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$\mathcal{PT}$-symmetry in one-dimensional quantum periodic potentials

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Abstract

A complete band structure is shown to exist for one-dimensional periodic non-Hermitian potentials exhibiting $\mathcal{PT}$-symmetry. The full band spectrum is exactly given and some of its properties discussed, specially those concerning the role of the imaginary parameters of the couplings. Infinite periodic arrays constructed with finite chains each one made of **N** different ultralocal couplings are used as models of this one-dimensional complex quantum wire.

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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 modeled 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 a **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 degree of accuracy due to the exact nature of the solution itself. The main physical motivation was indeed to modelate the band structure of a one-dimensional quantum wire. To our surprise 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 modeled at will by varying this parameter. The purpose of this Letter is to present this new solution as well as some preliminary graphics which show part of the rich structure that this model exhibits. Also the idea of performing band structure calculations 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 in aspects concerning the discrete spectrum and bound states ([4–7]) and are also far from an actual physical application. It is not the aim of the present Letter 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

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reference [3] and also to some work done recently in one-dimensional models [8] 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 parts are of primary importance in defining the transport properties of the one-dimensional quantum chain. Indeed band theory is just a small part of the main properties of the one-dimensional array. We should also be interested in localization and density of states. However a full research of the statistically correlated disorder in the presence of $\mathcal{PT}$-symmetry seems much more involved as the $\mathcal{PT}$-symmetry is hard to implement for random chains. Work in this direction is now in progress and will be the subject of a separate paper [10]. We shall describe in this Letter the quantum solution of the model for the band structure in the presence of $\mathcal{PT}$-symmetry and the role of the complex couplings in defining the band structure. Let us begin with a brief remainder of the solution presented in [1] corresponding to a 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

$$a_i = \frac{\hbar^2}{me_i^2} \tag{1}$$

is the length associated to each coupling, we define the matrices:

$$\mathbf{E} = \begin{pmatrix} e^{ika} & e^{-ika} \\ -ike^{ika} & ike^{-ika} \end{pmatrix}, \qquad \mathbf{A_j} = \begin{pmatrix} -1 & -1 \\ \left(ik - \frac{2}{a_j}\right) & -\left(ik + \frac{2}{a_j}\right) \end{pmatrix} \tag{2}$$

and the band structure is defined by the determinant of the following matrix:

$$\begin{pmatrix} \mathbf{E} & \mathbf{A_1} & 0_{2\times2} & \cdots & \cdots & \cdots & 0_{2\times2} \\ 0_{2\times2} & \mathbf{E} & \mathbf{A_2} & 0_{2\times2} & \cdots & \cdots & 0_{2\times2} \\ \vdots & 0_{2\times2} & \mathbf{E} & \mathbf{A_3} & 0_{2\times2} & \cdots & 0_{2\times2} \\ \vdots & \vdots & 0_{2\times2} & \cdots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \cdots & \cdots & \cdots & 0_{2\times2} \\ 0_{2\times2} & \vdots & \vdots & \cdots & \cdots & \mathbf{E} & \mathbf{A_{N-1}} \\ e^{iNQa}\mathbf{A_N} & 0_{2\times2} & 0_{2\times2} & \cdots & \cdots & 0_{2\times2} & \mathbf{E} \end{pmatrix}_{2N\times2N}, \tag{3}$$

where Q is an arbitrary real number which varies between $\frac{\pi}{Na}$ and $-\frac{\pi}{Na}$. It may appear at first glance that the determinant does not render any tractable expression at all. However this not actually the case. One can show after certain amount of algebra that for even **N** the following expression holds:

$$\cos(NQa) = B(\epsilon, a_1, a_2, \ldots, a_N), \tag{4}$$

$$B(\epsilon, a_1, a_2, \ldots, a_N) = 2^{N-1}\sum_P h_i \ldots (N) \ldots h_k - 2^{N-3}\sum_P h_i \ldots (N-2) \ldots h_k + 2^{N-5}\sum_P h_i \ldots (N-4) \ldots h_k - \cdots (-1)^{\frac{N}{2}-1}\sum_P h_i \ldots (2) \ldots h_k + (-1)^{\frac{N}{2}}. \tag{5}$$

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

The functions h_i have the universal form:

$$h_i(x) = \cos x + \left(\frac{a}{a_i}\right)\frac{\sin x}{x} \tag{6}$$

and the independent variable is a function of the energy (i.e., $x = ka$). In order to see that this condition looks much simpler than we could think at the beginning of the calculation let us list below, for the benefit of the reader, the first three conditions for $\mathbf{N} = \mathbf{2}$, **4** and **6**.

$$\cos(2Qa) = 2h_1h_2 - 1, \tag{7}$$

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

$$\begin{aligned}\cos(6Qa) = {} & 32h_1h_2h_3h_4h_5h_6 \\ & - 8(h_1h_2h_3h_4 + h_1h_2h_3h_6 + h_1h_2h_5h_6 + h_1h_4h_5h_6 + h_2h_3h_4h_5 + h_3h_4h_5h_6) \\ & + 2(h_1h_2 + h_1h_4 + h_1h_6 + h_2h_3 + h_2h_5 + h_3h_4 + h_3h_6 + h_4h_5 + h_5h_6) - 1.\end{aligned} \tag{9}$$

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* formula (5) is in itself quite easy to program for sequential calculations ([1,2]). The case of **N** *odd* will be treated separately at the end of this Letter.

Now the important remark regarding $\mathcal{PT}$-symmetry is the fact that expression (5) is still *real* if we use the following rules:

- Promote the couplings from *real* to *complex*, i.e., $e_i^2 \to R_i + i\,I_i$ for the first $\frac{\mathbf{N}}{2}$ $h_i(x)$-functions, where we are now using atomic units for which $\hbar = 2m = 1$;
- Order the potential in a $\mathcal{PT}$-invariant form. In our case this leads to the following identifications:

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

It is easy to check that Eq. (5) remains *real* under these identifications which make obviously the periodic potential *complex* but $\mathcal{PT}$-invariant. There has been an earlier attempt to generate *real* band condition from a complex but $\mathcal{PT}$-invariant potential [9]. However the results concerning the appearance and disappearance of forbidden and allowed bands was inconclusive. In our case this effect is clear and will be discussed at length below.

As is well known for years a Hermitian periodic potential cannot alter its band spectrum just by fine tunning the couplings. The bands can indeed be made wider or narrower but its number and quality (forbidden or allowed) remains 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 is simple. The question that the authors address in [9] was indeed whether this behaviour would be maintained if a $\mathcal{PT}$-invariant potential is used. For this purpose they use various analytical potentials carefully shifted to be $\mathcal{PT}$-invariant. They can prove that the band condition is real but in order to analyze the band structure they have 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 the expressions (7)–(9) (and in general (5)) exceeds $+1$ or goes below -1. In the case of [9] this appears a very hard task indeed as the authors do not have to 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*] ± 1".

But we do have such an exact band condition and in spite of the apparent formidable aspect of the expression (5) we can perform various kinds of numerical analysis 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.

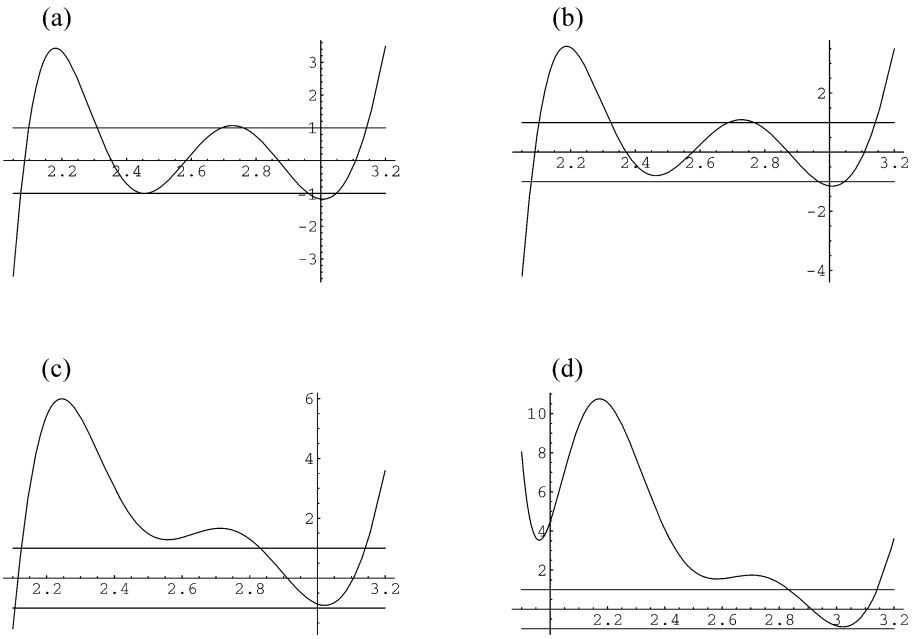

Fig. 1. Band structure for $\mathbf{N} = \mathbf{6}$ in the energy interval $2 < x < 3.3$ and couplings: (a) $\{5, 3, 1, 1, 3, 5\}$; (b) $\{5 + i, 3 + \frac{i}{2}, 1 + \frac{i}{5}, 1 - \frac{i}{5}, 3 - \frac{i}{2}, 5 - i\}$; (c) $\{5 + 3i, 3 + 2i, 1 + \frac{3}{5}i, 1 - \frac{3}{5}i, 3 - 2i, 5 - 3i\}$; (d) $\{5 + 3i, 3 + 2i, 1 + \frac{4}{5}i, 1 - \frac{4}{5}i, 3 - 2i, 5 - 3i\}$.

We have made a fairly complete survey of values and we have consistently observed the fact that even small values of I_i have a strong impact in the number, quality and form of the bands. In Fig. 1 we present the $\mathbf{N} = \mathbf{6}$ case. In a range between $x = 2$ and $x = 3.3$ we present four situations with parameters

$$(5, 3, 1, 1, 3, 5),$$
$$\left(5 + i, 3 + \frac{i}{2}, 1 + \frac{i}{5}, 1 - \frac{i}{5}, 3 - \frac{i}{2}, 5 - i\right),$$
$$\left(5 + 3i, 3 + 2i, 1 + \frac{3}{5}i, 1 - \frac{3}{5}i, 3 - 2i, 5 - 3i\right),$$
$$\left(5 + 3i, 3 + 2i, 1 + \frac{4}{5}i, 1 - \frac{4}{5}i, 3 - 2i, 5 - 3i\right)$$

and the band condition appears greatly distorted. First we have four allowed and three forbidden bands in this range. With the second set of parameters the structure remains the same but there is a pronounced dip in the second allowed band which does not show itself previously and *it is never present in the Hermitian case*. This is only an announcement of the drastic change that occurs when we use the third set of parameters. The allowed band between $x = 2.3$ and $x = 2.7$ has disappeared as well as the forbidden band around $x = 3$. More changes in the quality of the bands take place for the fourth set of parameters. No hyperfine calculations are needed to see qualitatively this dramatic change which shows itself to the naked eye. Notice that all this new band structure has been produced with a very moderate change in the imaginary parts of the couplings.

Let us now turn to a sequence of changes that erases all band structure in a given interval of energy. We shall be using the $\mathbf{N} = \mathbf{4}$ case. Let us take the following set of parameters:

$(5, 4, 4, 5)$,

$\left(5+i, 4+\frac{i}{2}, 4-\frac{i}{2}, 5-i\right)$,

$(5+2i, 4+i, 4-i, 5-2i)$,

$(5+3i, 4+2i, 4-2i, 5-3i)$,

$(5+4i, 4+3i, 4-3i, 5-4i)$,

$(5+200i, 4+150i, 4-150i, 5-200i)$.

In the interval $2.2 < x < 3.2$ we see in Fig. 2(a) the band structure for the first set of *real* parameters. Note the forbidden bands around $x = 2.3$ and $x = 2.9$. For the second set of parameters the forbidden band around $x = 2.3$ is no longer there but the second one exhibits the kind of effect described in [9]: we are unable to decide whether the forbidden band is still there or not. Fortunately a further small push to the parameters shows that the band gap has

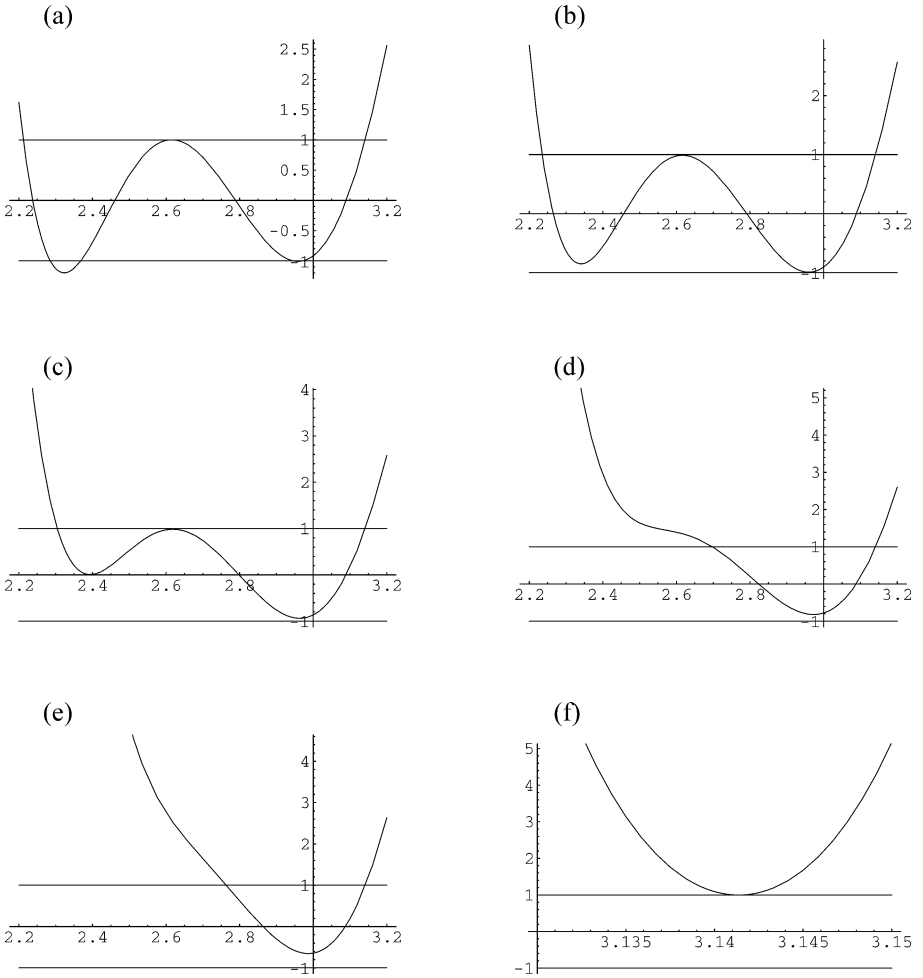

Fig. 2. Band structure for $\mathbf{N} = \mathbf{4}$ in the energy interval $2.2 < x < 3.2$ and couplings: (a) $\{5, 4, 4, 5\}$; (b) $\{5 + i, 4 + \frac{i}{2}, 4 - \frac{i}{2}, 5 - i\}$; (c) $\{5+2i, 4+i, 4-i, 5-2i\}$; (d) $\{5+3i, 4+2i, 4-2i, 5-3i\}$; (e) $\{5+4i, 4+3i, 4-3i, 5-4i\}$; (f) $\{5+200i, 4+150i, 4-150i, 5-200i\}$.

gone away definitely. Furthermore we can still make the remaining allowed band to disappear. The surprise is that the curve is extremely reluctant to move up and this can only be done with a drastic change in the imaginary parts. Even so, the last figure of the series shows that we cannot safely say whether the last allowed band has disappeared or a remaining infinitely narrow portion of the curve is still below $+1$. After this analysis there is no doubt that we can have changes in the band spectrum. There are however two kind of changes. If under a small variation of the parameters a definite and strong alteration in the structure and number of the bands occurs, we would be talking about "sudden changes" as those represented in Fig. 1(c). However other situations are more difficult to analyze since a large variation on the parameters does not necessarily means a different band structure or at least it seems hard to decide whether a definite band has clearly appeared (or disappeared) after this alteration. This is of course the case of the situation represented in Fig. 2(f) and very likely the one discussed in Ref. [9]. A comprehensive survey of the rigidity of the band structure with complex $\mathcal{PT}$-symmetric potentials is presently being written and will be reported elsewhere [10].

We would like to end up with some comments on the **N**-odd case. There is in fact another similar expression to (5) for odd **N** but since parity should be playing a crucial role in $\mathcal{PT}$-symmetry, we can either ignore the *odd* case or work with a central real coupling in the place $\frac{\mathbf{N}+1}{2}$ (**N** odd). We have done so for some particular cases in which the central atom or ion has a real coupling and the net effect of introducing complex couplings for the other delta potentials is essentially the same as the one described for the **N**-even case.

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