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A new integral representation for quasi-periodic fields and its application to two-dimensional band structure calculations

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ABSTRACT

In this paper, we consider band structure calculations governed by the Helmholtz or Maxwell equations in piecewise homogeneous periodic materials. Methods based on boundary integral equations are natural in this context, since they discretize the interface alone and can achieve high order accuracy in complicated geometries. In order to handle the *quasi-periodic* conditions which are imposed on the unit cell, the free-space Green's function is typically replaced by its quasi-periodic cousin. Unfortunately, the quasi-periodic Green's function diverges for families of parameter values that correspond to resonances of the empty unit cell. Here, we bypass this problem by means of a new integral representation that relies on the free-space Green's function alone, adding auxiliary layer potentials on the boundary of the unit cell itself. An important aspect of our method is that by carefully including a few neighboring images, the densities may be kept smooth and convergence rapid. This framework results in an integral equation of the second kind, avoids spurious resonances, and achieves spectral accuracy. Because of our image structure, inclusions which intersect the unit cell walls may be handled easily and automatically. Our approach is compatible with fast-multipole acceleration, generalizes easily to three dimensions, and avoids the complication of divergent lattice sums.

1. Introduction

A number of problems in wave propagation require the calculation of *quasi-periodic* solutions to the governing partial differential equation in the frequency domain. For concreteness, let us consider the two-dimensional (locally isotropic) Maxwell equations in what is called TM-polarization [27,28]. In this case, the Maxwell equations reduce to a scalar Helmholtz equation

$$\Delta u(x,y) + \omega^2 \epsilon \mu u(x,y) = 0, \tag{1}$$

where ϵ and μ are the permittivity and permeability of the medium, respectively, and we have assumed a time dependence of $e^{-i\omega t}$ at frequency $\omega > 0$. Given a solution u to (1), it is straightforward to verify that the corresponding electric and magnetic fields **E**,**H** of the form

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$$\mathbf{E}(x,y,z) = \mathbf{E}(x,y) = (0,0,u(x,y))$$
$$\mathbf{H}(x,y,z) = \mathbf{H}(x,y) = \frac{1}{i\omega\mu}(u_y(x,y), -u_x(x,y), 0)$$

satisfy the full system

$$\nabla \times \mathbf{E} = i\omega\mu\mathbf{H}$$
$$\nabla \times \mathbf{H} = -i\omega\epsilon\mathbf{E}.$$

We are particularly concerned with doubly periodic materials whose refractive index $n = \sqrt{\epsilon\mu}$ is piecewise constant (Fig. 1). Such structures are typical in solid state physics, and are of particular interest at present because of the potential utility of photonic crystals, where the obstacles are dielectric inclusions with a periodicity on the scale of the wavelength of light [28]. Photonic crystals allow for the control of optical wave propagation in ways impossible in homogeneous media, and are finding a growing range of exciting applications to optical devices, filters [21], sensors, negative-index and meta-materials [36], and solar cells [7].

We assume that the crystal consists of a periodic array of obstacles (Ω_Λ) with refractive index $n \neq 1$, embedded in a background material with refractive index $n = 1$ (denoted by $\mathbb{R}^2 \setminus \overline{\Omega_\Lambda}$). We then rewrite (1) as a system of Helmholtz equations

$$(\Delta + n^2\omega^2)u = 0 \quad \text{in } \Omega_\Lambda \tag{2}$$
$$(\Delta + \omega^2)u = 0 \quad \text{in } \mathbb{R}^2 \setminus \overline{\Omega_\Lambda} \tag{3}$$

The expression $\overline{\Omega_\Lambda}$, above, is used to denote the closure of the domain Ω_Λ (the union of the domain and its boundary $\partial\Omega_\Lambda$). In this formulation, we must also specify conditions at the material interfaces. These are derived from the required continuity of the tangential components of the electric and magnetic fields across $\partial\Omega_\Lambda$ [27,28], yielding

$$u, u_n \text{ continuous across } \partial\Omega_\Lambda \tag{4}$$

where $u_n = \partial u/\partial n$ is the outward-pointing normal derivative.

The essential feature of doubly periodic microstructures in 2D (or triply periodic microstructures in 3D) is that, at each frequency, there may exist traveling wave solutions (Bloch waves) propagating in some direction defined by a vector **k**.

Definition 1. *Bloch waves* are nontrivial solutions to (2)–(4), that are quasiperiodic, in the sense that

$$u(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\tilde{u}(\mathbf{x}), \tag{5}$$

where $\tilde{u}$ is periodic with the lattice period and $\mathbf{k} = (k_x, k_y)$ is real-valued. **k** is referred to as the *Bloch wavevector*.

Bloch waves characterize the bulk optical properties at frequency ω; they are analogous to plane waves for free space. If such waves are absent for all directions **k** for a given ω, then the material is said to have a *band-gap* [48]. The *size* of a band-gap is the length of the frequency interval $[\omega_1,\omega_2]$ in which Bloch waves are absent. Crystal structures with a large band-gap are 'optical insulators' in which defects may be used as guides [28], with the potential for enabling high-speed integrated optical computing and signal processing.

Definition 2. The *band structure* of a given crystal geometry is the set of parameter pairs (ω, **k**) for which nontrivial Bloch waves exist.

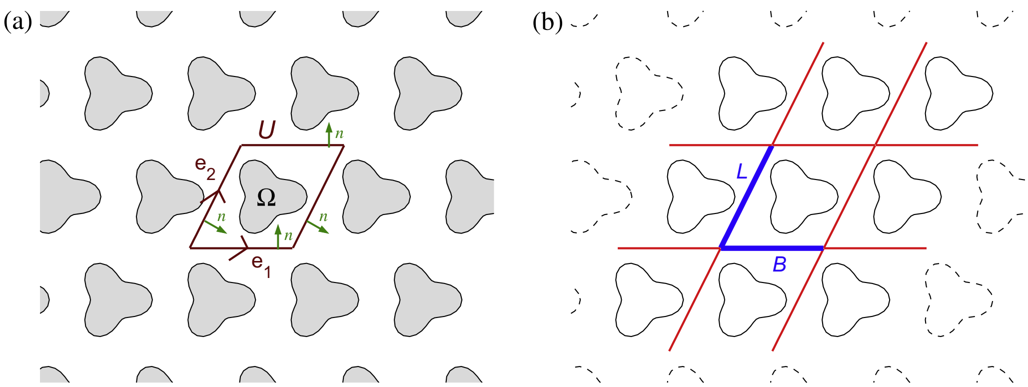

Fig. 1. (a) Problem geometry: an infinite dielectric crystal, in the case where the inclusion Ω lies within a parallelogram unit cell U. The (shaded) set of all inclusions in the lattice, denoted by Ω_Λ in the text, has refractive index n, while the white region has index 1. (b) Sketch of our quasi-periodizing scheme: we make use of layer potentials on the left (L) and bottom (B) walls, extended to the additional segments shown, which form a skewed 'tic-tac-toe' board, as well as the near neighbor images of Ω, outlined in solid lines.