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# The band spectrum of periodic potentials with $\mathcal{PT}$ -symmetry

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## Abstract

A *real* band condition is shown to exist for one-dimensional periodic *complex* non-Hermitian potentials exhibiting  $\mathcal{PT}$ -symmetry. We use an exactly solvable ultralocal periodic potential to obtain the band structure and discuss some spectral features of the model, specially those concerning the role of the imaginary parameters of the couplings. Analytical results as well as some numerical examples are provided.

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## 1. Introduction

In a previous series of papers [1, 2], we have presented the exact diagonalization of the Hermitian Schrödinger operator corresponding to a periodic potential composed of  $N$  atoms modelled by delta functions with different couplings for arbitrary  $N$ . This basic structure can repeat itself an infinite number of times giving rise to a periodic structure representing an  $N$ -species one-dimensional infinite chain of atoms. To our surprise this model is exactly solvable, and a far from straightforward calculation leads to an exact band condition. Due to the factorizable form of the solution, one has not only the advantage of closed form expressions but one can also perform computer calculations with an exceedingly high degree of accuracy due to the exact nature of the solution itself. The main physical motivation was indeed to model the band structure of a one-dimensional quantum wire. The model can be extended with a minimum amount of effort to the non-Hermitian but  $\mathcal{PT}$ -symmetric [3] quantum Hamiltonian, and the band condition becomes real although the potential is obviously a complex one. The imaginary parts of the couplings play a central role in defining the band structure which can be modelled at will by varying this parameter. The purpose of this paper is to present this new solution in a detailed fashion. In a previous paper, a preliminary analysis of the existence and properties of this exact band model solution was given [4]. Here we want to present a

careful study of the solution in a more rigorous manner paying due attention to the exciting properties that this rich structure seems to exhibit.

The idea of performing band structure calculations by using a non-Hermitian Hamiltonian is extremely promising as the examples of  $\mathcal{PT}$ -symmetric quantum Hamiltonians so far existing in the literature rely more on aspects concerning the discrete spectrum and bound states [5–8] and are also far from an actual physical application. It is not the aim of the present paper to provide a full discussion of the manifold aspects of the  $\mathcal{PT}$ -symmetry in quantum mechanics. We address the interested reader to the original reference [3], some recent interesting theoretical criticism [9] and also to some work done recently in one-dimensional models [10] which may help to understand better the role of  $\mathcal{PT}$ -symmetry in the framework of one-dimensional systems. In all these papers the imaginary part of the coupling plays a substantial role in defining the spectrum of bound states. We shall show that in the case of the band structure hereby presented, this imaginary part is of primary importance in defining the transport properties of the one-dimensional quantum chain.

The plan of the paper is as follows. In section 2 we shall be discussing the main features of the model just as a simple model for a quantum wire with only real couplings. Furthermore, the presence of  $\mathcal{PT}$ -symmetry and the role of the complex couplings will be introduced. The band spectrum remains analytical and real in spite of the complex non-Hermitian nature of the potential. In section 3 a thorough analysis of the band condition is made in order to clarify the effect of the imaginary parts of the couplings on the band spectrum. This analysis can be expressed analytically for some cases where  $N$  is not too large. Otherwise the equations appear to be intractable. Even in this case numerical calculations can always be performed with a high degree of accuracy. In section 4 we make some comments on the band spectrum and observe the form of the  $\mathcal{PT}$ -symmetric electronic states. Several pathologies plaguing the band spectrum for the complex coupling case are observed. This can be avoided working on a small range of energies for certain values of the imaginary couplings. The localization of the wavefunction over the primitive cell is also found to be altered manipulating only the imaginary parameters. We close with our conclusions in section 5.

## 2. The model and its band spectrum

Let us begin with a brief reminder of the solution presented in [1] corresponding to an infinite periodic potential composed of a basic structure made out of a *finite* number  $N$  of equally spaced deltas with different *real*  $N$  couplings, repeating itself an *infinite* number of times. If the spacing is  $a$  and

$$a_j = \frac{\hbar^2}{me_j^2} \quad (2.1)$$

is the length associated with each coupling ( $e_j^2$ ), the band structure can be written as

$$\cos(NQa) = \mathcal{B}(\varepsilon; a_1, a_2, \dots, a_N) \quad (2.2)$$

where  $Q$  is an arbitrary real number which varies between  $\frac{\pi}{Na}$  and  $-\frac{\pi}{Na}$  and

$$\begin{aligned} \mathcal{B}(\varepsilon; a_1, \dots, a_N) &= 2^{N-1} \sum_P h_i \cdots (N) \cdots h_k - 2^{N-3} \sum_P h_i \cdots (N-2) \cdots h_k \\ &+ 2^{N-5} \sum_P h_i \cdots (N-4) \cdots h_k - \cdots (-1)^{\frac{N}{2}-1} 2 \sum_P h_i \cdots (2) \cdots h_k \\ &+ (-1)^{\frac{N}{2}} \end{aligned} \quad (2.3)$$

$$\begin{aligned} \mathcal{B}(\varepsilon; a_1, \dots, a_N) &= 2^{N-1} \sum_P h_i \cdots (N) \cdots h_k - 2^{N-3} \sum_P h_i \cdots (N-2) \cdots h_k \\ &+ 2^{N-5} \sum_P h_i \cdots (N-4) \cdots h_k - \cdots (-1)^{\frac{N-3}{2}} 2^2 \sum_P h_i \cdots (3) \cdots h_k \\ &+ (-1)^{\frac{N-1}{2}} (h_1 + h_2 + \cdots + h_N) \end{aligned} \tag{2.4}$$

for even and odd  $N$ , respectively.

The symbol  $\sum_P h_i \cdots (M) \cdots h_k$  means a sum over all products of  $M$  different  $h_i$  with the following rule for each product: the indices must follow an increasing order and an odd index must always follow an even index and reciprocally.

The functions  $h_j$  have the universal form:

$$h_j(\varepsilon) = \cos(\varepsilon) + \left(\frac{a}{a_j}\right) \frac{\sin(\varepsilon)}{\varepsilon} \tag{2.5}$$

and the independent variable is a function of the energy (i.e.  $\varepsilon = ka$ ). In order to see that this condition looks much simpler than one might think at the beginning of the calculation let us list below, for the benefit of the reader, the first three conditions for the cases  $N = 2, 3$  and  $4$ .

$$\cos(2Qa) = 2h_1h_2 - 1 \tag{2.6}$$

$$\cos(3Qa) = 4h_1h_2h_3 - (h_1 + h_2 + h_3) \tag{2.7}$$

$$\cos(4Qa) = 8h_1h_2h_3h_4 - 2(h_1h_2 + h_1h_4 + h_2h_3 + h_3h_4) + 1. \tag{2.8}$$

It does not require too much time to write down the band conditions for fairly large  $N$ , but more important is the fact that the *exact* formulae (2.3) and (2.4) are in themselves quite easy to program for sequential calculations. Using the band condition we have been able not only to generate a full band spectrum but also to calculate the density of states for periodic one-dimensional lattices with a high degree of accuracy (see [1, 2]).

The next step is to include  $\mathcal{PT}$ -symmetry in this model. It is not hard to see that (2.2) is still *real* if we include the following changes:

- Promote the couplings from *real* to *complex*, i.e.  $\left(\frac{a}{a_j}\right) \rightarrow r_j + is_j$ .
- Order the potential in a  $\mathcal{PT}$ -invariant form that allows us to choose a  $\mathcal{PT}$ -symmetric primitive cell. This leads to the following identifications:

$$\begin{aligned} h_N &= h_1^* \\ h_{N-1} &= h_2^* \\ &\vdots \\ h_{\frac{N}{2}+1} &= h_{\frac{N}{2}}^* \quad \text{even } N \\ h_{\frac{N+1}{2}} &= h_{\frac{N+1}{2}}^* \quad \text{odd } N. \end{aligned}$$

It is easy to check that equations (2.3) and (2.4) remain *real* under these identifications, which make obviously the periodic potential *complex* but  $\mathcal{PT}$ -invariant. There has been an earlier attempt to generate a *real* band condition from a complex but  $\mathcal{PT}$ -invariant potential [11]. However, the results concerning the appearance and disappearance of forbidden and allowed bands were inconclusive. In our case this effect is clear and will be discussed at length below.

As has been well known for years, a Hermitian periodic potential cannot alter its band spectrum just by fine tuning the couplings. The bands can indeed be made wider or narrower but their number and quality (forbidden or allowed) remain unchanged. The theorems supporting

these statements are all based upon the intuitive idea that a Hermitian operator cannot change its spectrum that is basically given by the eigenvalues and eigenfunctions of the states at the edges of the bands. The mathematics can be hard but the physical idea was indeed whether this behaviour would be maintained if a  $\mathcal{PT}$ -invariant potential is used. For this purpose one can use various analytical potentials carefully shifted to be  $\mathcal{PT}$ -invariant. One can prove that the band condition is real but in order to analyse the band structure one has to assert with a very high degree of precision whether a given curve is above (below)  $+1$  ( $-1$ ) in a similar manner as we have to ascertain ourselves that expressions (2.6)–(2.8) (and in general (2.3) and (2.4)) exceed  $+1$  or go below  $-1$ . In the case of [11] this appears a very hard task indeed as the authors do not have at their disposal an analytical band condition, so they must carry out various kinds of approximations. The authors conclude that “despite this impressive precision, [ . . . its equations] (16) and (17) cannot be used directly to answer the crucial question of whether there are band gaps because these approximations to the discriminant [ . . . band condition] never cross the values [ . . . normalized to]  $\pm 1$ ”.

But we do have such an exact band condition and in spite of the apparent formidable aspect of expressions (2.3)–(2.4) we can perform various kinds of exact and numerical analyses in order to check the dependence of the band width and the band number on the exceptional parameter that arises in our model: the imaginary part of the complex couplings. This will be the subject of the next section.

### 3. The band condition for couplings with non-vanishing imaginary part

In order to understand the effect of the imaginary part of the couplings on the band spectrum, one must analyse in detail the behaviour of the band condition. Let us begin with the simplest  $\mathcal{PT}$ -symmetric chain including two deltas in the primitive cell characterized by the parameters  $(a/a_1) = r_1 + is_1$  and  $(a/a_1)^* = r_1 - is_1$ . This case has also been carefully studied considering different distances between the deltas in [12]. The band structure is entirely determined by the function  $\mathcal{B} = 2h_1 h_1^* - 1$ , which can be written as

$$\mathcal{B} = \mathcal{B}(s_1 = 0) + \frac{2s_1^2 \sin^2(\varepsilon)}{\varepsilon^2}. \quad (3.1)$$

The term due to the imaginary part is always positive and it has the effect of lifting up the band condition for all values of  $r_1$ . The position and width of the allowed (forbidden) bands come from the intersections at  $\mathcal{B} = 1, -1$ , which depend strongly on the position of the maxima and minima of the band condition. The changes on these limiting points can be analytically described in this case.

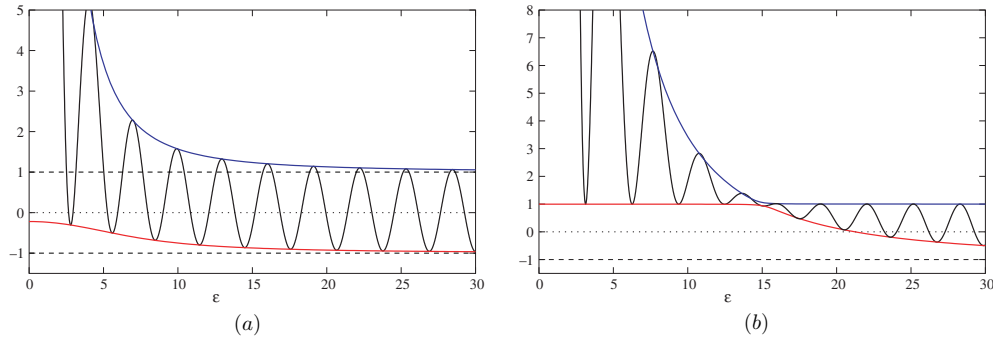
From the equation  $d\mathcal{B}/d\varepsilon = 0$  one can find the value of the oscillatory part of the band condition (i.e. the trigonometric functions) as a function of  $\varepsilon$  and substituting into  $\mathcal{B}$  with a proper choice of signs, will result in an analytical form for the curves crossing the extremal points of the band condition which reads

$$C_{\pm} = 2f_{\pm} f_{\pm}^* - 1 \quad (3.2)$$

where  $C_+$  ( $C_-$ ) lies on the maxima (minima) and the functions  $f_{\pm}$  are defined as follows:

$$f_{\pm} = \frac{1}{\sqrt{F_{\pm}}} \left[ \sqrt{2}r_1(r_1 - is_1) \pm (F_{\pm} - 2r_1^2\varepsilon^2)^{\frac{1}{2}} \right] \quad (3.3)$$

$$F_{\pm} = r_1^2 + (r_1^2 + s_1^2)^2 + 2(r_1 + r_1^2 - s_1^2)\varepsilon^2 + \varepsilon^4 \pm (r_1 - r_1^2 - s_1^2 + \varepsilon^2) \left[ (r_1 + r_1^2 + s_1^2)^2 + 2(r_1 + r_1^2 - s_1^2)\varepsilon^2 + \varepsilon^4 \right]^{\frac{1}{2}}. \quad (3.4)$$



**Figure 1.** Band condition for  $N = 2$  when  $s \sim r$  and  $s \gg r$ . The coloured lines correspond to  $C_{\pm}$ . (a)  $r_1 = 5, s_1 = 4$ ; (b)  $r_1 = 0.5, s_1 = 15$ .

Hence, the behaviour of the band condition can be studied through the evolution of  $C_{\pm}$ . Taking the limit  $s_1 \rightarrow 0$  we obtain

$$\lim_{s_1 \rightarrow 0} C_{\pm} = \begin{cases} 1 + \frac{2r_1^2}{\varepsilon^2} \frac{r_1(2+r_1) + \varepsilon^2}{r_1(2+r_1) + \varepsilon^2 + \frac{r_1^2}{\varepsilon^2}} & \\ -1. & \end{cases} \quad (3.5)$$

The real part of the couplings controls the amplitude of the oscillations (and therefore the distance between  $C_+$  and  $C_-$ ) but the minima will always lean on  $\mathcal{B} = -1$  unless the imaginary part is nonzero. Thus as we increase  $s_1$  the minima will rise, as can be seen in figure 1(a), and they never touch  $-1$  because  $\lim_{\varepsilon \rightarrow \infty} C_- = -1$ . On the other hand, considering  $r_1 \rightarrow 0$ , after some algebra one obtains

$$\lim_{r_1 \rightarrow 0} C_+ = \begin{cases} -1 + \frac{2s_1^2}{\varepsilon^2} \frac{s_1^4 + \varepsilon^4 + s_1^2(1 - 2\varepsilon^2)}{s_1^4 + \varepsilon^4 + s_1^2 \left( \frac{s_1^2}{\varepsilon^2} - 2\varepsilon^2 \right)} & \text{for } \varepsilon \leq s_1 \\ 1 & \text{for } \varepsilon > s_1 \end{cases} \quad (3.6)$$

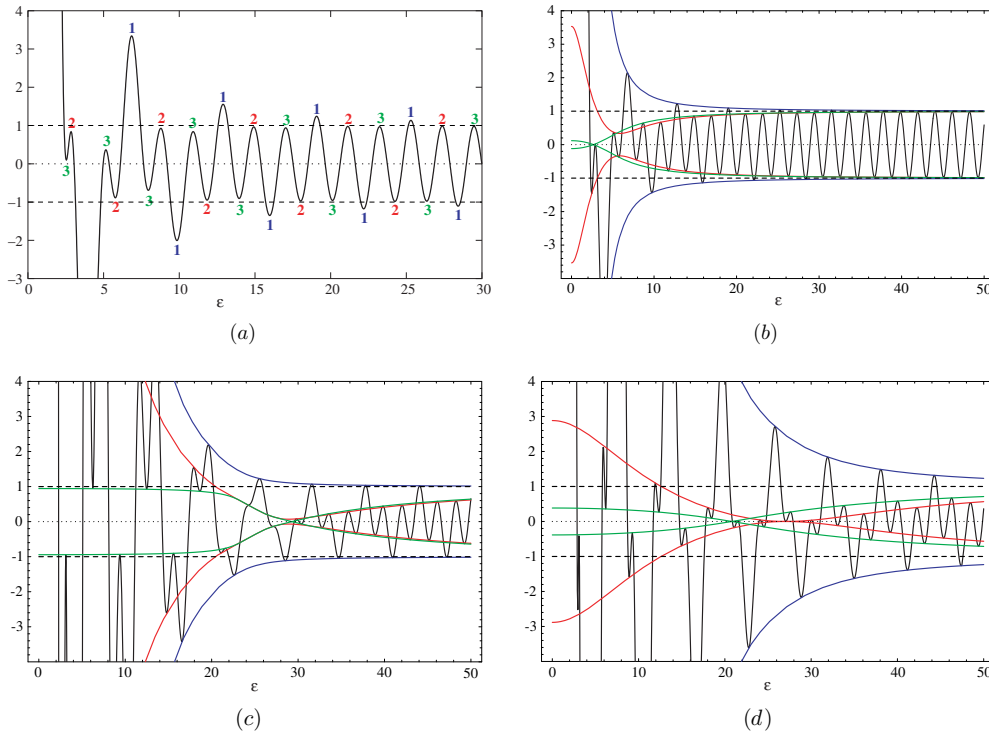
and for  $C_-$  the limit is the same as for  $C_+$  but interchanging with respect to the intervals in  $\varepsilon$ . Thus for an imaginary part of the coupling large enough compared to the real one the band condition goes above  $+1$  for energies below the value  $s_1$ . Figure 1(b) shows this last configuration. In fact the situation  $s_1 \gg r_1$  can be easily understood from the form of the band condition that can easily be written in this limit as

$$\mathcal{B} \simeq -1 + \frac{2s_1^2}{\varepsilon^2} + 2 \cos^2(x) \left( 1 - \frac{s_1^2}{\varepsilon^2} \right) \quad (3.7)$$

which shows clearly the boundaries when  $\varepsilon \leq s_1$ ;  $1 \leq \mathcal{B} \leq -1 + 2s_1^2/\varepsilon^2$  saturated at  $\varepsilon = n\pi$  and  $\varepsilon = (2n+1)\frac{\pi}{2}$  ( $n \in \mathbb{Z}$ ), respectively. For  $\varepsilon > s_1$  the boundaries simply interchange among them. Due to the nature of the functions  $h_j(\varepsilon)$  the band condition is always tied up to the value  $+1$  at every multiple of  $\pi$  for all  $r_1, s_1$ , as figure 1(b) clearly shows. Several configurations of the spectrum such as those in figure 1 can be built for different values of the complex coupling.

Let us now consider a  $\mathcal{PT}$ -symmetric chain whose primitive cell includes three atoms characterized by the parameters  $(a/a_1) = r_1 + is_1$ ,  $(a/a_2) = r_2$  and  $(a/a_1)^*$ . The band condition function reads  $\mathcal{B} = 4h_1 h_1^* h_2 - (h_1 + h_1^* + h_2)$ . This can be arranged as

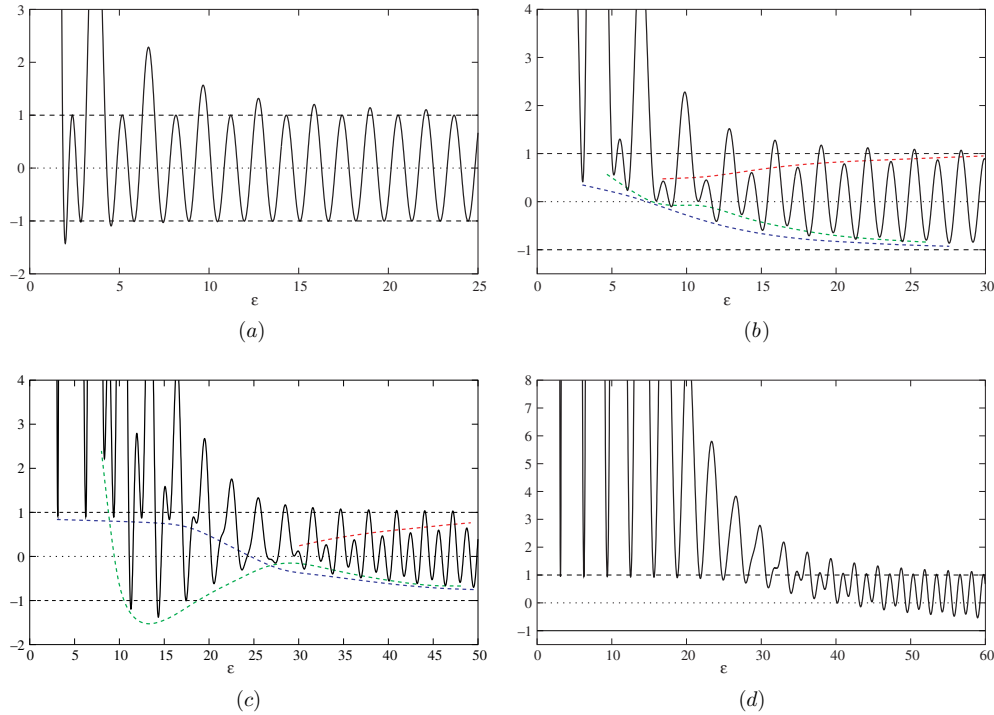
$$\mathcal{B} = \mathcal{B}(s_1 = 0) + \frac{4s_1^2 \sin^2(\varepsilon) [\varepsilon \cos(\varepsilon) + r_2 \sin(\varepsilon)]}{\varepsilon^3}. \quad (3.8)$$



**Figure 2.** Band condition for  $N = 3$  for different values of the couplings. Each type of extremal point is labelled with a different colour. (a)  $r_1 = 4, r_2 = 5, s_1 = 3$ ; (b)  $r_1 = 3, r_2 = 2, s_1 = 5$ ; (c)  $r_1 = 3, r_2 = 2, s_1 = 25$ ; (d)  $r_1 = 10, r_2 = 10, s_1 = 25$ .

The extra term arising from the imaginary part of the coupling can be either positive or negative depending on the value of  $r_2$  and the energy. The effect of  $s_1$  is different compared to the previous case although there is only one imaginary parameter. The structure of the band condition seems to be composed of pieces each one including three different types of extremal points, as figure 2(a) shows, each type apparently following a given pattern. The curves crossing the extremal points of the band condition can also be analytically calculated in the  $N = 3$  case but the expressions are quite hard to simplify and therefore we do not provide the explicit form of the equations. Three curves are obtained, one for each type of extremal point. Initially when  $s_1 = 0$  all the extremal points are outside or on the borders of the range  $[-1, 1]$ . As we increase the imaginary part, the amplitudes of two of the three types of extremal points begin to decrease (green and red in figure 2(b)). At the same time as  $s_1$  becomes larger the green and red curves get narrower with decreasing energy until  $\varepsilon \sim s_1$ . Below this value the curves broaden trying to expel the extremal points of the band condition outside the target range (figure 2(c)). From the form of  $\mathcal{B}$  it is clear that the even (odd) multiples of  $\pi$  will remain fixed to 1 ( $-1$ ). The efficiency of this expelling process depends upon the values of the real couplings as they control the amplitudes of the oscillations. One can stretch the maxima and minima (up and down, respectively) increasing  $r_1, r_2$ , as shown in figure 2(d).

Several configurations can be obtained among those shown in figure 2 and one important feature must be emphasized: the band condition always changes ‘symmetrically’ with respect to the abscissa axis. That is, there is the same amount of positive and negative function whatever the values of the couplings are. In fact the curves lying on the extremal points show

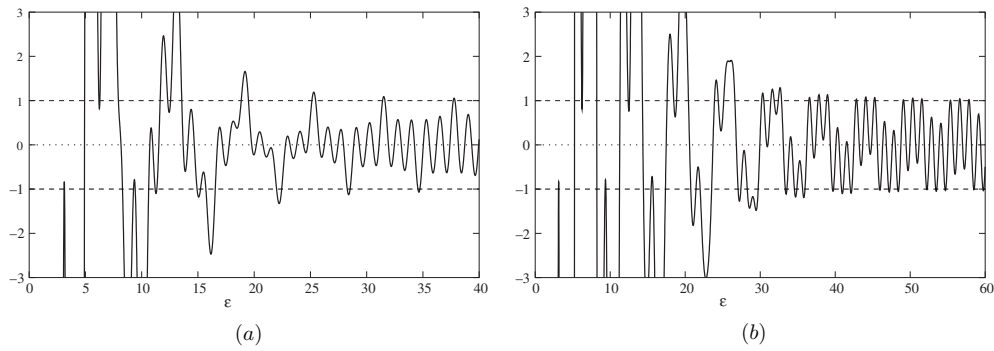


**Figure 3.** Band condition for  $N = 4$  with different values of the couplings. The coloured dashed lines are intended to clarify the behaviour of different groups of extremal points. (a)  $r_1 = 3, r_2 = 2, s_1 = 0, s_2 = 0$ ; (b)  $r_1 = 3, r_2 = 2, s_1 = 9, s_2 = 2$ ; (c)  $r_1 = 3, r_2 = 2, s_1 = 4, s_2 = 25$ ; (d)  $r_1 = 3, r_2 = 2, s_1 = 20, s_2 = 21$ .

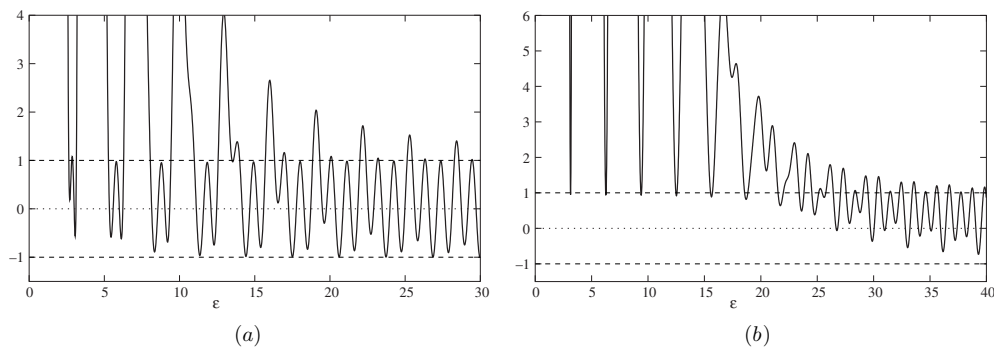
an exact reflection symmetry around the energy axis. This is in great contrast to the  $N = 2$  case where the band condition can be pushed up above  $+1$  for certain couplings. Thus when  $s_1 \gg r_1, r_2$  there will always remain a trace of the original permitted energy ranges in the form of ‘flat’ bands.

The first chain for which two different imaginary couplings can be manipulated is the one with  $N = 4$  atoms inside the primitive cell:  $(a/a_1) = r_1 + is_1, (a/a_2) = r_2 + is_2, (a/a_2)^*$  and  $(a/a_1)^*$ . In this case we have not calculated analytically the curves crossing the extremal points. Nevertheless a pictorial approach for some of the curves has been included in the graphics for a better understanding of the tendencies of change. The initial situation ( $s_1 = s_2 = 0$ ) is a common one for a periodic chain (figure 3(a)) and two different groups of extremal points can be distinguished. As we increase the imaginary part of the couplings one group of extremal points starts to decrease and the band condition lifts up globally (figure 3(b)). The effect of the two imaginary parts is quite similar. When both of them have comparable values the two groups of minima follow the same tendency moving the band condition upwards. However, if one imaginary part grows much more than the other one, several minima stretch down in a region of energy roughly included in  $s_{\text{small}} < \varepsilon < s_{\text{large}}$  (figure 3(c)). Finally, when  $s_1, s_2 \gg r_1, r_2$  one can force the band condition to go above  $+1$  (keeping our well-known knots at  $\varepsilon = n\pi$ ) in a certain energy range which depends on the values of the imaginary parts of the couplings (figure 3(d)) approximately the same way as for the  $N = 2$  case. Unlike the  $N = 3$  example the band condition can be unbalanced to positive values with a proper choice of the parameters.





**Figure 4.** Band condition for a  $\mathcal{PT}$ -symmetric chain with  $N = 5$ . (a)  $r_1 = 4, r_2 = 1, r_3 = 1, s_1 = 20, s_2 = 5$ ; (b)  $r_1 = 4, r_2 = 2, r_3 = 3, s_1 = 10, s_2 = 20$ .

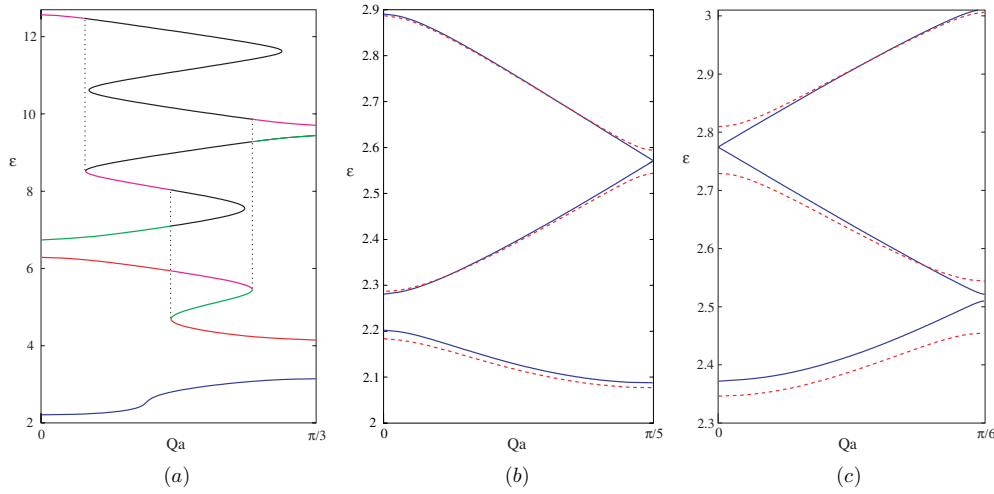


**Figure 5.** Band condition for a  $\mathcal{PT}$ -symmetric chain with  $N = 6$ . (a)  $r_1 = 5, r_2 = 3, r_3 = 4, s_1 = 2, s_2 = 5, s_3 = 4$ ; (b)  $r_1 = 1, r_2 = 2, r_3 = 0.5, s_1 = 10, s_2 = 11, s_3 = 12$ .

The band condition has also been studied in detail for  $N = 5$  and  $N = 6$ . Its behaviour gets really complex as the number of atoms grows. In figures 4 and 5 some characteristic examples are shown. For  $N = 5$  the band condition shows five types of extremal points that evolve ‘symmetrically’ around the abscissa axis as we change the imaginary couplings. For  $N = 6$  three types of maxima and minima appear and for large enough values of the imaginary couplings the band condition is greater than +1.

To summarize this mathematical analysis of the band condition let us now list some of the most salient features:

- the band condition is composed of pieces integrated by  $N$  ( $N/2$ ) extremal points for odd (even)  $N$ . Each extremal point belongs to a group that evolves differently according to the values of the imaginary parts of the couplings;
- for odd  $N$  the band condition is ‘symmetric’ around the abscissa axis for all values of the couplings. Therefore, some permitted levels always remain as a part of the spectrum;
- for even  $N$  the band condition can be expelled out of the target range for certain values of the couplings, so removing the allowed bands;
- for  $\varepsilon = n\pi$  the band condition is fixed to +1 or  $-1$  depending on the parity of  $N$  and  $n$  for all values of the couplings
- the real parts of the couplings are always proportional to the amplitude of the oscillations.



**Figure 6.** Band structure in the irreducible part of the first Brillouin zone for different chains: (a)  $N = 3$  with  $r_1 = 1, r_2 = 2, s_1 = 3$ . Different colours show the first four bands. (b)  $N = 5$  with  $r_1 = 4, r_2 = 2, r_3 = 1, s_1 = s_2 = 0$  (red) and  $s_1 = 0.775, s_2 = 0.1$  (blue). (c)  $N = 6$  with  $r_1 = 5, r_2 = 2, r_3 = 3, s_1 = s_2 = s_3 = 0$  (red) and  $s_1 = 1.613, s_2 = 0.12, s_3 = 0.3$  (blue).

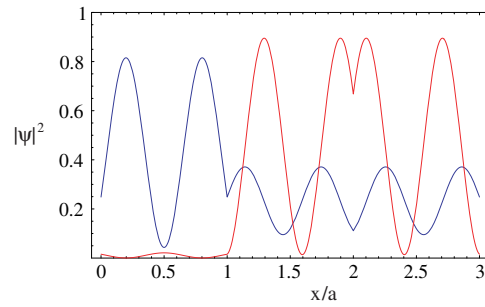
Even with all the included figures, it is hard to give a complete explanation of the behaviour of the band condition that otherwise can only be fully understood watching some proper animations of the function. This is the procedure we have followed to support the results. We encourage the interested reader to reproduce those animations, which can easily be done with Mathematica. Some example code lines are listed in the appendix.

#### 4. The band structure and the electronic states

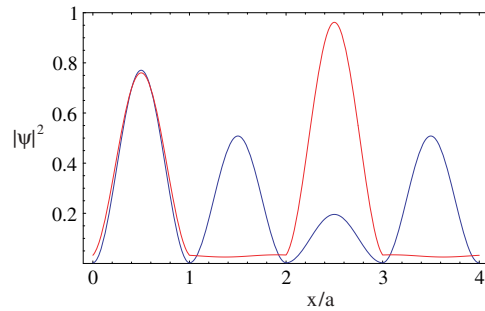
Let us now make some comments about the band structure. One important feature that stands out from the above examples is the presence of maxima (minima) inside the target range  $(-1, 1)$ . This fact involves the presence of points in the reciprocal space, where the gradient of the energy diverges, that makes the physical interpretation of the Hamiltonian not so straightforward. Probably some additional restrictions have to be imposed on the  $\mathcal{PT}$ -symmetric Hamiltonian. These special points also cause some changes in the form of the bands which are always understood as the ensembles of states and energies labelled with a certain index ( $n$  for the  $n$ th band). Every point of the Brillouin zone must represent a physical state on every band. Therefore for a certain value  $Qa$  let us label the eigenenergies of the Hamiltonian following an increasing order ( $\varepsilon_1(Qa) < \varepsilon_2(Qa) < \dots$ ). This procedure leads unavoidably to the definition of bands whose dispersion relations are not continuous over the reciprocal space as seen in figure 6(a). Of course the choice of the band indices is not unique but none of them will be free of these discontinuities.

On the other hand, those pathologies can be avoided if one restricts one's working scenario to a small range of energies. In that case the imaginary parts of the couplings can be tuned to modify essentially the spectrum of the system removing or decreasing gaps to virtually change its response to transport phenomena (figures 6(b) and (c)).

One can also wonder about the form of an electronic state belonging to such a characteristic spectrum. It is not hard to calculate analytically the wavefunction inside the primitive cell as a



**Figure 7.** Electronic wavefunction normalized to 1 inside the primitive cell of a  $\mathcal{PT}$ -symmetric chain for  $N = 3$  with  $r_1 = 5$ ,  $r_2 = 3$ ,  $s_1 = 0$  (blue) and  $s_1 = 19$  (red) at  $\varepsilon = 5.2$ .



**Figure 8.** Electronic wavefunction normalized to 1 inside the primitive cell of a  $\mathcal{PT}$ -symmetric chain for  $N = 4$  with  $r_1 = 3$ ,  $r_2 = 4$ ,  $s_1 = 5$ ,  $s_2 = 8.1$  for different energies:  $\varepsilon = 2.95$  (red) and  $\varepsilon = 3.13$  (blue).

function of the position and the energy with the help of the computer for low  $N$ . To our surprise we have found that the imaginary parts of the couplings behave as control parameters of the localization of the electrons inside the primitive cell. Thus one could tune these parameters to decrease the probability of presence in several sectors almost to zero or distribute it more homogeneously over the primitive cell, as shown in figure 7. Also for non-vanishing imaginary parts of the couplings, the dependence of the state on the energy seems quite strong as a small variation of this energy can involve an important change in the shape of the state (figure 8).

## 5. Conclusions

In this paper the band structure of a one-dimensional  $N$ -different coupling delta periodic potential is also assumed to be  $\mathcal{PT}$ -symmetric and hence the delta couplings can be made complex. In spite of the non-Hermitian nature of such a Hamiltonian, the band spectrum condition remains real. The imaginary parts of the couplings play an essential role in the variety of shapes and forms that the band spectrum and the wavefunctions may acquire in this new framework. Although the band condition is analytical for arbitrary  $N$ , we have studied carefully just some cases with a low number of couplings. A thorough study of the  $N = 2$  case is given with analytic expressions for the limiting points of the bands. The cases  $N = 3, 4, 5$  and  $6$  are solved graphically and conclusive results for the band spectrum are also offered. In all these cases, the control of the imaginary parts plays an essential role in the way the band spectrum gets distorted and reshaped. As we have been able to discuss the evolution of this

band spectrum, we are now planning to apply these results to more physical situations in which localization and de-localization may be tuned on and off by means of a judicious control of the imaginary parts. We have been able to show how wavefunction de-localization actually takes place for particular cases such as those discussed in section 4. However, a manifold of interesting questions remains to be answered such as: could a random (non-periodical) calculation with this sort of potential be carried out in the case of  $\mathcal{PT}$ -symmetry? Does the de-localization property hold for more general cases? These and related research subjects are now being investigated and will be reported elsewhere.

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### Appendix

Here are some example lines for animating the band condition. First load the package 'Animation' and define the band conditions for  $N = 2$  and  $N = 3$ .

```
<< Graphics 'Animation'
h[r_., s_] = Cos[x] + (r + I*s) * Sin[x] / x;
B2[r1_., s1_] = 2*h[r1, s1] * h[r1, -s1] - 1;
B3[r1_., r2_., s1_] = 4*h[r1, s1] * h[r2, 0] * h[r1, -s1]
                    - (h[r1, s1] + h[r2, 0] + h[r1, -s1]);
```

To see the evolution of the band condition for  $N = 3$  versus the imaginary part  $s_1$  for  $r_1 = 2$  and  $r_2 = 3$ , one would write

```
Animate[Plot[Evaluate[{B3[2, 3, t], 1, -1}], {x, 0, 30},
           PlotRange -> {-3, 3}], {t, 0, 30}]
```

and finally one must group and compress the cells with all the generated plot, and by double clicking on the image, the animation will start.

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