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Unstable Surface Modes in Finite Chain Computations: Deficiency of Reflection Coefficient Approach

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Abstract. In this paper, we investigate the stability for a finite harmonic lattice under a certain class of boundary conditions. A rigorous eigenvalue study clarifies that the invalidity of Fourier modes as the basis results in the deficiency of standard reflection coefficient approach for stability analysis. In a certain parameter range, unstable surface modes exist in the form of exponential decay in space, and exponential growth in time. An approximate eigen-polynomial is proposed to ease the stability analysis. Moreover, the eigenvalues with small positive real part quantitatively explain the long time instability in wave propagation computations. Numerical results verify the analysis.

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Key words: Unstable surface mode, reflection coefficient, finite chain.

1 Introduction

Interfaces/surfaces are of fundamental importance in materials science and engineering. Substantial understanding of the physics has been obtained through studies on wave propagations across an interface/surface. Generally speaking, the two materials across an interface/surface yield different dispersion relations. Continuity of the wave function requires a certain combination of waves with different propagation directions. Wave features are then usually characterized by the reflection and transmission coefficients. In the mean time, interfaces/surfaces also play an important role in numerical computations. For instance, in a multi-scale computation that couples atomistic dynamics and continuum deformation, atomistic fluctuations need to be damped out through suitable boundary conditions. As it is virtually impossible to cleanly transmit all fluctuations, the reflected part enters back and cause spurious wave interactions inside the atomistic

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domain. Hence a key ingredient for a multi-scale algorithm is the design of interfacial conditions for reflection reduction. In the literature, numerical absorption treatments have been proposed, including a perfect matched layer, or a time history kernel convolution, or a velocity interfacial condition, etc [1,5,20,23–25]. Most of these methods adopt a sinusoidal Fourier mode viewpoint, and are validated or analyzed through the resulted reflection coefficients. A dynamic atomistic-continuum algorithm is even designed by minimizing the reflection coefficient within a certain range of wave-numbers [6]. In addition, for continuous wave propagation in an unbounded domain, one assigns a finite computing domain. Numerical boundary conditions are then also analyzed and optimized through the reflection coefficient approach [3,7,10,12,13,17,27]. We remark that rigorous analysis had also been performed for continuous wave equations by Kreiss and others [8,14], and for discrete schemes by Halpern, Li, and others [9,15].

In this paper, we study carefully the validity of the reflection coefficient approach for wave propagation applications. As is known for a long time, the Fourier modes do not completely or accurately describe the wave features for finite lattice chains. We quantitatively demonstrate, with a velocity interfacial condition, that this invalidity results in the deficiency of the reflection coefficient approach and incorrect stability results. We observe unstable surface modes in a parameter range where the reflection coefficient approach claims to be stable. An approximate eigen-polynomial is proposed, which has a much lower order than the full problem. This may greatly ease a rigorous stability analysis. The eigen modes are classified into unstable surface modes, absorption modes, and vibration/propagation modes. Our results reveal the complexity of wave propagations in multiple media, and urges for substantiating numerical analysis for multi-scale computations. We remark that the finite size effects may lead to possible discoveries for micro-/nano-materials, similar to those for electronic states in a finite crystal [22].

The rest of the paper is arranged as follows. We describe the governing equations and the reflection coefficient approach for a finite chain in Section 2. Then a full eigen-problem study is performed in Section 3. Numerical tests are also presented. In Section 4, we discuss long time instability, which is a subtle issue in numerical simulations and quantitatively explained by the current eigen-problem results. We make some concluding remarks in Section 5.

2 Reflection coefficient

We consider a harmonic lattice consisting $(N+2)$ atoms. The n-th atom deviates from its equilibrium by a displacement $u_n(t)$, and a velocity $v_n(t)=\dot{u}_n(t)$. We impose the same type of boundary conditions at both ends. The governing system is as follows.

$$\dot{u}_0=\alpha u_0+\beta u_1, \tag{2.1a}$$

$$\dot{u}_n=v_n, \quad n=1,\cdots,N, \tag{2.1b}$$

$$\dot{v}_n=u_{n-1}-2u_n+u_{n+1}, \quad n=1,\cdots,N, \tag{2.1c}$$