}\int_\Omega \varphi(z,x)\epsilon^3\sum_{\xi\in\Omega_\epsilon^*} e^{\imath\xi\cdot(x-X_i)}\imath\xi dzdx + \mathrm{err}_1(X_i)\\
=&-\sum_{\xi\in\Omega_\epsilon^*}\int_\Omega e^{\imath\xi\cdot X_i}\frac{1}{|\Omega|}\int_\Omega e^{-\imath\xi\cdot x}\varphi(z,x)dx\imath\xi dz + \mathrm{err}_1(X_i)\\
=&-\int_\Omega\sum_{\xi\in\Omega_\epsilon^*} e^{\imath\xi\cdot X_i}\hat{\varphi}(z,\xi)\imath\xi dz + \mathrm{err}_1(X_i)\\
=&-\int_\Omega\sum_{\xi\in\mathbb{L}^*} e^{\imath\xi\cdot X_i}\hat{\varphi}(z,\xi)\imath\xi dz + \mathrm{err}_1(X_i) + \mathrm{err}_2(X_i)\\
=&-\int_\Omega \mathrm{div}_x\varphi(z,X_i)dz + \mathrm{err}_1(X_i) + \mathrm{err}_2(X_i)
\end{aligned}$$

where

$$\mathrm{err}_1(X_i) = \int_\Omega \varphi(\frac{x}{\epsilon},x)\sum_{\xi\in\Omega_\epsilon^*} e^{\imath\xi\cdot(x-X_i)}\imath\xi dx - \int_\Omega\frac{1}{|\Omega|}\int_\Omega\varphi(z,x)\sum_{\xi\in\Omega_\epsilon^*} e^{\imath\xi\cdot(x-X_i)}\imath\xi dzdx \tag{6.5}$$

$$\mathrm{err}_2(X_i) = -\int_\Omega\sum_{\xi\in\mathbb{L}^*\backslash\Omega_\epsilon^*} e^{\imath\xi\cdot X_i}\hat{\varphi}(z,\xi)\imath\xi dz \tag{6.6}$$

We first estimate err_1,

$$\begin{aligned}
&\mathrm{err}_1(X_i)\\
=&\int_\Omega \varphi(\frac{x}{\epsilon},x)\sum_{\xi\in\Omega_\epsilon^*} e^{\imath\xi\cdot(x-X_i)}\imath\xi dx-\int_\Omega\frac{1}{|\Omega|}\int_\Omega\varphi(z,x)\sum_{\xi\in\Omega_\epsilon^*} e^{\imath\xi\cdot(x-X_i)}\imath\xi dzdx\\
=&\sum_{\xi\in\Omega_\epsilon^*} e^{-\imath\xi\cdot X_i}\int_\Omega e^{\imath\xi\cdot x}[\varphi(\frac{x}{\epsilon},x)-\frac{1}{|\Omega|}\int_\Omega\varphi(z,x)dz]dx\imath\xi\\
=&\sum_{\xi\in\Omega_\epsilon^*,\xi'\in\mathbb{L}^*} e^{-\imath\xi\cdot X_i}\int_\Omega e^{\imath\xi\cdot x}e^{\imath\xi'\cdot x}[\hat\varphi(\frac{x}{\epsilon},\xi')-\frac{1}{|\Omega|}\int_\Omega\hat\varphi(z,\xi')dz]dx\imath\xi\\
=&\sum_{\xi\in\Omega_\epsilon^*,\xi'\in\mathbb{L}^*,\xi''\in\mathbb{L}^*\backslash\{0\}} e^{-\imath\xi\cdot X_i}\int_\Omega e^{\imath\xi\cdot x}e^{\imath\xi'\cdot x}e^{\imath\xi''\cdot\frac{x}{\epsilon}}\hat{\hat\varphi}(\xi'',\xi')dx\imath\xi\\
=&|\Omega|\sum_{\xi,\xi',\xi''}\frac{1}{|\Omega|}\int_\Omega e^{\imath(\frac{\xi''}{\epsilon}+\xi'+\xi)\cdot x}dx\hat{\hat\varphi}(\xi'',\xi')e^{-\imath\xi\cdot X_i}\imath\xi\\
=&|\Omega|\sum_{\xi,\xi''}\hat{\hat\varphi}(\xi'',-\xi-\frac{\xi''}{\epsilon})e^{\imath\xi\cdot X_i}\imath\xi
\end{aligned}$$

So

$$\begin{aligned}
&\|\mathrm{err}_1\|_{\epsilon,5}\\
\leqslant&|\Omega|\sum_{\xi,\xi''}\frac{C_{N_1}}{|\xi''|^{N_1}}\frac{C_{N_2}}{|\xi+\frac{\xi''}{\epsilon}|^{N_2}}\cdot C\epsilon^{-6}\\
=&C\epsilon^{N_2-9}(\epsilon^3\sum_{\xi\in\Omega_\epsilon^*})\sum_{\xi''}\frac{1}{|\xi''|^{N_1}}\frac{1}{|\epsilon\xi+\xi''|^{N_2}}\\
\lesssim&\epsilon^{N_2-9}\sum_{\xi''\in\mathbb{L}^*\backslash\{0\}}\frac{1}{|\xi''|^{N_1+N_2}}\\
\lesssim&\epsilon^k
\end{aligned}$$

if $\varphi(z,\cdot)\in C^{N_2}, N_2\geqslant 9+k$, so that $\sum_{\xi''\in\mathbb{L}^*\backslash\{0\}}\frac{1}{|\xi''|^{N_1+N_2}}\leqslant M<\infty$, where M is independent of ϵ. Notice $\epsilon\xi+\xi''$: $\xi''\in\mathbb{L}^*\backslash\{0\}$, so $\xi''=\sum c_jb_j, c_j\neq 0\in\mathbb{Z}$; $\xi\in\Omega_\epsilon^*$, so $\epsilon\xi=\sum c_jb_j$, $c_j\in\epsilon\mathbb{Z}\cap[-\frac{1}{2},\frac{1}{2})$. Therefore $|\epsilon\xi+\xi''|\sim|\xi''|$.

Next, let us estimate

$$\begin{aligned}&\mathrm{err}_2(X_i)\\&=-\int_\Omega\sum_{\xi\in\mathbb{L}^*\backslash\Omega^*_\epsilon}e^{\imath\xi\cdot X_i}\hat{\varphi}(z,\xi)\imath\xi dz,\end{aligned}$$

so

$$\begin{aligned}\|\mathrm{err}_2\|_{\epsilon,5}\lesssim&\sum_{\xi\in\mathbb{L}^*\backslash\Omega^*_\epsilon}\int_\Omega|\hat{\varphi}(z,\xi)|dz|\imath\xi|^6\\\lesssim&\sum_{\xi\in\mathbb{L}^*\backslash\Omega^*_\epsilon}\frac{1}{|\xi|^{p-6}}\\=&\epsilon^k\sum_{\xi\in\mathbb{L}^*\backslash\Omega^*_\epsilon}\frac{1}{|\xi|^{p-6-k}}\\\lesssim&\epsilon^k\end{aligned}$$

if $\varphi(z,\cdot)\in C^p, p>9+k$. By the Sobolev embedding $H^k\subset C^{k-2,\frac{1}{2}}$, we need $\varphi(z,\cdot)\in H^{12+k}$ which is satisfied by the condition. So we can conclude

$$\|\epsilon^{-3}\int_\Omega\varphi(\frac{x}{\epsilon},x)\partial_{Y_i}\nabla\tau(x)dx+\int_\Omega\mathrm{div}_x\varphi(z,X_i)dz\|_{\epsilon,5}\lesssim\epsilon^k.$$

□

6.4 Proof of the consistency estimate

We compute

$$\begin{aligned}&\mathcal{F}_{\mathrm{at}}[Y_{\mathrm{CB}}](X_i)\\=&-\epsilon^{-3}\int_\Omega JV_{\mathrm{exa},\epsilon}\partial_{Y_i}\rho_b^\epsilon dx-f(X_i)\\=&-\epsilon^{-3}\int_\Omega JV_{\mathrm{exa},\epsilon}\sum_{X\in\mathbb{L}_\epsilon}\nabla m_a(\frac{\tau_{\mathrm{CB}}(x)-\tau_{\mathrm{CB}}(X)}{\epsilon})\frac{1}{\epsilon}(\partial_{Y_i}\tau_{\mathrm{CB}}(x)-\partial_{Y_i}\tau_{\mathrm{CB}}(X))dx-f(X_i)\end{aligned}$$

$$
\begin{aligned}
=& -\epsilon^{-3}\frac{1}{\epsilon}\int_{\Omega} JV_{\text{exa},\epsilon}\sum_{X\in\mathbb{L}_\epsilon}\nabla m_a\Big(\frac{\tau_{\text{CB}}(x)-\tau_{\text{CB}}(X)}{\epsilon}\Big)\epsilon^3\sum_{\xi\in\Omega_\epsilon^*}e^{\imath\xi(x-X_i)}dx\\
&+\epsilon^{-3}\frac{1}{\epsilon}\int_{\Omega} JV_{\text{exa},\epsilon}\sum_{r\in\mathbb{L}_\epsilon}\nabla m_a\Big(\frac{\tau_{\text{CB}}(x)-\tau_{\text{CB}}(X_i)+r}{\epsilon}\Big)dx - f(X_i)\\
=&T_1(X_i)+T_2(X_i),
\end{aligned}
$$

where τ_{CB} is the Fourier interpolation of Y_{CB}. It is not the same as the Cauchy-Born solution u_{CB} we solved from the continuum elasticity model. Moreover, $\mathcal{V}_{\text{exa},\epsilon}(x) = \mathcal{V}_{\text{ext}}(\frac{x}{\epsilon})$.

6.4.1 General approximation of the background charge

The idea of analyzing $\mathcal{F}_{\text{at}}[Y_{\text{CB}}]$ is to use Taylor expansions of $\nu_{\text{exa},\epsilon}, V_{\text{exa},\epsilon}, \rho_b^\epsilon$, for which we need to first have the expansion of the deformation in hand. For $x\in\Omega$ close to $X\in\Omega_\epsilon$, expand τ_{CB} around x:

$$
\begin{aligned}
&\frac{1}{\epsilon}[\tau_{\text{CB}}(x)-\tau_{\text{CB}}(X)]\\
=&\nabla\tau_{\text{CB}}(x)\Big(\frac{x-X}{\epsilon}\Big)+\sum_{k=2}^{l}(-1)^{k-1}\epsilon^{k-1}\sum_{|\beta|=k}\frac{1}{\beta!}\nabla^\beta\tau_{\text{CB}}(x)\Big(\frac{x-X}{\epsilon}\Big)^\beta+\epsilon^l\tau_{\text{err}}(x,X)\\
=&\nabla\tau_{\text{CB}}(x)\Big(\frac{x-X}{\epsilon}\Big)+\sum_{k=1}^{l-1}\epsilon^k\tau_k(x,X)+\epsilon^l\tau_{\text{err}}(x,X)
\end{aligned}
$$

where $\tau_k(x,X) = (-1)^k\sum_{|\beta|=k+1}\frac{1}{\beta!}\nabla^\beta\tau_{\text{CB}}(x)(\frac{x-X}{\epsilon})^\beta$ and $\tau_{\text{err}} = \tau_{\text{err}}(\nabla^{l_1}\tau_{\text{CB}}; l_1 = 1,\cdots,l+1)$.

Next we expand ∇m_a:

$$
\nabla m_a\Big(\frac{\tau_{\text{CB}}(x)-\tau_{\text{CB}}(X)}{\epsilon}\Big) = P_{\text{CB}}\Big(\frac{x-X}{\epsilon},x\Big)+\sum_{k=1}^{l}\epsilon^k P_k\Big(\frac{x-X}{\epsilon},x\Big)+\epsilon^{l+1}P_{\text{err}}(x,X)
$$

where

$$
P_{\text{CB}}\Big(\frac{x-X}{\epsilon},x\Big)=\nabla m_a\Big(\nabla\tau_{\text{CB}}(x)\Big(\frac{x-X}{\epsilon}\Big)\Big)
$$

and

$$\begin{aligned}
&P_k(\frac{x-X}{\epsilon},x)\\
=&P_k(\nabla^{l_1}m_a,\tau_{l_2};l_1=2,\dots,k+1,l_2=1,\dots,k)\\
=&P_k(\nabla^{l_1}m_a(\nabla\tau_{\mathrm{CB}}(x)(\frac{x-X}{\epsilon})),\nabla^{\beta}\tau_{\mathrm{CB}}(x),\frac{x-X}{\epsilon};\\
&l_1=2,\dots,k+1,|\beta|=1,\dots,k+1)
\end{aligned}$$

$$P_{\mathrm{err}}=P_{\mathrm{err}}(\tau_{\mathrm{err}},\nabla^{l_1}m_a,\nabla^{l_2}\tau_{\mathrm{CB}};l_1=2,\cdots,l+2,l_2=1,\cdots,l).$$

6.4.2 Analysis of T_1

We plug the above expansions into T_1, so

$$\begin{aligned}
&T_1(X_i)\\
=&-\frac{1}{\epsilon}\int_{\Omega}JV_{\mathrm{exa},\epsilon}\sum_{X\in\mathbb{L}_\epsilon}\nabla m_a(\frac{\tau_{\mathrm{CB}}(x)-\tau_{\mathrm{CB}}(X)}{\epsilon})\sum_{\xi\in\Omega_\epsilon^*}e^{\imath\xi(x-X_i)}dx\\
=&-\frac{1}{\epsilon}\int_{\Omega}J(V_{\mathrm{CB}}+\sum_{k=1}^{10}\epsilon^kV_k+\epsilon^{11}V_{\mathrm{err}})\sum_{X\in\mathbb{L}_\epsilon}(P_{\mathrm{CB}}+\sum_{k=1}^{10}\epsilon^kP_k+\epsilon^{11}P_{\mathrm{err}})\sum_{\xi\in\Omega_\epsilon^*}e^{\imath\xi(x-X_i)}dx\\
=&-\frac{1}{\epsilon}\int_{\Omega}JV_{\mathrm{CB}}\sum_{X\in\mathbb{L}_\epsilon}P_{\mathrm{CB}}(\frac{x-X}{\epsilon},x)\sum_{\xi\in\Omega_\epsilon^*}e^{\imath\xi(x-X_i)}dx\\
&-\int_{\Omega}J\sum_{X\in\mathbb{L}_\epsilon}(V_{\mathrm{CB}}P_1(\frac{x-X}{\epsilon},x)+V_1P_{\mathrm{CB}}(\frac{x-X}{\epsilon},x))\sum_{\xi\in\Omega_\epsilon^*}e^{\imath\xi(x-X_i)}dx\\
&-\epsilon\int_{\Omega}J\sum_{X\in\mathbb{L}_\epsilon}[V_{\mathrm{CB}}P_2(\frac{x-X}{\epsilon},x)+V_1P_1(\frac{x-X}{\epsilon},x)+V_2P_{\mathrm{CB}}(\frac{x-X}{\epsilon},x)]\\
&\cdot\sum_{\xi\in\Omega_\epsilon^*}e^{\imath\xi(x-X_i)}dx\\
&-\sum_{k=2}^{9}\epsilon^k\int_{\Omega}J\sum_{X\in\mathbb{L}}\varphi_k(\frac{x-X}{\epsilon},x)dx
\end{aligned}$$

$$
\begin{aligned}
&- \epsilon^{10} \int_\Omega J \sum_{X\in\mathbb{L}_\epsilon} [V_{\text{err}}\varphi_P(\frac{x-X}{\epsilon}, x) + \varphi_V(\frac{x}{\epsilon}, x) P_{\text{err}}(x, X)] \sum_{\xi\in\Omega_\epsilon^*} e^{\imath\xi(x-X_i)} dx \\
= &- \frac{1}{\epsilon} \int_\Omega J(X_i) V_{\text{CB}}(z, X_i) \sum_{X\in\mathbb{L}} \nabla m_a(\nabla\tau_{\text{CB}}(X_i)(z-X)) dz \\
&- \int_\Omega J(X_i) \sum_{X\in\mathbb{L}} [V_{\text{CB}}(z, X_i) P_1(z-X, X_i) + V_1(z, X_i) P_{\text{CB}}(z-X, X_i)] dz \\
&- \epsilon \int_\Omega J(X_i) \sum_{X\in\mathbb{L}} [V_{\text{CB}} P_2 + V_1 P_1 + V_2 P_{\text{CB}}](z, X, X_i) dz \\
&- \sum_{k=2}^{9} \epsilon^k \int_\Omega J(X_i) \sum_{X\in\mathbb{L}} \varphi_k(z-X, X_i) dz + \text{err}_{\text{Hom}}(X_i) + \epsilon^{10}\Phi_{1,\text{err}}(X_i)
\end{aligned}
$$

where

$$
\begin{aligned}
\varphi_k =& V_{\text{CB}} P_{k+1} + \sum_{l=1}^{k} V_l P_{k+1-l} + V_{k+1} P_{\text{CB}} \\
\varphi_P =& P_{\text{CB}} + \sum_{k=1}^{10} \epsilon^k P_k \\
\varphi_V =& V_{\text{CB}} + \sum_{k=1}^{10} \epsilon^k V_k \\
\Phi_{1,\text{err}} =& - \int_\Omega J \sum_{X\mathbb{L}_\epsilon} [V_{\text{err}}\varphi_P + \varphi_V P_{\text{err}}] \sum_{\xi\in\Omega_\epsilon^*} e^{\imath\xi(x-X_i)} dx
\end{aligned}
$$

and

$$
\begin{aligned}
&\text{err}_{\text{Hom}}(X_i) \\
= &\sum_{k=0}^{10} \text{err}_{k,\text{Hom}}(X_i) \\
= &- \frac{1}{\epsilon} [\epsilon^{-3} \int_\Omega J(x) V_{\text{CB}}(\frac{x}{\epsilon}, x) \sum_{X\in\mathbb{L}_\epsilon} P_{\text{CB}}(\frac{x-X}{\epsilon}, x) \partial_{Y_i} \nabla\tau_{\text{CB}}(x) dx \\
&- \int_\Omega J(X_i) V_{\text{CB}}(z, X_i) \sum_{X\in\mathbb{L}} P_{\text{CB}}(z-X, X_i) dz]
\end{aligned}
$$

$$+\sum_{k=1}^{10}\epsilon^{k-1}[\epsilon^{-3}\int_\Omega J(x)\sum_{X\in\mathbb{L}_\epsilon}\varphi_{k-1}(\frac{x-X}{\epsilon},x)\partial_{Y_i}\nabla\tau_{\rm CB}(x)dx$$

$$-\int_\Omega J(X_i)\sum_{X\in\mathbb{L}}\varphi_{k-1}(z-X,X_i)dz]$$

So

$$\|\mathrm{err}_{\rm Hom}+\epsilon^{10}\Phi_{1,\mathrm{err}}\|_{\epsilon,5}\lesssim\epsilon^2$$

provided

$$J(\cdot)V_{\rm CB}(z,\cdot)\sum_{X\in\mathbb{L}}P(z-X,\cdot)\in H^{15}$$

$$J(\cdot)\sum_{X\in\mathbb{L}}\varphi_0(z-X,\cdot)\in H^{14}$$

$$J(\cdot)\sum_{X\in\mathbb{L}}\varphi_1(z-X,\cdot)\in H^{13}$$

$$J(\cdot)\sum_{X\in\mathbb{L}}\varphi_k(z-X,\cdot)\in H^{12},\quad k=2,\dots,9,$$

or more specifically, $u\in H_1^{23}$ and $m_a\in H^{23}$.

6.4.3 Analysis of T_2

We have the following expression for T_2

$$\begin{aligned}
&T_2(X_i)\\
=&\epsilon^{-3}\frac{1}{\epsilon}\int_\Omega JV_{\rm exa}^\epsilon\sum_{r\in\mathbb{L}_\epsilon}\nabla m_a(\frac{\tau_{\rm CB}(x)-\tau_{\rm CB}(X_i+r)}{\epsilon})dx-f(X_i)\\
=&\frac{1}{\epsilon}\epsilon^{-3}\int_\Omega J(V_{\rm CB}+\sum_{k=1}^{10}\epsilon^kV_k+\epsilon^{11}V_{\rm err})\sum_{r\in\mathbb{L}}(P_{\rm CB}(X_i+r)+\sum_{k=1}^{10}\epsilon^kP_k(X_i+r)\\
&+\epsilon^{11}P_{\rm err}(X_i+r))dx-f(X_i)\\
=&\epsilon^{-3}\int_\Omega\sum_{r\in\mathbb{L}}\frac{1}{\epsilon}JV_{\rm CB}P_{\rm CB}(X_i+r)+J(V_{\rm CB}P_1(X_i+r)+V_1P_{\rm CB}(X_i+r))
\end{aligned}$$

$$+\epsilon J(V_{\text{CB}}P_2(X_i+r)+V_1P_1(X_i+r)+V_2P_{\text{CB}}(X_i+r))$$

$$+\sum_{k=2}^{9}\epsilon^k J\varphi_k(X_i+r)+\epsilon^{10}[V_{\text{err}}\varphi_P(X_i+r)+\varphi_V P_{\text{err}}(X_i+r)]dx-f(X_i)$$

Recall our purpose is to derive the Euler-Lagrange equation of the continuum elasticity model which thus vanishes, and use inversion symmetry to show the ϵ-order terms also vanish.

Let us analyze the first term, while others except the error terms are similar. So expand the term around X_i,

$$\epsilon^{-3}\int_\Omega \frac{1}{\epsilon}JV_{\text{CB}}\sum_{r\in\mathbb{L}}P_{\text{CB}}(X_i+r)dx$$

$$=\frac{1}{\epsilon}\epsilon^{-3}\int_\Omega J(x)V_{\text{CB}}(\frac{x}{\epsilon},x)\sum_{r\in\mathbb{L}}\nabla m_a(\nabla\tau_{\text{CB}}(x)(\frac{x-X_i-r}{\epsilon}))dx$$

$$=\frac{1}{\epsilon}\epsilon^{-3}\int_\Omega J(X_i)V_{\text{CB}}(\frac{x}{\epsilon},X_i)\sum_{r\in\mathbb{L}}\nabla m_a(\nabla\tau_{\text{CB}}(X_i)(\frac{x-X_i-r}{\epsilon}))dx$$

$$+\sum_{k=0}^{9}\epsilon^k\epsilon^{-3}\int_\Omega\sum_{|\beta|=k+1}\frac{1}{\beta!}\nabla_x^\beta[J(X_i)V_{\text{CB}}(\frac{x}{\epsilon},X_i)\sum_{r\in\mathbb{L}}\nabla m_a(\nabla\tau_{\text{CB}}(X_i)(\frac{x-X_i-r}{\epsilon}))]$$

$$\cdot(\frac{x-X_i-r}{\epsilon})^\beta dx$$

$$+\epsilon^{10}\epsilon^{-3}\int_\Omega\sum_{|\beta|=11}\frac{1}{\beta!}\nabla_x^\beta[J(x^*)V_{\text{CB}}(\frac{x}{\epsilon},x^*)\sum_{r\in\mathbb{L}}\nabla m_a(\nabla\tau_{\text{CB}}(x^*)(\frac{x-X_i-r}{\epsilon}))]$$

$$\cdot(\frac{x-X_i-r}{\epsilon})^\beta dx$$

$$=\frac{1}{\epsilon}\int_{n\Omega}J(X_i)V_{\text{CB}}(z,X_i)\sum_{r\in\mathbb{L}}\nabla m_a(\nabla\tau_{\text{CB}}(X_i)(z-\frac{X_i+r}{\epsilon}))dz+\epsilon^{10}\text{err}_0(X_i)$$

$$+\sum_{k=0}^{9}\epsilon^k\int_{n\Omega}\sum_{|\beta|=k+1}\frac{1}{\beta!}\nabla_x^\beta[J(X_i)V_{\text{CB}}(z,X_i)$$

$$\cdot \sum_{r\in\mathbb{L}} \nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z - \frac{X_i + r}{\epsilon}))] \cdot (z - \frac{X_i + r}{\epsilon})^\beta dz$$

$$= \frac{1}{\epsilon} \sum_{X\in\Omega_\epsilon} \int_\Omega J(X_i) V_{\mathrm{CB}}(z + \frac{X}{\epsilon}, X_i) \sum_{r\in\mathbb{L}} \nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z - \frac{X_i - X + r}{\epsilon}))dz$$

$$+ \sum_{k=0}^{9} \epsilon^k \sum_{X\in\Omega_\epsilon} \int_\Omega \sum_{|\beta|=k+1} \frac{1}{\beta!} \nabla_x^\beta [J(X_i) V_{\mathrm{CB}}(z + \frac{X}{\epsilon}, X_i)$$

$$\cdot \sum_{r\in\mathbb{L}} \nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z - \frac{X_i - X + r}{\epsilon}))] \cdot (z - \frac{X_i - X + r}{\epsilon})^\beta dz$$

$$+ \epsilon^{10} \mathrm{err}_0(X_i)$$

$$= \frac{1}{\epsilon} \int_\Omega J(X_i) V_{\mathrm{CB}}(z, X_i) \sum_{X\in\mathbb{L}} \nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z - X))dz$$

$$+ \sum_{k=0}^{9} \epsilon^k \int_\Omega \sum_{|\beta|=k+1} \frac{1}{\beta!} \nabla_x^\beta [J(X_i) V_{\mathrm{CB}}(z, X_i) \sum_{X\in\mathbb{L}} \nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z - X))](z - X)^\beta dz$$

$$+ \epsilon^{10} \mathrm{err}_0(X_i)$$

$$= \frac{1}{\epsilon} \int_\Omega J(X_i) V_{\mathrm{CB}}(z, X_i) \sum_{X\in\mathbb{L}} \nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z - X))dz$$

$$+ \int_\Omega \nabla_x [J(X_i) V_{\mathrm{CB}}(z, X_i) \sum_{X\in\mathbb{L}} \nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z - X))](z - X)dz$$

$$+ \sum_{k=2}^{9} \epsilon^k \int_\Omega \sum_{|\beta|=k+1} \frac{1}{\beta!} \nabla_x^\beta [J(X_i) V_{\mathrm{CB}}(z, X_i) \sum_{X\in\mathbb{L}} \nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z - X))](z - X)^\beta dz$$

$$+ \epsilon^{10} \mathrm{err}_0(X_i)$$

where

$$\epsilon^{10} \mathrm{err}_0(X_i)$$

$$= \epsilon^{10} \epsilon^{-3} \int_\Omega \sum_{|\beta|=11} \frac{1}{\beta!} \nabla_x^\beta [J(x^*) V_{\mathrm{CB}}(\frac{x}{\epsilon}, x^*) \sum_{r\in\mathbb{L}} \nabla m_a(\nabla\tau_{\mathrm{CB}}(x^*)(\frac{x - X_i - r}{\epsilon}))]$$

$$\cdot (\frac{x - X_i - r}{\epsilon})^\beta dx$$

with $x^* = tX_i + (1-t)x$ for some $0 < t < 1$.

Similarly we have

$$\epsilon^{-3}\int_\Omega \sum_{r\in\mathbb{L}} J(V_{\rm CB}P_1(X_i+r) + V_1 P_{\rm CB}(X_i+r))dx$$

$$= \int_\Omega J(X_i) \sum_{X\in\mathbb{L}} [V_{\rm CB}(z,X_i)P_1(z-X,X_i) + V_1(z,X_i)P_{\rm CB}(z-X,X_i)]dz$$

$$+ \epsilon \int_\Omega \sum_{X\in\mathbb{L}} \nabla_x [J(X_i)V_{\rm CB}(z,X_i)P_1(z-X,X_i) + J(X_i)V_1(z,X_i)P_{\rm CB}(z-X,X_i)]$$

$$\cdot (z-X)dz + \sum_{k=2}^{9} \epsilon^k \int_\Omega \sum_{|\beta|=k} \frac{1}{\beta!}\nabla_x^\beta [J(X_i)V_{\rm CB}(z,X_i)P_1(z-X,X_i)$$

$$+ J(X_i)V_1(z,X_i)P_{\rm CB}(z-X,X_i)](z-X)^\beta dz + \epsilon^{10}\mathrm{err}_1(X_i)$$

$$= \int_\Omega J(X_i)[V_{\rm CB}(z,X_i)P_1(z-X,X_i) + V_1(z,X_i)P_{\rm CB}(z-X,X_i)]dz$$

$$+ \sum_{k=2}^{9} \epsilon^k \int_\Omega \sum_{|\beta|=k+1} \frac{1}{\beta!}\nabla_x^\beta [J(X_i)V_{\rm CB}(z,X_i)P_1(z-X,X_i)$$

$$+ J(X_i)V_1(z,X_i)P_{\rm CB}(z-X,X_i)](z-X)^\beta dz + \epsilon^{10}\mathrm{err}_1(X_i)$$

where

$$\epsilon^{10}\mathrm{err}_1(X_i)$$

$$=\epsilon^{10}\epsilon^{-3}\int_\Omega \sum_{|\beta|=11} \frac{1}{\beta!}\nabla_x^\beta \sum_{r\in\mathbb{L}} [J(x^*)(V_{\rm CB}(\frac{x}{\epsilon},x^*)P_1(\frac{x-X_i-r}{\epsilon},x^*)$$

$$+ V_1(\frac{x}{\epsilon},x^*)P_{\rm CB}(\frac{x-X_i-r}{\epsilon},x^*))](\frac{x-X_i-r}{\epsilon})^\beta dx$$

with $x^* = tX_i + (1-t)x$ for some $0 < t < 1$.

$$\epsilon^{-3}\int_\Omega \sum_{r\in\mathbb{L}} \epsilon J(V_{\rm CB}P_2(X_i+r) + V_1 P_1(X_i+r) + V_2 P_{\rm CB}(X_i+r))dx$$

$$=\epsilon \int_\Omega J(X_i) \sum_{X\in\mathbb{L}} [V_{\rm CB}(z,X_i)P_2(z-X,X_i) + V_1(z,X_i)P_1(z-X,X_i) + V_2(z,X_i)$$

$$\cdot P_{\mathrm{CB}}(z-X,X_i)]dz + \sum_{k=2}^{9}\epsilon^k \int_\Omega \sum_{|\beta|=k-1} \frac{1}{\beta!}\nabla_x^\beta[V_{\mathrm{CB}}(z,X_i)P_2(z-X,X_i)$$

$$+ V_1(z,X_i)P_1(z-X,X_i) + V_2(z,X_i)P_{\mathrm{CB}}(z-X,X_i)](z-X)^\beta dz + \epsilon^{10}\mathrm{err}_2(X_i)$$

where

$$\epsilon^{10}\mathrm{err}_2(X_i)$$

$$=\epsilon^{10}\epsilon^{-3}\int_\Omega \sum_{|\beta|=8}\frac{1}{\beta!}\nabla_x^\beta \sum_{r\in\mathbb{L}}[J(x^*)(V_{\mathrm{CB}}(\frac{x}{\epsilon},x^*)P_2(\frac{x-X_i-r}{\epsilon},x^*)$$

$$+ V_1(\frac{x}{\epsilon},x^*)P_1(\frac{x-X_i-r}{\epsilon},x^*)) + V_2(\frac{x}{\epsilon},x^*)P_{\mathrm{CB}}(\frac{x-X_i-r}{\epsilon},x^*))](\frac{x-X_i-r}{\epsilon})^\beta dx$$

with $x^* = tX_i + (1-t)x$ for some $0 < t < 1$.

$$\sum_{k=2}^{9}\epsilon^k\epsilon^{-3}\int_\Omega \sum_{r\in\mathbb{L}} J\varphi_k(X_i+r)dx$$

$$=\sum_{k=2}^{9}\epsilon^k[\sum_{r=0}^{9-k}\epsilon^r\int_\Omega\sum_{|\beta|=r}\frac{1}{\beta!}\nabla_x^\beta[J(X_i)\sum_{X\in\mathbb{L}}\varphi_k(z,z-X,X_i)](z-X)^\beta dz + \epsilon^{10-k}\mathrm{err}_{k+1}(X_i)]$$

where

$$\mathrm{err}_{k+1}(X_i)$$

$$=\epsilon^{-3}\int_\Omega\sum_{|\beta|=11}\frac{1}{\beta!}\nabla_x^\beta\sum_{r\in\mathbb{L}}[J(x^*)\varphi_{3,k}(\frac{x}{\epsilon},\frac{x-X_i-r}{\epsilon},x^*)](\frac{x-X_i-r}{\epsilon})^\beta dx, \quad k=2,\dots,9$$

with $x^* = tX_i + (1-t)x$ for some $0 < t < 1$.

6.4.4 Final estimate

Now we combine all the terms in the above expressions of $T_1(X_i)$ and $T_2(X_i)$ to get

$$\mathcal{F}_{\mathrm{at}}[Y](X_i) = T_1(X_i) + T_2(X_i)$$

$$
\begin{aligned}
=&\int_\Omega \nabla_x[J(X_i)V_{\mathrm{CB}}(z,X_i)\sum_{X\in\mathbb{L}}\nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z-X))](z-X)dz - f(X_i)\\
&+\sum_{k=2}^{9}\epsilon^k\int_\Omega\sum_{|\beta|=k+1}\frac{1}{\beta!}\nabla_x^\beta[J(X_i)V_{\mathrm{CB}}(z,X_i)\sum_{X\in\mathbb{L}}\nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z-X))](z-X)^\beta dz\\
&+\sum_{k=2}^{9}\epsilon^k\int_\Omega\sum_{|\beta|=k+1}\frac{1}{\beta!}\nabla_x^\beta[J(X_i)V_{\mathrm{CB}}(z,X_i)P_1(z-X,X_i)\\
&+J(X_i)V_1(z,X_i)P_{\mathrm{CB}}(z-X,X_i)](z-X)^\beta dz\\
&+\sum_{k=2}^{9}\epsilon^k\int_\Omega\sum_{|\beta|=k-1}\frac{1}{\beta!}\nabla_x^\beta[J(X_i)V_{\mathrm{CB}}(z,X_i)P_2(z-X,X_i)+J(X_i)V_1(z,X_i)\\
&\cdot P_1(z-X,X_i)\\
&+J(X_i)V_2(z,X_i)P_{\mathrm{CB}}(z-X,X_i)](z-X)^\beta dz+\epsilon^{10}\Phi_{1,\mathrm{err}}(X_i)+\mathrm{err}_{\mathrm{Hom}}(X_i)\\
&+\sum_{k=2}^{9}\epsilon^k[\sum_{r=0}^{9-k}\epsilon^r\int_\Omega\sum_{|\beta|=r}\frac{1}{\beta!}\nabla_x^\beta[J(X_i)\sum_{X\in\mathbb{L}}\varphi_k(z-X,X_i)](z-X)^\beta dz\\
&+\epsilon^{10-k}\mathrm{err}_{k+1}(X_i)]\\
=&\int_\Omega \nabla_x[J(X_i)V_{\mathrm{CB}}(z,X_i)\sum_{X\in\mathbb{L}}\nabla m_a(\nabla\tau_{\mathrm{CB}}(X_i)(z-X))](z-X)dz - f(X_i)\\
&+\epsilon^2\Phi(X_i)+\mathrm{err}_{\mathrm{Hom}}(X_i)+\epsilon^{10}(\Phi_{1,\mathrm{err}}(X_i)+\Phi_{2,\mathrm{err}}(X_i))\\
=&\epsilon^2\Phi(X_i)+\mathrm{err}_{\mathrm{Hom}}(X_i)+\epsilon^{10}(\Phi_{1,\mathrm{err}}(X_i)+\Phi_{2,\mathrm{err}}(X_i))
\end{aligned}
$$

where

$$\epsilon^{10}\Phi_{2,\mathrm{err}}(X_i)=\epsilon^{10}\sum_{k=0}^{10}\mathrm{err}_k(X_i)$$

and

$$\|\epsilon^{10}\Phi_{2,\mathrm{err}}\|_{\epsilon,5}\lesssim\epsilon^2$$

provided

$$\varphi_k(z,z-X,\cdot)\in W^{16,\infty},\quad k=2,\dots,9$$

or more specifically, if $u \in H_1^{29}(\Omega), m_a \in C_0^\infty$.

Now we analyze $\epsilon^2\Phi(X_i)$ which is the shorthand notation for

$$
\begin{aligned}
&\epsilon^2\Phi(X_i)\\
&= \sum_{k=2}^{9} \epsilon^k \int_\Omega \sum_{|\beta|=k+1} \frac{1}{\beta!} \nabla_x^\beta [J(X_i)V_{\mathrm{CB}}(z, X_i) \sum_{X\in\mathbb{L}} \nabla m_a(\nabla \tau_{\mathrm{CB}}(X_i)(z-X))](z-X)^\beta dz\\
&+ \sum_{k=2}^{9} \epsilon^k \int_\Omega \sum_{|\beta|=k+1} \frac{1}{\beta!} \nabla_x^\beta [J(X_i)V_{\mathrm{CB}}(z, X_i)P_1(z-X, X_i)\\
&+ J(X_i)V_1(z, X_i)P_{\mathrm{CB}}(z-X, X_i)](z-X)^\beta dz\\
&+ \sum_{k=2}^{9} \epsilon^k \int_\Omega \sum_{|\beta|=k-1} \frac{1}{\beta!} \nabla_x^\beta [J(X_i)V_{\mathrm{CB}}(z, X_i)P_2(z-X, X_i)\\
&+ J(X_i)V_1(z, X_i)P_1(z-X, X_i) + J(X_i)V_2(z, X_i)P_{\mathrm{CB}}(z-X, X_i)](z-X)^\beta dz\\
&+ \sum_{k=2}^{9} \epsilon^k \sum_{r=0}^{9-k} \epsilon^r \int_\Omega \sum_{|\beta|=r} \frac{1}{\beta!} \nabla_x^\beta [J(X_i) \sum_{X\in\mathbb{L}} \varphi_k(z-X, X_i)](z-X)^\beta dz
\end{aligned}
$$

from which we can see that $\|\epsilon^2\Phi\|_{\epsilon,5} \lesssim \epsilon^2$ if $u \in H_1^{29}(\Omega), m_a \in C_0^\infty$.

So finally we have the consistency estimate

$$\|\mathcal{F}_{\mathrm{at}}[Y]\|_{\epsilon,5} \leqslant C(\|u\|_{H_1^{29}(\Omega)})\epsilon^2.$$

7

Stability Conditions

7.1 The Atomistic Hessian

Recall the atomistic functional

$$\begin{aligned}\mathcal{I}_{\rm at}(Y) &= I(\nu_{\rm exa}(\tau_Y), V_{\rm exa}(\tau_Y), \rho_b(Y)) \\ &= \int_{n\Omega} \nu_{\rm exa}^{\frac{10}{3}} + |\nabla \nu_{\rm exa}|^2 - \nu_{\rm exa}^{\frac{8}{3}} + \frac{1}{2} V_{\rm exa}(\nu_{\rm exa}^2 - \rho_b) dy\end{aligned} \tag{7.1}$$

and the corresponding Euler-Lagrange equation

$$\mathcal{F}_{\rm at}[Y](X_i) = -\int_{n\Omega} V_{\rm exa} \frac{\partial \rho_b}{\partial Y_i} dy = f(X_i) \tag{7.2}$$

The Hessian is defined as

$$\mathcal{H}_{\rm at}[Y]Z = \lim_{t\to 0} \frac{\partial \mathcal{F}_{\rm at}}{\partial t}[Y + tZ]. \tag{7.3}$$

So

$$
\begin{aligned}
\mathcal{H}_{\mathrm{at}}[Y](i,j) :=& \frac{\delta^2}{\delta Y_i \delta Y_j}\mathcal{I}(\nu_{\mathrm{exa}}, V_{\mathrm{exa}}, \rho_b) \\
=& \frac{\partial}{\partial Y_j}\mathcal{F}_{\mathrm{at}}[Y](X_i) \\
=& -\int_{n\Omega} \frac{\partial V_{\mathrm{exa}}}{\partial Y_j}\frac{\partial \rho_b}{\partial Y_i} + V_{\mathrm{exa}}\frac{\partial^2 \rho_b}{\partial Y_j \partial Y_i} dy \\
=& -\int_{n\Omega} J_\epsilon(\tau_Y)\frac{\partial V_{\mathrm{exa}}}{\partial Y_j}\frac{\partial \rho_b}{\partial Y_i} + J_\epsilon(\tau_Y) V_{\mathrm{exa}}\frac{\partial^2 \rho_b}{\partial Y_j \partial Y_i} dx
\end{aligned}
\tag{7.4}
$$

Similarly in undeformed case $Y = \mathrm{Id}$, we have

Proposition 7.1.1.

$$
\begin{aligned}
\mathcal{H}_{at}[Id](i,j) =& -\epsilon^{-2}\int_{n\Omega} \delta_{ij} V_{per}\sum_{r\in\mathbb{L}} \nabla^2 m_a(x - \frac{X_j}{\epsilon} + \frac{r}{\epsilon}) \\
&+ \frac{1}{2}\sum_{r_1\in\mathbb{L}} \nabla m_a(x - \frac{X_i}{\epsilon} + \frac{r_1}{\epsilon})(\mathcal{L}^{-1}_{per})_{22}[\sum_{r_2\in\mathbb{L}} \nabla m_a(\cdot - \frac{X_j}{\epsilon} + \frac{r_2}{\epsilon})]dx
\end{aligned}
$$

Proof. We have

$$
\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](i,j) = -\int_{n\Omega} \frac{\partial V_{\mathrm{per}}}{\partial Y_j}\frac{\partial \rho_{b,\mathrm{per}}}{\partial Y_i} + V_{\mathrm{per}}\frac{\partial^2 \rho_{b,\mathrm{per}}}{\partial Y_j \partial Y_i} dx,
$$

then it suffices to show

$$
\partial_{Y_j} V_{\mathrm{per}}(x) = \frac{1}{2}(\mathcal{L}^{-1}_{\mathcal{V}_{\mathrm{per}}(x)})_{22}(\partial_{Y_j}\rho_{b,\mathrm{per}})(x). \tag{7.5}
$$

Denote

$$
\mathcal{F}(\mathcal{V}_{\mathrm{per}}) = \begin{pmatrix} -\epsilon^2\Delta\nu_{\mathrm{per}} + \frac{5}{3}\nu_{\mathrm{per}}^{\frac{7}{3}} - \frac{4}{3}\nu_{\mathrm{per}}^{\frac{5}{3}} + V_{\mathrm{per}}\nu_{\mathrm{per}} \\ \frac{1}{8\pi}\epsilon^2\Delta V_{\mathrm{per}} + \frac{1}{2}\nu_{\mathrm{per}}^2 \end{pmatrix} \tag{7.6}
$$

Then

$$
\mathcal{F}(\mathcal{V}_{\mathrm{per}}(Y)) = \begin{pmatrix} 0 \\ \frac{1}{2}\rho_{b,\mathrm{per}}(Y) \end{pmatrix}. \tag{7.7}
$$

Take derivative with respect to Y_j, we get

$$\mathcal{L}_{\mathcal{V}_{\text{per}}(x)} \begin{pmatrix} \partial_{Y_j} \nu_{\text{per}}(x) \\ \partial_{Y_j} V_{\text{per}}(x) \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{1}{2} \partial_{Y_j} \rho_{b,\text{per}}(x) \end{pmatrix} \tag{7.8}$$

then it is straightforward to calculate the formula. □

Now we begin to further analyze the Hessian $\mathcal{H}_{\text{at}}[\text{Id}]$ by diagonalizing it and derive the eigenvalues for its dynamical matrix. We first show that $\mathcal{H}_{\text{at}}[\text{Id}]$ is translation invariant, next diagonalize it by using the plane wave functions, then we show the dynamical matrix is Hermitian so that its eigenvalues are real, finally we give the **Stability Condition B** and its equivalent interpretations.

7.1.1 Translation invariant

For fixed $\alpha, \beta \in \{1, 2, 3\}$, we regard $\mathcal{H}_{\text{at}}^{\alpha\beta}[\text{Id}]$ as an operator $\mathcal{H}_{\text{at}}^{\alpha\beta}[\text{Id}] : L^2(\Omega_\epsilon, \mathbb{R}) \to L^2(\Omega_\epsilon, \mathbb{R})$ given by $\mathcal{H}_{\text{at}}^{\alpha\beta}[\text{Id}](Z)(X_i) = \sum_{X_j \in \Omega_\epsilon} \mathcal{H}_{\text{at}}^{\alpha\beta}[\text{Id}](X_i, X_j) Z(X_j)$.

Lemma 7.1.2. *The operator $\mathcal{H}_{at}^{\alpha\beta}[Id](X_i, X_j)$ is translation invariant:*

$$\mathcal{H}_{at}^{\alpha\beta}[Id](X_i, X_j) = \mathcal{H}_{at}^{\alpha\beta}[Id](X_i + r, X_j + r), \quad \forall X_i, X_j \in \Omega_\epsilon, r \in \epsilon\mathbb{L}. \tag{7.9}$$

Proof. For $X_i \in \Omega_\epsilon$,

$$\begin{aligned} &\mathcal{H}_{\text{at}}^{\alpha\beta}[\text{Id}](X_i, X_i) \\ &= -\frac{1}{\epsilon^2} \int_{n\Omega} \sum_{r_1 \in \mathbb{L}} V_{\text{per}}(x) \nabla_\alpha \nabla_\beta m_a(x - \frac{X_i}{\epsilon} + \frac{r_1}{\epsilon}) dx \\ &\quad - \frac{1}{2\epsilon^2} \int_{n\Omega} \sum_{r_2 \in \mathbb{L}} \nabla_\beta m_a(x - \frac{X_i}{\epsilon} + \frac{r_2}{\epsilon}) \big[(\mathcal{L}_{\text{per}}^{-1})_{22} [\sum_{r_3 \in \mathbb{L}} \nabla_\alpha m_a(\cdot - \frac{X_i}{\epsilon} + \frac{r_3}{\epsilon})](x)\big]^T dx \end{aligned}$$

for $X_i \neq X_j$,

$$\mathcal{H}_{\text{at}}^{\alpha\beta}[\text{Id}](X_i, X_j)$$

$$= -\frac{1}{2\epsilon^2}\int_{n\Omega}\sum_{r_2\in\mathbb{L}}\nabla_\beta m_a(x-\frac{X_i}{\epsilon}+\frac{r_2}{\epsilon})\big[(\mathcal{L}_{\rm per}^{-1})_{22}[\sum_{r_3\in\mathbb{L}}\nabla_\alpha m_a(\cdot-\frac{X_j}{\epsilon}+\frac{r_3}{\epsilon})](x)\big]^T dx$$

Recall

$$\mathcal{L}_{\rm per} = \begin{pmatrix} \mathcal{L}_{1,\rm per} & \nu_{\rm per} \\ \nu_{\rm per} & \frac{\Delta}{8\pi} \end{pmatrix}$$

where $\mathcal{L}_{1,\rm per} = -\Delta + \frac{35}{9}\nu_{\rm per}^{\frac{4}{3}} - \frac{20}{9}\nu_{\rm per}^{\frac{2}{3}} + V_{\rm per}$. Since Δ, any power of $\nu_{\rm per}$ and $V_{\rm per}$ commute with the translation τ_r for $r\in\mathbb{L}$, we have $\mathcal{L}_{\rm per}\tau_r = \tau_r\mathcal{L}_{\rm per}$, therefore $\mathcal{L}_{\rm per}^{-1}\tau_r = \tau_r\mathcal{L}_{\rm per}^{-1}$. This implies $\tau_r(\mathcal{L}_{\rm per}^{-1})_{22}\tau_{-r} = (\mathcal{L}_{\rm per}^{-1})_{22}$, which says

$$(\mathcal{L}_{\rm per}^{-1})_{22}(\sum_{r_1\in\mathbb{L}}\nabla_\alpha m_a(\cdot-\frac{X_j}{\epsilon}+\frac{r_1}{\epsilon}-\frac{r}{\epsilon}))(x+\frac{r}{\epsilon}) = (\mathcal{L}_{\rm per}^{-1})_{22}(\sum_{r_2\in\mathbb{L}}\nabla_\alpha m_a(\cdot-\frac{X_j}{\epsilon}+\frac{r_2}{\epsilon}))(x)$$

for $r\in\epsilon\mathbb{L}$.

So for $r\in\epsilon\mathbb{L}$,

$$\int_{n\Omega}\sum_{r_2\in\mathbb{L}}\nabla_\beta m_a(x-\frac{X_i+r}{\epsilon}+\frac{r_2}{\epsilon})\big[(\mathcal{L}_{\rm per}^{-1})_{22}[\sum_{r_3\in\mathbb{L}}\nabla_\alpha m_a(\cdot-\frac{X_j+r}{\epsilon}+\frac{r_3}{\epsilon})](x)\big]^T dx$$

$$=\int_{n\Omega-r}\sum_{r_2\in\mathbb{L}}\nabla_\beta m_a(x-\frac{X_i}{\epsilon}+\frac{r_2}{\epsilon})\big[(\mathcal{L}_{\rm per}^{-1})_{22}[\sum_{r_3\in\mathbb{L}}\nabla_\alpha m_a(\cdot-\frac{X_j}{\epsilon}+\frac{r_3}{\epsilon}-\frac{r}{\epsilon})](x+\frac{r}{\epsilon})\big]^T dx$$

$$=\int_{n\Omega-r}\sum_{r_2\in\mathbb{L}}\nabla_\beta m_a(x-\frac{X_i}{\epsilon}+\frac{r_2}{\epsilon})\big[(\mathcal{L}_{\rm per}^{-1})_{22}[\sum_{r_3\in\mathbb{L}}\nabla_\alpha m_a(\cdot-\frac{X_j}{\epsilon}+\frac{r_3}{\epsilon})](x)\big]^T dx$$

$$=\int_{n\Omega}\sum_{r_2\in\mathbb{L}}\nabla_\beta m_a(x-\frac{X_i}{\epsilon}+\frac{r_2}{\epsilon})\big[(\mathcal{L}_{\rm per}^{-1})_{22}[\sum_{r_3\in\mathbb{L}}\nabla_\alpha m_a(\cdot-\frac{X_j}{\epsilon}+\frac{r_3}{\epsilon})](x)\big]^T dx.$$

The last equality holds because the integrand is periodic in $n\Omega$.

Similarly for the diagonal part

$$\int_{n\Omega}V_{\rm per}(x)\sum_{r_1\in\mathbb{L}}\nabla_\beta\nabla_\alpha m_a(x-\frac{X_i+r}{\epsilon}+\frac{r_1}{\epsilon})dx$$

$$=\int_{n\Omega-r}V_{\rm per}(x+nr)\sum_{r_1\in\mathbb{L}}\nabla_\beta\nabla_\alpha m_a(x-\frac{X_i}{\epsilon}+\frac{r_1}{\epsilon})dx$$

$$= \int_{n\Omega - r} V_{\mathrm{per}}(x) \sum_{r_1 \in \mathbb{L}} \nabla_\beta \nabla_\alpha m_a(x - \frac{X_i}{\epsilon} + \frac{r_1}{\epsilon}) dx$$

$$= \int_{n\Omega} V_{\mathrm{per}}(x) \sum_{r_1 \in \mathbb{L}} \nabla_\beta \nabla_\alpha m_a(x - \frac{X_i}{\epsilon} + \frac{r_1}{\epsilon}) dx$$

□

7.1.2 Diagonalization

Theorem 7.1.3. *The operator $\mathcal{H}_{at}[Id]$ satisfies*

$$\mathcal{H}_{at}[Id](e^{\imath X \cdot \xi})(X) = \mathcal{D}_{at}^{Id}[\xi] e^{\imath X \cdot \xi}, \quad X \in \Omega_\epsilon \tag{7.10}$$

for any $\xi \in \Omega_\epsilon^*$, where $\mathcal{D}_{at}^{Id}[\xi]$ is a 3×3 matrix.

Proof. Assume $\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](e^{\imath X \cdot \xi_n})(X) = \sum_{\xi_m \in \Omega_\epsilon^*} \lambda_m(\xi_n) e^{\imath X \cdot \xi_m}$. Then for any $a \in \epsilon\mathbb{L}$, we have

$$\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](e^{\imath (X+a) \cdot \xi_n})(X_i) = e^{\imath a \cdot \xi_n} \mathcal{H}_{\mathrm{at}}[\mathrm{Id}](e^{\imath X \cdot \xi_n})(X_i) = e^{\imath a \cdot \xi_n} \sum_{\xi_m \in \Omega_\epsilon^*} \lambda_m(\xi_n) e^{\imath X_i \cdot \xi_m}.$$

On the other hand, we have

$$\begin{aligned}
&\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](e^{\imath (X+a) \cdot \xi_n})(X_i) \\
=& \sum_{X_j \in \Omega_\epsilon} \mathcal{H}_{\mathrm{at}}[\mathrm{Id}](X_i, X_j) e^{\imath (X_j + a) \cdot \xi_n} \\
=& \sum_{X_j \in \Omega_\epsilon} \mathcal{H}_{\mathrm{at}}[\mathrm{Id}](X_i + a, X_j + a) e^{\imath (X_j + a) \cdot \xi_n} \\
=& \mathcal{H}_{\mathrm{at}}[\mathrm{Id}](e^{\imath X \cdot \xi_n})(X_i + a) \\
=& \sum_{\xi_m \in \Omega_\epsilon^*} \lambda_m(\xi_n) e^{\imath (X_i + a) \cdot \xi_m}
\end{aligned}$$

These imply

$$\sum_{\xi_m \in \Omega_\epsilon^*} \lambda_m(\xi_n) e^{\imath X_i \cdot \xi_m} (e^{\imath a \cdot \xi_m} - e^{\imath a \cdot \xi_n}) = 0, \quad \forall a \in \epsilon\mathbb{L}.$$

So $\lambda_m(\xi_n) = 0$ for $m \neq n$. Denote $\lambda_n(\xi_n) = \mathcal{D}_{\rm at}^{\rm Id}[\xi_n]$, then we have

$$\mathcal{H}_{\rm at}[\mathrm{Id}](e^{\imath X\cdot\xi})(X) = \mathcal{D}_{\rm at}^{\rm Id}[\xi]e^{\imath X\cdot\xi},$$

from which we can also get the formula for the dynamical matrix $\mathcal{D}_{\rm at}^{\rm Id}[\xi]$:

$$\mathcal{D}_{\rm at}^{\rm Id}[\xi] = \epsilon^3 \sum_{X_i, X_j \in \Omega_\epsilon} \mathcal{H}_{\rm at}[\mathrm{Id}](X_i, X_j)e^{\imath(X_j - X_i)\cdot\xi}. \tag{7.11}$$

□

7.1.3 Hermitian property

Lemma 7.1.4. *For each $\xi \in \Omega_\epsilon^*$, $\mathcal{D}_{at}^{Id}[\xi]$ is Hermitian, so its eigenvalues are real and it is diagonalizable.*

Proof. Check $(\mathcal{D}_{\rm at}^{\rm Id}[\xi])^{\alpha\beta} = \overline{(\mathcal{D}_{\rm at}^{\rm Id}[\xi])^{\beta\alpha}}$.

$$\begin{aligned}\overline{(\mathcal{D}_{\rm at}^{\rm Id}[\xi])^{\beta\alpha}} =& \overline{\epsilon^3 \sum_{X_i, X_j \in \Omega_\epsilon} \mathcal{H}_{\rm at}^{\beta\alpha}[\mathrm{Id}](X_i, X_j)e^{\imath(X_j - X_i)\cdot\xi}} \\ &= \epsilon^3 \sum_{X_i, X_j \in \Omega_\epsilon} \overline{\mathcal{H}_{\rm at}^{\beta\alpha}[\mathrm{Id}](X_i, X_j)}e^{\imath(X_i - X_j)\cdot\xi} \\ &= \epsilon^3 \sum_{X_i, X_j \in \Omega_\epsilon} \mathcal{H}_{\rm at}^{\beta\alpha}[\mathrm{Id}](X_j, X_i)e^{\imath(X_j - X_i)\cdot\xi}\end{aligned}$$

So it suffices to prove $\mathcal{H}_{\rm at}^{\beta\alpha}[\mathrm{Id}](X_j, X_i) = \mathcal{H}_{\rm at}^{\alpha\beta}[\mathrm{Id}](X_i, X_j)$. Knowing that $\nabla^2 m_a$ is a symmetric matrix, we analyze the non-diagonal part

$$-\frac{1}{2\epsilon^2}\int_{n\Omega} \sum_{r_2 \in \mathbb{L}} \nabla m_a(x - \frac{X_i}{\epsilon} + \frac{r_2}{\epsilon})\big[(\mathcal{L}_{\rm per}^{-1})_{22}[\sum_{r_3 \in \mathbb{L}} \nabla m_a(\cdot - \frac{X_j}{\epsilon} + \frac{r_3}{\epsilon})](x)\big]^T dx$$

Thus we need to show

$$\begin{aligned}&\sum_{r_2, r_3 \in \mathbb{L}} \int_{n\Omega} \partial_p m_a(x - \frac{X_i}{\epsilon} + \frac{r_2}{\epsilon})(\mathcal{L}_{\rm per}^{-1})_{22}\big(\partial_q m_a(\cdot - \frac{X_j}{\epsilon} + \frac{r_3}{\epsilon})\big)(x)dx \\ =& \sum_{r_2, r_3 \in \mathbb{L}} \int_{n\Omega} \partial_q m_a(x - \frac{X_j}{\epsilon} + \frac{r_2}{\epsilon})(\mathcal{L}_{\rm per}^{-1})_{22}\big(\partial_p m_a(\cdot - \frac{X_i}{\epsilon} + \frac{r_3}{\epsilon})\big)(x)dx\end{aligned}$$

$$= \sum_{r_2, r_3 \in \mathbb{L}} \int_{n\Omega} \partial_q m_a(x - \frac{X_j}{\epsilon} + \frac{r_3}{\epsilon})(\mathcal{L}_{\text{per}}^{-1})_{22}\big(\partial_p m_a(\cdot - \frac{X_i}{\epsilon} + \frac{r_2}{\epsilon})\big)(x)dx$$

where the second equality holds because $r_2, r_3 \in \mathbb{L}$ are arbitrary. So it suffices to prove

$$\int_{n\Omega} \partial_p m_a(x - \frac{X_i}{\epsilon} + \frac{r_2}{\epsilon})(\mathcal{L}_{\text{per}}^{-1})_{22}\big(\partial_q m_a(\cdot - \frac{X_j}{\epsilon} + \frac{r_3}{\epsilon})\big)(x)dx$$
$$= \int_{n\Omega} \partial_q m_a(x - \frac{X_j}{\epsilon} + \frac{r_3}{\epsilon})(\mathcal{L}_{\text{per}}^{-1})_{22}\big(\partial_p m_a(\cdot - \frac{X_i}{\epsilon} + \frac{r_2}{\epsilon})\big)(x)dx$$

which is equivalent to $(\mathcal{L}_{\text{per}}^{-1})_{22}$ being a symmetric operator on $(L_n^2)^2$.

Recall

$$\mathcal{L}_{\text{per}} = \begin{pmatrix} \mathcal{L}_{1,\text{per}} & \nu_{\text{per}} \\ \nu_{\text{per}} & \frac{\Delta}{8\pi} \end{pmatrix}$$

where $\mathcal{L}_{1,\text{per}} = -\epsilon^2\Delta + \frac{35}{9}\nu_{\text{per}}^{\frac{4}{3}} - \frac{20}{9}\nu_{\text{per}}^{\frac{2}{3}} + V_{\text{per}}$. Since Δ, any power of ν_{per}, and V are symmetric operators, so is $\mathcal{L}_{\text{per}}$:

$$\langle \mathcal{L}_{\text{per}} \begin{pmatrix} \omega^1 \\ W^1 \end{pmatrix}, \begin{pmatrix} \omega^2 \\ W^2 \end{pmatrix} \rangle_{(L_n^2)^2} = \langle \begin{pmatrix} \omega^1 \\ W^1 \end{pmatrix}, \mathcal{L}_{\text{per}} \begin{pmatrix} \omega^2 \\ W^2 \end{pmatrix} \rangle_{(L_n^2)^2}.$$

Rewrite the above equality as

$$\langle \mathcal{L}_{\text{per}} \begin{pmatrix} \omega^1 \\ W^1 \end{pmatrix}, \mathcal{L}_{\text{per}}^{-1}\mathcal{L}_{\text{per}} \begin{pmatrix} \omega^2 \\ W^2 \end{pmatrix} \rangle_{(L_n^2)^2} = \langle \mathcal{L}_{\text{per}}^{-1}\mathcal{L}_{\text{per}} \begin{pmatrix} \omega^1 \\ W^1 \end{pmatrix}, \mathcal{L}_{\text{per}} \begin{pmatrix} \omega^2 \\ W^2 \end{pmatrix} \rangle_{(L_n^2)^2}.$$

Since $\mathcal{L}_{\text{per}}$ is invertible, we have

$$\langle \begin{pmatrix} \omega^1 \\ W^1 \end{pmatrix}, \mathcal{L}_{\text{per}}^{-1} \begin{pmatrix} \omega^2 \\ W^2 \end{pmatrix} \rangle_{(L_n^2)^2} = \langle \mathcal{L}_{\text{per}}^{-1} \begin{pmatrix} \omega^1 \\ W^1 \end{pmatrix}, \begin{pmatrix} \omega^2 \\ W^2 \end{pmatrix} \rangle_{(L_n^2)^2}.$$

□

7.1.4 Eigenvalues

We have shown that $\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi]$ is Hermitian, so it is diagonalizable $\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi] = P_\xi \Lambda_\xi P_\xi^{-1}$, where $P_\xi = (P_\xi^1, P_\xi^2, P_\xi^3)$ consists of the eigenvectors which form a basis, $\Lambda_\xi = \mathrm{diag}(w_1^{\mathrm{Id}}(\xi), w_2^{\mathrm{Id}}(\xi), w_3^{\mathrm{Id}}(\xi))$ contains the eigenvalues.

Then

$$
\begin{aligned}
&\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](P_\xi^j e^{\imath X\cdot\xi})(X) \\
=&\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi] P_\xi^j e^{\imath X\cdot\xi} \\
=&P_\xi \Lambda_\xi P_\xi^{-1} P_\xi^j e^{\imath X\cdot\xi} \\
=&w_j^{\mathrm{Id}}(\xi) P_\xi^j e^{\imath X\cdot\xi}.
\end{aligned}
$$

for any $X \in \Omega_\epsilon, \xi \in \Omega_\epsilon^*$. Therefore $\mathcal{H}_{\mathrm{at}}[\mathrm{Id}]$ has eigenfunctions $P_\xi^j e^{\imath X\cdot\xi}$ with the corresponding eigenvalues $w_j^{\mathrm{Id}}(\xi)$, for $j = 1, 2, 3$, $\xi \in \Omega_\epsilon^*$.

7.1.5 Stability Condition

We introduce **Stability Condition B** for the atomistic TFDW model, which states that

$$|w_k^{\mathrm{Id}}(\xi)| \geqslant \Lambda|\xi|^2, \tag{7.12}$$

where $w_k^{\mathrm{Id}}, k = 1, 2, 3$ are eigenvalues of $\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi]$, for any $\xi \in \Omega_\epsilon^*$ and some constant $\Lambda > 0$.

It is straightforward to see that the following two statements are equivalent

1. $|w_k^{\mathrm{Id}}(\xi)| \geqslant \Lambda|\xi|^2, \forall \xi \in \Omega_\epsilon^*, k = 1, 2, 3,$

2. $\det \mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi] \geqslant a_{\mathrm{at}} \Lambda_{0,\epsilon}^6(\xi), \forall \xi \in \Omega_\epsilon^*,$

where Λ, a_{at} are some positive constants and $\Lambda_{0,\epsilon}^2(\xi) = 1 + |\xi|^2$.

7.2 The Stability Condition For The Continuum Elasticity Model

Up to now we have introduced **Stability Condition A** for the electronic TFDW model and **Stability Condition B** for the atomistic TFDW model. These two stability conditions are independent. We still need a stability condition for the Cauchy-Born continuum elasticity model. However, this stability condition is not independent. In fact, we have

Theorem 7.2.1. Stability Condition *B implies* **Stability Condition** *C for the continuum elasticity model*

$$D_A^2 W_{CB}(0)(\xi \otimes \eta, \xi \otimes \eta) \geqslant \Lambda |\xi|^2 |\eta|^2 \tag{7.13}$$

where W_{CB} is the stored energy density function, and ξ, η are arbitrary vectors in $\mathbb{R}^3$.

Proof. Let us compute $D_A W_{\mathrm{CB}}(A)$ in Eulerian coordinates,

$$\begin{aligned}
& D_A W_{\mathrm{CB}}(A) \\
=& D_A \frac{1}{|\Omega|} \int_\Omega F_{\mathrm{CB}}(z, A) dz \\
=& D_A \frac{1}{|\Omega|} \int_\Omega \nu_{\mathrm{CB}}^{\frac{10}{3}}(y; A) + |\nabla_y \nu_{\mathrm{CB}}(y; A)|^2 - \nu_{\mathrm{CB}}^{\frac{8}{3}}(y; A) \\
& + \frac{1}{2} V_{\mathrm{CB}}(y; A) \big(\nu_{\mathrm{CB}}^2(y; A) - \rho_{b,0}(y; A)\big) dy \\
=& \frac{2}{|\Omega|} \int_\Omega \big(-\Delta \nu_{\mathrm{CB}} + \frac{5}{3} \nu_{\mathrm{CB}}^{\frac{7}{3}} - \frac{4}{3} \nu_{\mathrm{CB}}^{\frac{5}{3}} + V_{\mathrm{CB}} \nu_{\mathrm{CB}}\big) D_A \nu_{\mathrm{CB}}(y; A) dy \\
& - \frac{1}{|\Omega|} \int_\Omega V_{\mathrm{CB}}(y) D_A \rho_{b,0}(y, A) dy \\
=& - \frac{1}{|\Omega|} \int_\Omega V_{\mathrm{CB}}(y; A) D_A \rho_{b,0}(y; A) dy
\end{aligned}$$

Then

$$D_{A_{kl}} D_{A_{ij}} W_{\mathrm{CB}}(0) = -\frac{1}{|\Omega|} \int_\Omega D_{A_{kl}} V_{\mathrm{per}} D_{A_{ij}} \rho_{b,\mathrm{per}} + V_{\mathrm{per}} D_{A_{kl}} D_{A_{ij}} \rho_{b,\mathrm{per}} dx \tag{7.14}$$

We derive $D_{A_{kl}} V_{\text{per}}$ as follows. The system of Euler-Lagrange equations for $\mathcal{V}_{\text{CB}}$ in Eulerian coordinates is

$$\mathcal{F}(\mathcal{V}_{\text{CB}}, A) = \begin{pmatrix} -\Delta\nu_{\text{CB}} + \frac{5}{3}\nu_{\text{CB}}^{\frac{7}{3}} - \frac{4}{3}\nu_{\text{CB}}^{\frac{5}{3}} + V_{\text{CB}}\nu_{\text{CB}} \\ \frac{1}{8\pi}\Delta V_{\text{CB}} + \frac{1}{2}\nu_{\text{CB}}^2 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{1}{2}\rho_{b,0} \end{pmatrix} \tag{7.15}$$

Take derivative of $\mathcal{F}(\mathcal{V}_{\text{CB}}, A)$ with respect to A and evaluate at $A = 0$, we get

$$\mathcal{L}_{\text{per}} D_{A_{kl}} \mathcal{V}_{\text{per}} = \partial_{A_{kl}} \mathcal{F}(\mathcal{V}_{\text{per}}, 0) = \begin{pmatrix} 0 \\ \frac{1}{2} D_{A_{kl}} \rho_{b,\text{per}} \end{pmatrix} \tag{7.16}$$

Thus

$$D_{A_{kl}} V_{\text{per}} = (\mathcal{L}_{\text{per}}^{-1})_{22}[\frac{1}{2} D_{A_{kl}} \rho_{b,\text{per}}]. \tag{7.17}$$

Therefore

$$D_{A_{kl}} D_{A_{ij}} W_{\text{CB}}(0) = -\frac{1}{|\Omega|}\int_\Omega V_{\text{per}} D_{A_{kl}} D_{A_{ij}} \rho_{b,\text{per}} + D_{A_{ij}} \rho_{b,\text{per}} (\mathcal{L}_{\text{per}}^{-1})_{22} \frac{1}{2} D_{A_{kl}} \rho_{b,\text{per}} dx \tag{7.18}$$

Recall

$$\rho_{b,0}(x; A) = \sum_{X \in \Omega_\epsilon, r \in \mathbb{L}} m_a(x - \frac{(I+A)X}{\epsilon} + \frac{r}{\epsilon}) \tag{7.19}$$

so

$$D_{A_{ij}} \rho_{b,0}(x; 0) = -\sum_{X \in \Omega_\epsilon, r \in \mathbb{L}} \nabla_i m_a(x - \frac{X}{\epsilon} + \frac{r}{\epsilon}) X^j \tag{7.20}$$

$$D_{A_{kl}} D_{A_{ij}} \rho_{b,0}(x; 0) = \sum_{X \in \Omega_\epsilon, r \in \mathbb{L}} \nabla_k \nabla_i m_a(x - \frac{X}{\epsilon} + \frac{r}{\epsilon}) X^j X^l \tag{7.21}$$

So

$$D_{A_{kl}} D_{A_{ij}} W_{\text{CB}}(0) \tag{7.22}$$

$$= -\frac{1}{|\Omega|}\int_\Omega V_{\text{per}} \sum_{X \in \Omega_\epsilon, r \in \mathbb{L}} \nabla_k \nabla_i m_a(x - \frac{X}{\epsilon} + \frac{r}{\epsilon}) dx X^j X^l \tag{7.23}$$

$$- \frac{1}{2|\Omega|} \int_\Omega \sum_{X_p \in \Omega_\epsilon, r \in \mathbb{L}} \nabla_i m_a (x - \frac{X_p}{\epsilon} + \frac{r}{\epsilon}) (\mathcal{L}_{\text{per}}^{-1})_{22} \tag{7.24}$$

$$\cdot [\sum_{X_q \in \Omega_\epsilon, r \in \mathbb{L}} \nabla_k m_a (\cdot - \frac{X_q}{\epsilon} + \frac{r}{\epsilon})]^T (x) dx X_p^j X_q^l \tag{7.25}$$

$$= - \frac{\epsilon^{-2}}{|\Omega|} \int_\Omega V_{\text{per}} \sum_{X \in \Omega_\epsilon, r \in \mathbb{L}} \nabla_k \nabla_i m_a (\frac{x - X + r}{\epsilon}) dx X^j X^l \tag{7.26}$$

$$- \frac{\epsilon^{-2}}{2|\Omega|} \int_\Omega \sum_{X_p \in \Omega_\epsilon, r \in \mathbb{L}} \nabla_i m_a (\frac{x - X + r}{\epsilon}) (\mathcal{L}_{\text{per}}^{-1})_{22} \tag{7.27}$$

$$\cdot [\sum_{X_q \in \Omega_\epsilon, r \in \mathbb{L}} \nabla_k m_a (\frac{\cdot - X + r}{\epsilon})]^T (x) dx X_p^j X_q^l \tag{7.28}$$

Next we compute

$$\sum_{jl} D_{A_{kl}} D_{A_{ij}} W_{\text{CB}}(0) \xi^j \xi^l$$

$$= - \frac{\epsilon^{-2}}{|\Omega|} \int_\Omega V_{\text{per}} \sum_{X \in \Omega_\epsilon, r \in \mathbb{L}} \nabla^2 m_a (\frac{x - X + r}{\epsilon}) dx (X \cdot \xi)^2$$

$$- \frac{\epsilon^{-2}}{2|\Omega|} \int_\Omega \sum_{X_p \in \Omega_\epsilon, r \in \mathbb{L}} \nabla m_a (\frac{x - X_p + r}{\epsilon}) (\mathcal{L}_{\text{per}}^{-1})_{22}$$

$$\cdot [\sum_{X_q \in \Omega_\epsilon, r \in \mathbb{L}} \nabla m_a (\frac{\cdot - X_q + r}{\epsilon})]^T (x) dx (X_p \cdot \xi)(X_q \cdot \xi)$$

$$= \epsilon^3 \sum_{X_i, X_j \in \Omega_\epsilon} \mathcal{H}_{\text{at}}[\text{Id}](i,j) (X_i \cdot \xi)(X_j \cdot \xi)$$

By translation invariance of the lattice, we have

$$\sum_{X_j \in \Omega_\epsilon} \mathcal{H}_{\text{at}}[\text{Id}](i,j) = 0, \qquad \sum_{X_i \in \Omega_\epsilon} \mathcal{H}_{\text{at}}[\text{Id}](i,j) = 0. \tag{7.29}$$

So

$$- \frac{1}{2} \sum_{X_j \in \Omega_\epsilon} \mathcal{H}_{\text{at}}[\text{Id}](0,j) |X_j \cdot \xi|^2$$

$$=-\frac{1}{2}\sum_{X_j-X_i\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j-i)|X_j\cdot\xi-X_i\cdot\xi|^2$$

$$=-\frac{\epsilon^3}{2}\sum_{X_i,X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](i,j)\big(|X_j\cdot\xi|^2-2(X_i\cdot\xi)(X_j\cdot\xi)+|X_i\cdot\xi|^2\big)$$

$$=\epsilon^3\sum_{X_i,X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](i,j)(X_i\cdot\xi)(X_j\cdot\xi)-\frac{\epsilon^3}{2}\sum_{X_i,X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](i,j)\big(|X_i\cdot\xi|^2+|X_j\cdot\xi|^2\big)$$

$$=\epsilon^3\sum_{X_i,X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](i,j)(X_i\cdot\xi)(X_j\cdot\xi)-0$$

On the other hand, let us compute $\mathcal{D}^{\mathrm{Id}}_{\mathrm{at}}[\xi]$. Notice that by translation invariance we have $\sum_{X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j)=0$. Then

$$\mathcal{D}^{\mathrm{Id}}_{\mathrm{at}}[\xi]$$

$$=\epsilon^3\sum_{X_j,X_l\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](j,l)e^{\imath(X_j-X_l)\cdot\xi}$$

$$=\sum_{X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j)e^{\imath X_j\cdot\xi}$$

$$=\frac{1}{2}\sum_{X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j)(e^{\imath X_j\cdot\xi}+e^{-\imath X_j\cdot\xi})$$

$$=\sum_{X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j)\cos(X_j\cdot\xi)$$

$$=\sum_{X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j)(\cos(X_j\cdot\xi)-1)$$

$$=-2\sum_{X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j)\sin(\frac{X_j\cdot\xi}{2})$$

$$=-\frac{1}{2}\sum_{X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j)(\xi\cdot X_j)^2+2\sum_j\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j)[(\frac{X_j\cdot\xi}{2})^2-\sin(\frac{X_j\cdot\xi}{2})]$$

$$=|\Omega|\sum_{X_j,X_l\in\Omega_\epsilon}D_{A_{kl}}D_{A_{ij}}W_{\mathrm{CB}}(0)\xi_j\xi_l+2\sum_{X_j\in\Omega_\epsilon}\mathcal{H}_{\mathrm{at}}[\mathrm{Id}](0,j)[(\frac{X_j\cdot\xi}{2})^2-\sin(\frac{X_j\cdot\xi}{2})]$$

From $\cos(x) \leqslant 1 - \frac{x^2}{2} + \frac{x^4}{4!}, \forall x \in \mathbb{R}$, we have

$$0 \leqslant (\frac{X_j \cdot \xi}{2})^2 - \sin(\frac{X_j \cdot \xi}{2}) \leqslant \frac{|\xi|^4 |X_j|^4}{12}. \tag{7.30}$$

Then since $\mathcal{H}_{\text{at}}[\text{Id}](0, j) = \mathcal{O}(\epsilon^{-2})$, we have

$$\begin{aligned} &2 \sum_{X_j \in \Omega_\epsilon} \mathcal{H}_{\text{at}}[\text{Id}](0, j)[(\frac{X_j \cdot \xi}{2})^2 - \sin(\frac{X_j \cdot \xi}{2})] \\ \leqslant &\frac{1}{6} \sum_{X_j \in \Omega_\epsilon} |\mathcal{H}_{\text{at}}[\text{Id}](0, j)||\xi|^4 |X_j|^4 \end{aligned}$$

Recall $\mathcal{H}_{\text{at}}[\text{Id}](i, k) = \mathcal{H}_{\text{at}}[\text{Id}](0, k-i)$ is nonzero if $|X_k - X_i| \leqslant 2\epsilon M$ since m_a has compact support $m_a(x) = 0, \forall |x| \geqslant M$. So in the above sum over Ω_ϵ only those with $|X_j| \leqslant 2\epsilon M$ is nonzero. This means the number of those X_j is $\mathcal{O}(1)$, and $|X_j|^4 \leqslant C\epsilon^4$. Therefore

$$2 \sum_j \mathcal{H}_{\text{at}}[\text{Id}](0, j)[(\frac{X_j \cdot \xi}{2})^2 - \sin(\frac{X_j \cdot \xi}{2})] \leqslant C\epsilon^2 |\xi|^4. \tag{7.31}$$

Now assume we only consider those $\xi \in \Omega_\epsilon^*$ that satisfy $\xi = \mathcal{O}(1)$, then for any $\eta \in \mathbb{R}^3$, we have

$$\begin{aligned} |\Omega| D_A^2 W_{\text{CB}}(0)(\xi \otimes \eta, \xi \otimes \eta) \geqslant &\eta^T \mathcal{D}_{\text{at}}^{\text{Id}}[\xi]\eta - C\epsilon^2 |\xi|^4 |\eta|^2 \\ \geqslant &(\Lambda - C\epsilon^2 |\xi|^2)|\xi|^2 |\eta|^2 \\ \geqslant &\frac{\Lambda}{2} |\xi|^2 |\eta|^2. \end{aligned}$$

The above inequality is homogeneous with respect to ξ, so it is valid for any $\xi \in \mathbb{R}^3$.

□

8

The Continuum Elasticity Model

In this chapter, we analyze the Cauchy-Born continuum elasticity model to derive the corresponding solution Y_{CB}. Recall

$$X = \left\{ v : \Omega \to \mathbb{R}^3 | v \in W^{m+2,p}(\Omega;\mathbb{R}^3) \cap W^{1,p}_{\sharp}(\Omega;\mathbb{R}^3), \int_{\Omega} v = 0 \right\} \tag{8.1}$$

for $m \geqslant 0, p > 3$.

The Cauchy-Born continuum elasticity problem is formulated as follows: find a deformation function $u \in X$ such that

$$u = \mathrm{argmin}_{v \in X} I_{\mathrm{CB}}(v) \tag{8.2}$$

where

$$I_{\mathrm{CB}}(v) = \int_{\Omega} W_{\mathrm{CB}}(\nabla v(x)) - f(x)(v(x) - x)dx, \tag{8.3}$$

where the Cauchy-Born stored energy density W_{CB} is

$$\begin{aligned} W_{\mathrm{CB}}(A) = & \frac{1}{|\Omega|} \int_{\Omega} J^{-\frac{2}{3}}(A) \nu_{\mathrm{CB}}^{\frac{10}{3}}(A) - \nu_{\mathrm{CB}} a^{ij}(A) \partial_{z_i} \partial_{z_j} \nu_{\mathrm{CB}}(A) \\ & - J^{-\frac{1}{3}}(A) \nu_{\mathrm{CB}}^{\frac{8}{3}}(A) + \frac{1}{2} V_{\mathrm{CB}}(A)(\nu_{\mathrm{CB}}^2(A) - J(A)\rho_{b,0}(A)) dz \end{aligned}$$

The corresponding Euler-Lagrange equation is

$$\mathcal{F}_{\mathrm{CB}}(u(x)) = f(x), \quad x \in \Omega \tag{8.4}$$

where

$$\mathcal{F}_{\mathrm{CB}}(u(x)) = -\nabla \cdot (D_A W_{\mathrm{CB}}(\nabla u(x))). \tag{8.5}$$

Theorem 8.0.1. *If Stability Condition C holds*

$$D_A^2 W_{CB}(0)(\xi \otimes \eta, \xi \otimes \eta) \geqslant \Lambda |\xi|^2 |\eta|^2, \tag{8.6}$$

and $p > 3, m \geqslant 0$, *then there exist constants* $\delta, \kappa_1, \kappa_2$, *such that for any* $B \in \mathbb{R}_+^{3\times 3}$ *with* $\|B\| \leqslant \kappa_1$ *and* $\|f\|_{W^{m,p}(\Omega)} \leqslant \kappa_2$, *there exists a unique solution* $u_{CB} \in X$ *such that the following properties hold*

1. u_{CB} *satisfies the Euler-Lagrange equation*

$$\mathcal{F}_{CB}(u_{CB}(x)) = f(x), \quad x \in \Omega; \tag{8.7}$$

2. u_{CB} *is a* $W^{1,\infty}$ *local minimizer of the Cauchy-Born continuum elasticity functional* $\mathcal{I}_{CB}(v)$.

3. $\|u_{CB} - B \cdot x\|_{W^{m+2,p}} \leqslant \delta$, *for any* $x \in \Omega$.

Proof. We will use the implicit function theorem to derive the solution. We first prove that

$$\int_\Omega \nabla v \cdot D_A^2 W_{\mathrm{CB}}(B) \cdot \nabla v dx \geqslant \frac{C_1}{2} ||v||_1^2.$$

Rewrite v as

$$v(x) = \sum_{n \in \mathbb{Z}^3} a_n e^{2\pi \imath n \cdot x}, \quad a_n = \int_\Omega v(x) e^{-2\pi \imath n \cdot x} dx,$$

and denote

$$C_{\alpha\beta\gamma\delta} = \frac{\partial^2 W_{\text{CB}}}{\partial A_{\alpha\beta}\partial A_{\gamma\delta}}(0),$$

then

$$\begin{aligned}
&\int_\Omega \nabla v \cdot D_A^2 W_{\text{CB}}(0) \cdot \nabla v dx \\
=&4\pi^2 \sum_{\alpha\beta\gamma\delta} \sum_{n,m\in\mathbb{Z}^3} C_{\alpha\beta\gamma\delta} n_\alpha m_\gamma a_{n_\beta} a_{m_\delta} \int_\Omega e^{2\pi\imath(n-m)\cdot x} dx \\
=&4\pi^2 \sum_{\alpha\beta\gamma\delta} \sum_{n\in\mathbb{Z}^3} C_{\alpha\beta\gamma\delta} n_\alpha n_\gamma a_{n_\beta} a_{n_\delta} \\
\geqslant&4\pi^2 \Lambda \sum_{n\in\mathbb{Z}^3} |n|^2 |a_n|^2 \\
=&\Lambda \int_\Omega |\nabla v|^2 dx \\
\geqslant&\frac{\Lambda\pi^2}{1+\pi^2} ||v||_1^2.
\end{aligned}$$

The last inequality comes from Poincaré's inequality and $\int_\Omega v = 0$.

Let $C_1 = \frac{\Lambda\pi^2}{1+\pi^2}, M = \max_{A\in\mathbb{R}^{3\times 3}} |D_A^3 W_{\text{CB}}(A)|, \kappa_1 = \min(C_1/(2M), 1)$, then $\|B\| \leqslant \kappa_1$ implies

$$|D_A^2 W_{\text{CB}}(B) - D_A^2 W_{\text{CB}}(0)| \leqslant M\|B\| \leqslant \frac{C_1}{2}.$$

Therefore

$$\int_\Omega \nabla v \cdot D_A^2 W_{\text{CB}}(B) \cdot \nabla v dx \geqslant \frac{C_1}{2} \|v\|_1^2.$$

Define $T : Y \times X \to \mathbb{R}^3$ by

$$T(f, v) = \mathcal{L}(v + B \cdot x) - f,$$

then

1. $T(0, 0) = 0$;

2. $D_vT(0,0)$ is a bijection from X to Y;

3. $D_AW_{\text{CB}} \in C^2(\mathbb{R}^{3\times 3}_+, \mathbb{R}^{3\times 3})$, since $W^{k,p}(\Omega;\mathbb{R}^3)$ is a Banach algebra for $p > 3, k \geqslant 1$.

So we can apply the implicit function theorem: there exist constants R, r such that for any $\|f\|_{W^{m,p}} \leqslant r$, there exists a unique $v(f) \in X$ such that $T(f, v(f)) = 0$, $\|v(f)\|_{W^{m+2,p}} \leqslant R$, and $v(0) = 0$.

Define $u_{\text{CB}} = v(f) + B \cdot x$, then u_{CB} satisfies the Euler-Lagrange equation and $\|u_{\text{CB}} - B \cdot x\|_{W^{m+2,p}} \leqslant R$.

Next we show u_{CB} is a $W^{1,\infty}$ local minimizer of $I_{\text{CB}}(v)$.

$$I_{\text{CB}}(v) - I_{\text{CB}}(u_{\text{CB}}) = \int_\Omega \nabla(v - u_{\text{CB}})\Big(\int_0^1 (1-t)D_A^2W_{\text{CB}}(\nabla u^t)dt\Big) \cdot \nabla(v - u_{\text{CB}})dx$$

where $u^t = tv + (1-t)u_{\text{CB}}$. Since

$$\nabla u^t - B = t\nabla(v - u_{\text{CB}}) + \nabla v(f),$$

there exist κ_2, δ such that for any $\|f\|_{L^p} \leqslant \kappa_2$, and $\|v - u_{\text{CB}}\|_{1,\infty} \leqslant \delta$, we have

$$\int_\Omega \nabla(v - u_{\text{CB}})D_A^2W_{\text{CB}}(\nabla u^t) \cdot \nabla(v - u_{\text{CB}})dx \geqslant \frac{C_1}{4}\|v - u_{\text{CB}}\|_1^2$$

for any $0 \leqslant t \leqslant 1$. Hence

$$I_{\text{CB}}(v) - I_{\text{CB}}(u_{\text{CB}}) \geqslant \frac{C_1}{4}\|v - u_{\text{CB}}\|_1^2.$$

Therefore u_{CB} is a $W^{1,\infty}$ local minimizer of $I_{\text{CB}}(v)$.

□

9

The Atomistic Model

9.1 Introduction

In this final chapter, we are going to finish our proof of the main theorem stated in Chapter 3:

Theorem 9.1.1. *Given* $m_a \in C_0^\infty(\mathbb{R}^3)$*,* $\|f\|_{W_1^{27,p}} \leqslant h_f$ *for some constants* $h_f > 0, p > 3$*, assume* **Stability Conditions** *A and B hold (then* **Stability Condition** *C also holds), we have the following estimate for the discrete form* Y_{CB} *of the solution of the continuum elasticity model and the solution* Y_{at} *of the atomistic TFDW model with some positive constant* $M > 0$ *and all sufficiently small* $\epsilon > 0$ *on a simple crystal lattice:*

$$\|Y_{at} - Y_{CB}\|_{\epsilon,7} \leqslant M\epsilon^2. \tag{9.1}$$

To prove the theorem we need to analyze the stability conditions and the consistence estimate. In Chapter 7, we have derived the consistence estimate:

Given $Y_{\rm CB} \in H_\epsilon^{29}$, the Fourier interpolation satisfies $\tau_{\rm CB} \in H_1^{29}$. Moreover, assume $m_a \in H^{23}$. then with these assumptions, we have the estimate

$$\|\mathcal{F}_{\rm at}[Y_{\rm CB}]\|_{\epsilon,5} \leqslant C(\|u_{\rm CB}\|_{H_1^{29}})\epsilon^2. \tag{9.2}$$

For stability, we analyze the perturbation of the eigenvalues of the dynamical matrices with nearby deformations:

Given **Stability Condition B**, i.e. the eigenvalues of the dynamical matrix $\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi]$ without deformation satisfy

$$|w_j^{\mathrm{Id}}\xi|^2 \geqslant \Lambda|\xi|^2, \quad j = 1, 2, 3 \tag{9.3}$$

$$\tag{9.4}$$

for every $\xi \in \Omega_\epsilon^*$, then the eigenvalues of the dynamical matrix $\mathcal{D}_{\mathrm{at}}^{Y^t}[\xi]$ satisfy

$$|w_j^{Y^t}\xi|^2 \geqslant C\Lambda|\xi|^2, \quad j = 1, 2, 3 \tag{9.5}$$

$$\tag{9.6}$$

for every $\xi \in \Omega_\epsilon^*$. $Y^t = tY + (1-t)Y_{\mathrm{CB}}$, and $Y \in B$.

9.2 Stability Condition

Define the dynamical matrix

$$\mathcal{D}_{\mathrm{at}}^{Y}[\xi] = \frac{1}{N}\sum_{X_i, X_j} \mathcal{H}_{\mathrm{at}}^{Y}(i,j)e^{\imath(X_i - X_j)\cdot\xi} \tag{9.7}$$

Then

$$\mathcal{H}_{\mathrm{at}}[Y]e_k e^{\imath X\cdot\xi} = \mathcal{D}_{\mathrm{at}}^{Y}[\xi]e_k e^{\imath X\cdot\xi} \tag{9.8}$$

and

$$z^T\mathcal{H}_{\mathrm{at}}[\mathrm{Id}]z = \frac{1}{N}\sum_{\xi} \hat{z}^T[\xi]\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi]\hat{z}[\xi]$$

Diagonalize $\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi]$ which is Hermitian

$$\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi] = Q^T[\xi]\mathrm{diag}(w_1^{\mathrm{Id}}[\xi], w_2^{\mathrm{Id}}[\xi], w_3^{\mathrm{Id}}[\xi])Q[\xi] \tag{9.9}$$

Stability Condition B states that the eigenvalues of the dynamical matrix $\mathcal{D}_{\mathrm{at}}^{\mathrm{Id}}[\xi]$ without deformation satisfy

$$|w_j^{\mathrm{Id}}\xi|^2 \geqslant \Lambda|\xi|^2, \quad j = 1, 2, 3 \tag{9.10}$$

$$(9.11)$$

for every $\xi \in \Omega_\epsilon^*$.

9.3 Estimates of norms

Define the following norms that we will use

$$\|z\|^2_{\mathcal{H}_{\mathrm{at}}[\mathrm{Id}]} := \epsilon^3 z^T \mathcal{H}_{\mathrm{at}}[\mathrm{Id}] z \tag{9.12}$$

$$\|z\|^2_{\epsilon,1} = \sum_{|\alpha|=1} \epsilon^3 \sum_{X \in \Omega_\epsilon} |\mathcal{D}^\alpha_\epsilon(X)|^2 \tag{9.13}$$

$$\|z\|^2_a = \epsilon^3 \epsilon^{-2} \sum_{X_i, X_j \in \Omega_\epsilon} e^{-\frac{\gamma}{\epsilon}|X_i - X_j|} |z(X_i) - z(X_j)|^2. \tag{9.14}$$

Lemma 9.3.1.

$$\|z\|^2_{\epsilon,1} \leqslant C \|z\|^2_{\mathcal{H}_{at}[Id]} \tag{9.15}$$

Proof.

$$\|z\|^2_{\mathcal{H}_{\mathrm{at}}[\mathrm{Id}]} = \epsilon^3 z^T \mathcal{H}_{\mathrm{at}}[\mathrm{Id}] z$$

$$= \epsilon^3 \sum_{X_i, X_j \in \Omega_\epsilon} z_i^T H_{\mathrm{at}}[\mathrm{Id}](i,j) z_j$$

$$= \epsilon^3 \sum_{i,j} \sum_{\xi, \xi', \xi'' \in \Omega_\epsilon^*} e^{-\imath X_i \xi} \hat{z}^T[\xi] \epsilon^3 \mathcal{D}^{\mathrm{Id}}_{\mathrm{at}}[\xi'] e^{-\imath (X_j - X_i)\xi'} e^{\imath X_j \xi''} \hat{z}[\xi'']$$

$$= \sum_{\xi, \xi', \xi''} \hat{z}^T[\xi] \mathcal{D}^{\mathrm{Id}}_{\mathrm{at}}[\xi'] \hat{z}[\xi''] \big(\epsilon^3 \sum_i e^{\imath X_i(\xi' - \xi)}\big) \big(\epsilon^3 \sum_j e^{\imath X_j (\xi'' - \xi')}\big)$$

$$= \sum_\xi \hat{z}^T[\xi] \mathcal{D}^{\mathrm{Id}}_{\mathrm{at}}[\xi] \hat{z}[\xi]$$

$$= \sum_\xi \hat{z}^T[\xi] P^T[\xi] \mathrm{diag}(\omega_l^2[\xi]) P[\xi] \hat{z}[\xi]$$

$$\geqslant \sum_\xi \Lambda |\xi|^2 |P[\xi] \hat{z}[\xi]|^2$$

$$= \sum_\xi \Lambda |\xi|^2 |\hat{z}[\xi]|^2$$

$$\geqslant C\|z\|_{\epsilon,1}^2.$$

□

Lemma 9.3.2.

$$\|z\|_a^2 \leqslant C\|z\|_{\epsilon,1}^2 \tag{9.16}$$

Proof. Assume

$$X_k = n_k^1\epsilon a_1 + n_k^2\epsilon a_2 + n_k^3\epsilon a_3 \tag{9.17}$$

then $n_k^1, n_k^2, n_k^3 = 1, 2, \cdots, \frac{1}{\epsilon} = n$.

Recall

$$\begin{aligned}\|z\|_a^2 =&\epsilon^3 \sum_{X_i, X_j\in\Omega_\epsilon} e^{-\frac{\gamma}{\epsilon}|X_i-X_j|}\left|\frac{z(X_i)-z(X_j)}{\epsilon}\right|^2\\ =&2^3\epsilon^3 \sum_{n_j^s\geqslant n_i^s, s=1,2,3} e^{-\frac{\gamma}{\epsilon}|X_i-X_j|}\left|\frac{z(X_i)-z(X_j)}{\epsilon}\right|^2\end{aligned}$$

Decompose $|\frac{z(X_i)-z(X_j)}{\epsilon}|^2$ as below

$$\begin{aligned}&\left|\frac{z(X_i)-z(X_j)}{\epsilon}\right|^2\\ \leqslant&(n_j^1-n_i^1)\Big[\sum_{k=0}^{n_j^1-n_i^1-1}|D_{\epsilon,a_1}^+ z(X_i+k\epsilon a_1)|^2 + \left|\frac{z(X_i+(n_j^1-n_i^1-1)\epsilon a_1)-z(X_j)}{\epsilon}\right|^2\Big]\\ \leqslant&(n_j^1-n_i^1)\left(\begin{array}{c}\sum_{k=0}^{n_j^1-n_i^1-1}|D_{\epsilon,a_1}^+ z(X_i+k\epsilon a_1)|^2\\ +(n_j^2-n_i^2)\left(\begin{array}{c}\sum_{k=0}^{n_j^2-n_i^2-1}|D_{\epsilon,a_2}^+ z(X_i+(n_j^1-n_i^1-1)\epsilon a_1+k\epsilon a_2)|^2\\ +|\frac{z(X_i+(n_j^1-n_i^1-1)\epsilon a_1+(n_j^2-n_i^2-1)\epsilon a_2)-z(X_j)}{\epsilon}|^2\end{array}\right)\end{array}\right)\\ \leqslant&(n_j^1-n_i^1)\big(A_1+(n_j^2-n_i^2)(A_2+(n_j^3-n_i^3)A_3)\big)\\ \leqslant&\prod_{s=1}^3(n_j^s-n_i^s)(A_1+A_2+A_3)\end{aligned}$$

where

$$A_1 = \sum_{k=0}^{n_j^1-n_i^1-1}|D_{\epsilon,a_1}^+ z(X_i+k\epsilon a_1)|^2$$

$$A_2 = \sum_{k=0}^{n_j^2-n_i^2-1} |D^+_{\epsilon,a_2} z(X_i + (n_j^1 - n_i^1 - 1)\epsilon a_1 + k\epsilon a_2)|^2$$

$$A_3 = \sum_{k=0}^{n_j^3-n_i^3-1} |D^+_{\epsilon,a_3} z(X_i + (n_j^1 - n_i^1 - 1)\epsilon a_1 + (n_j^2 - n_i^2 - 1)\epsilon a_2 + k\epsilon a_3)|^2$$

Group coefficients of each $|D^+_{\epsilon,a_s} z(X_k)|$, we get

$$\|z\|_a^2$$

$$\leqslant 2^3\epsilon^3 \sum_{X_k\in\Omega_\epsilon} \begin{pmatrix} \sum_{n_i^1\leqslant n_k^1\leqslant n_j^1, n_i^2=n_k^2\leqslant n_j^2, n_i^3=n_k^3\leqslant n_j^3} \prod_{s=1}^3 (n_j^s - n_i^s) e^{-\frac{\gamma}{\epsilon}|X_i-X_j|} |D^+_{\epsilon,a_1} z(X_k)|^2 \\ + \sum_{n_i^1\leqslant n_k^1=n_j^1, n_i^2\leqslant n_k^2\leqslant n_j^2, n_i^3=n_k^3\leqslant n_j^3} \prod_{s=1}^3 (n_j^s - n_i^s) e^{-\frac{\gamma}{\epsilon}|X_i-X_j|} |D^+_{\epsilon,a_2} z(X_k)|^2 \\ + \sum_{n_i^1\leqslant n_k^1=n_j^1, n_i^2\leqslant n_k^2=n_j^2, n_i^3\leqslant n_k^3\leqslant n_j^3} \prod_{s=1}^3 (n_j^s - n_i^s) e^{-\frac{\gamma}{\epsilon}|X_i-X_j|} |D^+_{\epsilon,a_3} z(X_k)|^2 \end{pmatrix}$$

Analysis of the three sums are the same, so we analyze the first one in detail. Notice

$$\begin{aligned} |X_i - X_j| &= \frac{1}{\sqrt{3}}\sqrt{3|X_i - X_j|^2} \\ &= \frac{1}{\sqrt{3}}\sqrt{3[(n_i^1 - n_j^1)^2\epsilon^2 a_1^2 + (n_i^2 - n_j^2)^2\epsilon^2 a_2^2 + (n_i^3 - n_j^3)^2\epsilon^2 a_3^2]} \\ &\geqslant \frac{1}{\sqrt{3}}\sqrt{\left(|n_i^1 - n_j^1|\epsilon a_1 + |n_i^2 - n_j^2|\epsilon a_2 + |n_i^3 - n_j^3|\epsilon a_3\right)^2} \\ &= \frac{1}{\sqrt{3}}\left(|n_i^1 - n_j^1|\epsilon a_1 + |n_i^2 - n_j^2|\epsilon a_2 + |n_i^3 - n_j^3|\epsilon a_3\right) \end{aligned}$$

So

$$e^{-\frac{\gamma}{\epsilon}|X_i-X_j|} \leqslant e^{-\frac{\gamma a_1}{\sqrt{3}}|n_i^1-n_j^1|} e^{-\frac{\gamma a_2}{\sqrt{3}}|n_i^2-n_j^2|} e^{-\frac{\gamma a_3}{\sqrt{3}}|n_i^3-n_j^3|} \tag{9.18}$$

Now consider the sum in the coefficient of $|D^+_{\epsilon,a_1} z(X_k)|^2$

$$\sum_{n_i^1\leqslant n_k^1\leqslant n_j^1, n_i^2=n_k^2\leqslant n_j^2, n_i^3=n_k^3\leqslant n_j^3} \prod_{s=1}^3 (n_j^s - n_i^s) e^{-\frac{\gamma}{\epsilon}|X_i-X_j|}|$$

$$\leqslant \sum_{n_i^1\leqslant n_k^1\leqslant n_j^1} (n_j^1 - n_i^1) e^{-\frac{\gamma a_1}{\sqrt{3}}(n_j^1-n_i^1)} \sum_{n_i^2=n_k^2\leqslant n_j^2} (n_j^2 - n_i^2) e^{-\frac{\gamma a_2}{\sqrt{3}}(n_j^2-n_i^2)}$$

$$\cdot \sum_{n_i^3 = n_k^3 \leqslant n_j^3} (n_j^3 - n_i^3) e^{-\frac{\gamma a_3}{\sqrt{3}}(n_j^3 - n_i^3)}$$

We analyze the first factor

$$\sum_{n_i^1 \leqslant n_k^1 \leqslant n_j^1} (n_j^1 - n_i^1) e^{-\frac{\gamma a_1}{\sqrt{3}}(n_j^1 - n_i^1)}$$

$$= \sum_{n_i^1=0}^{n_k^1} \sum_{n_j^1 = n_k^1}^{n} (n_j^1 - n_i^1) e^{-\frac{\gamma a_1}{\sqrt{3}}(n_j^1 - n_i^1)}$$

$$= \sum_{n_i^1=0}^{n_k^1} \int_{n_k^1}^{n} (x - n_i^1) e^{-\frac{\gamma a_1}{\sqrt{3}}(x - n_i^1)} dx + O(1)$$

$$= \sum_{n_i^1=0}^{n_k^1} \int_{n_k^1 - n_i^1}^{n - n_i^1} x e^{-\frac{\gamma a_1}{\sqrt{3}} x} dx + O(1)$$

$$= \sum_{n_i^1=0}^{n_k^1} \left(\begin{array}{c} -\frac{\sqrt{3}}{\gamma a_1} \left((n - n_i^1) e^{-\frac{\gamma a_1}{\sqrt{3}}(n - n_i^1)} - (n_k^1 - n_i^1) e^{-\frac{\gamma a_1}{\sqrt{3}}(n_k^1 - n_i^1)} \right) \\ -\frac{3}{(\gamma a_1)^2} \left(e^{-\frac{\gamma a_1}{\sqrt{3}}(n - n_i^1)} - e^{-\frac{\gamma a_1}{\sqrt{3}}(n_k^1 - n_i^1)} \right) \end{array} \right) + O(1)$$

$$= \int_0^{n_k^1} \left(\begin{array}{c} -\frac{\sqrt{3}}{\gamma a_1} \left((n - x) e^{-\frac{\gamma a_1}{\sqrt{3}}(n - x)} - (n_k^1 - x) e^{-\frac{\gamma a_1}{\sqrt{3}}(n_k^1 - x)} \right) \\ -\frac{3}{(\gamma a_1)^2} \left(e^{-\frac{\gamma a_1}{\sqrt{3}}(n - x)} - e^{-\frac{\gamma a_1}{\sqrt{3}}(n_k^1 - x)} \right) \end{array} \right) dx + O(1)$$

$$= -\frac{3}{(\gamma a_1)^2} n_k^1 e^{-\frac{\gamma a_1}{\sqrt{3}} n_k^1} - \frac{3\sqrt{3}}{(\gamma a_1)^3} (e^{-\frac{\gamma a_1}{\sqrt{3}} n_k^1} - 1)$$

$$+ \frac{3}{(\gamma a_1)^2} \left(n e^{-\frac{\gamma a_1}{\sqrt{3}} n} - (n - n_k^1) e^{-\frac{\gamma a_1}{\sqrt{3}}(n - n_k^1)} \right)$$

$$+ \frac{3\sqrt{3}}{(\gamma a_1)^3} \left(e^{-\frac{\gamma a_1}{\sqrt{3}} n} - e^{\frac{\gamma a_1}{\sqrt{3}}(n - n_k^1)} \right) - \frac{3\sqrt{3}}{(\gamma a_1)^3} (e^{-\frac{\gamma a_1}{\sqrt{3}} n_k^1} - 1)$$

$$+ \frac{3\sqrt{3}}{(\gamma a_1)^3} (e^{-\frac{\gamma a_1}{\sqrt{3}} n} - 1) + O(1)$$

$$= O(1).$$

Similarly

$$\sum_{n_i^2=n_k^2\leqslant n_j^2}(n_j^2-n_i^2)e^{-\frac{\gamma a_2}{\sqrt{3}}(n_j^2-n_i^2)}=O(1)$$

$$\sum_{n_i^3=n_k^3\leqslant n_j^3}(n_j^3-n_i^3)e^{-\frac{\gamma a_3}{\sqrt{3}}(n_j^3-n_i^3)}=O(1).$$

So

$$\sum_{n_i^1\leqslant n_k^1\leqslant n_j^1,n_i^2=n_k^2\leqslant n_j^2,n_i^3=n_k^3\leqslant n_j^3}\prod_{s=1}^{3}(n_j^s-n_i^s)e^{-\frac{\gamma}{\epsilon}|X_i-X_j|}|\leqslant C, \tag{9.19}$$

C is a positive constant independent of ϵ.

The same results hold for the other two sums $\sum_{n_i^1\leqslant n_k^1=n_j^1,n_i^2\leqslant n_k^2\leqslant n_j^2,n_i^3=n_k^3\leqslant n_j^3}$ and $\sum_{n_i^1\leqslant n_k^1=n_j^1,n_i^2\leqslant n_k^2=n_j^2,n_i^3\leqslant n_k^3\leqslant n_j^3}$.

Therefore

$$\|z\|_a^2\leqslant 2^3\epsilon^3C\sum_{X_k\in\Omega_\epsilon}\left(|D^+_{\epsilon,a_1}z(X_k)|^2+|D^+_{\epsilon,a_2}z(X_k)|^2+|D^+_{\epsilon,a_3}z(X_k)|^2\right)\leqslant C\|z\|_{\epsilon,1}^2.$$

□

9.4 Perturbation of the Hessian

Lemma 9.4.1.

$$\|\mathcal{H}_{at}[Y_2](i,j)-\mathcal{H}_{at}[Y_1](i,j)\|\leqslant C\epsilon^{-2}e^{-\frac{\gamma}{\epsilon}|X_i-X_j|}\|Y_2-Y_1\|_{W_\epsilon^{1,\infty}} \tag{9.20}$$

Proof.

$$\begin{aligned}\mathcal{H}_{\rm at}[Y](i,j)=&\frac{\partial^2\mathcal{I}_{\rm at}(Y)}{\partial Y_i\partial Y_j}\\ =&\frac{\partial}{\partial Y_j}\big(\frac{\delta\mathcal{I}_{\rm at}}{\delta\nu}\frac{\partial\nu_{\rm exa}}{\partial Y_i}+\frac{\delta\mathcal{I}_{\rm at}}{\delta V}\frac{\partial V_{\rm exa}}{\partial Y_i}+\frac{\delta\mathcal{I}_{\rm at}}{\delta\rho_b}\frac{\partial\rho_b}{\partial Y_i}\big)\\ =&\frac{\partial}{\partial Y_j}\big(\int_{n\Omega}0\frac{\partial\nu_{\rm exa}}{\partial Y_i}dy+\frac{1}{2}\int_{n\Omega}(\nu_{\rm exa}^2-\rho_b)\frac{\partial V_{\rm exa}}{\partial Y_i}dy-\frac{1}{2}\int_{n\Omega}V_{\rm exa}\frac{\partial\rho_b}{\partial Y_i}dy\big)\end{aligned}$$

$$= -\frac{\partial}{\partial Y_j}\int_{n\Omega} V_{\text{exa}}\frac{\partial \rho_b}{\partial Y_i}dy$$

$$= -\int_{n\Omega}\frac{\partial V_{\text{exa}}}{\partial Y_j}\frac{\partial \rho_b}{\partial Y_i} + \int_{n\Omega} V_{\text{exa}}\frac{\partial^2 \rho_b}{\partial Y_j \partial Y_i}dy$$

$$= -\int_{n\Omega} J_\epsilon(\tau_Y)\frac{\partial V_{\text{exa}}}{\partial Y_j}\frac{\partial \rho_b}{\partial Y_i} + \int_{n\Omega} J_\epsilon(\tau_Y) V_{\text{exa}}\frac{\partial^2 \rho_b}{\partial Y_j \partial Y_i}dx$$

Then we have

$$\|\mathcal{H}_{\text{at}}[Y_2](i,j) - \mathcal{H}_{\text{at}}[Y_1](i,j)\|$$

$$\leqslant \int_{n\Omega}\|J_\epsilon(\tau_{Y_2})V_{\text{exa}}(Y_2)\partial_i\partial_j\rho_b(Y_2) - J_\epsilon(\tau_{Y_1})V_{\text{exa}}(Y_1)\partial_i\partial_j\rho_b(Y_1)\|dx$$

$$+ \frac{1}{2}\int_{n\Omega}\|J_\epsilon(\tau_{Y_2})\partial_j V_{\text{exa}}(Y_2)\partial_i\rho_b^\epsilon(Y_2) - J_\epsilon(\tau_{Y_1})\partial_j V_{\text{exa}}(Y_1)\partial_i\rho_b^\epsilon(Y_1)\|dx$$

$$\leqslant \int_{n\Omega}\|(J_\epsilon(\tau_{Y_2}) - J_\epsilon(\tau_{Y_1}))V_{\text{exa}}(Y_2)\partial_i\partial_j\rho_b(Y_2)\|dx$$

$$+ \int_{n\Omega}\|J_\epsilon(\tau_{Y_1})(V_{\text{exa}(Y_2)} - V_{\text{exa}(Y_1)})\partial_i\partial_j\rho_b(Y_2)\|dx$$

$$+ \int_{n\Omega}\|J_\epsilon(\tau_{Y_1})V_{\text{exa}(Y_1)}(\partial_i\partial_j\rho_b(Y_2) - \partial_i\partial_j\rho_b(Y_1))\|dx$$

$$+ \int_{n\Omega}\|(J_\epsilon(\tau_{Y_2}) - J_\epsilon(\tau_{Y_1}))\partial_j V_{\text{exa}}(Y_2)\partial_i\rho_b(Y_2)\|dx$$

$$+ \int_{n\Omega}\|J_\epsilon(\tau_{Y_1})(\partial_j V_{\text{exa}}(Y_2) - \partial_j V_{\text{exa}}(Y_1))\partial_i\rho_b(Y_2)\|dx$$

$$+ \int_{n\Omega}\|J_\epsilon(\tau_{Y_1})\partial_j V_{\text{exa}}(Y_1)(\partial_i\rho_b(Y_2) - \partial_i\rho_b(Y_1))\|dx$$

Recall

$$\|\partial_i\rho_b(x,Y)\| \leqslant \frac{C}{\epsilon}e^{-\gamma|x+\frac{-X_i+r_{i,\epsilon x}}{\epsilon}|}$$

$$\|\partial_i V_{\text{exa}}(x,Y)\| \leqslant \frac{C}{\epsilon}e^{-\gamma|x+\frac{-X_i+r_{i,\epsilon x}}{\epsilon}|}$$

$$\|J_\epsilon(\tau_{Y_2}) - J_\epsilon(\tau_{Y_1})\|_{L^\infty(n\Omega)} \leqslant C\|Y_2 - Y_1\|_{W^{1,\infty}_\epsilon}$$

$$\|\rho_b(Y_2)-\rho_b(Y_1)\|_{L^\infty(n\Omega)} \leqslant C\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}$$

$$|\partial_j\rho_b(x,Y_2)-\partial_j\rho_b(x,Y_1)| \leqslant C\epsilon^{-1}e^{-\gamma|x-\frac{X_j+r_{j,\epsilon x}}{\epsilon}|}\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}$$

$$|\partial_i\partial_j\rho_b(x,Y_2)-\partial_i\partial_j\rho_b(x,Y_1)| \leqslant C\epsilon^{-2}e^{-\gamma|x-\frac{X_i+r_{i,\epsilon x}}{\epsilon}|}e^{-\gamma|x-\frac{X_j+r_{j,\epsilon x}}{\epsilon}|}\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}$$

$$\|V_{\text{exa}}(Y_2)-V_{\text{exa}}(Y_1)\|_{L^\infty(n\Omega)} \leqslant C\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}$$

$$|\partial_jV_{\text{exa}}(x,Y_2)-\partial_jV_{\text{exa}}(x,Y_1)| \leqslant C\epsilon^{-1}e^{-\gamma|x-\frac{X_j+r_{j,\epsilon x}}{\epsilon}|}\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}$$

Therefore we get

$$\begin{aligned}
&\|\mathcal{H}_{\text{at}}[Y_2](i,j)-\mathcal{H}_{\text{at}}[Y_1](i,j)\|\\
\leqslant& C\epsilon^{-2}\int_{n\Omega}e^{-\gamma|x-\frac{X_i+r_{i,\epsilon x}}{\epsilon}|}e^{-\gamma|x-\frac{X_j+r_{j,\epsilon x}}{\epsilon}|}dx\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}\\
\leqslant& C\epsilon^{-2}\sum_{r\in S}\int_{n\Omega}e^{-\gamma|x-\frac{X_i+r}{\epsilon}|}e^{-\gamma|x-\frac{X_j+r}{\epsilon}|}dx\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}\\
\leqslant& C\epsilon^{-2}\sum_{r\in S}e^{-\frac{\gamma}{\epsilon}|X_i-X_j|}\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}\\
\leqslant& C\epsilon^{-2}e^{-\frac{\gamma}{\epsilon}|X_i-X_j|}\|Y_2-Y_1\|_{W^{1,\infty}_\epsilon}
\end{aligned}$$

□

Proposition 9.4.2. *Given $\epsilon^3 z^T\mathcal{H}_{at}[Y_1]z \geqslant \kappa\|z\|^2_{\mathcal{H}_{at}[Id]}$ and $\|Y_1-Y_2\|_{W^{1,\infty}_\epsilon} \leqslant \delta$ with δ sufficiently small, we have $\epsilon^3 z^T\mathcal{H}_{at}[Y_2]z \geqslant \frac{\kappa}{2}\|z\|^2_{\mathcal{H}_{at}[Id]}$*

Proof. By translation invariance,

$$\sum_{X_j\in\Omega}H_{\text{at}}[Y](i,j)=0$$

so

$$z^T\mathcal{H}_{\text{at}}[Y]z=-\frac{1}{2}\sum_{X_i,X_j\in\Omega_\epsilon}(z_i^T-z_j^T)H_{\text{at}}[Y](i,j)(z_i-z_j).$$

Thus

$$|\sum_{X_i,X_j\in\Omega_\epsilon}(z_i^T-z_j^T)(H_{\text{at}}[Y_2](i,j)-H_{\text{at}}[Y_1](i,j))(z_i-z_j)|$$

$$\leqslant C\epsilon^{-2}\|Y_1 - Y_2\|_{W_\epsilon^{1,\infty}} \sum_{X_i, X_j \in \Omega_\epsilon} e^{-\frac{\gamma}{\epsilon}|X_i - X_j|}|z_i - z_j|^2$$

$$\leqslant C\delta\epsilon^{-2} \sum_{X_i, X_j \in \Omega_\epsilon} e^{-\frac{\gamma}{\epsilon}|X_i - X_j|}|z_i - z_j|^2$$

$$\leqslant C\delta\epsilon^{-3}\|z\|_a^2$$

$$\leqslant C\delta\epsilon^{-3}\|z\|_{H_{\mathrm{at}}[\mathrm{Id}]}^2$$

Therefore

$$\epsilon^3 z^T H_{\mathrm{at}}[Y_2]z = \epsilon^3 z^T H_{\mathrm{at}}[Y_1]z + \epsilon^3 z^T (H_{\mathrm{at}}[Y_2] - H_{\mathrm{at}}[Y_1])z$$

$$\geqslant \kappa\|z\|_{H_{\mathrm{at}}[\mathrm{Id}]} - C\delta\|z\|_{H_{\mathrm{at}}[\mathrm{Id}]}^2$$

$$\geqslant \frac{\kappa}{2}\|z\|_{H_{\mathrm{at}}[\mathrm{Id}]}^2.$$

□

Corollary 9.4.3.

$$\epsilon^3 z^T \mathcal{H}_{at}[Y_{CB}]z \geqslant \kappa\|z\|_{\mathcal{H}_{at}[Id]}^2 \tag{9.21}$$

$$\epsilon^3 z^T \mathcal{H}_{at}[Y^t]z \geqslant \kappa\|z\|_{\mathcal{H}_{at}[Id]}^2 \tag{9.22}$$

where $Y^t = tY_{CB} + (1-t)Y$, *for* $Y \in B$.

Proposition 9.4.4. *If*

$$\epsilon^3 z^T \mathcal{H}_{at}[Y]z \geqslant \kappa\|z\|_{\mathcal{H}_{at}[Id]}^2$$

then

$$w_k^Y[\xi] \geqslant C\kappa\Lambda|\xi|^2, \quad \forall \xi \in \Omega_\epsilon^*, k = 1, 2, 3.$$

where $w_k^Y[\xi]$ *are eigenvalues of* $\mathcal{D}_{at}^Y[\xi]$.

Proof. For a given $\xi \in \Omega_\epsilon^*$, we have

$$\mathcal{D}_{\mathrm{at}}^Y = P_{\xi,Y}^T \mathrm{diag}(w_k^Y[\xi]) P_{\xi,Y}$$

let $z(X_j) = P^T_{\xi,Y} e_k e^{\imath X_j \xi}$, then

$$\epsilon^3 z^T \mathcal{H}_{\rm at}[Y] z = e_k^T P_{\xi,Y} \mathcal{D}^Y_{\rm at}[\xi] P^T_{\xi,Y} e_k = w^Y_k[\xi]$$

On the other hand, if $z(X_j) = P^T_{\xi,Y} e_k e^{\imath X_j \xi}$, then $\hat{z}[\xi'] = (P^T_{\xi,Y} e_k \delta_{\xi\xi'})$, so

$$\begin{aligned}
\|z\|^2_{\mathcal{H}_{\rm at}[\rm Id]} = &\sum_{\xi'} \hat{z}^T[\xi'] \mathcal{D}^{\rm Id}_{\rm at}[\xi'] \hat{z}[\xi'] \\
=& \hat{z}^T[\xi] \mathcal{D}^{\rm Id}_{\rm at}[\xi] \hat{z}[\xi] \\
=& e_k^T P_{\xi,Y} \mathcal{D}^{\rm Id}_{\rm at}[\xi] P^T_{\xi,Y} e_k \\
=& e_k^T P_{\xi,Y} P^T_{\xi,\rm Id} {\rm diag}(w^{\rm Id}_k[\xi]) P_{\xi,\rm Id} P^T_{\xi,Y} e_k \\
\geqslant& C\Lambda |\xi|^2.
\end{aligned}$$

Therefore

$$w^Y_k[\xi] = \epsilon^3 z^T \mathcal{H}_{\rm at}[Y] z \geqslant \kappa \|z\|^2_{\mathcal{H}_{\rm at}[\rm Id]} \geqslant C\kappa\Lambda|\xi|^2.$$

□

9.5 The atomistic model

Theorem 9.5.1. *Under Stability Condition B, i.e., the dynamical matrix $\mathcal{D}^{Id}_{at}[\xi]$ of the Hessian $\mathcal{H}_{at}[Id]$ of the above Euler-Lagrange equation in the undeformed state, i.e., $Y = Id$ or $u = 0$, satisfies*

$$\det \mathcal{D}^{Id}_{at}[\xi] \geqslant a_{at} \Lambda^6_{0,\epsilon}(\xi), \quad \xi \in \Omega^*_\epsilon, \tag{9.23}$$

further assume $m_a \in C^\infty, f_\epsilon \in H^{27}_\epsilon$, then there exists unique $Y_{at} \in H^5_\epsilon \cap X_\epsilon$ with the properties

Y_{at} satisfies the Euler-Lagrange equation

$$\mathcal{F}_{at}[Y_{at}](X) = f_\epsilon(X), \quad X \in \Omega_\epsilon \tag{9.24}$$

Consistency of Cauchy-Born rule holds

$$\|\mathcal{F}_{at}[Y_{CB}]\|_{\epsilon,5} \leqslant C(\|u_{CB}\|_{W^{29,\infty}})\epsilon^2 \tag{9.25}$$

Y_{at} is a $W^{1,\infty}_\epsilon$ local minimizer of the functional I_{at}.

Finally, there exists a positive constant C such that

$$\|Y_{at} - Y_{CB}\|_{\epsilon,7} \leqslant C\epsilon^2. \tag{9.26}$$

Proof. To solve $\mathcal{F}_{\rm at}[Y] = f_\epsilon$ in $B_{\kappa,7}(Y_{\rm CB}) = \{Y | \|Y - Y_{\rm CB}\|_{\epsilon,7} \leqslant \epsilon^\kappa, \sum_{X\in\Omega_\epsilon} Y(X) = 0\}$, $\kappa \in (\frac{3}{2}, 2)$, consider

$$\mathcal{F}_{\rm at}[Y] = \mathcal{F}_{\rm at}[Y_{\rm CB}] + \int_0^1 \mathcal{H}_{\rm at}[Y^t]dt(Y - Y_{\rm CB}) \tag{9.27}$$

in which $Y_{\rm CB}(X) = X + u_{\rm CB}(X), X \in \Omega_\epsilon$, $Y^t = tY_{\rm CB} + (1-t)Y$, for some $0 < t < 1$, and $\|Y - Y_{\rm CB}\|_{\epsilon,7} \leqslant \epsilon^\kappa$. So it is equivalent to find a fixed point $F(Y) = Y$ for

$$\int_0^1 \mathcal{H}_{\rm at}[Y^t]dt(F(Y) - Y_{\rm CB}) = -\mathcal{F}_{\rm at}[Y_{\rm CB}] \tag{9.28}$$

in $B_{\kappa,7}(Y_{\rm CB})$.

Take discrete Fourier transform, we get

$$\int_0^1 \widehat{\mathcal{H}_{\rm at}[Y^t]dt(F(Y) - Y_{\rm CB})}[\xi] = -\widehat{\mathcal{F}_{\rm at}[Y_{\rm CB}]}[\xi], \quad \forall \xi \in \Omega^*_\epsilon \tag{9.29}$$

Using the dynamical matrix, we get

$$\int_0^1 \mathcal{D}^{Y^t}_{\rm at}[\xi]dt\widehat{(F(Y) - Y_{\rm CB})}[\xi] = -\widehat{\mathcal{F}_{\rm at}[Y_{\rm CB}]}[\xi], \quad \forall \xi \in \Omega^*_\epsilon \tag{9.30}$$

Multiply both sides by $\widehat{(F(Y) - Y_{\rm CB})}^T[\xi]$

$$\widehat{(F(Y) - Y_{\rm CB})}^T[\xi] \int_0^1 \mathcal{D}^{Y^t}_{\rm at}[\xi]dt\widehat{(F(Y) - Y_{\rm CB})}[\xi] = -\widehat{(F(Y) - Y_{\rm CB})}^T[\xi]\widehat{\mathcal{F}_{\rm at}[Y_{\rm CB}]}[\xi] \tag{9.31}$$

By our perturbation of the Hessian above, i.e. Proposition 9.4.2, Corollary 9.4.3, Proposition 9.4.4 and Stability Condition C, we get

$$\Lambda|\xi|^2|(\widehat{F(Y)-Y_{\mathrm{CB}}})[\xi]|^2 \leqslant |(\widehat{F(Y)-Y_{\mathrm{CB}}})[\xi]||\widehat{\mathcal{F}_{\mathrm{at}}[Y_{\mathrm{CB}}]}[\xi]| \tag{9.32}$$

Multiply both sides by $|\xi|^{12}$, then sum over ξ and use Cauchy-Schwartz inequality on the RHS

$$\begin{aligned}\Lambda\sum_{\xi}|\xi|^{14}|(\widehat{F(Y)-Y_{\mathrm{CB}}})[\xi]|^2 &\leqslant \sum_{\xi}|\xi|^7|(\widehat{F(Y)-Y_{\mathrm{CB}}})[\xi]||\xi|^5|\widehat{\mathcal{F}_{\mathrm{at}}[Y_{\mathrm{CB}}]}[\xi]| \\ &\leqslant \Big(\sum_{\xi}|\xi|^{14}|(\widehat{F(Y)-Y_{\mathrm{CB}}})[\xi]|^2\Big)^{\frac{1}{2}}\Big(\sum_{\xi}|\xi|^{10}|\widehat{\mathcal{F}_{\mathrm{at}}[Y_{\mathrm{CB}}]}[\xi]|^2\Big)^{\frac{1}{2}}\end{aligned} \tag{9.33}$$

then by Lemma 2.3.1 we get

$$\Lambda\|F(Y)-Y_{\mathrm{CB}}\|_{\epsilon,7}^2 \leqslant \|F(Y)-Y_{\mathrm{CB}}\|_{\epsilon,7}\|\mathcal{F}_{\mathrm{at}}[Y_{\mathrm{CB}}]\|_{\epsilon,5} \tag{9.34}$$

So if $F(Y)-Y_{\mathrm{CB}}\neq 0$, then

$$\|F(Y)-Y_{\mathrm{CB}}\|_{\epsilon,7} \leqslant \Lambda^{-1}\|\mathcal{F}_{\mathrm{at}}[Y_{\mathrm{CB}}]\|_{\epsilon,5} \leqslant \Lambda^{-1}C\epsilon^2\|u_{\mathrm{CB}}\| \leqslant \epsilon^{\kappa}. \tag{9.35}$$

Thus we use Brouwer fixed point theorem to conclude that there is a unique solution $Y_{\mathrm{at}} \in B_{\kappa,7}(Y_{\mathrm{CB}})$. In fact, from the last inequality (9.35), we have the stricter estimate

$$\|Y_{\mathrm{at}}-Y_{\mathrm{CB}}\|_{\epsilon,7} \leqslant C\epsilon^2. \tag{9.36}$$

The consistency of Cauchy-Born rule was proved in Chapter 6. Now we show Y_{at} is a $W_{\epsilon}^{1,\infty}$ local minimizer of the functional I_{at} by Proposition 9.4.2.

Given any $Y:\Omega_{\epsilon}\to\mathbb{R}^3$ with $\|Y-Y_{\mathrm{at}}\|_{W_{\epsilon}^{1,\infty}} \leqslant \frac{\delta}{2}$, write

$$\mathcal{F}_{\mathrm{at}}(Y)-\mathcal{F}_{\mathrm{at}}(Y_{\mathrm{at}}) = (Y-Y_{\mathrm{at}})\cdot\int_0^1\mathcal{H}_{\mathrm{at}}[Y^t]dt\cdot(Y-Y_{\mathrm{at}}).$$

Note that

$$|Y^t-Y_{\mathrm{CB}}|_{W_{\epsilon}^{1,\infty}} \leqslant t|Y_{\mathrm{at}}-Y_{\mathrm{CB}}|_{W_{\epsilon}^{1,\infty}}+|Y-Y_{\mathrm{CB}}|_{W_{\epsilon}^{1,\infty}} \leqslant \delta$$

for sufficiently small ϵ. Then there exists a constant C such that

$$\mathcal{F}_{\mathrm{at}}(Y) - \mathcal{F}_{\mathrm{at}}(Y_{\mathrm{at}}) \geqslant C\epsilon^{-3}\|Y - Y_{\mathrm{at}}\|^2_{\mathcal{H}_{\mathrm{at}[\mathrm{Id}]}} > 0.$$

Therefore Y_{at} is a $W^{1,\infty}_{\epsilon}$ local minimizer.

□

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