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Vanishing Gaps in Photonic Crystals and Other Periodic Potentials

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ABSTRACT
Using Floquet-Bloch theory, we find incipient bands (vanishing gaps) in the band structures of one-dimensional photonic crystals with a piece-wise constant profile of the refractive index, and in the band structures of continuously differentiable periodic potentials. The emphasis is on potentials that allow solutions in an exact analytical form.

Keywords: Floquet-Bloch theory, band structure of periodic potentials, vanishing gaps (incipient bands).

1. INTRODUCTION

The mathematical description of many physical problems, involving periodic variations either in space or time, reduces to Hill's differential equation in the form

$$\frac{d^2\Psi(z)}{dz^2} + Q(z)\Psi(z) = 0, \quad Q(z) = Q(z+d). \tag{1}$$

This includes, for example, light propagation in a one-dimensional (1D) photonic crystal, or the motion of electrons in a 1D superlattice.

According to Floquet-Bloch theory, see [1-3], among the fundamental systems of solutions of equation (1) there is a special one called the Floquet-Bloch system. This special fundamental system typically consists of two particular solutions $F_{1,2}(z)$, called Bloch waves, with the property under translation

$$F_{1,2}(z+d) = \rho_{1,2} F_{1,2}(z), \tag{2}$$

where the constants $\rho_{1,2}$ are non-zero, generally complex-valued numbers, called Floquet multipliers. They obey the relation

$$\rho_1 \rho_2 = 1, \tag{3}$$

In the allowed bands (regions of stability) both Bloch waves are bounded propagating functions. In the bandgaps (regions of instability) one Bloch wave decreases along the axis of propagation, while the other grows exponentially. That growing wave is an unphysical solution in case of an infinite periodic structure. Accordingly, in the bandgaps the multipliers $\rho_{1,2}$ become real-valued numbers.

On the boundaries (bandedges) between allowed bands and bandgaps, the two Bloch waves coincide, i.e. $F_2(z) = F_1(z) \equiv F(z)$. The constants $\rho_{1,2}$ also coincide, i.e. $\rho_1 = \rho_2 \equiv \rho$ and, in accordance with equation (3), either $\rho = 1$ or $\rho = -1$. In the former case the function $F(z)$ has a period d while in the latter case it has a period $2d$. Then, to complete the fundamental system of equation (1) another particular solution is required. That particular solution is often taken in the form of a hybrid Floquet mode, with the property

$$G(z+d) = \rho G(z) + \rho d\, G(z). \tag{4}$$

In practice, Bloch waves, hybrid Floquet modes, Floquet multipliers are all expressed in terms of normalized solutions $u(z)$ [$u(0)=1, u'(0)=0$] and $v(z)$ [$v(0)=0, v'(0)=1$]. The structure of allowed bands and bandgaps is defined by the dispersion equation

$$\cos(\mu d) = [u(d) + v'(d)]/2, \tag{5}$$

where μ is the Bloch wave number related to the Floquet multipliers by $\rho_{1,2} = \exp(\pm i\mu d)$. One can see that in the allowed bands $-1 < \cos(\mu d) < 1$, in the bandgaps $|\cos(\mu d)| > 1$, and at the bandedges $\cos(\mu d) = \pm 1$.

In the spectrum of Floquet-Bloch solutions, a case of special interest is so-called incipient bands (or vanishing gaps). Those are points of contact between distinct allowed bands (i.e. a special type of band crossing). Mathematically, in that case $\rho_1 = \rho_2 \equiv \rho = \pm 1$, but the two Bloch waves are independent periodic functions, with

the same periodicity (d if $\rho=1$, or $2d$ if $\rho=-1$), accordingly at those points $\cos(\mu d)=\pm 1$ and, in addition, $\nu(d)=0$, $u'(d)=0$.

It is known that vanishing gaps do not occur for the Dirac comb, nor the Mathieu potential, nor for a sawtooth potential [4, 5]. In this paper we summarize our recent findings on certain periodic potentials for which incipient bands do exist. This includes not only a well-known case of a binary photonic crystal (analogue of the Kronig-Penney model in quantum mechanics) but also a small set of periodic potentials having a continuously-differentiable function $Q(z)$ in equation (1).

2. VANISHING GAPS IN BINARY PHOTONIC CRYSTALS

In this section, we illustrate existence of incipient bands in a spectrum of light impinging normally on a binary crystal, illustrated in Fig. 1, for the case $d_1=d_2=d/2$ (basis layers of the same thickness). The dispersion equation (5) takes the form

$$\cos(\mu d)=\frac{\cos(kn_{\text{av}}d)-r_{21}^2\cos(r_{21}kn_{\text{av}}d)}{1-r_{21}^2}, \tag{6}$$

where $k=2\pi/\lambda$ is the vacuum wavenumber of impinging light and $r_{21}=(n_2-n_1)/(n_2+n_1)$ is the amplitude Fresnel reflection coefficient on the boundary between the layers n_2 and n_1. The results are shown in Fig. 2. The incipient bands are a set of points defined by either

$$\begin{cases} kn_{\text{av}}d=2m\pi, & m=2,3,\ldots, \\ r_{21}=\pm l/m, & l=1,\ldots,m-1, \end{cases} \tag{7}$$

where the Bloch waves have periodicity d, or by

$$\begin{cases} kn_{\text{av}}d=(2m-1)\pi, & m=2,3,\ldots, \\ r_{21}=\pm(2l-1)/(2m-1), & l=1,\ldots,m-1, \end{cases} \tag{8}$$

where the Bloch waves have periodicity $2d$.

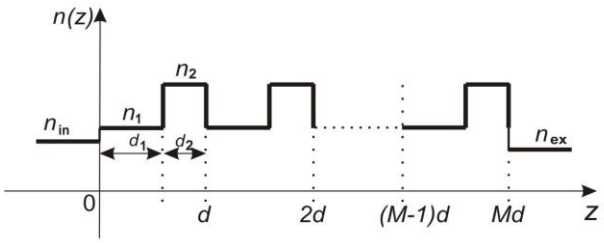

Fig. 1. Binary photonic crystal with the layers of refractive indices n_1, n_2 and thicknesses d_1, d_2, M is the number of periods.

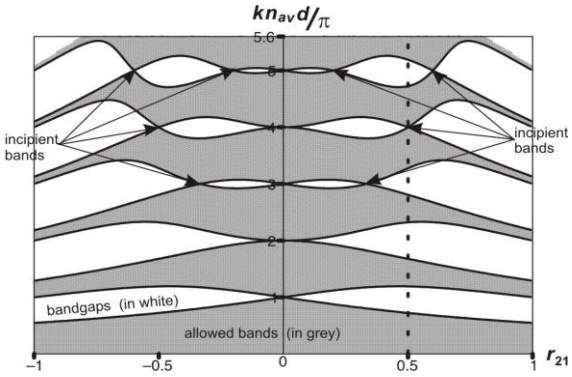

Fig. 2. Band structure of a binary crystal for normal incidence for the case $d_1=d_2=d/2$, $r_{21}=(n_2-n_1)/(n_2+n_1)$, $n_{\text{av}}=(n_2d_2+n_1d_1)/d$.

The above problem about light normally incident on a binary photonic crystal with layers of equal geometrical thicknesses $(d_1=d_2)$ is just one example of incipient bands (vanishing gaps) in the band structure of piece-wise constant periodic potentials. Other confirmed examples where incipient bands occur, include normal incidence of light on a binary crystal with layers of equal optical thicknesses $(n_1d_1=n_2d_2)$, see [6], oblique incidence of light on an arbitrary binary crystal, see [7], etc. We should note that in all those problems the incipient bands (vanishing gaps) appear in the form of a discrete set of points.

3. VANISHING GAPS IN CONTINUOUS PERIODIC POTENTIALS

In this section we illustrate existence of incipient bands for three periodic potentials with continuously-differentiable functions $Q(z)$. The first example is the Casperson potential [8, 9], see Fig. 3, given by

$$Q_c=\frac{a}{(1+q\cos 2z)^4}+\frac{4q\cos(2z)}{1+q\cos 2z}, \quad -1<q<1. \tag{9}$$

For this potential the dispersion equation (5) takes the form

$$\cos(\mu d) = \cos\left[\pi\sqrt{\frac{a}{(1-q^2)^3}}\right], \tag{10}$$

where $d = \pi$ is the period of the potential. The band structure is shown in Fig. 4. There is only one allowed band ($a > 0$) separated by a bandedge ($a = 0$) from a single bandgap ($a < 0$). The incipient bands are curves defined by

$$\frac{a}{(1-q^2)^3} = m^2, \quad m = 1,2,3,4,\ldots, \tag{11}$$

where the Bloch waves have periodicity $d = \pi$ for $m = 2,4,\ldots$, and $2d = 2\pi$ for $m = 1,3,\ldots$.

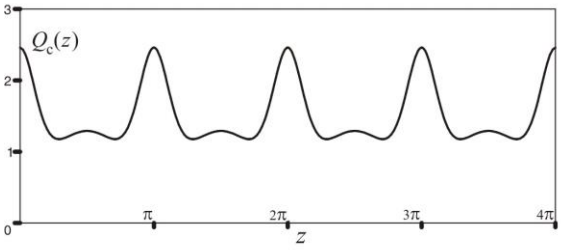

Fig. 3. Casperson potential for $q = -0.25$, $a = 1.20$.

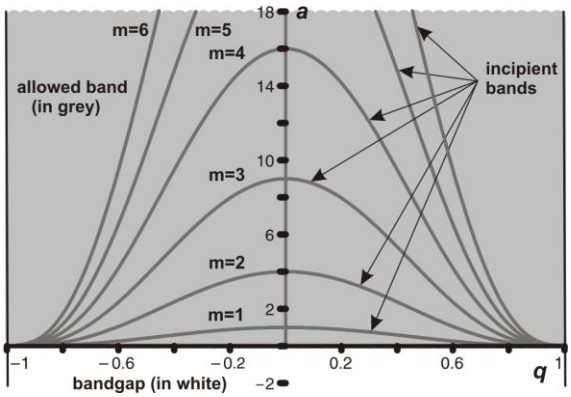

Fig. 4. Band structure of the Casperson potential, only the first six incipient bands are shown.

The next example is the Wu potential [9, 10], see Fig. 5, which is somewhat similar to the Casperson one. It is given by the function

$$Q_w = \frac{a + q^2\sin^2 2z}{(1+q\cos 2z)^2} + \frac{2q\cos(2z)}{1+q\cos 2z}, \quad -1 < q < 1, \tag{12}$$

with the dispersion equation (5) taking the form

$$\cos(\mu d) = \cos\left[\pi\sqrt{\frac{a}{1-q^2}}\right]. \tag{13}$$

The band structure is shown in Fig. 6. Similar to the Casperson potential, there is a single allowed band ($a > 0$) separated by a bandedge ($a = 0$) from a single bandgap ($a < 0$). The incipient bands are curves defined by

$$\frac{a}{1-q^2} = m^2, \quad m = 1,2,3,4,\ldots, \tag{14}$$

where the Bloch waves have periodicity $d = \pi$ for $m = 2,4,\ldots$, and $2d = 2\pi$ for $m = 1,3,\ldots$.

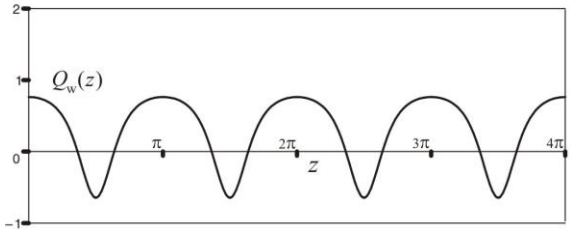

Fig. 5. Wu potential for $q = 0.45$, $a = 0.30$.

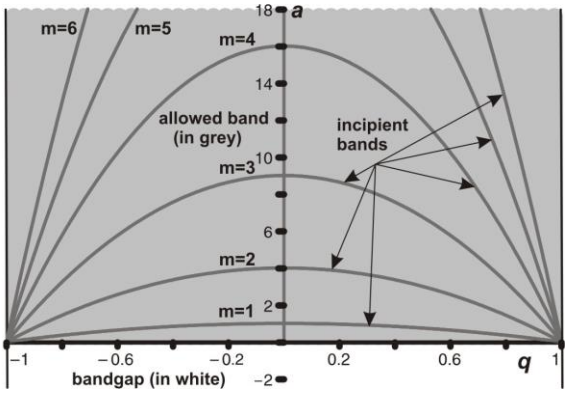

Fig. 6. Band structure of the Wu potential, only the first six incipient bands are shown.

The final example is the Takayama potential [11, 12], see Fig. 7, given by the function

$$Q_t = 1 + \frac{a\left(1-q^2\right)}{\left(1+q\cos 2z\right)^2}, \qquad -1 < q < 1, \tag{15}$$

with the dispersion equation (5)

$$\cos\left(\mu d\right) = \cos\left[\pi\sqrt{a+1}\right]. \tag{16}$$

The band structure is shown in Fig. 8. An allowed band ($a > -1$) is separated by a bandedge ($a = -1$) from a single bandgap ($a < -1$). The incipient bands are straight lines defined by

$$a = m^2 - 1, \qquad m = 1,2,3,4,\ldots, \tag{17}$$

where the Bloch waves have periodicity $d = \pi$ for $m = 2,4,\ldots$, and $2d = 2\pi$ for $m = 1,3,\ldots$.

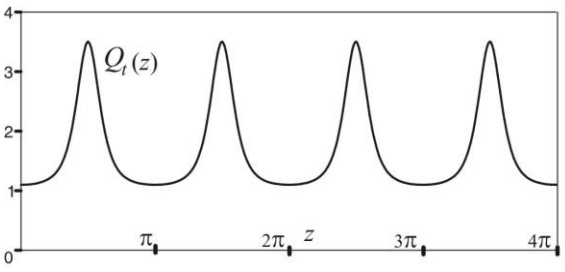

Fig. 7. Takayama potential for $q = 2/3$, $a = 1/2$.

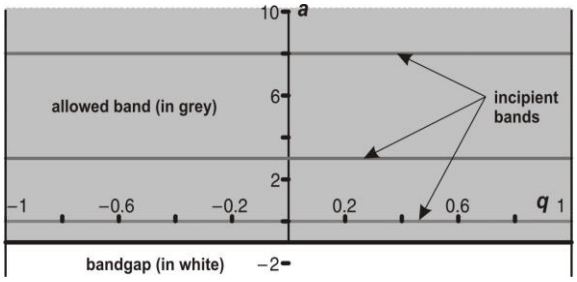

Fig. 8. Band structure of the Takayama potential, only the first three incipient bands are shown.

The above three continuous periodic potentials add to the set of exactly solvable Hill's equations. The band structure of each potential features a single bandgap separated by a bandedge from a single allowed band, which is divided into pieces by incipient bands (vanishing gaps). Those incipient bands are a set of continuous curves, rather than a set of points as was observed for the piece-wise constant periodic potential.

4. CONCLUSIONS

We analysed the band structures of certain exactly solvable Hill's equations with both piece-wise constant and continuously-differentiable periodic potentials. Particular attention was given to the incipient bands (vanishing gaps) where all solutions of Hill's equation become periodic functions. A further logical step would be to obtain an analytical criterion for the existence of incipient bands in an arbitrary periodic potential.

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