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PDE Constrained Optimization and Design of Frozen Mode Crystals

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Abstract. We explore the use of PDE constrained nonlinear optimization techniques to optimize and design electromagnetic crystals which exhibit frozen mode behavior. This is characterized by Van Hove singularities in the dispersion relation, e.g., stationary reflection points and degenerate band edge points. Hence, the optimization process modifies the dispersion relation by adjusting the geometries and material parameters. The resulting algorithm is found to be capable of recovering all known crystal configurations as well as many new configurations, some of which display dramatically improved properties over previously used configuration. We investigate both gyrotropic photonic crystals and degenerate band edge crystals as well as the more complex case of the oblique incidence. In this latter case, we extend the investigation to the three-dimensional case to identify the first three-dimensional crystal exhibiting frozen mode behavior.

AMS subject classifications: 65M60, 78A48, 78M10, 93M25

Key words: PDE constrained optimization, method of matched asymptotics, frozen mode, photonic crystal.

1 Introduction

Controlling the flow of electromagnetic waves in materials has been at the frontier of significant research efforts during the last decade. Well known examples rely on the ability to prohibit wave propagation or generation of strongly localize electromagnetic energy, both utilized in photonic bandgap devises. Furthermore, recent studies of periodic structures of anisotropic materials have demonstrated the ability to produce unexpected electromagnetic phenomena such as a dramatic slow-down of the wave and a significant increase in field amplitude without adversely affecting the ability to transmit energy

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into these crystals [3–5]. Under ideal circumstances, this has been shown to a allow a dramatic compression of the electromagnetic energy inside the crystal with a vanishing group velocity at the carrier frequency. This phenomenon has been called a frozen mode and these unique features of this are attractive for numerous practical applications. Recent studies [1] have confirmed the robustness of these phenomena, further increasing the practicality of manufacturing such devises.

Initially, the frozen mode was regarded as a distinctive phenomenon related to stationary inflection points of the dispersion relations $\omega(k)$ such as,

$$\frac{\partial\omega}{\partial k}=0; \quad \frac{\partial^2\omega}{\partial k^2}=0; \quad \frac{\partial^3\omega}{\partial k^3}\neq 0 \quad \text{at } \omega=\omega_0.$$

These properties of the dispersion relation are special cases of what is known as Van Hove singularities [7] as points where the first derivative of the dispersion relation $\omega(k)$ vanishes, i.e.,

$$\frac{\partial\omega}{\partial k}=0 \quad \text{at } \omega=\omega_0.$$

This nomenclature is related to the density of state (DOS), as it is known that the DOS is inversely proportional to $\partial\omega/\partial k$ [8].

All previous studies have focused on the analysis of crystal configurations found by a trial-and-error technique. Due to complexity of finding useful configurations, this clearly limits the number of parameters one can freely manage to vary. This naturally again impact that parameter space one can practically search and leaves open questions of whether it is generally possible to achieve the properties in the dispersion relation, e.g., given some specific materials, can modify the geometric properties of the crystal as needed?

To address this problem in a more systematic way, we consider the implementation of a PDE constrained optimization approach where we use the dispersion relation, given by the transfer matrix method or by solving the Maxwell eigenproblem, in combination with the algorithm of Method of Moving Asymptote (MMA) [9–13]. This allows us to recreate and to optimize known configurations as well as to design entirely new crystal arrangements.

We consider the optimization and design of three different types of crystals all of which exhibit the frozen mode phenomena. The first one is a gyrotropic photonic crystal consisting of two misaligned anisotropic layers and one magnetic layer. Its dispersion relation has a stationary inflection point in the 2nd band. The second class of crystals consists of two misaligned anisotropic layers and vacuum between them. Its dispersion relation has a degenerate band edge in the first band. The final structure consists of only one anisotropic layer with $\varepsilon_{xz}\neq 0$ and vacuum between them. However, the frozen mode phenomenon only emerges when the incident wave propagates into this layer at an oblique angle. This latter case is quite different from the previous two cases. The dispersion relation was originally computed by a one-dimensional transfer matrix method