TE band structure for honeycomb media in a high contrast regime

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Abstract

We consider the propagation of Transverse Electric (TE) waves in a 2D photonic crystal made of an homogeneous bulk containing high permittivity identical inclusions localized at the vertices of a honeycomb lattice [1, 2]. In this high contrast regime, we analyse the band structure of the underlying elliptic operator. We prove global results on the evolution of the band structure with respect to the contrast as well as detailed local information such as the existence of Dirac points, which are conical crossings between consecutive dispersion surfaces. Our study is illustrated by numerical simulations. Moreover, essential differences between this electromagnetic setting and the quantum model of graphene [3] will be discussed during the talk.

Keywords: Honeycomb photonic crystals, high contrast regime, band structure, Dirac points

1 Introduction and mathematical model

Honeycomb media such as graphene have been recently intensively studied for the new physical properties. These properties such as the existence of topological protected edge states rely on the existence of Dirac points, conical crossings of dispersion surfaces. The existence of such points has been demonstrated for Schrödinger equations in the strong binding (high contrast) regime model of graphene [3]. In this work, we study (see [1,2]) a similar configuration for photonic crystals and show many differences with the quantum case analysed in [3].

We consider a 2D honeycomb photonic crystal (cf. figure 1) with constant permeability μ_0 made of a two phase dielectric material: an homogeneous bulk of permittivity ε_0 that contains identical inclusions with high permittivity $\varepsilon_0 g$. The inclusions centers are localized on the vertices of a honeycomb lattice $(\boldsymbol{v}_A + \Lambda) \cup (\boldsymbol{v}_B + \Lambda)$, where $\Lambda := \mathbb{Z}\boldsymbol{v}_1 \oplus \mathbb{Z}\boldsymbol{v}_2$. The crystal is partitioned into diamond-shaped periodic cells that contains two inclusions: a A-site (in red) and a B-site (in blue). The fundamental cell Ω encloses two inclusions centered at $\boldsymbol{v}_A$ and $\boldsymbol{v}_B$ whose shape is assumed invariant by a rotation of $\pi/6$ with respect to $\boldsymbol{v}_A$ or $\boldsymbol{v}_B$.

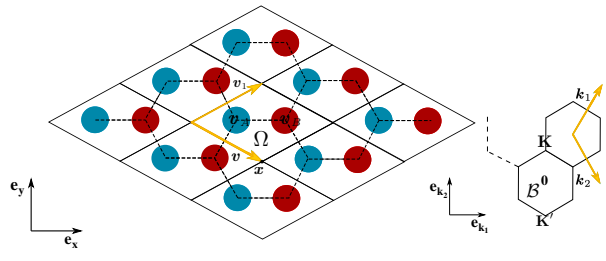


Figure 1: Honeycomb media in the case of disk shaped inclusions (left). Dual lattice Λ^*, hexagonal Brillouin zone $\mathcal{B}$, dual basis $(\boldsymbol{k}_1, \boldsymbol{k}_2)$ and high symmetry quasimomenta $\mathbf{K}$ and $\mathbf{K}'$ (right).

In this structure, we analyse the propagation of (TE) modes (E_x, E_y, H_z). For such modes and a circular frequency $\omega \neq 0$, the magnetic component H_z is solution of $-\nabla \cdot \varepsilon_g^{-1} \nabla H_z = \omega^2 \mu_0 H_z$ where the permittivity function ε_g takes two values: $\varepsilon_0 g$ within the inclusions and ε_0 in the bulk. The transverse field (E_x, E_y) is then computed explicitly from H_z. After of multiplication of the H_z- equation by $\varepsilon_0 g$, we obtain an equivalent spectral problem for the self-adjoint elliptic unbounded operator $\mathbb{A}_g = -\nabla \cdot \sigma_g \nabla$:

$$\mathbb{A}_g H_z = \lambda H_z \text{ where } \lambda = g\Big(\frac{\omega}{c}\Big)^2, \; c = (\mu_0 \varepsilon_0)^{-\frac{1}{2}},$$

and the function σ_g takes two values: 1 in the inclusions and g in the bulk.

As $\mathbb{A}_g$ commutes with lattice (Λ) translations, its spectrum is obtained via a family of Floquet-Bloch eigenvalue problems. More precisely, for each $\boldsymbol{k} \in \mathcal{B}$, the hexagonal Brillouin zone (cf. figure 1), we denote by $\lambda_1(\boldsymbol{k}; g) \leq \cdots \leq \lambda_n(\boldsymbol{k}; g) \leq \ldots$ the sequence of eigenvalues (listed with multiplicity) of $\mathbb{A}_g$ subject to $\boldsymbol{k}$-quasiperiodic boundary conditions. The graphs of the Lipschitz continuous maps $\boldsymbol{k} \mapsto \lambda_n(\boldsymbol{k}; g)$, $n \geq 1$, are called *dispersion surfaces*. The $L^2(\mathbb{R}^2)$ spectrum of $\mathbb{A}_g$ is the union of closed real intervals, that are

swept out by its dispersion maps as $\boldsymbol{k}$ varies over $\mathcal{B}$. The collection of all Floquet-Bloch eigenpairs is referred to as the *band structure* of $\mathbb{A}_g$.

2 Summary of our main results

We analyse the band structure of $\mathbb{A}_g$ in the high contrast regime: $g \gg 1$. We summarize our results for the two first dispersion maps. However, we point out that they hold in some configurations for dispersion surfaces arbitrary high in the spectrum, see [1].

a) High contrast global behavior. We show that:
• The first dispersion map $\lambda_1(\cdot;g)$ converges uniformly as $g \to +\infty$ on any compact set of $\mathcal{B}\backslash\{0\}$ to the constant function $\delta_1 > 0$ equal to the first Dirichlet eigenvalue on a single inclusion. The uniform convergence on all $\mathcal{B}$ fails since $\lambda_1(0;g) = 0$ for all $g > 0$. Unlike, $\lambda_1(\cdot;g)$, $\lambda_2(\cdot;g)$ converges uniformly to δ_1 on all $\mathcal{B}$.
• For g large enough, there exists a gap between the second and third dispersion surfaces.

b) Existence of Dirac point for $g \gg 1$. A Dirac points is as an energy / quasimomentum pair $(\lambda_D, \boldsymbol{k}_D) \in \mathbb{R}^+ \times \mathcal{B}$ where $\lambda_D = \lambda_-(\boldsymbol{k}_D;g) = \lambda_+(\boldsymbol{k}_D;g)$ is of multiplicity two and the consecutive dispersion maps $\lambda_-(\cdot;g) \leq \lambda_+(\cdot;g)$ touch conically. Namely, there exists a constant $v_D(g) > 0$, referred to as the Dirac velocity, such that:

$$\lambda_\pm(\boldsymbol{k};g) = \lambda_D \pm v_D(g)\,|\boldsymbol{k}-\boldsymbol{k}_D| + o(|\boldsymbol{k}-\boldsymbol{k}_D|). \quad (1)$$

In [1], we establish (for $g > 0$ fixed) sufficient conditions for the existence of Dirac points at any of the six vertices $\mathbf{K}_*$ of $\mathcal{B}$. In addition, we show that $v_D(g)$ in (1) is explicitly given in terms of a basis of the two dimensional eigenspace $\mathcal{V}_{g,\boldsymbol{k}_D} := \ker(\mathbb{A}_g - \lambda_D \mathrm{I})$ of Floquet-Bloch modes at $k_D = \mathbf{K}_*$. Furthermore, we show (under the hypothesis $v_D(g) \neq 0$, satisfied numerically) that these conditions hold for large contrast for the two first dispersion maps. Thus, there exists a Dirac point $(\lambda_D, \boldsymbol{k}_D)$ between $\lambda_-(\cdot;g) = \lambda_1(\cdot;g)$ and $\lambda_+(\cdot;g) = \lambda_2(\cdot;g)$ at the six vertices $\mathbf{K}_*$ of $\mathcal{B}$. We refer to the figure 2 for a numerical illustration of the results described in a) and b) at $g = 50$ and $\mathbf{K}_* = \mathbf{K}$.

c) Asymptotic expansions of Floquet-Bloch eigen–elements at the Dirac point. We obtain at $\boldsymbol{k}_D = \mathbf{K}_*$ asymptotic expansions at any order in powers of g^{-1} of the Dirac energy $\lambda_D(g)$ and a basis $\{\Phi_1, \Phi_2\}$ of the two-dimensional space $\mathcal{V}_{g,\boldsymbol{k}_D}$ of FloquetBloch modes. At leading order $\lambda_D(g) = \delta_1 + O(g^{-1})$ and $\{\Phi_1, \Phi_2\}$ satisfies $\Phi_1(\cdot;g) = P_{\boldsymbol{k}_D,A} + O(g^{-1})$ and $\Phi_2(\cdot;g) = P_{\boldsymbol{k}_D,B} + O(g^{-1})$. Here, $P_{\boldsymbol{k}_D,A}$ and $P_{\boldsymbol{k}_D,B}$ are $\boldsymbol{k}_D$-quasiperiodic superpositions of single inclusion Dirichlet states; supported respectively on the A-inclusions and on the B-inclusions. They play the role of *atomic orbitals* in the strong-binding Schrödinger regime; see [3]. Unlike ground state quantum atomic orbitals, they are compactly and disjointly supported, rather than exponentially localized in the well-depth parameter. The disjointness of the supports of $\Phi_j(\cdot;g)$ at leading order (cf. figure 3 for disks inclusions with $R = 0.2$) implies that $v_D(g) = v_D^{(1)} g^{-1} + O(g^{-2})$, where we have verified that $v_D^{(1)} > 0$ numerically. It explains why the "Dirac cones" flatten as g becomes large (see figure 2 for $g = 50$).

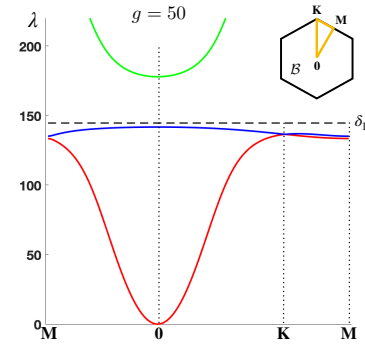


Figure 2: $\boldsymbol{k} \mapsto \lambda_1(\boldsymbol{k};50)$, $\lambda_2(\boldsymbol{k};50)$, $\lambda_3(\boldsymbol{k};50)$ plotted along the (yellow) contour: **M-0-K-M** of $\mathcal{B}$ for disks inclusions of radius $R = 0.2$.

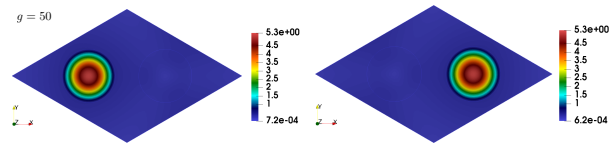


Figure 3: $|\Phi_1(\cdot;50)|$ and $|\Phi_1(\cdot;50)|$ on Ω at $\mathbf{K}$.

References

[1] M. Cassier and M. I. Weinstein, High contrast elliptic operators in honeycomb structures, *MMS* **19** (4) (2021), pp. 1784–1856.

[2] M. Cassier and M. I. Weinstein, TE Band Structure for High Contrast Honeycomb Media, in 2020 Fourteenth International Congress on Artificial Materials for Novel Wave Phenomena (Metamaterials), IEEE 2020, pp. 479–481.

[3] C. L. Fefferman, J. P. Lee-Thorp and M. I. Weinstein, Honeycomb Schrödinger operators in the strong binding regime, *Comm. in Pure and Appl. Math* **71** (6) (2018), pp. 1178–1270.