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On the Effect of Ghost Force in the Quasicontinuum Method: Dynamic Problems in One Dimension

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Abstract. Numerical error caused by "ghost forces" in a quasicontinuum method is studied in the context of dynamic problems. The error in the discrete $W^{1,\infty}$ norm is analyzed for the time scale $\mathcal{O}(\varepsilon)$ and the time scale $\mathcal{O}(1)$ with ε being the lattice spacing.

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Key words: Quasicontinuum methods, ghost force, dynamic problems.

1 Introduction

The present paper is concerned with the error caused by ghost forces in quasicontinuum (QC) type of multiscale coupling methods for crystalline solids. In these methods, one reduces the degrees of freedom of an atomic level description by replacing part of the system with continuum mechanics models [2,15,25,38,39]. Such integrated methods have been very useful in studying mechanical properties of solids. It allows one to simulate a relatively large system while still able to keep the atomistic description around the critical areas, such as crack tips and dislocation cores. These methods have also drawn much attention from numerical analysts. We refer to [6, 7, 11, 12, 21, 27, 30, 36] and references therein for a list of representative works. Nevertheless, many challenges in the analysis of these methods still remain. Examples include full three-dimensional problems, systems with line or wall defects, and problems with bifurcation. We refer to [22, 31] for a review

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of the recent progress in this area. A critical issue that arises in the numerical analysis is *ghost forces*, which is the non-zero forces on the atoms near the atomistic/continuum interface at an equilibrium state [38]. For statics problems, the removal of ghost forces is a necessary ingredient to achieve uniform accuracy [11,30]. For one-dimensional models, the influence of ghost forces has been explicitly characterized in [6, 26, 27]. They found that the ghost force induces a negligible error on the solution, which is usually as small as the lattice spacing. But it may lead to an $\mathcal{O}(1)$ error on the gradient of the solution at the interface, which decays to $\mathcal{O}(\varepsilon)$ at distance $\mathcal{O}(\varepsilon|\ln\varepsilon|)$ from the interface with ε being the lattice spacing. The influence of the ghost force for a two-dimensional model and a three-dimensional model with a planar interface has recently been studied in [4,5]. It was found that the ghost forces still lead to an $\mathcal{O}(\varepsilon)$ error on the solution, while the gradient of the error is $\mathcal{O}(1)$, which decays from the interface to $\mathcal{O}(\varepsilon)$ over a distance at most $\mathcal{O}(\sqrt{\varepsilon})$. The decay rates seem to be much smaller than that of the one-dimensional problems.

The QC method can be extended to dynamic problems using the coarse-grained energy and the Hamilton's principle [33,37]. The dynamic QC method couples an elastodynamics model with a molecular dynamics model. Many dynamic coupling methods with similar goals have recently been developed, see [1, 2, 8–10, 17, 18, 20, 32, 35, 40, 41, 43–45]. However, very little has been done to study the stability and accuracy of these methods. Most numerical studies have been focused on the artificial reflections at the interface. The reflection is caused by the drastic change in the dispersion relation across the interface, which is often due to the difference between the mesh size in the continuum region and the lattice spacing in the molecular dynamics model. The reflection can be studied by considering an incident wave packet traveling toward the interface and examine the amplitude of the reflected waves [8,19]. The issue of ghost forces for the dynamic problems, however, has not yet been addressed.

The purpose of this paper is to study the effect of ghost forces in the context of *dynamic problems*. To focus primarily on the issue of ghost forces, we consider the dynamic models in [33, 37] derived from the original QC method when the mesh size coincides with the lattice spacing. In addition, the initial displacement is given by a uniform deformation. This allows us to compute the error caused only by the ghost forces. The error will be studied in the discrete $W^{1,\infty}$-norm as done for static problems [4,6,26,27]. The maximum norm for the gradient of the error is particularly suited for the ghost force issue because it controls the pointwise accuracy, while the error measured in the discrete $W^{1,p}$ norm or in the discrete L^p norm with $1<p<\infty$ is often insufficient because it cannot fully reflect the local oscillatory nature of the ghost force. From a practical viewpoint, the discrete gradient measures the relative atomic displacement. Therefore, a pointwise measure is more indicative of the local lattice distortion and it is extremely useful for understanding how the error influences the structures of local defects. Our study shows that the error, which is initially zero, grows dramatically quickly, and already becomes $\mathcal{O}(1)$ at the $\mathcal{O}(\varepsilon)$ time scale. The error exhibits fast oscillations, with amplitude of the order of ε. On the $\mathcal{O}(1)$ time scale, which is typically the time scale of interest, the amplitude of the oscillations grows, and it is bounded by an $\mathcal{O}(\sqrt{\varepsilon})$ quantity. The average of the oscillations has a peak at the interface. In contrast to the static case, where the error is mainly concentrated at the interface, the error in the dynamic case is observed in the entire domain on the time scale $\mathcal{O}(1)$. These observations are quite different from those of wave reflections, and it indicates that the effect of ghost forces is a separate numerical issue.

The proof of our results starts with an explicit representation of the error, and the discrete $W^{1,\infty}$-norm of the error is reduced to estimating certain exponential sums, which is achieved by the truncated Poisson summation formula of Van der Corput [42]. Our approach differs from the standard way for estimating the solution of the discrete dispersive equations as in [24, 34]. The main reason is that the problem under study has an oscillatory source term that is orthogonal to a constant, which plays a key role for obtaining the sharp estimate of the error as suggested in [6, 27]. We do not know presently how to adapt the arguments in [24, 34] to deal with the oscillatory term. Moreover, the main concern in [24, 34] is the solution instead of the gradient of the solution, which is our main concerns.

The rest of the paper is organized as follows. In Section 2 we describe the one-dimensional atomistic model and the derivation of the QC model, and briefly demonstrate the appearance of ghost forces. In Section 3 we show results from several numerical tests. They provide certain insight into the evolution of the error. The next three sections are devoted to the analysis of the error for short and long time scales. We draw some conclusions in the last section.

2 Motivation and the formulation of the problem

As in [13], we consider the dynamic problem of a one-dimensional chain of atoms. The interatomic interaction is assumed to be among the nearest and the next nearest neighbors. Let x be the reference position of an atom, and $\widetilde{y}(x,t)$ be the current position at time t. The equations of motion for the atoms in the chain read as

$$\begin{cases} \ddot{\widetilde{y}}(x,t) - \mathcal{L}_{\rm at}[\widetilde{y}](x,t) = 0, \quad x \in \mathbb{L}, \\ \widetilde{y}(x,0) = x, \quad \dot{\widetilde{y}}(x,0) = x, \\ \widetilde{y}(x,t) - x \text{ is periodic with period 1.} \end{cases} \tag{2.1}$$

Here, we have set the mass to unity, and $\mathbb{L} \equiv \{j\varepsilon, j \in \mathbb{N}\} \cap (-1/2, 1/2]$ with ε being the lattice spacing. The operator $\mathcal{L}_{\rm at}$ is defined as

$$\begin{aligned} \mathcal{L}_{\rm at}[z](x,t) \equiv \varepsilon^{-2} \big[&\kappa_2 z(x-2\varepsilon,t) + \kappa_1 z(x-\varepsilon,t) + \kappa_1 z(x+\varepsilon,t) + \kappa_2 z(x+2\varepsilon,t) \\ &- 2(\kappa_1+\kappa_2) z(x,t) \big]. \end{aligned} \tag{2.2}$$

Since the ghost force arises from interactions beyond nearest neighbors instead of the nonlinearity, we consider a linear model, which may be viewed as a harmonic approximation of a fully nonlinear model. In (2.2), κ_1 and κ_2 are the force constants computed from an interatomic potential. For example, for a pairwise potential φ, the total energy is given by

$$E=\sum_x\left[\varphi\left(\frac{y(x+\varepsilon)-y(x)}{\varepsilon}\right)+\varphi\left(\frac{y(x+2\varepsilon)-y(x)}{\varepsilon}\right)\right].$$

A direct calculation yields

$$\kappa_1=\varphi''(1),\qquad \kappa_2=\varphi''(2).$$

One commonly used potential function is the Lennard-Jones potential [16]:

$$\varphi(r)=(\sigma/r)^{12}-(\sigma/r)^6,$$

where σ is a length scale parameter. If only the nearest and the next nearest neighborhood interactions are considered, the lattice spacing is given by

$$\varepsilon=\sigma/K^{1/6}\quad\text{with}\quad K=(1+2^{-6})/[2(1+2^{-12})].$$

The force constants are

$$\begin{aligned}\kappa_1&=156K^2-42K\approx 18.886,\\ \kappa_2&=2^{-6}(156K^2 2^{-6}-42K)\approx -0.323.\end{aligned}$$

Throughout this paper, we shall assume the following stability condition

$$\kappa_1>0,\qquad \kappa_1+4\kappa_2>0.$$

With the harmonic approximation, the total energy takes the form of

$$E=\sum_x\left[\frac{\kappa_1}{2}\left(\frac{y(x+\varepsilon)-y(x)}{\varepsilon}\right)^2+\frac{\kappa_2}{2}\left(\frac{y(x+2\varepsilon)-y(x)}{\varepsilon}\right)^2\right].$$

The dynamic model (2.1) can be derived from this energy using Hamilton's principle. The total energy can be written as the sum of the energy at each atom site, i.e., $E=\sum_x E(x)$ with

$$\begin{aligned}E(x)=&\frac{\kappa_2}{4}\left(\frac{y(x+2\varepsilon)-y(x)}{\varepsilon}\right)^2+\frac{\kappa_1}{4}\left(\frac{y(x+\varepsilon)-y(x)}{\varepsilon}\right)^2\\ &+\frac{\kappa_1}{4}\left(\frac{y(x)-y(x-\varepsilon)}{\varepsilon}\right)^2+\frac{\kappa_2}{4}\left(\frac{y(x)-y(x-2\varepsilon)}{\varepsilon}\right)^2.\end{aligned}$$

In the QC method, one defines a local region where the atomistic model is approximated by the Cauchy-Born elasticity model [3]. One also defines a nonlocal region where the atomistic description is kept. Without loss of generality, we assume that the interface is located at $x=0$ and the nonlocal region is in the domain $x<0$. We further assume that the mesh size is equal to the lattice parameter to primarily focus on the effect of ghost forces. The Cauchy-Born approximation of the energy in the local region is given by

$$E_{\rm CB}(x)=\frac{\kappa_1+4\kappa_2}{4}\left(\frac{y(x+\varepsilon)-y(x)}{\varepsilon}\right)^2+\frac{\kappa_1+4\kappa_2}{4}\left(\frac{y(x)-y(x-\varepsilon)}{\varepsilon}\right)^2.$$

At the interface $x=0$, the energy takes a mixed form:

$$\begin{aligned}E(0)=&\frac{\kappa_2}{4}\left(\frac{y(x)-y(x-2\varepsilon)}{\varepsilon}\right)^2+\frac{\kappa_1}{4}\left(\frac{y(x)-y(x-\varepsilon)}{\varepsilon}\right)^2\\&+\frac{\kappa_1+4\kappa_2}{4}\left(\frac{y(x+\varepsilon)-y(x)}{\varepsilon}\right)^2.\end{aligned}$$

With such energy summation rule, we may write the QC approximation of $\mathcal{L}_{\rm at}$ as $\mathcal{L}_{\rm qc}$, with $\mathcal{L}_{\rm qc}$ given below. For $x\le -2\varepsilon$,

$$\begin{aligned}\mathcal{L}_{\rm qc}[z](x,t)\equiv\varepsilon^{-2}\big[&\kappa_2 z(x-2\varepsilon,t)+\kappa_1 z(x-\varepsilon,t)+\kappa_1 z(x+\varepsilon,t)+\kappa_2 z(x+2\varepsilon,t)\\&-2(\kappa_1+\kappa_2)z(x,t)\big],\end{aligned}$$

and for $x\ge 2\varepsilon$,

$$\mathcal{L}_{\rm qc}[z](x,t)=\mathcal{L}_{\rm CB},\quad \mathcal{L}_{\rm CB}\equiv\varepsilon^{-2}(\kappa_1+4\kappa_2)[z(x-\varepsilon,t)-2z(x,t)+z(x+\varepsilon,t)].$$

This is exactly the operator corresponding to the Cauchy-Born approximation.

At the interface, we have for $x=-\varepsilon$,

$$\begin{aligned}\mathcal{L}_{\rm qc}[z](x,t)\equiv\varepsilon^{-2}\Big[&\kappa_2 z(x-2\varepsilon,t)+\kappa_1 z(x-\varepsilon,t)+\kappa_1 z(x+\varepsilon,t)+\frac{\kappa_2}{2}z(x+2\varepsilon,t)\\&-(2\kappa_1+3\kappa_2/2)z(x,t)\Big],\end{aligned}$$

for $x=0$,

$$\begin{aligned}\mathcal{L}_{\rm qc}[z](x,t)\equiv\varepsilon^{-2}\Big[&\kappa_2 z(x-2\varepsilon,t)+\kappa_1 z(x-\varepsilon,t)+(\kappa_1+4\kappa_2)z(x+\varepsilon,t)\\&-(2\kappa_1+5\kappa_2)z(x,t)\Big],\end{aligned}$$

and for $x=\varepsilon$,

$$\begin{aligned}\mathcal{L}_{\rm qc}[z](x,t)\equiv\varepsilon^{-2}\Big[&\frac{\kappa_2}{2}z(x-2\varepsilon,t)+(\kappa_1+4\kappa_2)z(x-\varepsilon,t)+(\kappa_1+4\kappa_2)z(x+\varepsilon,t)\\&-(2\kappa_1+17\kappa_2/2)z(x,t)\Big].\end{aligned}$$

Using the Hamilton's principle, we write the QC model as

$$\begin{cases}\ddot{\widetilde{y}}(x,t)-\mathcal{L}_{\rm qc}[\widetilde{y}](x,t)=0, & x\in\mathbb{L},\\ \widetilde{y}(x,0)=x,\quad \dot{\widetilde{y}}(x,0)=x,\\ \widetilde{y}(x,t)-x \text{ is periodic with period 1.}\end{cases}\tag{2.3}$$

We scaled the mass to be unity for simplicity. The initial and boundary conditions have been chosen as a uniform deformation in order to identify the effect of the ghost force. We will compute the deviation of the solution away from the equilibrium. For this purpose, we define the error $y(x,t) = \widetilde{y}(x,t) - x$, and the error satisfies

$$\begin{aligned}\ddot{y}(x,t) - \mathcal{L}_{\rm qc}[y](x,t) &= \ddot{\widetilde{y}}(x,t) - \mathcal{L}_{\rm qc}[\widetilde{y} - x](x,t)\\ &= \mathcal{L}_{\rm qc}[x](x,t) \equiv f(x,t)\end{aligned} \tag{2.4}$$

with f given by

$$f(x,t) = \begin{cases} 0 & \text{if } \ |x| \geq 2\varepsilon, \\ -\dfrac{\kappa_2}{\varepsilon} & \text{if } \ x = -\varepsilon, \\ \dfrac{2\kappa_2}{\varepsilon} & \text{if } \ x = 0, \\ -\dfrac{\kappa_2}{\varepsilon} & \text{if } \ x = \varepsilon. \end{cases} \tag{2.5}$$

The function $f(x,t)$ is precisely the ghost force. Since it is independent of the temporal variable, we denote it by $f(x)$ for simplicity. Finally, we supplement the above problem with the homogeneous initial condition and periodic boundary condition as

$$\begin{cases} y(x,0) = 0 \ \text{ and } \ \dot{y}(x,0) = 0, \quad x \in \mathbb{L}. \\ y(x,t) \ \text{ is periodic with period 1.} \end{cases} \tag{2.6}$$

3 Observations from numerical results

In this section we show several numerical results. Since the operator $\mathcal{L}_{\rm qc}$ coincides with $\mathcal{L}_{\rm CB}$ in the local region, and with $\mathcal{L}_{\rm at}$ in the nonlocal region, it is natural to look at models similar to (2.4), in which $\mathcal{L}_{\rm qc}$ is replaced by either $\mathcal{L}_{\rm CB}$ or $\mathcal{L}_{\rm at}$ in the entire domain. Therefore, our numerical experiments are conducted for the following three models:

- Model I: $\mathcal{L}_{\rm qc}$ is approximated by $\mathcal{L}_{\rm CB}$: $\ddot{y} - \mathcal{L}_{\rm CB}[y] = f$.
- Model II: $\mathcal{L}_{\rm qc}$ is approximated by $\mathcal{L}_{\rm at}$: $\ddot{y} - \mathcal{L}_{\rm at}[y] = f$.
- Model III: The quasicontinuum model (2.4).

In all these models, we impose homogeneous initial condition and periodic boundary condition (2.6).

As an example, the force constants are obtained from the Morse potential [29]. In particular, we choose $\kappa_1 = 4.4753$ and $\kappa_2 = 0.4142$. All the simulations are performed in the domain $x \in (-1/2, 1/2]$, and the ODEs are integrated using the Verlet's method. Since all three models are Hamiltonian systems, this method is particularly suitable.

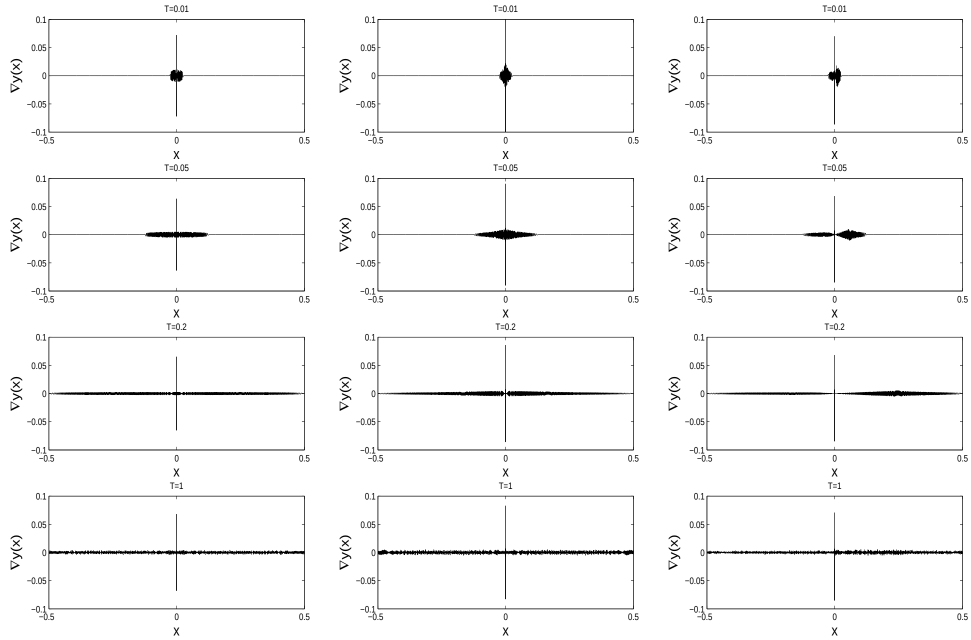

Figure 1: The gradient of the error. Left to right: Solution computed from Model I, II and III. From top to bottom: The solutions at time $t=0.01, 0.05, 0.2$ and 1. $\varepsilon=1/2000$.

First we show the solutions computed from the three models at different time step. The results are shown in Fig. 1. For this set of numerical tests, we have chosen $\varepsilon=1/2000$. We observe that the error firstly develops at the interface, and then it starts to spread toward the local and nonlocal region for all three models. Another noticeable feature is that the error exhibits a peak at the interface, and the peak remains for all later time. At $t=1$, the error is observed in the entire domain. Our main observations here can be summarized as following:

(1) In the presence of ghost forces, the error grows very quickly. It reaches $\mathcal{O}(1)$ on the time scale $\mathcal{O}(\varepsilon)$;

(2) On the time scales $t=\mathcal{O}(\varepsilon)$ and $t=\mathcal{O}(1)$, the solutions of all three models are qualitatively the same.

Next we monitor the solution for those atoms near the interface. In Fig. 2, we show the time history for those atoms. We observe that for most of the time, the error oscillates around certain constant values, and the constant values depend on the location of the atom. These constant values show a peak at the interface $x=0$.

In Figs. 3 and 4, we show the time history of the solution at the interface for various values of ε. The observation is that the amplitude of the oscillation decrease as ε gets small. However, the constant values around which the solutions oscillate do not change as ε varies.

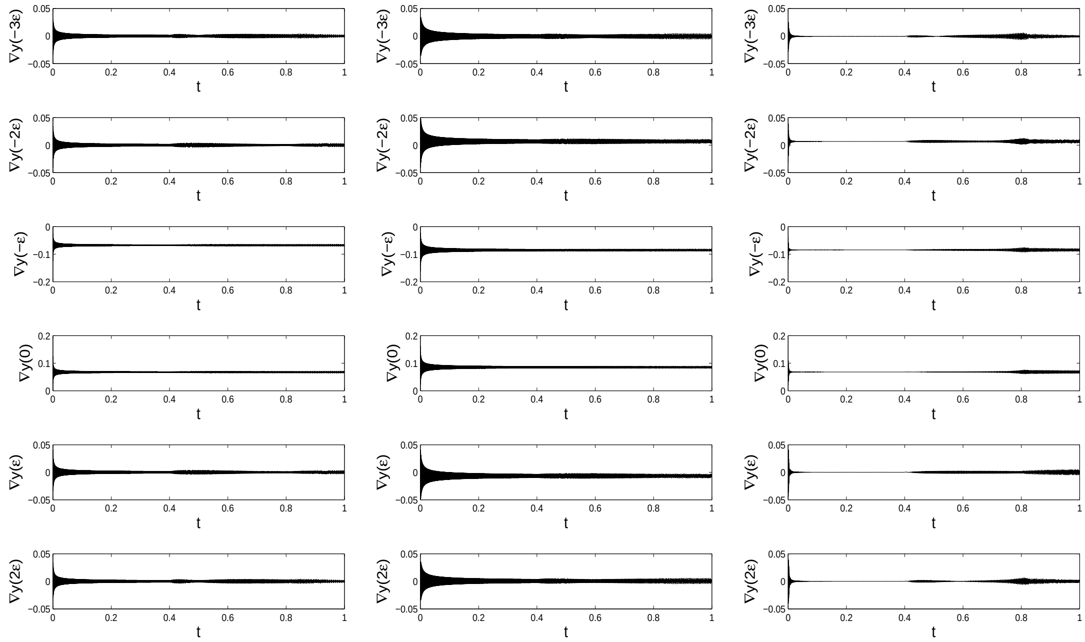

Figure 2: The time history of the gradient of the error near the interface. Left to right: Solution computed from Model I, II and III. From top to bottom: The solutions near the interface: $x=-3\varepsilon, x=-2\varepsilon, x=-\varepsilon, x=0, x=\varepsilon$ and $x=2\varepsilon$.

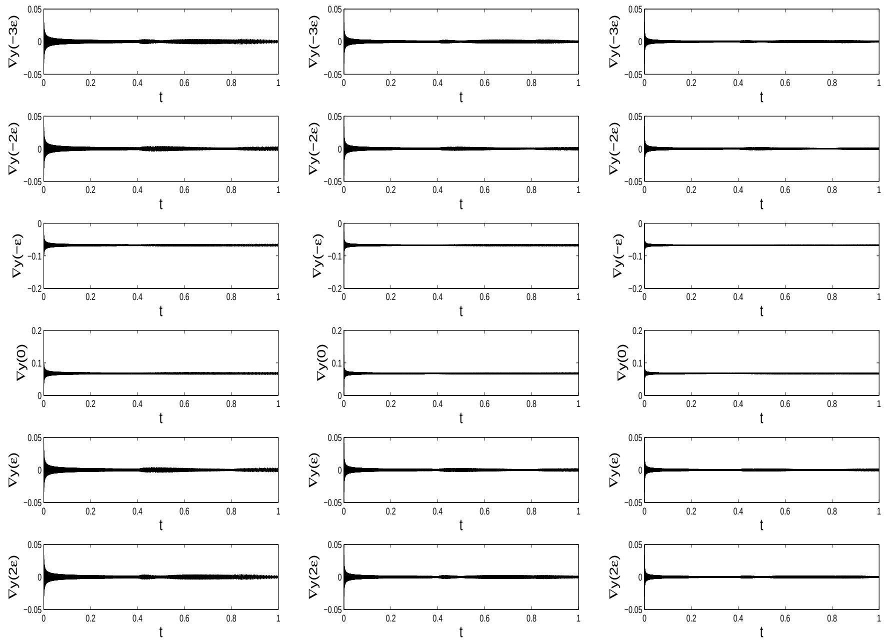

Figure 3: The gradient of the error. The solutions are computed from Model I with different choice of ϵ. Left to right: Solution computed for $\varepsilon=1/2000$, $\varepsilon=1/4000$ and $\varepsilon=1/8000$. From top to bottom: The solutions near the interface: $x=-3\varepsilon$, $x=-2\varepsilon$, $x=-\varepsilon$, $x=0$, $x=\varepsilon$ and $x=2\varepsilon$.

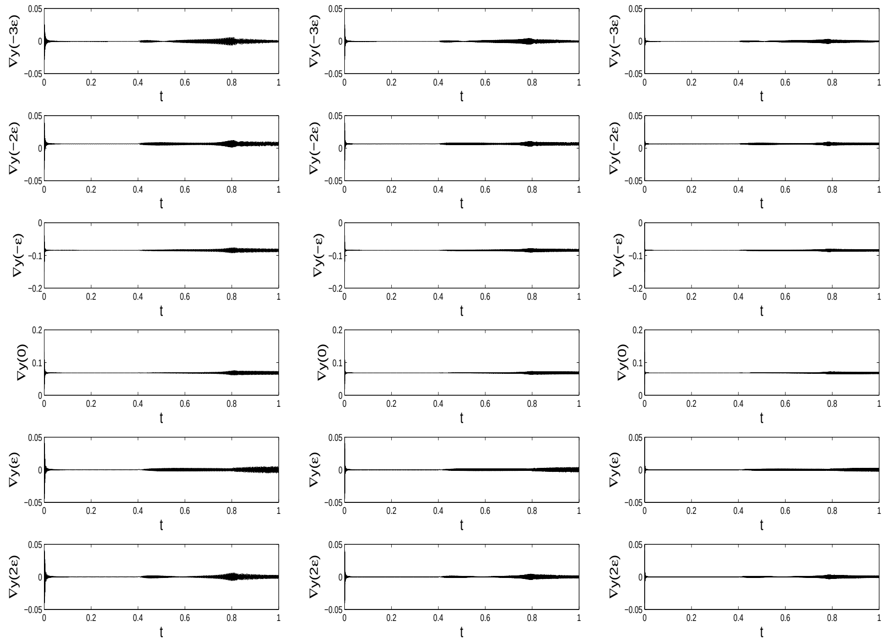

Figure 4: The gradient of the error. The solutions are computed from Model III with different choices of ε. Left to right: Solution computed for $\varepsilon=1/2000$, $\varepsilon=1/4000$ and $\varepsilon=1/8000$. From top to bottom: The solutions near the interface: $x=-3\varepsilon$, $x=-2\varepsilon$, $x=-\varepsilon$, $x=0$, $x=\varepsilon$ and $x=2\varepsilon$.

4 Explicit solutions for the approximating model

In view of the numerical results, we have observed that the dynamical behavior of model I bears is similar to that of the original problem (2.4) at both the time scale $\mathcal{O}(\varepsilon)$ and time scale $\mathcal{O}(1)$. Therefore, we will turn to this model to study the effect of ghost forces. Model I is convenient to analyze, particularly because it admits an explicit representation of the solution. Recall that in Model I, we solve the following problem:

$$\begin{cases} \ddot{y}(x,t)-\mathcal{L}_{\rm CB}[y](x,t)=f(x), \quad x\in\mathbb{L}, \\ y(x,0)=0, \quad \dot{y}(x,0)=0, \\ y(x,t) \text{ is periodic with period } 1. \end{cases} \tag{4.1}$$

Without loss of generality, we let $\mathbb{L}=(-1/2,1/2]$ with N atoms, and N is assumed to be an even integer for technical simplicity. Obviously, $\varepsilon=1/N$, and we will switch to the notation

$$w(n,t)=w(-1/2+n\varepsilon,t), \quad n=1,2,\cdots,N. \tag{4.2}$$

We express the solution of (4.1) in terms of the lattice Green's function [23], which is defined as the solution of the ODEs:

$$\begin{cases} \ddot{G}(n,t)-\mathcal{L}_{\mathrm{CB}}[G](n,t)=0, \quad n=0,\cdots,N, \\ G(n,0)=0, \quad \dot{G}(n,0)=\delta_n, \\ G(n,t)=G(n+N,t). \end{cases} \tag{4.3}$$

The solution of (4.1) is given by

$$y(n,t)=\int_0^t \left(\sum_{m=1}^N G(n-m,t-s)f(m)\right)\mathrm{d}s,$$

where f is given by (2.5) under the transform (4.2). As a result, we have

$$\sum_{m=1}^N G(n-m,t)f(m)=\frac{\kappa_2}{\varepsilon}\big(2G(n-L,t)-G(n-L-1,t)-G(n-L+1,t)\big),$$

where we have set $L=N/2$.

Using the method of separation of variables, we have the following explicit form for the lattice Green's function G:

$$G(n,t)=\frac{t}{N}+\frac{1}{N}\sum_{k=1}^{N-1}\frac{\sin[\omega_k t]}{\omega_k}\cos\frac{2kn\pi}{N} \tag{4.4}$$

with ω_k being the dispersion relation given by $\omega_k=(2/\varepsilon)\sqrt{\kappa_1+4\kappa_2}\sin(k\pi/N)$.

Using the fact that $\sum_{m=1}^N f(m)=0$, we write

$$\sum_{m=1}^N G(n-m,t-s)f(m)=\frac{4\kappa_2}{N\varepsilon}\sum_{k=1}^{N-1}\frac{\sin[\omega_k(t-s)]}{\omega_k}\sin^2\frac{k\pi}{N}\cos\frac{2k\pi}{N}(n-L).$$

This leads to

$$y(n,t)=\frac{\varepsilon}{N}\frac{2\kappa_2}{\kappa_1+4\kappa_2}\sum_{k=1}^{N-1}\sin^2\frac{\omega_k t}{2}\cos\frac{2k\pi}{N}(n-L).$$

Using the above expression we bound $y(n,t)$ as follows,

$$|y(n,t)|\le\frac{2|\kappa_2|}{\kappa_1+4\kappa_2}\varepsilon. \tag{4.5}$$

This estimate shows that the magnitude of the error $y(n,t)$ is as small as $\mathcal{O}(\varepsilon)$ for all n and all time t. This in turn suggests that the magnitude of the error caused by the ghost force is small, which is consistent with that of the statics problem [4,6,27].

A direct calculation gives the discrete gradient of the error:

$$
\begin{aligned}
Dy(n,t) &\equiv \frac{y(n+1,t)-y(n,t)}{\varepsilon} \\
&= -\frac{1}{N}\frac{4\kappa_2}{\kappa_1+4\kappa_2}\sum_{k=1}^{N-1}\sin\frac{2k\pi}{N}(n+1/2-L)\sin\frac{k\pi}{N}\sin^2\frac{\omega_k t}{2}.
\end{aligned}
$$

Clearly we may write $Dy(n,t)$ as

$$
Dy(n,t) = -\frac{1}{N}\frac{4\kappa_2}{\kappa_1+4\kappa_2}\sum_{k=0}^{N}\sin\frac{2k\pi}{N}(n+1/2-L)\sin\frac{k\pi}{N}\sin^2\frac{\omega_k t}{2}. \tag{4.6}
$$

It follows from the above expression that $Dy(n,t)$ is anti-symmetric in the sense that

$$
Dy(n,t) = -Dy(N-n-1,t).
$$

Therefore, we only consider the case $n \geq L$. By (4.5) we bound $Dy(n,t)$ trivially as

$$
|Dy(n,t)| \leq \frac{4|\kappa_2|}{\kappa_1+4\kappa_2}.
$$

This shows that $Dy(n,t)$ is uniformly bounded for all n and all time t. In the next two sections, we seek a refined pointwise estimate of $Dy(n,t)$ in the case when t is of the order $\mathcal{O}(1)$ and $\mathcal{O}(\varepsilon)$. The same method can be employed to obtain a refined pointwise estimate of $y(n,t)$, and we leave it to the interested readers.

5 Estimate of the error over long time scale

In this section, we estimate the error for $t = \mathcal{O}(1)$. By (4.6), we write $Dy(L,t)$ as

$$
Dy(L,t) = -\frac{1}{N}\frac{4\kappa_2}{\kappa_1+4\kappa_2}\sum_{k=0}^{N}\sin^2\frac{k\pi}{N}\sin^2\frac{\omega_k t}{2}.
$$

Using the identity $\sum_{k=0}^{N}\sin^2(k\pi/N) = N/2$, we write

$$
\begin{aligned}
Dy(L,t) &= -\frac{1}{N}\frac{2\kappa_2}{\kappa_1+4\kappa_2}\sum_{k=0}^{N}\sin^2\frac{k\pi}{N} + \frac{1}{N}\frac{2\kappa_2}{\kappa_1+4\kappa_2}\sum_{k=0}^{N}\sin^2\frac{k\pi}{N}\cos(\omega_k t) \\
&= -\frac{\kappa_2}{\kappa_1+4\kappa_2} + \frac{1}{N}\frac{2\kappa_2}{\kappa_1+4\kappa_2}\sum_{k=0}^{N}\sin^2\frac{k\pi}{N}\cos(\omega_k t).
\end{aligned} \tag{5.1}
$$

When $n \neq L$, we use the fact that

$$
\sum_{k=0}^{N}\sin\frac{2k\pi}{N}(n+1/2-L)\sin\frac{k\pi}{N} = 0,
$$

and we write the expression of $Dy(n,t)$ in (4.6) as

$$Dy(n,t)=\frac{1}{N}\frac{2\kappa_2}{\kappa_1+4\kappa_2}\sum_{k=0}^{N}\sin\frac{2k\pi}{N}(n+1/2-L)\sin\frac{k\pi}{N}\cos(\omega_k t),$$

which can be further decomposed into

$$\begin{aligned}Dy(n,t)=\frac{1}{N}\frac{\kappa_2}{\kappa_1+4\kappa_2}\sum_{k=0}^{N}\sin\frac{k\pi}{N}\Big\{\sin\Big(\omega_k t+\frac{2k\pi}{N}(n+1/2-L)\Big)\\ -\sin\Big(\omega_k t-\frac{2k\pi}{N}(n+1/2-L)\Big)\Big\}.\end{aligned}\tag{5.2}$$

To bound $Dy(n,t)$, we need to estimate an exponential sum as $\sum_{k=0}^{N} e\big(f(k)\big)$, where the shorthand notation $e\big(f(k)\big)\equiv\exp\big(2\pi\imath f(k)\big)$ is assumed. The basic tool is the truncated form of the Poisson summation formula of Van der Corput [42]. The following form with an explicit estimate for the remainder term can be found in [14, Lemma 7].

Theorem 5.1. (Truncated Poisson) *Let f and ϕ be real-valued functions satisfying the following conditions on a closed interval $[a,b]$:*

1. *f'' and $\phi'(x)$ are continuous;*
2. *$0<f''(x)\le C_0$;*
3. *There are positive constants $H,U,\phi_0,\phi_1,\lambda$ such that $U\ge 1, 0<b-a\le\lambda U$ and*

$$|\phi(x)|\le\phi_0 H,\quad |\phi'(x)|\le\phi_1 H/U.$$

For any $\Delta, 0<\Delta<1$, the equation

$$\sum_{a<n\le b}\phi(n)e\big(f(n)\big)=\sum_{\alpha-\Delta\le\nu\le\beta+\Delta}\int_a^b\phi(x)e(f(x)-\nu x)\,\mathrm{d}x+\theta R\tag{5.3}$$

holds, where $\alpha=f'(a)$, $\beta=f'(b)$ and

$$\begin{aligned}R=(\phi_0+\lambda\phi_1)H\Big(9.42+9C_0+12\Delta+\pi^{-1}\big(10\Delta^{-1}+2\ln\Delta^{-1}\\ +4.5(1+\Delta)^{-1}-4.5\ln(1+\Delta)+6.5\ln(\beta-\alpha+2)\big)\Big).\end{aligned}$$

Here θ is a function such that $|\theta|\le 1$.

The assumption $f''>0$ can be relaxed to either $f''\ge 0$ or $f''\le 0$. In the latter case, the second condition is replaced by $-C_0\le f''(x)\le 0$.

5.1 The estimate for $Dy(N/2,t)$

To bound $Dy(N/2,t)$, we start with the representation (5.1). Using Theorem 5.1, we transform the exponential sum in (5.1) to a shorter sum with a bounded remainder. To clarify the dependance of the constant, we denote $\gamma = t\sqrt{\kappa_1+4\kappa_2}$, and assume that $1\le\gamma\le N$ since $t=\mathcal{O}(1)$ and $N\ge 2$. We also denote by $\lfloor p\rfloor$ the integer part of a real number p, and denote its fractional part by $\{p\}=p-\lfloor p\rfloor$.

Lemma 5.1. *Let $\phi(x)=\sin^2(\pi x/N)$ and $f(x)=\gamma/(\pi\varepsilon)\sin(\pi x/N)$. There holds*

$$\begin{aligned}\frac{1}{N}\left|\sum_{k=0}^{N}\phi(k)e\big(f(k)\big)\right| \le &\left|\frac{2}{N}\sum_{\alpha-1/2\le\nu\le\gamma+1/2}\int_0^{N/2}\phi(x)e\big(f(x)-\nu x\big)\,\mathrm{d}x\right|\\ &+C\varepsilon\big(1+\varepsilon\gamma+\log(\gamma+2)\big),\end{aligned}\tag{5.4}$$

where C is independent of N,t and γ.

Proof. It is easy to write the exponential sum as follows,

$$\sum_{k=0}^{N}\phi(k)e\big(f(k)\big)=2\sum_{k=0}^{N/2}\phi(k)e\big(f(k)\big)-\phi(N/2)e\big(f(N/2)\big).$$

With such choice of f and ϕ, we have

$$\begin{aligned}&a=0,\quad b=N/2,\quad \alpha=0,\quad \beta=\gamma,\\ &\phi_0=\phi_1=1,\quad H=\pi,\quad \lambda=1,\quad U=N/2.\end{aligned}$$

Setting $\Delta=1/2$ and using Theorem 5.1, we obtain

$$\frac{1}{N}\sum_{k=0}^{N/2}\phi(k)e\big(f(k)\big)=\frac{1}{N}\sum_{\alpha-1/2\le\nu\le\gamma+1/2}\int_0^{N/2}\phi(x)e\big(f(x)-\nu x\big)\,\mathrm{d}x+\theta\frac{R}{N},$$

where

$$R=2\pi\Big(9.42+9\pi\gamma/N+6+\pi^{-1}\big(20+2\ln 2+3-4.5\ln(3/2)+6.5\ln(\gamma+2)\big)\Big).$$

This immediately implies that there exists a constant C such that

$$|\theta R/N|\le C\varepsilon(1+\varepsilon\gamma+\ln(\gamma+2)).$$

We obtain (5.4) by combining the above two inequalities. □

Remark 5.1. The choice of Δ is not unique. However, it cannot be too small. Otherwise, the remainder term blows up as $\Delta\to 0$.

To bound the shorter sum in (5.4), we rely on the following first derivative test.

Lemma 5.2 (First derivative test)**.** [28, Lemma 1, p. 47] *Let $r(x)$ and $\theta(x)$ be real-valued functions on $[a,b]$ such that $r(x)$ and $\theta'(x)$ are continuous. Suppose that $\theta'(x)/r(x)$ is positive and monotonically increasing in this interval. If $0<\lambda_1\le\theta'(a)/r(a)$, then*

$$\left|\int_a^b r(x)e\big(\theta(x)\big)\,\mathrm{d}x\right|\le\frac{1}{\pi\lambda_1}.$$

Remark 5.2. If $\theta'(x)/r(x)$ is negative and monotonically decreasing on $[a,b]$ and

$$\theta'(a)/r(a)\le\lambda_1<0,$$

then we obtain the same bound by taking complex conjugates. Moreover, if $\theta'(x)/r(x)$ is monotone on $[a,b]$ and

$$|\theta'(x)/r(x)|\ge\lambda_1>0,\quad x\in(a,b),$$

we obtain the same bound by combining the above two cases.

We write

$$\frac{1}{N}\int_0^{N/2}\phi(x)e\big(f(x)-\nu x\big)\,\mathrm{d}x=\frac{1}{\pi}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y,$$

where $\varphi(y)=\sin^2 y$, and $G_\nu(y)=(N/\pi)(\gamma\sin y-\nu y)$ for any $\nu\in\mathbb{N}$. By Lemma 5.1, it remains to estimate the integral $\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y$ for $\nu=0,\cdots,\lfloor\gamma+1/2\rfloor$. The three cases $\nu=0,\nu=1,\cdots,\lfloor\gamma+1/2\rfloor-1$ and $\nu=\lfloor\gamma+1/2\rfloor$ will be treated separately in the following lemmas. We denote $F_\nu(y)=G'_\nu(y)/\varphi(y)$.

Lemma 5.3. *There holds*

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\le 2(N\gamma)^{-1/2}. \tag{5.5}$$

Proof. For any $\delta\in(0,\pi/2)$ to be chosen later, we have, for any $y\in(0,\pi/2-\delta)$,

$$F_0(y)\ge F_0(\pi/2-\delta)=\frac{N\gamma}{\pi}\frac{\sin\delta}{\cos^2\delta}\ge\frac{N\gamma}{\pi}\tan\delta\ge\frac{N\gamma\delta}{\pi},$$

where we have used the fact that $\tan x\ge x$ for $x\in[0,\pi/2]$. Using Lemma 5.2 with $\lambda_1=N\gamma\delta/\pi$, we obtain

$$\left|\int_0^{\pi/2-\delta}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\le\frac{1}{N\gamma\delta}.$$

The integral over the complementary portion of the interval can be bounded as

$$\left|\int_{\pi/2-\delta}^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\le\int_{\pi/2-\delta}^{\pi/2}\mathrm{d}y\le\delta.$$

On adding the two estimates we deduce that

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\le\frac{1}{N\gamma\delta}+\delta.$$

This is minimized by taking $\delta=(N\gamma)^{-1/2}\in(0,\pi/2)$, and we obtain (5.5). $\square$

The second case is more involved because F_ν changes sign over $(0,\pi/2)$.

Lemma 5.4. *If* $1\le\nu<\gamma$, *then*

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{3\pi}{\sqrt{N\gamma}}. \tag{5.6}$$

Proof. For $1\le\nu<\gamma$, there exists $y_\nu\in(0,\pi/2)$ such that $F_\nu(y_\nu)=0$ with $\cos y_\nu=\nu/\gamma$. For any $\eta\in\big(0,\min(y_\nu,\pi/2-y_\nu)\big)$ that will be chosen later, we write

$$\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y=\left(\int_0^{y_\nu-\eta}+\int_{y_\nu+\eta}^{\pi/2}+\int_{y_\nu-\eta}^{y_\nu+\eta}\right)\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y.$$

We deal with the three integrals separately.

Using Lemma 5.2 with $\lambda_1=|F_\nu(y_\nu-\eta)|$, we obtain

$$\left|\int_0^{y_\nu-\eta}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{1}{\pi|F_\nu(y_\nu-\eta)|},$$

and

$$\begin{aligned}|F_\nu(y_\nu-\eta)|&=\frac{N\gamma}{\pi}\frac{\cos(y_\nu-\eta)-\cos y_\nu}{\sin^2(y_\nu-\eta)}=\frac{2N\gamma}{\pi}\frac{\sin(y_\nu-\eta/2)\sin(\eta/2)}{\sin^2(y_\nu-\eta)}\\&\ge\frac{2N\gamma}{\pi}\frac{\sin(\eta/2)}{\sin y_\nu}\ge\frac{2N\gamma\eta}{\pi^2\sin y_\nu},\end{aligned}$$

where we have used Jordan's inequality

$$\sin x\ge\frac{2}{\pi}x,\quad x\in[0,\pi/2]. \tag{5.7}$$

This gives

$$\left|\int_0^{y_\nu-\eta}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{\pi\sin y_\nu}{2N\gamma\eta}.$$

Using Lemma 5.2 again with $\lambda_1=|F_\nu(y_\nu+\eta)|$, we have, for the second integral,

$$\left|\int_{y_\nu+\eta}^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{1}{\pi|F_\nu(y_\nu+\eta)|}.$$

Furthermore,

$$\begin{aligned}|F_\nu(y_\nu+\eta)|&=\frac{N\gamma}{\pi}\frac{\cos y_\nu-\cos(y_\nu+\eta)}{\sin^2(y_\nu+\eta)}\\&=\frac{2N\gamma}{\pi}\frac{\sin(y_\nu+\eta/2)\sin(\eta/2)}{\sin^2(y_\nu+\eta)}\\&\ge\frac{2N\gamma\eta}{\pi^2}\frac{\sin(y_\nu+\eta/2)}{\sin^2(y_\nu+\eta)}.\end{aligned}$$

This leads to

$$\left|\int_{y_\nu+\eta}^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{\pi}{2N\gamma\eta}\frac{\sin^2(y_\nu+\eta)}{\sin(y_\nu+\eta/2)}.$$

If $y_\nu\in(0,\pi/4]$, we would require that $\eta\in(0,y_\nu)$. We will have, $\sin(y_\nu+\eta)\le\sin 2y_\nu\le 2\sin y_\nu$ and $\sin y_\nu<\sin(y_\nu+\eta/2)$ since $y_\nu<y_\nu+\eta/2<2y_\nu\le\pi/2$. The bound for the above integral is changed to

$$\left|\int_{y_\nu+\eta}^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{2\pi\sin y_\nu}{N\gamma\eta}.$$

We estimate the remaining integral trivially:

$$\left|\int_{y_\nu-\eta}^{y_\nu+\eta}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le 2\eta.$$

Summing up all the above estimates, we obtain

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{5\pi\sin y_\nu}{2N\gamma\eta}+2\eta.$$

Taking $\eta=(N\gamma)^{-1/2}\sin y_\nu$, which is less than y_ν, we obtain

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{5\pi}{2\sqrt{N\gamma}}+\frac{2\sin y_\nu}{\sqrt{N\gamma}}\le\frac{5\pi/2+\sqrt{2}}{\sqrt{N\gamma}}<\frac{3\pi}{\sqrt{N\gamma}}.$$

On the other hand, if $y_\nu\in(\pi/4,\pi/2]$, we would require that $\eta\in(0,\pi/2-y_\nu)$. We will have $\sin y_\nu<\sin(y_\nu+\eta/2)$ since $y_\nu<y_\nu+\eta/2<y_\nu+\eta\le\pi/2$, and $\sin^2(y_\nu+\eta)\le 1\le 2\sin^2 y_\nu$ since $\sin^2 y_\nu\ge 1/2$. We bound the second integral as

$$\left|\int_{y_\nu+\eta}^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{\pi\sin y_\nu}{N\gamma\eta}.$$

This yields

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{3\pi\sin y_\nu}{2N\gamma\eta}+2\eta.$$

In this case, we can choose $\eta=(N\gamma)^{-1/2}$ provided that

$$\eta<\pi/2-y_\nu. \tag{5.8}$$

This immediately implies that

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{3\pi}{\sqrt{N\gamma}}.$$

Such choice of η is feasible since $\nu\ge 1>\sqrt{\gamma/N}$, which yields $\nu>\gamma\eta$, or equivalently, $\eta<\cos y_\nu=\sin(\pi/2-y_\nu)\le\pi/2-y_\nu$. This directly gives (5.8). Finally we get (5.6). $\square$

Next we consider the endpoint case $\nu=\lfloor\gamma+1/2\rfloor$.

Lemma 5.5. *Let $\nu=\lfloor\gamma+1/2\rfloor$. If $\nu\geq\gamma$, then*

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\leq\frac{4}{N\gamma}. \tag{5.9}$$

If $\nu<\gamma$, then

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\leq\frac{3\pi}{\sqrt{N\gamma}}. \tag{5.10}$$

Proof. If $\nu\geq\gamma$, then there exists a stationary point y_ν of $F_\nu(y)$ with $\cos y_\nu=\nu/\gamma-\sqrt{(\nu/\gamma)^2-1}$. Because $F_\nu(y)$ is monotonically increasing over $(0,y_\nu)$ and monotonically decreasing over $(y_\nu,\pi/2)$, we get $\min_{y\in(0,\pi/2)}|F_\nu(y)|\geq|F_\nu(y_\nu)|$. To each of the two intervals we apply Lemma 5.2 with $\lambda_1=|F_\nu(y_\nu)|$. On adding these estimates we deduce that

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\leq\frac{2}{\pi|F_\nu(y_\nu)|}, \tag{5.11}$$

which yields (5.9) by using

$$|F_\nu(y_\nu)|=\frac{N\gamma}{2\pi}\left(\nu/\gamma+\sqrt{\nu^2/\gamma^2-1}\right)\geq\frac{N\gamma}{2\pi}.$$

When $\nu=\lfloor\gamma+1/2\rfloor<\gamma$, we invoke the estimate (5.6) to get (5.10). □

Summing up the above estimates for the shorter sum, we obtain the estimate for the exponential sum in (5.4).

Lemma 5.6. *There holds*

$$\frac{1}{N}\left|\sum_{k=0}^{N}\phi(k)e\big(f(k)\big)\right|\leq C\left(\varepsilon(1+\varepsilon\gamma+\log(\gamma+2))+\sqrt{\frac{\varepsilon}{\gamma}}(1+\gamma)\right), \tag{5.12}$$

where C is independent of N, t and γ.

Proof. Denote $\nu_0=\lfloor\gamma+1/2\rfloor$. If $\nu_0\geq\gamma$, then

$$\sum_{\nu=0}^{\nu_0}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y=\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y+\sum_{\nu=1}^{\nu_0-1}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y$$
$$+\int_0^{\pi/2}\varphi(y)e\big(G_{\nu_0}(y)\big)\,\mathrm{d}y.$$

Using the estimates (5.5), (5.6), and (5.9), we bound the above sum as

$$\begin{aligned}\left|\sum_{\nu=0}^{\nu_0}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|&\leq2(N\gamma)^{-1/2}+3\pi\sum_{\nu=1}^{\nu_0-1}(N\gamma)^{-1/2}+4(N\gamma)^{-1}\\&\leq\pi(N\gamma)^{-1/2}(3\gamma+1)+4(N\gamma)^{-1}.\end{aligned} \tag{5.13}$$

If $\nu_0<\gamma$, then we have $\nu_0=\lfloor\gamma\rfloor$ and

$$\sum_{\nu=0}^{\nu_0}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y=\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y+\sum_{\nu=1}^{\nu_0}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y.$$

Proceeding along the same line that leads to (5.13), we obtain

$$\left|\sum_{\nu=0}^{\nu_0}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le 2(N\gamma)^{-1/2}+3\pi(\gamma/N)^{1/2}. \tag{5.14}$$

Combining the estimates (5.13), (5.14) and (5.4), we obtain (5.12). $\square$

Substituting the estimates (5.12) and (5.4) into (5.1), we obtain the pointwise estimate for $D(N/2,t)$ as follows.

Theorem 5.2. *If $t=\mathcal{O}(1)$ and $n=N/2$ or $N/2-1$, then*

$$\left|Dy(n,t)+\frac{\kappa_2}{\kappa_1+4\kappa_2}\right|\le C\frac{|\kappa_2|}{\kappa_1+4\kappa_2}\left(\varepsilon[1+\varepsilon\gamma+\log(\gamma+2)]+\sqrt{\frac{\varepsilon}{\gamma}}(1+\gamma)\right), \tag{5.15}$$

where C is independent of N,t and γ.

The above estimate means that $Dy(n,t)$ is in the $\mathcal{O}(\sqrt{\varepsilon})-$neighborhood of $-\kappa_2/(\kappa_1+4\kappa_2)$ when $n=N/2$ or $n=N/2-1$.

5.2 The estimate for $Dy(n,t)$ with $n\neq L$

By (5.2), we need to estimate two exponential sums $\sum_{k=0}^{N}\phi(k)e\big(f(k)\big)$ with

$$\phi(x)=\sin\frac{\pi x}{N},\quad f(x)=\frac{\gamma}{\pi\varepsilon}\sin\frac{\pi x}{N}+\frac{n+1/2-L}{N}x,$$

and

$$\phi(x)=\sin\frac{\pi x}{N},\quad f(x)=\frac{\gamma}{\pi\varepsilon}\sin\frac{\pi x}{N}-\frac{n+1/2-L}{N}x.$$

In what follows we only give the full details for estimating of the first exponential sum, and the same proof works for the second exponential sum. Denote by $\varrho=(n+1/2-L)/N$, proceeding along the same line that leads to (5.4) and choosing $\Delta=\max(1/2,1-\{\gamma+\varrho\})$, we get

$$\begin{aligned}\frac{1}{N}\left|\sum_{k=0}^{N}\phi(k)e\big(f(k)\big)\right|\le&\left|\frac{2}{\pi}\sum_{\nu=0}^{\lfloor\gamma+\varrho\rfloor+1}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\\&+C\varepsilon(1+\varepsilon\gamma+\log(\gamma+2)),\end{aligned} \tag{5.16}$$

where C is independent of N,t and γ. Here $\varphi(y)=\sin y$ and $G_\nu(y)=(N/\pi)(\gamma\sin y+\varrho y-\nu y)$.

Lemma 5.7. *There holds*

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\le\min\left(2(N\gamma)^{-1/2},\frac{1}{n+1/2-L}\right).\tag{5.17}$$

Proof. If $2(N\gamma)^{-1/2}<1/(n+1/2-L)$, then we proceed in the same way that leads to Lemma 5.3 to obtain

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\le 2(N\gamma)^{-1/2}.$$

Otherwise, using Lemma 5.2 with $\lambda=(n+1/2-L)/\pi$, we obtain

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\le\frac{1}{n+1/2-L}.$$

The combination of the above two inequalities gives (5.17). $\square$

Lemma 5.8. *Let $\nu=\lfloor\gamma+\varrho\rfloor+1$, then*

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le 4(N\gamma)^{-2/3}.\tag{5.18}$$

Proof. The function F_ν has a stationary point y_ν that satisfies $\cos y_\nu=\gamma/(\nu-\varrho)$. In this case, applying the *first derivative test* directly to the integral may yield a bound of the form $1/(N\sin y_\nu)$, which is undesirable since y_ν can be very close to zero when ν is close to $\gamma+\varrho$. Instead, for any $\delta\in(0,\pi/2)$ to be determined later on, we have

$$\left|\int_0^{\delta}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\int_0^{\delta}\varphi(y)\,\mathrm{d}y\le\int_0^{\delta}y\,\mathrm{d}y=\frac{\delta^2}{2}.$$

If $y_\nu\le\delta$, then we use Lemma 5.2 with $\lambda_1=|F_\nu(\delta)|$. This gives

$$\left|\int_\delta^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{1}{\pi|F_\nu(\delta)|}.$$

If $y_\nu>\delta$, then we proceed along the same line that leads to (5.11) to get

$$\left|\int_\delta^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{2}{\pi\min_{y\in[\delta,\pi/2]}|F_\nu(y)|}=\frac{2}{\pi|F_\nu(y_\nu)|}.$$

A direct calculation gives

$$\begin{aligned}|F_\nu(\delta)|&=\frac{N}{\pi}(\nu-\varrho)\frac{1-\cos y_\nu\cos\delta}{\sin\delta}\ge\frac{N}{\pi}(\nu-\varrho)\frac{1-\cos\delta}{\sin\delta}\\&=\frac{N}{\pi}(\nu-\varrho)\tan\frac{\delta}{2}\ge\frac{N(\nu-\varrho)}{2\pi}\delta,\end{aligned}$$

and for $y_\nu > \delta$,

$$|F_\nu(y_\nu)| = \frac{N}{\pi}(\nu-\varrho)\sin y_\nu \geq \frac{2N(\nu-\varrho)}{\pi^2} y_\nu > \frac{2N(\nu-\varrho)}{\pi^2}\delta. \tag{5.19}$$

Combining the above four inequalities, we obtain, for any $\delta \in (0,\pi/2)$,

$$\left| \int_\delta^{\pi/2} \varphi(y) e\big(G_\nu(y)\big)\,\mathrm{d}y \right| \leq \max\left(\frac{1}{\pi|F_\nu(\delta)|}, \frac{2}{\pi|F_\nu(y_\nu)|} \right) \leq \frac{\pi}{N(\nu-\varrho)\delta}.$$

Summing up, we have

$$\left| \int_0^{\pi/2} \varphi(y) e\big(G_\nu(y)\big)\,\mathrm{d}y \right| \leq \frac{\delta^2}{2} + \frac{\pi}{N(\nu-\varrho)\delta}.$$

Taking $\delta = \pi^{1/3}(N(\nu-\varrho))^{-1/3} \in (0,\pi/2)$, we get

$$\left| \int_0^{\pi/2} \varphi(y) e\big(G_\nu(y)\big)\,\mathrm{d}y \right| \leq \frac{3}{2}\pi^{2/3}[N(\nu-\varrho)]^{-2/3} \leq 4[N(\nu-\varrho)]^{-2/3}, \tag{5.20}$$

which yields (5.18) by using the fact that $\nu-\varrho \geq \gamma+\varrho-\varrho = \gamma$. $\square$

Proceeding in the same way that led to (5.10), we obtain a parallel result of Lemma 5.4. The proof is postponed to the appendix.

Lemma 5.9. *If* $1 \leq \nu < \lfloor \gamma+\varrho \rfloor$, *then*

$$\left| \int_0^{\pi/2} \varphi(y) e\big(G_\nu(y)\big)\,\mathrm{d}y \right| \leq \frac{3\pi}{\sqrt{N\gamma}\sin y_\nu}. \tag{5.21}$$

The estimate for the endpoint case $\nu = \lfloor \gamma+\varrho \rfloor$ is essentially the same with the argument that leads to (5.21). However, the root y_ν varies with the magnitude of the fractional part of $\gamma+\varrho$. Therefore, a more careful treatment is required to obtain a bound that is independent of the magnitude of $\{\gamma+\varrho\}$. The proof is also postponed to the appendix.

Lemma 5.10. *If* $\nu = \lfloor \gamma+\varrho \rfloor$, *then*

$$\left| \int_0^{\pi/2} \varphi(y) e\big(G_\nu(y)\big)\,\mathrm{d}y \right| \leq 4\pi(N\gamma)^{-1/2}. \tag{5.22}$$

Combining these lemmas, we have the following estimate.

Theorem 5.3. *If* $t = \mathcal{O}(1)$, *and* $n \neq N/2, N/2-1$, *then*

$$|Dy(n,t)| \leq C\frac{|\kappa_2|}{\kappa_1+4\kappa_2}\left(\sqrt{\frac{\varepsilon}{\gamma}}(1+\gamma) + \varepsilon(1+\varepsilon\gamma+\log(\gamma+2)) \right), \tag{5.23}$$

where C *is independent of* N,t *and* γ.

Proof. Summing up the above three lemmas, we obtain

$$\begin{aligned}&\left|\sum_{\nu=0}^{\lfloor\gamma+\varrho\rfloor+1}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\\&\le 2(N\gamma)^{-1/2}+\sum_{\nu=1}^{\lfloor\gamma+\varrho\rfloor-1}\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|+4\pi(N\gamma)^{-1/2}+4(N\gamma)^{-2/3}\\&\le 3\pi(N\gamma)^{-1/2}\sum_{\nu=1}^{\lfloor\gamma+\varrho\rfloor-1}\frac{1}{\sin y_\nu}+5\pi(N\gamma)^{-1/2}+4(N\gamma)^{-2/3}.\end{aligned}$$

A direct calculation gives

$$\begin{aligned}&\sum_{\nu=1}^{\lfloor\gamma+\varrho\rfloor-1}\frac{1}{\sin y_\nu}=\sum_{\nu=1}^{\lfloor\gamma+\varrho\rfloor-1}\frac{1}{\sqrt{1-(\nu-\varrho)^2/\gamma^2}}\\&\le\sum_{\nu=1}^{\lfloor\gamma+\varrho\rfloor-1}\int_\nu^{\nu+1}\frac{1}{\sqrt{1-(x-\varrho)^2/\gamma^2}}\,\mathrm{d}x=\int_1^{\lfloor\gamma+\varrho\rfloor}\frac{1}{\sqrt{1-(x-\varrho)^2/\gamma^2}}\,\mathrm{d}x\\&\le\int_\varrho^{\gamma+\varrho}\frac{1}{\sqrt{1-(x-\varrho)^2/\gamma^2}}\,\mathrm{d}x=\gamma.\end{aligned}$$

Combining the above two inequalities, we obtain

$$\left|\sum_{\nu=0}^{\lfloor\gamma+\varrho\rfloor+1}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le 5\pi(N\gamma)^{-1/2}(1+\gamma)+4(N\gamma)^{-2/3}. \tag{5.24}$$

It remains to estimate the integral $\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y$ with

$$\varphi(y)=\sin y \quad\text{and}\quad G_\nu(y)=(N/\pi)(\gamma\sin y-\varrho y-\nu y).$$

We choose $\Delta=1/2$. The remainder is still bounded by $\mathcal{O}(\varepsilon(1+\varepsilon\gamma+\log(\gamma+2)))$. Obviously, there holds $-\varrho-\Delta>-1$ since $|\varrho|\le 1/2$. It now remains to estimate the shorter sum with $\nu=0,\cdots,\lfloor\gamma-\varrho+1/2\rfloor$. We deal with the cases when $\nu=\lfloor\gamma-\varrho\rfloor+1,\nu=\lfloor\gamma-\varrho\rfloor$ and $\nu=0,\cdots,\lfloor\gamma-\varrho\rfloor-1$ exactly the same with those of Lemmas 5.8, 5.10 and 5.9, respectively. This results in

$$\left|\sum_{\nu=0}^{\lfloor\gamma-\varrho\rfloor+1}\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le 5\pi(N\gamma)^{-1/2}(1+\gamma)+4(N\gamma)^{-2/3},$$

which together with (5.24) gives the final estimate (5.23). $\square$

6 Estimate the error over short time

In this section, we estimate the solution over a shorter time interval $t=\mathcal{O}(\varepsilon)$. This is motivated by the previous observation that the error already develops to finite magnitude within this short time scale.

Lemma 6.1. *If $t=\mathcal{O}(\varepsilon)$ and $n\neq N/2,N/2-1$, then*

$$|Dy(n,t)|\leq C\frac{|\kappa_2|}{\kappa_1+4\kappa_2}\Big(|n+1/2-N/2|^{-2/3}+\varepsilon^{2/3}\Big). \tag{6.1}$$

where C is independent of N and t.

The proof of this lemma is essentially the same with that of Theorem 5.3.

Proof. As to $f(x)=\gamma/(\pi\varepsilon)\sin(\pi x/N)+\varrho x$, we have $\alpha=\varrho$ and $\beta=\gamma+\varrho$. We choose $\Delta=1/2$, and the remainder term is bounded by $\mathcal{O}(\varepsilon+\log(\gamma+2)\varepsilon)=\mathcal{O}(\varepsilon)$. There are only two terms in the shorter sum (5.3), i.e., $\nu=0$ and $\nu=1$, since $t=\mathcal{O}(\varepsilon)$. When $\nu=0$, using Lemma 5.2 when $\lambda=(n+1/2-L)/\pi$, we obtain

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\leq\frac{1}{n+1/2-L}.$$

Using (5.20) when $\nu=1$, we obtain

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_1(y)\big)\,\mathrm{d}y\right|\leq 4[N-(n+1/2-L)]^{-2/3}\leq 8N^{-2/3}.$$

As to $f(x)=\gamma/(\pi\varepsilon)\sin(\pi x/N)-\varrho x$, we still take $\Delta=1/2$, and the remainder is still bounded by $\mathcal{O}(\varepsilon)$. There is only one term in the shorter sum, i.e., $\nu=0$. Proceeding along the same line that leads to (5.20), we get, for any $\delta\in(0,\pi/2)$,

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\leq\frac{\delta^2}{2}+\frac{\pi}{(n+1/2-L)\delta},$$

which is minimized by taking $\delta=\pi^{1/3}(n+1/2-L)^{-1/3}\in(0,\pi/2)$. This gives

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_0(y)\big)\,\mathrm{d}y\right|\leq 4(n+1/2-L)^{-2/3}.$$

Summing up the above estimates, we get (6.1). □

We use Euler-MacLaurin formula instead of the truncated Poisson summation formula to bound $Dy(N/2,t)$, because this approach gives a more explicit bound for the remainder. The starting point is the following first-derivative form of Euler-MacLaurin formula. For any real valued function $f(x)$ in $[a,b]$ with continuous first derivative, we have

$$\begin{aligned}\int_a^b f(x)\,\mathrm{d}x=&\frac{b-a}{2N}(f(a)+f(b))+\frac{b-a}{N}\sum_{k=1}^{N-1} f\left(a+k\frac{b-a}{N}\right)\\&-\frac{b-a}{N}\int_a^b\left(\frac{(x-a)N}{b-a}-\left\lfloor\frac{(x-a)N}{b-a}\right\rfloor-\frac{1}{2}\right)f'(x)\,\mathrm{d}x.\end{aligned}\tag{6.2}$$

Starting with (5.1), and applying Euler-MacLaurin formula (6.2) to

$$f(x)=\sin^2 x\cos[(2\gamma/\varepsilon)\sin x]$$

with $a=0$ and $b=\pi$, we obtain

$$\frac{1}{N}\sum_{k=0}^{N}\sin^2\frac{k\pi}{N}\cos(\omega_k t)=\fint_0^\pi f(x)\,\mathrm{d}x+\frac{1}{N}\int_0^\pi\left(\frac{Nx}{\pi}-\left\lfloor\frac{Nx}{\pi}\right\rfloor-\frac{1}{2}\right)f'(x)\,\mathrm{d}x.$$

The remainder can be directly bounded as

$$\left|\frac{1}{N}\int_0^\pi\left(\frac{Nx}{\pi}-\left\lfloor\frac{Nx}{\pi}\right\rfloor-\frac{1}{2}\right)f'(x)\,\mathrm{d}x\right|\le\frac{\pi}{N}(2+2\gamma/\varepsilon).$$

The integral $\fint_0^\pi f(x)\,\mathrm{d}x$ can be calculated as follows.

$$\begin{aligned}\fint_0^\pi f(x)\,\mathrm{d}x=\fint_0^{\pi/2} f(x)\,\mathrm{d}x&=\fint_0^{\pi/2}\sin^2 x\sum_{m=0}^{\infty}(-1)^m\left(\frac{2\gamma}{\varepsilon}\right)^{2m}\frac{1}{(2m)!}\sin^{2m}x\,\mathrm{d}x\\&=\sum_{m=0}^{\infty}(-1)^m\left(\frac{2\gamma}{\varepsilon}\right)^{2m}\frac{1}{(2m)!}\fint_0^{\pi/2}\sin^{2m+2}x\,\mathrm{d}x\\&=\sum_{m=0}^{\infty}(-1)^m\left(\frac{2\gamma}{\varepsilon}\right)^{2m}\frac{1}{(2m)!}\frac{(2m+1)!!}{(2m+2)!!}\\&=\sum_{m=0}^{\infty}(-1)^m\left(\frac{\gamma}{\varepsilon}\right)^{2m}\frac{1}{(m!)^2}\frac{2m+1}{2m+2}.\end{aligned}$$

This implies the following estimate for $Dy(N/2,t)$ when $t=\mathcal{O}(\varepsilon)$.

Lemma 6.2. *If $t=\mathcal{O}(\varepsilon)$ and $n=N/2$ or $n=N/2-1$, then*

$$\left|Dy(n,t)-\sum_{m=1}^{\infty}(-1)^m\left(\frac{\gamma}{\varepsilon}\right)^{2m}\frac{1}{(m!)^2}\frac{2m+1}{2m+2}\right|\le 2\pi(\varepsilon+\gamma).\tag{6.3}$$

The above estimate means that $Dy(N/2,t)$ is in an $\mathcal{O}(\varepsilon)-$neighborhood of a constant that depends on the ratio t/ε.

Remark 6.1. We cannot directly use the above approach to estimate $Dy(n,t)$ because an undesirable term $\mathcal{O}(n/N)$ may appear in the bound.

7 Discussion

The issue of ghost forces frequently arises from multiscale coupling methods in both static and dynamic problems. As a first step to understand this critical issue in dynamic problems, we have considered the original quasicontinuum method applied to a one-dimensional atom chain model. Based on numerical simulations and direct analysis, we show that the error caused by ghost forces develops rather quickly. On the $\mathcal{O}(1)$ time scale, the error is observed in the entire domain, and the gradient of the error is $\mathcal{O}(1)$ at the atomistic/continuum interface. Therefore, the effect of ghost forces is more significant than that of the static case. Our study also suggests that the issue of the ghost force may even be more severe than the artificial reflections at the atomistic/continuum interface. The order of the error obtained from this analysis has been confirmed by numerical tests, shown in Fig. 5, and seems to be sharp. In the analysis, we have considered a *surrogate* model that is an approximation to the quasicontinuum model. The surrogate model is more amenable to analysis, and it correctly predicts the short time and the long time behavior of the error caused by ghost forces of the original model. The analysis of the original dynamic QC model would require a different method, and it will be pursued in our future works.

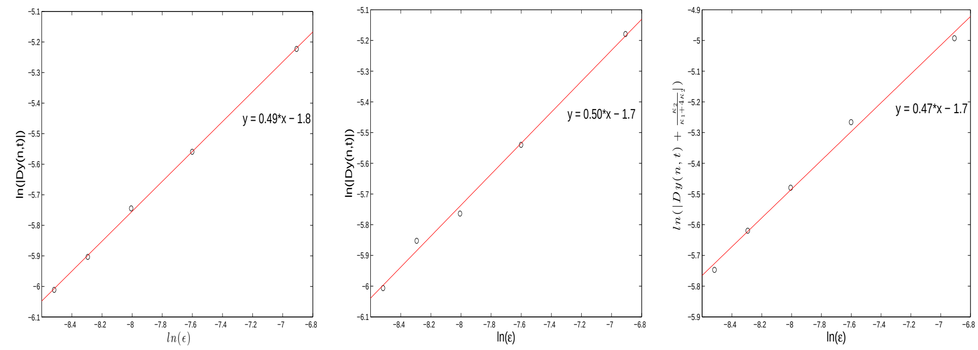

Figure 5: The maximum of the gradient of the error over $\mathcal{O}(1)$ time scale. Left to right: $n=L-3$, $n=L-2$ and $n=L-1$. The linear fitting is based on results obtained from the cases $\varepsilon=1/1000,1/2000,1/3000,1/4000$, and $1/5000$, on a log-log scale. In all the three cases, the rate is close to one half.

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A Proof of Lemma 5.9

The proof of this lemma is essentially the same with that of Lemma 5.4.

Proof. For $1\le\nu<\gamma$, there exists $y_\nu\in(0,\pi/2)$ such that $F_\nu(y_\nu)=0$ with $\cos y_\nu=(\nu-\varrho)/\gamma$. For any $\eta\in(0,\min(y_\nu,\pi/2-y_\nu))$ that will be chosen later, we write

$$\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y=\bigg(\int_0^{y_\nu-\eta}+\int_{y_\nu+\eta}^{\pi/2}+\int_{y_\nu-\eta}^{y_\nu+\eta}\bigg)\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y.$$

Using Lemma 5.2 with $\lambda_1=|F_\nu(y_\nu-\eta)|$, we obtain

$$\bigg|\int_0^{y_\nu-\eta}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\bigg|\le\frac{1}{\pi|F_\nu(y_\nu-\eta)|},$$

and

$$\begin{aligned}|F_\nu(y_\nu-\eta)|&=\frac{N\gamma}{\pi}\frac{\cos(y_\nu-\eta)-\cos y_\nu}{\sin(y_\nu-\eta)}=\frac{2N\gamma}{\pi}\frac{\sin(y_\nu-\eta/2)\sin(\eta/2)}{\sin(y_\nu-\eta)}\\&\ge\frac{2N\gamma}{\pi}\sin(\eta/2)\ge\frac{2N\gamma\eta}{\pi^2},\end{aligned}$$

where we have used Jordan's inequality (5.7) in the last step. This gives

$$\bigg|\int_0^{y_\nu-\eta}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\bigg|\le\frac{\pi}{2N\gamma\eta}.$$

Using Lemma 5.2 again with $\lambda_1=|F_\nu(y_\nu+\eta)|$, we have

$$\bigg|\int_{y_\nu+\eta}^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\bigg|\le\frac{1}{\pi|F_\nu(y_\nu+\eta)|}.$$

Furthermore,

$$\begin{aligned}|F_\nu(y_\nu+\eta)|&=\frac{N\gamma}{\pi}\frac{\cos y_\nu-\cos(y_\nu+\eta)}{\sin(y_\nu+\eta)}=\frac{2N\gamma}{\pi}\frac{\sin(y_\nu+\eta/2)\sin(\eta/2)}{\sin(y_\nu+\eta)}\\&\ge\frac{2N\gamma\eta}{\pi^2}\frac{\sin(y_\nu+\eta/2)}{\sin(y_\nu+\eta)},\end{aligned}$$

which yields

$$\bigg|\int_{y_\nu+\eta}^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\bigg|\le\frac{\pi\sin(y_\nu+\eta)}{2N\gamma\eta\sin(y_\nu+\eta/2)}.$$

If $y_\nu\in(0,\pi/4]$, we would require that $\eta\in(0,y_\nu)$. We will have, $\sin(y_\nu+\eta)\le\sin 2y_\nu\le 2\sin y_\nu$, and $\sin y_\nu<\sin(y_\nu+\eta/2)$ since $y_\nu<y_\nu+\eta/2<2y_\nu\le\pi/2$. The bound for the above integral is simplified to

$$\left|\int_{y_\nu+\eta}^{\pi/2}\phi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{\pi}{N\gamma\eta}.$$

A trivial bound for the remaining integral yields

$$\left|\int_{y_\nu-\eta}^{y_\nu+\eta}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le 2\eta.$$

Summing up all the above estimates, we obtain

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{3\pi}{2N\gamma\eta}+2\eta. \tag{A.1}$$

Taking $\eta=(N\gamma)^{-1/2}\sin y_\nu$, which is less than y_ν, we obtain

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{3\pi}{2\sqrt{N\gamma}\sin y_\nu}+\frac{2\sin y_\nu}{\sqrt{N\gamma}}\le\frac{3\pi}{\sqrt{N\gamma}\sin y_\nu}.$$

Now, if $y_\nu\in(\pi/4,\pi/2]$, we would require that $\eta\in(0,\pi/2-y_\nu)$. We will have $\sin(y_\nu+\eta)>\sin y_\nu$ since $y_\nu<y_\nu+\eta/2<y_\nu+\eta\le\pi/2$, and $\sin(y_\nu+\eta)\le 1\le\sqrt{2}\sin y_\nu$ since $\sin y_\nu\ge 1/\sqrt{2}$. We bound the second integral as

$$\left|\int_{y_\nu+\eta}^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{\sqrt{2}\pi}{N\gamma\eta},$$

This yields

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{(1+\sqrt{2})\pi}{2N\gamma\eta}+2\eta.$$

In this case, we might choose $\eta=\frac{1}{2}(N\gamma)^{-1/2}$ provided that

$$\eta<\pi/2-y_\nu. \tag{A.2}$$

With such choice of η, we have

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{3\pi}{\sqrt{N\gamma}}.$$

This choice of η is feasible since

$$\nu-\varrho\ge 1/2>(1/2)\sqrt{\gamma/N}=\gamma\eta,$$

which yields $\eta<\cos y_\nu\le\pi/2-y_\nu$, this gives (A.2) and completes the proof. $\square$

B Proof of Lemma 5.10

Proof. There exists $y_\nu \in (0,\pi/2)$ such that $F_\nu(y_\nu)=0$, and

$$\cos y_\nu = \frac{\nu-\varrho}{\gamma} = \frac{\gamma-\{\gamma+\varrho\}}{\gamma}.$$

Using the elementary inequality

$$1-\frac{2x}{\pi} \le \cos x \le 1-\frac{x^2}{\pi}, \quad x\in[0,\pi/2], \tag{B.1}$$

we obtain

$$\frac{\pi}{2}\frac{\{\gamma+\varrho\}}{\gamma} \le y_\nu \le \sqrt{\frac{\pi\{\gamma+\varrho\}}{\gamma}}. \tag{B.2}$$

Proceeding along the same line that leads to (A.1), we get for any $\eta\in(0,y_\nu)$,

$$\left|\int_0^{\pi/2} \varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right| \le \frac{3\pi}{N\gamma\eta}+2\eta.$$

We take $\eta=(N\gamma)^{-1/2}$, which yields

$$\left|\int_0^{\pi/2} \varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right| \le \frac{3\pi+2}{\sqrt{N\gamma}} \le \frac{4\pi}{\sqrt{N\gamma}}.$$

If $\{\gamma+\varrho\}$ satisfies

$$\frac{\{\gamma+\varrho\}}{\gamma} > \frac{2}{\pi}(N\gamma)^{-1/2},$$

then using the left hand side of (B.2), we obtain $\eta\in(0,y_\nu)$.

On the other hand, if

$$\frac{\{\gamma+\varrho\}}{\gamma} \le \frac{2}{\pi}(N\gamma)^{-1/2},$$

then letting $\delta=2(N\gamma)^{-1/4}$, we have

$$\frac{\{\gamma+\varrho\}}{\gamma} \le \frac{\delta^2}{2\pi} \le \frac{1-\cos\delta}{2}, \tag{B.3}$$

where we have used the right hand side inequality of (B.1). It follows from the above inequality and the right hand side of (B.2) that $y_\nu \le \delta/\sqrt{2} < \delta$. Using Lemma 5.2 again with $\lambda_1=|F_\nu(\delta)|$, we get

$$\left|\int_\delta^{\pi/2} \varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right| \le \frac{1}{\pi|F_\nu(\delta)|}.$$

We estimate the contribution of the complementary portion of the integral trivially:

$$\left|\int_0^{\delta}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\int_0^{\delta}y\,\mathrm{d}y=\frac{\delta^2}{2}.$$

On adding the above estimates we deduce that

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{\delta^2}{2}+\frac{1}{\pi|F_\nu(\delta)|}.$$

A direct calculation gives

$$|F_\nu(\delta)|=\frac{N\gamma}{\pi}\frac{\cos y_\nu-\cos\delta}{\sin\delta}=\frac{N\gamma}{\pi}\frac{1-\cos\delta-\{\gamma+\varrho\}/\gamma}{\sin\delta}.$$

Using (B.3), we obtain

$$|F_\nu(\delta)|\ge\frac{N\gamma}{2\pi}\frac{1-\cos\delta}{\sin\delta}=\frac{N\gamma}{2\pi}\tan\frac{\delta}{2}\ge\frac{N\gamma\delta}{4\pi}.$$

This gives

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\frac{\delta^2}{2}+\frac{4}{N\gamma\delta}=2(N\gamma)^{-1/2}+2(N\gamma)^{-3/4}\le4(N\gamma)^{-1/2}.$$

Finally, we have

$$\left|\int_0^{\pi/2}\varphi(y)e\big(G_\nu(y)\big)\,\mathrm{d}y\right|\le\max(4\pi(N\gamma)^{-1/2},4(N\gamma)^{-1/2})=4\pi(N\gamma)^{-1/2}.$$

The proof is complete. $\square$

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