The energy spectrum of complex periodic potentials of the Kronig-Penney type

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Abstract

We consider a complex periodic PT-symmetric potential of the Kronig-Penney type, in order to elucidate the peculiar properties found by Bender et al. for potentials of the form \( V = i(\sin x)^{2N+1} \), and in particular the absence of anti-periodic solutions. In this model we show explicitly why these solutions disappear as soon as \( V^*(x) \neq V(x) \), and spell out the consequences for the form of the dispersion relation.

In a recent paper Bender et al. [1] showed that periodic potentials which were complex but obeyed PT symmetry possessed real band spectra, with, however, one striking difference from the case of real periodic potentials, namely that there were no antiperiodic solutions, i.e. Bloch waves with lattice wave vector \( k = (2n + 1)\pi/a \). This result was obtained from detailed numerical studies of potentials of the form \( V(x) = i\sin^{2N+1}(x) \), and it was found necessary to work to extremely high accuracy to detect the absence of such solutions. In the present note we supplement this work by an analytical solution to a complex, PT-symmetric version of the Kronig-Penney model, which illustrates the phenomenon very clearly. It therefore seems a generic property of non-Hermitian, but PT symmetric potentials, although an analytic proof is still not available.

In the standard Kronig-Penney model [2] the potential consists of a periodic string of delta functions of the form

\[
V(x) = \alpha \sum_n \delta(x - na).
\]

The simplest way to find the energy eigenvalues is the Floquet procedure, described in [1], based on two solutions which in the region \( 0 \leq x < a \) are

\[
u_1(x) = \cos \kappa x, \quad \nu_2 = (1/\kappa) \sin \kappa x.
\]

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The lattice wave vector $k$, which occurs in the phase $e^{ika}$ of the Bloch wave function at $x = a_+$, is given by

$$\cos ka = \frac{1}{2}(u_1(a) + u'_2(a)).$$

(3)

Crossing the delta function at $x = a$, $u'_2$ has the discontinuity $\alpha u_2(a_-)$, giving the well-known condition

$$\cos ka = \cos \kappa a + \frac{\alpha}{2\kappa} \sin \kappa a.$$

(4)

We can construct a non-Hermitian PT-symmetric version of this model by taking the coefficients of the delta functions to be pure imaginary and alternating in sign, and arranging them symmetrically about the origin:

$$V(x) = i\alpha \sum_n (-1)^n \delta(x - \frac{1}{2}(n + \frac{1}{2})a).$$

(5)

The periodicity of the potential is still $a$. To perform the Floquet analysis it is easier to shift the origin to $-\frac{1}{4}a$, so that the two wave functions initially take the same form as in Eq. (2) and then track their discontinuities through the delta functions at $x = \frac{1}{2}a$ and $x = a$. The net result is that the Kronig-Penney expression for $\cos ka$ is replaced by

$$\cos ka = \cos \kappa a + \frac{\alpha^2}{2\kappa^2} \sin^2 \frac{1}{2} \kappa a,$$

(6)

from which it is immediately apparent that $\cos ka$ is strictly greater than -1, and in particular that there are no antiperiodic solutions with $k = (2n+1)\pi/a$.

A generalization of Eq. (5) is the potential

$$V(x) = \alpha \sum_n e^{(-1)^n i\theta} \delta(x - \frac{1}{2}(n + \frac{1}{2})a),$$

(7)

which reduces to Eq. (5) for $\theta = \pi/2$ and to the standard Kronig-Penney model, with spacing $\frac{1}{2}a$, for $\theta = 0$. It is then a reasonable question to ask at what value of $\theta$ the antiperiodic solutions disappear: the answer is perhaps surprising.

Beginning, as before, with the two solutions of Eq. (2), and tracking the discontinuities of their derivatives through the (shifted) delta functions at $x = \frac{1}{2}a$ and $x = a$, we arrive at the equation

$$\cos ka = \cos \kappa a + \frac{\alpha}{\kappa} \sin \kappa a \cos \theta + \frac{\alpha^2}{2\kappa^2} \sin^2 \frac{1}{2} \kappa a,$$

(8)
which reduces to (6) for $\theta = \pi/2$. It implies the following relation for $\cos ka + 1$:

$$\cos ka + 1 = 2 \left| \cos \frac{1}{2} \kappa a + \frac{\alpha}{2\kappa} e^{i\theta} \sin \frac{1}{2} \kappa a \right|^2,$$

(9)

which is non-zero as soon as $\theta \neq 0$, $m\pi$. Thus the antiperiodic solution disappears immediately, rather than at some finite critical angle between 0 and $\pi/2$.

As noted above, whereas for $\theta \neq 0$ the repeat distance is $a$, it reduces to $\frac{1}{2}a$ at $\theta = 0$. Correspondingly (8) can be rewritten as

$$\cos \frac{1}{2} ka = \cos \frac{1}{2} \kappa a + \frac{\alpha}{2\kappa} \sin \frac{1}{2} \kappa a,$$

(10)

which starts off positive, passes through $\cos \frac{1}{2} ka = 0$ and then becomes negative. However, the moment $\theta$ becomes non-zero this solution disappears, and by continuity $\cos \frac{1}{2} ka$ must always remain positive, i.e.

$$\cos \frac{1}{2} ka = \left| \cos \frac{1}{2} \kappa a + \frac{\alpha}{2\kappa} e^{i\theta} \sin \frac{1}{2} \kappa a \right|.$$

(11)

The situation is illustrated in Fig. 1, where we have taken $\theta = 0.1^\circ$.

![Fig. 1. Eq. (10) (solid line) and Eq. (11) (dashed line). Where both expressions are positive the two curves are barely distinguishable.](image)

In Fig. 2 we show the resulting band structure for the same value of $\theta$. The Brillouin zone boundary is at $k = \pi/a$, in the middle of the Brillouin zone for $\theta = 0$. In contrast to the usual situation, as exemplified by the dispersion relation for phonons in a diatomic molecule, where a gap appears at the
boundary, here the energy levels merge together before reaching the boundary, thus forming one continuous, double-valued band. At the point where the levels merge the effective mass is zero.

![Diagram](image-url)

Fig. 2. The structure of the lowest band resulting from Eq. (9). Energy in arbitrary units.

Consideration of this toy model seems to show that there is something generic about the dispersion relations for periodic potentials with $V^*(x) = V(-x) \neq V(x)$. In this case we have an analytic demonstration that as soon as $\theta \neq 0$ there is no antiperiodic solution and the energy levels do not reach the Brillouin zone boundaries. A general proof of this property, not depending on the specific form of $V$, would be very welcome.

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**References**

[1] C. M. Bender, G. V. Dunne and P. N. Meisinger, Phys. Lett. A 252 (1999) 272.

[2] C. Kittel, Introduction to Solid State Physics, 7th Ed. (Wiley, New York, 1996).