SUPPLEMENTARY MATERIALS: STABILITY OF A FORCE-BASED HYBRID METHOD WITH PLANAR SHARP INTERFACE

JIANFENG LU* AND PINGBING MING†

S1. Lattice function and norms. We will consider only Bravais lattices in this work, which is denoted as $\mathbb{L}$. Let $\{a_j\}_{j=1}^d \subset \mathbb{R}^d$ be the basis vectors of $\mathbb{L}$, and d be the dimension,

$$\mathbb{L} = \Big\{ x \in \mathbb{R}^d \,\Big|\, x = \sum_j n_j a_j,\, n \in \mathbb{Z}^d \Big\}.$$

Let $\{b_j\}_{j=1}^d \subset \mathbb{R}^d$ be the reciprocal basis vectors satisfying $a_j \cdot b_k = 2\pi\delta_{jk}$,where δ_{jk} is the standard Kronecker delta symbol. The reciprocal lattice $\mathbb{L}^*$ is

$$\mathbb{L}^* = \Big\{ x \in \mathbb{R}^d \,\Big|\, x = \sum_j n_j b_j,\, n \in \mathbb{Z}^d \Big\}.$$

We take a computational domain

$$\Omega = \Big\{ \sum_j x_j a_j \,\Big|\, x \in [0,1)^d \Big\},$$

and let Ω_ε be a grid mesh in Ω with mesh size $\varepsilon = 1/(2N)$, $N \in \mathbb{Z}_+$:

$$\Omega_\varepsilon = \Big\{ x_\nu = \varepsilon \sum_j \nu_j a_j \,\Big|\, \nu \in \mathbb{Z}^d,\, 0 \le \nu_j < 2N \Big\}.$$

Using the reciprocal basis $\{b_j\}$, we define

$$\mathbb{L}^*_\varepsilon = \Big\{ \xi = \sum_j k_j b_j \,\Big|\, k \in \mathbb{Z}^d,\, -N \le k_j < N \Big\}.$$

We will identify functions defined on Ω_ε with their periodic extensions in this work, i.e., we consider the periodic boundary condition. General boundary conditions will be left for future work.

For $\mu \in \mathbb{Z}^d$, we define the translation operator T^μ_ε as

$$(T^\mu_\varepsilon u)(x) = u(x + \varepsilon \mu_j a_j) \quad \text{for } x \in \mathbb{R}^d,$$

where the index summation convention is used. We define the forward and backward difference operators as

$$D^+_{\varepsilon,\mu} = \varepsilon^{-1}(T^\mu_\varepsilon - I) \qquad \text{and} \qquad D^-_{\varepsilon,\mu} = \varepsilon^{-1}(I - T^{-\mu}_\varepsilon),$$

*Department of Mathematics, Physics, and Chemistry, Duke University, Box 90320, Durham, NC, 27708 USA. Email: jianfeng@math.duke.edu

†LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, AMSS, Chinese Academy of Sciences, No. 55, Zhong-Guan-Cun East Road, Beijing 100190, China. Email: mpb@lsec.cc.ac.cn

where I denotes the identity operator. We say α is a multi-index, if $\alpha \in \mathbb{Z}^d$ and $\alpha \geq 0$. We will use the notation $|\alpha| = \sum_{j=1}^d \alpha_j$. For a multi-index α, the difference operator D_ε^α is given by

$$D_\varepsilon^\alpha = \prod_{j=1}^d (D_{\varepsilon,e_j}^+)^{\alpha_j},$$

where $\{e_j\}_{j=1}^d$ are the canonical basis of $\mathbb{R}^d$ (columns of a $d \times d$ identity matrix).

We will use various norms for functions defined on Ω_ε. For integer $k \geq 0$, define the difference norm

$$\|u\|_{\varepsilon,k}^2 = \sum_{0\leq|\alpha|\leq k} \varepsilon^d \sum_{x\in\Omega_\varepsilon} |(D_\varepsilon^\alpha u)(x)|^2 .$$

It is clear that $\|\cdot\|_{\varepsilon,k}$ is a discrete analog of Sobolev norm associated with $H^k(\Omega)$. Hence, we denote the corresponding spaces of lattice functions as $H_\varepsilon^k(\Omega)$ and $L_\varepsilon^2(\Omega)$ when $k = 0$. We also need the uniform norms on Ω_ε, which are defined as

$$\begin{aligned}
\|u\|_{L_\varepsilon^\infty} &= \max_{x\in\Omega_\varepsilon} |u(x)| , \\
\|u\|_{W_\varepsilon^{k,\infty}} &= \sum_{0\leq|\alpha|\leq k} \max_{x\in\Omega_\varepsilon} |(D_\varepsilon^\alpha u)(x)| .
\end{aligned}$$

Recall that we identify lattice function u with its periodic extension to function defined on $\varepsilon\mathbb{L}$, and hence differences of the lattice functions are well-defined. These norms may be extended to vector-valued functions as usual. For $k > d/2$, we have the discrete Sobolev inequality $\|u\|_{L_\varepsilon^\infty} \lesssim \|u\|_{\varepsilon,k}$. Here and throughout this paper, we denote $A \lesssim B$ if $A \leq CB$ with C an absolute constant.

The discrete Fourier transform for a lattice function u is given for $\xi \in \mathbb{L}_\varepsilon^*$ by

$$\widehat{u}(\xi) = \Big(\frac{\varepsilon}{2\pi}\Big)^d \sum_{x\in\Omega_\varepsilon} e^{-\imath\xi\cdot x} u(x).$$

By the Fourier inversion formula, for $x \in \Omega_\varepsilon$,

$$u(x) = \sum_{\xi\in\mathbb{L}_\varepsilon^*} e^{\imath x\cdot\xi}\widehat{u}(\xi).$$

We will use a symbol introduced by Nirenberg in [2626, 26], which plays the same role for the difference operators as $\Lambda^2(\xi) = 1 + \Lambda_0^2(\xi) = 1 + |\xi|^2$ for the differential operators. For $\varepsilon > 0$, let

$$\Lambda_{j,\varepsilon}(\xi) = \frac{1}{\varepsilon}\left|e^{\imath\varepsilon\xi_j} - 1\right|, \qquad j = 1, \cdots, d,$$

and

$$\Lambda_\varepsilon^2(\xi) = 1 + \Lambda_{0,\varepsilon}^2(\xi) = 1 + \sum_{j=1}^d \Lambda_{j,\varepsilon}^2(\xi) = 1 + \sum_{j=1}^d \frac{4}{\varepsilon^2}\sin^2\Big(\frac{\varepsilon\xi_j}{2}\Big).$$

It is not hard to check for any $\xi \in \mathbb{L}_\varepsilon^*$, there holds

$$c\Lambda^2(\xi) \leq \Lambda_\varepsilon^2(\xi) \leq \Lambda^2(\xi),$$

where the positive constant c depends on $\{b_j\}$.

S2. Proof of Lemma 3.2. Let us first recall the following consistency lemma proved in [2222; 22, Section 2] (proofs of these results do not depend on the smoothness of ϱ).

LEMMA S2.1 (Consistency). *For any u smooth, we have*

$$\|\mathcal{F}_{\rm at}[u]-\mathcal{F}_{\rm CB}[u]\|_{L^\infty_\varepsilon} \le C\varepsilon^2 \|u\|_{W^{18,\infty}}, \tag{S2.1}$$

$$\|\mathcal{F}_{\varepsilon}[u]-\mathcal{F}_{\rm CB}[u]\|_{L^\infty_\varepsilon} \le C\varepsilon^2 \|u\|_{W^{18,\infty}}, \tag{S2.2}$$

$$\|\mathcal{F}_{\rm hy}[u]-\mathcal{F}_{\rm at}[u]\|_{L^\infty_\varepsilon} \le C\varepsilon^2 \|u\|_{W^{18,\infty}}, \tag{S2.3}$$

where the constant C depends on V and $\|u\|_{L^\infty}$, but is independent of ε.

Proof. [Proof of Lemma 3.2] The proof for (3.6) and (3.7) are analogous, and hence we will only prove the latter. By definition, for $1 \le j,k \le d$,

$$(h_{\rm at})_{jk}(\xi) = e^{-\imath x\cdot\xi}(\mathcal{H}_{\rm at}(e_k f_\xi))_j(x),$$
$$(h_{\rm hy})_{jk}(x,\xi) = e^{-\imath x\cdot\xi}(\mathcal{H}_{\rm hy}(e_k f_\xi))_j(x),$$

where $f_\xi(x) = e^{\imath x\cdot\xi}$ for $x\in\Omega$. Taking difference of the above two equations, we obtain the bound

$$|h_{\rm at}(\xi)-h_{\rm hy}(x,\xi)| \le C \sup_{1\le k\le d} \|\mathcal{H}_{\rm at}(e_k f_\xi)-\mathcal{H}_{\rm hy}(e_k f_\xi)\|_{L^\infty_\varepsilon}.$$

Note that by the definition of linearized operators $\mathcal{H}_{\rm at}$ and $\mathcal{H}_{\rm hy}$, we have

$$\mathcal{H}_{\rm at}(e_k f_\xi)-\mathcal{H}_{\rm hy}(e_k f_\xi) = \lim_{t\to 0^+}\frac{1}{t}\big(\mathcal{F}_{\rm at}[t(e_k f_\xi)]-\mathcal{F}_{\rm hy}[t(e_k f_\xi)]\big).$$

Hence,

$$\begin{aligned}\|\mathcal{H}_{\rm at}(e_k f_\xi)-\mathcal{H}_{\rm hy}(e_k f_\xi)\|_{L^\infty_\varepsilon} &= \lim_{t\to 0^+}\frac{1}{t}\|\mathcal{F}_{\rm at}[t(e_k f_\xi)]-\mathcal{F}_{\rm hy}[t(e_k f_\xi)]\|_{L^\infty_\varepsilon}\\ &\lesssim \varepsilon^2\|e_k f_\xi\|_{W^{18,\infty}} \lesssim \varepsilon^2\|e_k f_\xi\|_{H^s} \lesssim \varepsilon^2(1+|\xi|^2)^{s/2},\end{aligned}$$

where s is chosen so that the Sobolev inequality $\|f\|_{W^{18,\infty}(\Omega)} \le C\|f\|_{H^s(\Omega)}$ holds for any $f\in H^s(\Omega)$ (s depends on the dimension). Here, we have used Lemma S2.1 in the first inequality, noticing that $\|te_k f_\xi\|_{L^\infty}$ is uniformly bounded for ξ as $t\to 0$. This concludes the proof. ∎

S3. Additional details for Example 1. LEMMA S3.1. *z_1, z_2 and z_3 are distinct roots.*

Proof. It is clear that

$$z_2 = w_2\zeta^{1/2} \quad\text{and}\quad z_3 = w_3\zeta^{1/2}$$

with $-1 < w_3 < 0 < w_2 < 1$, this implies $z_2 \ne z_3$.

A direct calculation gives

$$\begin{aligned} z_1 &= \frac{6-\zeta-\bar\zeta-\sqrt{\left(4-\zeta-\bar\zeta\right)\left(2-\zeta-\bar\zeta\right)}}{2(1+\bar\zeta)}\\ &= \frac{6-\zeta-\bar\zeta-\sqrt{\left(4-\zeta-\bar\zeta\right)\left(2-\zeta-\bar\zeta\right)}}{2(1+\zeta)\left(1+\bar\zeta\right)}(1+\zeta)\\ &= \frac{6-\zeta-\bar\zeta-\sqrt{\left(4-\zeta-\bar\zeta\right)\left(2-\zeta-\bar\zeta\right)}}{2\left(2+\zeta+\bar\zeta\right)}\left(\zeta^{1/2}+\bar\zeta^{1/2}\right)\zeta^{1/2}.\end{aligned}$$

Recalling $\zeta = e^{\imath\theta}$ with $\theta \in (-\pi, \pi)$, and we may write

$$z_1 = \frac{2\cos(\theta/2)}{3 - \cos\theta + \sqrt{(7-\cos\theta)(1-\cos\theta)}}\, e^{\imath\theta/2}.$$

Note that

$$\frac{2\cos(\theta/2)}{3 - \cos\theta + \sqrt{(7-\cos\theta)(1-\cos\theta)}} > 0 > w_3,$$

this implies $z_1 \neq z_3$.

It remains to prove $z_1 \neq z_2$. Note that

$$z_2 = \frac{1}{2}\left(B - \sqrt{B^2-4}\right) e^{\imath\theta/2}$$

with

$$B = -A/2 + \sqrt{A^2/4 + 14 - \left(\zeta + \bar{\zeta}\right)}.$$

Using

$$A = \zeta + \bar{\zeta} + \zeta^3 + \bar{\zeta}^3 = \left(\zeta + \bar{\zeta}\right)\left(\zeta^2 + \bar{\zeta}^2\right) = 4\cos(\theta/2)\cos\theta,$$

we write

$$\begin{aligned} A^2/4 + 14 - \left(\zeta + \bar{\zeta}\right) &= 16\cos^2(\theta/2)\cos^2\theta + 14 - 2\cos\theta \\ &= 16\cos^2(\theta/2)\cos^2\theta + 14 - 2(2\cos^2(\theta/2) - 1) \\ &= 16 - 4\cos^2(\theta/2)\sin^2\theta. \end{aligned}$$

This gives

$$B = 2\sqrt{4 - \cos^2(\theta/2)\sin^2\theta} - 2\cos(\theta/2)\cos\theta.$$

To prove $z_1 \neq z_2$, it remains to show $|z_1| \neq |z_2|$, i.e.,

$$\frac{1}{2}\left(B - \sqrt{B^2-4}\right) \neq \frac{2\cos(\theta/2)}{3 - \cos\theta + \sqrt{(7-\cos\theta)(1-\cos\theta)}}.$$

Actually, we shall prove that for $\theta \in (-\pi, \pi)$ and $\theta \neq 0$, there holds

$$\frac{1}{2}\left(B - \sqrt{B^2-4}\right) > \frac{2\cos(\theta/2)}{3 - \cos\theta + \sqrt{(7-\cos\theta)(1-\cos\theta)}}. \tag{S3.1}$$

The above inequality is equivalent to

$$3 - \cos\theta + \sqrt{(7-\cos\theta)(1-\cos\theta)} > \cos(\theta/2)\left(B + \sqrt{B^2-4}\right). \tag{S3.2}$$

Denote by $t = \cos(\theta/2)$, we write the above inequality as

$$2 - t^2 + \sqrt{(4-t^2)(1-t^2)} > t\left(g(t) + \sqrt{g^2(t) - 1}\right), \qquad t \in [0, 1), \tag{S3.3}$$

where

$$g(t) := t - 2t^3 + 2\sqrt{1 - t^4 + t^6}.$$

To prove (S3.3), we firstly prove

$$2 - t^2 > tg(t) \qquad t \in [0, 1). \tag{S3.4}$$

A direct calculation gives

$$\begin{aligned} 2 - t^2 - tg(t) &= 2(1 - t^2) + 2t\left(t^3 - \sqrt{1 - t^4 + t^6}\right) \\ &= 2(1 - t^2) + \frac{2t(t^4 - 1)}{\sqrt{1 - t^4 + t^6} + t^3} \\ &= 2(1 - t^2)\left(1 - \frac{t + t^3}{\sqrt{1 - t^4 + t^6} + t^3}\right). \end{aligned}$$

Note that

$$\sqrt{1 - t^4 + t^6} > t,$$

which follows from $(1 - t^2)(1 - t^4) > 0$. Combining the above two inequalities, we obtain (S3.4).

Next, by (S3.4) and note $g(t) \geq 0$, we obtain

$$(4 - t^2)(1 - t^2) = (2 - t^2)^2 - t^2 \geq t^2(g^2(t) - 1).$$

A direct calculation gives that $g(t) \geq 1$. Therefore,

$$\sqrt{(4 - t^2)(1 - t^2)} \geq t\sqrt{g^2(t) - 1},$$

which together with (S3.4) gives (S3.3). This implies $z_1 \neq z_2$ and completes the proof. □