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Parameterized and systematically assembled operators for lattice defect dynamics

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ABSTRACT

In this paper, we develop a calculation method for determining the phonon or vibration spectra of lattices with defects. The dynamical matrices of lattices containing defects are calculated by introducing defects systematically into the dynamical matrices of pristine, defect-free lattices using linear operators. Each operation effectively modifies or removes an individual bond or mass. Then, complex defect configurations can be constructed through reiterative application of the operators. The proposed method may be applied to systems containing any interaction type or bond order, is amenable to parameterization with continuous variables, and is suited to the study of periodic structures and atomic lattices. For verification, the method is used to calculate the dilute limit in the optical mode of a point vacancy and the periodic-to-aperiodic convergence rate as a function of the increasing unit cell size. Additional demonstrations are then shown using two dimensional lattices containing a vacancy point defect and a tri-vacancy defect cluster.

1. Introduction

Defects can significantly alter important properties such as failure response, carrier mobilities, or vibration spectra of lattices across all length scales–nano, micro, or macroscopic. As a result, non-destructive defect detection (Feldman et al., 1966; Nakashima et al., 2001; Ruiz et al., 2013) and defect design or phononics (Hussein et al., 2014), have become increasingly popular areas of study. However, across all systems that have a lattice basis and all types of defects that can exist in those lattices, there are an infinite number of possible defect configurations. Yet few methods enable systematic investigation or offer a basis for design in an otherwise infinite parameter space. Namely, each model of a defect configuration is discrete and independent of other configurations, and subsequent study of variations in the configuration must be analyzed anew. Thus, while it is a straightforward matter of calculating, say, the phonon spectrum given the configuration and properties of a lattice, it can be quite challenging to determine the changes to eigenvalues, even from small perturbations or adjustments in configuration, due to the presence of a non-linear secular equation. This paper describes an approach for relating defect variants to the same pristine reference lattice, thereby enabling the construction of dynamical matrices of defect configurations in a continuously parameterizable way that is also amenable to computer implementation.

This work relates to, and draws from, the enormous literature in the fields of both lattice and structural dynamics. The approaches for studying phonon behavior in complex material lattices at the atomic scale are not fundamentally different from those used to investigate the vibrational response of periodic structures (Colquitt et al., 2011), or material micro-structure analyses (Hutchinson and Fleck, 2006). A primary reason for this is in the use of the harmonic approximation in atomic lattices which essentially makes the problems analogous. Even when atomic lattices contain bond-order effects and long-range non-bonded interactions that are usually absent in macroscopic structures, analogous pair and/or many-body interactions and internal couples could be used in the latter to emulate such effects. Thus an approach that quantifies the effects of defects in vibration spectra is applicable to both atomic as well as engineered lattices.

Analytical tools for quantifying the effect of defects on phonon spectra of atomic lattices originate from the Green's function-based techniques initially proposed by Montroll and Potts (1955). Their method calculates the localized changes in frequency due to point defects. Recognizing the $r^{-1}\exp(-Ar)$ decay of the effect of point defects at large distances, they developed a Green's function-based technique to study single defects and defect pairs in 1D chains with extended arguments for 3D lattices. Lifshitz and Kosevich (1966) developed a more expansive approach, enabling the calculation of both local modes as well as continuous mode changes

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of the bulk spectra due to point, line, and planar defects. Each of these articles helped to create a rigorous, physical understanding of the modal properties of defective lattices. However, both rely on Green's functions which make extensions to complex lattice structures challenging. More recently, Grimm and Wagner (1994) expanded the Lifshitz formalism of Lifšic (1956), to calculate the effect of densely populated 1D defects on the thermodynamic properties of 3D crystalline materials. Grimm and Wagner's methods increased the efficiency of Lifshitz formulae by defining 'mesoscopic' coordinates, effectively reducing the rank of the tensors. The proposed method increased the breadth and computability of the Lifshitz formalism, but continued to utilize Green's functions for calculations, the exact forms of which may be challenging to determine for arbitrary and general complex geometries, and the derivation of the approach assumed central force, pair potentials. In studies of the static behaviors of lattices (Tewary, 1973; Migoni et al., 1980; Thomson and Zhou, 1994; Yang and Tewary, 2005) unique Green's function have been developed for point defects and surfaces in the myriad combinations involving lattice types.

With the advent of "smart" materials, and an increase in computational power, several works (Theocharis et al., 2009; Boechler et al., 2011; Nolde et al., 2011) analyzed the effects of periodic lattice parameters on the vibrational response of macro-level systems. Theocharis et al. (2009) developed a systematic continuum-level method for analyzing the stability of localized modes in granular crystals. They studied continuum-scale grains and developed simple matrices to manipulate the pristine system into one containing defective grains of dissimilar masses, radii, or elastic moduli. The matrix equations were derived to include anharmonic effects, assuming 1D chains of uniform grains interacting only with their nearest neighbors. Later work by Boechler et al. (2010) expanded the theory to include diatomic granular crystals. Nolde et al. (2011) developed a methodology for examining the vibrational modes of materials with non-homogeneous micro-structure. The chosen geometry was a 2D square lattice composed of non-homogeneous elastic strings. By employing lattice dynamics, the authors were able to calculate the changes in high frequency modes as the elastic constants of the strings varied, whereas prior continuum-level approaches were only accurate for wavelengths larger than the micro-structure of the material. Similarly, Chen et al. (2004) demonstrated that continuum-level approaches could be used to calculate the optical regime of material phonon spectra only when coupled with Micromorphic theory, which accounts for the micro-structure of the material. Other works on elastic bodies have examined the consequences of singular perturbations on eigenvalues (Maz'ya et al., 2016) and localized waves in layered media with composite defects (Andrianov et al., 2014).

In this work we propose a general approach for modeling defects in any system that can be modeled as a periodic lattice or periodic structure. In traditional lattice dynamics, the dynamical matrix is obtained from a fixed lattice configuration. The dynamical matrices of defect lattices are mapped to the dynamical matrix of a pristine reference lattice. Traditional lattice dynamic calculations or finite element methods can be used to generate the matrix for the pristine, defect-free lattices. Then simple, sparse operators can be applied reiteratively to "build" defects of complex arrangements into the pristine structure. Thus a clear relationship exists between each defect configuration and its pristine lattice and, therefore, each defect configuration to each other. The systematic approach avoids having to repeatedly re-calculate dynamical matrices and thereby allows simple and efficient parametric study of the effects of defect configurations. In a manner of speaking, this also enables a computable framework for the Lifshitz formalism (Lifšic, 1956) and an extension to the theory of Montroll and Potts (1955) that avoids the use of Green's functions. At present, we adopt the assumption of no relaxation in the neighborhood of the defect, as also employed in the atomic models of Montroll and Potts (1955); Lifshitz and Kosevich (1966), and Grimm and Wagner (1994), and periodic structures such as Theocharis et al. (2009); Hutchinson and Fleck (2006), and Nolde et al. (2011).

The paper is organized as follows. In Section 2 the operator method is derived for defects in atomic systems with central or non-central forces as well as progressive damage in periodic structures. The explicit form of the operators are then derived for central force potentials in Section 3, and the calculation approach is demonstrated to recover the solution of Montroll and Potts (1955) in Section 4.1. In particular, through the parameterization afforded by the method, we numerically determine the critical exponent for finite scale effects caused by defect interactions. The formulae are then applied to 2D rectangular lattices in Section 4 for examples containing an atomic point defect, a structural truss defect, and an atomic tri-vacancy. Then, the conclusions are drawn in Section 5.

2. Methodology

The present developments are intended to be applicable to both periodic structures and material lattices. For the sake of this generality, the terminology we use presently is nodes and interactions. Thus a node may be either a feature of a finite element mesh or an atom, while an interaction may be from the interactions between atoms or through the structural interactions between two material points. In this section, we will first briefly overview the main idea for defect operators and then provide details in Sections 3.

Consider an n-dimensional lattice. The lattice is composed from a space-filling periodic unit cell containing N nodes. The vibration or phonon spectrum of the lattice ($\boldsymbol{\omega} \in \mathbb{R}^{nN}$ for stable systems, or $\boldsymbol{\omega} \in \mathbb{C}^{nN}$ for unstable systems) can be computed through the eigenvalue problem

$$\boldsymbol{\omega} = \left(Eigenvalues(\mathbf{M}^{-1}\mathbf{D})\right)^{1/2} \tag{1}$$

where $\mathbf{D} \in \mathbb{C}^{nN\times nN}$ is the dynamical matrix, $\mathbf{M} \in \mathbb{R}^{nN\times nN}$ is the mass matrix, and the square root is taken over individual terms in the column vector. Here, the mass matrix can be composed of point or continuous masses. The dynamical matrix contains all information about geometric and kinematic relations between nodes.

Our problem statement is as follows: Find $\mathbf{A} \in \mathbb{C}^{nN\times nN}$ and $\mathbf{B} \in \mathbb{R}^{nN\times nN}$ such that the spectrum of the **defective** lattice can be directly computed from the pristine system through

$$\boldsymbol{\omega}_d = \left(Eigenvalues\left(\mathbf{B}\mathbf{M}_p^{-1}(\mathbf{A}\mathbf{D}_p)\right)\right)^{1/2} \tag{2}$$

The script "p" is used to indicate quantities associated with the pristine lattice, and "d" the defective lattice. **A** and **B** may be interpreted as operators that map the pristine dynamical and mass matrices into their respective "defect space".

The main point is that although **A** and **B** are not the same from one defect to another, we show that they can be assembled using fundamental interactions that do not differ from one defect to another. Consider a pristine lattice that has an additively decomposable potential energy function, E_p, such that

$$E_p = \sum_i E_{p_i} \tag{3}$$

where each E_{p_i} is the energy associated with a single interaction (be it one, two, or many-bodied) and the sum is taken over every individual interaction in the system. Each potential energy term may be an atomic interaction, or any finite element discretization of elasticity between two or more nodes (e.g. truss, beam, plate, etc).

The dynamical matrix is the Fourier transform of the second derivative of the potential energy with respect to state variables.