Research Proposal - Vibrational modes of materials with topological defects

Assaf Zohar

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1 Introduction

A material property is considered topological when such property is invariant under continuous deformations. One interesting subclass of topological properties are topological defects. In 2D two particular defects can be described as dislocations, when an atom in the lattice has an extra neighbour while another atom is missing one, and disclinations, which can be achieved by making removing an angular section of the lattice and gluing its sides together[1].

While some properties such as electrical conductivity and stress response are an active area of research[2][3], the vibrational modes of lattices with topological defects is currently an unsolved problem.

In a Bravais lattice (with or without a basis), translational symmetry dictates the vibrational modes and limits the problem to the first Brilouin Zone[4]. In materials hosting topological defects such symmetry is broken and modes can no longer be considered solely in the unit cell. Furthermore introducing a defect results in system pre-strain (i.e thinking of the system as a set of coupled masses on springs - the system's minimal energy is not the state where all springs are relaxed), in the disclination described earlier it results in non trivial strain gradient emerging from the defect center.

2 Research Goals

In order to develop a theory of vibrational modes in such materials we will attempt to find these modes numerically and derive a Hamiltonian of the system. Once a Hamiltonian is derived we shall find its eigenvalues and modes in order to create a basis for every wave in the lattice. Our research will focus on 2-dimensional materials, where topological defects are characterized as discilinations and dislocations.

We will begin by simulating the out of plane vibrational modes of a simple triangular Bravais lattice, in a way not dependent on the lattice translational symmetry, later modifying the simulation to such a lattice hosting a defect. We expect adding defects will change the system's spectrum, perhaps creating modes that are coupled to it, similar to electronic systems with a defect.

3 References

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[3] Ran, Y., Zhang, Y. Vishwanath, A. One-dimensional topologically protected modes in topological insulators with lattice dislocations. Nature Phys 5, 298–303 (2009). https://doi.org/10.1038/nphys1220
[4] https://arxiv.org/pdf/cond-mat/0307616v2.pdf