Use of equivalent Hermitian Hamiltonian for $PT$-symmetric sinusoidal optical lattices

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Abstract
We show how the beam dynamics of non-Hermitian $PT$-symmetric sinusoidal optical lattices can be approached from the point of view of the equivalent Hermitian problem, obtained by an analytic continuation in the transverse spatial variable $x$. In this latter problem the eigenvalue equation reduces to the Mathieu equation, whose eigenfunctions and properties have been well studied. That being the case, the beam propagation, which parallels the time-development of the wave-function in quantum mechanics, can be calculated using the equivalent of the method of stationary states. We also discuss a model potential that interpolates between a sinusoidal and periodic square well potential, showing that some of the striking properties of the sinusoidal potential, in particular birefringence, become much less prominent as one goes away from the sinusoidal case.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The recent surge of interest in quantum Hamiltonians which are not Hermitian but which nonetheless possess a completely real energy spectrum, due to an unbroken $PT$ symmetry, stems from the pioneering paper of Bender and Boettcher [1], in which they showed that the Hamiltonians

$$ H = p^2 - (ix)^N $$

had that property for $N \geq 2$.

Since then there has been intensive investigation into the properties of Hamiltonians of this kind, which is summarized in the reviews by Bender [2] and Mostafazadeh [3]. In particular, it was realized by Mostafazadeh [4] that the Hamiltonians of equation (1) were quasi-Hermitian,
i.e. they could be related to equivalent isospectral Hermitian Hamiltonians $h$ by a similarity transformation:

$$H = e^{i\theta} h e^{-i\theta},$$

(2)

where $Q$ is a Hermitian operator, related to the $C$ operator of [5] by $C = e^{i\theta} P$.

The corresponding action of the similarity transformation on states is just

$$|\psi\rangle = e^{i\theta} |\phi\rangle,$$

(3)

where $|\psi\rangle$ is a state of the non-Hermitian system governed by $H$ and $|\phi\rangle$ is the corresponding state in the Hermitian system governed by $h$.

A surprising recent development has been the application of these ideas to classical optics [6–14]. That such a transfer is possible is due to the fact that under certain approximations the equation of propagation of electromagnetic waves reduces to the paraxial wave equation, which has the same form as the Schrödinger equation, but with different roles for the objects appearing there. The equation takes the form

$$i\frac{\partial \psi}{\partial z} = -\left(\frac{\partial^2}{\partial x^2} + V(x)\right) \psi,$$

(4)

where now $\psi(x, z)$ represents the envelope function of the amplitude of the electric field, where $z$ is a scaled propagation distance, and $V(x)$ is the optical potential, proportional to the variation in the refractive index of the material through which the wave is passing. A complex $V$ corresponds to a complex refractive index, whose imaginary part represents either loss or gain. In principle the loss and gain regions can be carefully configured so that $V$ is $PT$ symmetric, that is $V^*(x) = V(-x)$.

Reference [8], where, apart from an overall additive constant, the periodic optical potential was taken to be of the form

$$V = \frac{1}{2} A \left(\cos 2x + 2iV_0 \sin 2x\right),$$

and with $z$-dependence $\psi \propto e^{i\beta z}$. It was recognized in [15] that the threshold for $PT$-symmetry breaking at $V_0 = \frac{1}{2}$, showing unusual features, such as non-reciprocity, power oscillations and bifurcation. In what follows we attempt to cast light on these phenomena from the point of view of the equivalent Hermitian system.

In section 2 we discuss the spectrum (band structure) of $h$ and the corresponding Bloch wave-functions, and in section 3 we show how the method of stationary states can be implemented to generate the $z$-development, first in the Hermitian case, and then in the non-Hermitian case by means of the similarity transformation, which here amounts to a complex shift in the argument $x$ of the Bloch functions. In section 4, by introducing a potential that can interpolate between the sinusoidal potential and a periodic square well, we show that the phenomenon of birefringence may depend rather sensitively on the exact form of the potential. Finally, in section 5 we give a brief discussion of the significance of our results.

2. Equivalent Hermitian Hamiltonian

For the potential used in [8], the analogue Schrödinger equation takes the form

$$-\psi'' - \frac{1}{2} A \left(\cos 2x + 2iV_0 \sin 2x\right) \psi = -\beta \psi,$$

(5)

for an eigenstate of $H$, with eigenvalue $\beta$ and $z$-dependence $\psi \propto e^{i\beta z}$. It was recognized in [15] that the threshold for $PT$-symmetry breaking was $V_0 = \frac{1}{2}$, and that for $V_0 < 1/2$ the real and imaginary parts of the potential can be combined into a cosine of complex argument.
satisfying
\( \cos 2x + 2iV_0 \sin 2x = \sqrt{(1 - 4V_0^2)} \cos (2x - i\theta), \)
where \( \theta = \arctan(2V_0) \). Thus, the non-Hermitian Hamiltonian
\[
H = p^2 - \frac{1}{2}A(\cos 2x + 2iV_0 \sin 2x)
\]
can be converted into the equivalent Hermitian Hamiltonian
\[
h = p^2 - \frac{1}{2}A\sqrt{(1 - 4V_0^2)} \cos 2x
\]
by the complex shift \( x \to x + \frac{1}{2}i\theta \). This can be implemented by the similarity transformation of equation (2), namely
\[
h = e^{-\frac{1}{2}i\theta} H e^{\frac{1}{2}i\theta}
\]
with \( Q = \theta \hat{p} \equiv -i\theta \mathrm{d}/\mathrm{dx} \), which ensures that the spectra of the two Hamiltonians are identical for \( V_0 < 1/2 \) (and real), one of the principal results of [15].

In what follows we shall choose \( A = 4 \), the value taken in [8]. Then the analogue Schrödinger equation for \( h \) is the Mathieu equation [17]:
\[
\varphi'' + (a - 2q \cos 2x)\varphi = 0,
\]
with \( q = -\sqrt{(1 - 4V_0^2)} \) and \( a = -\beta \).

The canonical method for determining the Bloch eigenfunctions and energy levels is the Floquet method, whereby we take two independent solutions \( u_1(x) \) and \( u_2(x) \) with the respective initial conditions \( u_1(0) = 1, \ u'_1(0) = 0 \) and \( u_2(0) = 0, \ u'_2(0) = 1 \) and integrate up to the Brillouin zone boundary at \( x = \pi \) to form the discriminant
\[
D(\beta) = \frac{1}{2}(u_1(\pi) + u'_2(\pi)).
\]
If \( |D| \leq 1 \), there exists a periodic Bloch-Floquet solution of the form
\[
\varphi_k(x) = c_1u_1(x) + d_2u_2(x),
\]
satisfying
\[
\varphi_k(x + \pi) = e^{ik\pi} \varphi_k(x),
\]
where \( k = (1/\pi) \arccos D \). This procedure gives \( k \) as a function of \( \beta \), a relation that has to be inverted to give the band structure \( \beta = \beta(k) \).

In the standard notation for the Mathieu equation, \( k(\beta) \) is called the characteristic exponent. The values of \( \beta \) where \( k \) is an integer \( r \), i.e. at the Brillouin zone boundaries, are termed characteristic values, and are of two types, \( a_r \) or \( b_r \), depending on whether the Bloch wave-function is even or odd. In fact in Mathematica these functions have been extended to \( k \) non-integral (the functions MathieuA and MathieuB), effectively mapping out the whole band structure \( \beta(k) \) without the need to go through the Floquet procedure explicitly. Using this method we show in figure 1 the band structure in both the reduced and extended zone schemes for the potential of equation (7), or equation (5), for \( V_0 = 0.45 \). Similar results were previously obtained in [8] by numerical application of the Floquet procedure to the original non-Hermitian potential of equation (5).

In the present case it turns out that the Floquet functions \( u_1 \) and \( u_2 \) are precisely the even and odd Mathieu functions \( ce(a, q, x) \) and \( se(a, q, x) \) respectively, up to a normalization factor. For a given value of \( k \), we know \( a \) and hence, using equation (12), can determine the value of the ratio \( c_1/d_2 \) in the equation (11) for the Bloch wave-function. Away from the Brillouin

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1 This is essentially the same transformation as was used in the discussion of the PT-symmetric version of the Sine–Gordon theory.
zone boundaries neither $c_k$ nor $d_k$ vanishes, but precisely at those boundaries one or other is zero, making the solution purely symmetric or antisymmetric. Thus, for example, at $k = 1$ the wave-function corresponding to the lowest band is symmetric, whereas the wave-function corresponding to the next band is antisymmetric.

The Bloch wave-functions can be individually normalized in the extended zone scheme according to

$$\int_0^\pi |\psi_k(x)|^2 \, dx = 1. \quad (13)$$

For $k \neq k' \mod 2$ the orthogonality arises from the different periodicities of $\psi_k(x)$ and $\psi_{k'}(x)$. If we use periodic boundary conditions in $-N\pi \leq x \leq N\pi$, so that $k \rightarrow k_r = r/N$,

$$\int_{-N\pi}^{N\pi} \psi_{k_r}^*(x)\psi_{k_s} (x) \, dx = e^{-i\pi/\Delta} \sin \frac{N\pi \Delta}{\sin \frac{\pi \Delta}{2}} \int_0^\pi \psi_{k_r}^*(x)\psi_{k_s} (x) \, dx, \quad (14)$$

where $\Delta = k_r - k_s = (r-s)/N$. The second factor gives the orthogonality for $r \neq s \mod 2$, while the remaining integral gives the orthogonality at the BZ boundaries.

3. Method of stationary states

In quantum mechanics a standard method of implementing time development is the method of stationary states. That is, the initial wave-function $\psi(x, t = 0)$ is expanded as a superposition of orthonormalized energy eigenstates $\psi_i(x)$:

$$\psi(x, t = 0) = \sum_i c_i \psi_i(x), \quad (15)$$

with

$$c_i = \int \psi_i^*(x)\psi(x, t = 0) \, dx, \quad (16)$$

and then

$$\psi(x, t) = \sum_i c_i \psi_i(x) e^{-E_i t}. \quad (17)$$

In the optical problem exactly the same method can be applied, with $z$ taking over the role of $t$, and the eigenstates being the Bloch wave-functions. We first apply this method to the Hermitian
problem of equation (7) and then show how it can be adapted to give the $z$-development for equation (5).

3.1. Propagation in Hermitian case

The initial envelope $\psi(x, z = 0) \equiv g(x)$ is to be expanded in terms of the $\varphi_k(x)$, according to

$$g(x) = \sum c_r \varphi_k(x),$$

(18)

with the coefficients $c_r$ given by

$$c_r = \int_{-N\pi}^{N\pi} \varphi_k^*(x) g(x) \, dx.$$  

(19)

Using the translational property of the Bloch wave-functions we can reduce the integration range to the standard cell 0 to $\pi$:

$$c_r = \int_0^\pi \varphi_k^*(x) G(x) \, dx,$$

(20)
where \( G(x) = \sum_{q=-N}^{N-1} e^{-i\pi q^2} g(x + q\pi) \), and then \( \varphi(x, z) \) is given by
\[
\varphi(x, z) = \sum_r c_r \varphi_k(x) e^{-i\pi kr g(x)}.
\] (21)

For definiteness let us take \( g(x) \) to be a broad Gaussian, \( g(x) = e^{-\left(x/w\right)^2} \), with \( w = 6\pi \), a function used in [8, 11]. In this case the absolute values of the coefficients are given in figure 2, which reveals that they fall off rapidly with \( |k| \), and are essentially negligible for \( |k| > 3 \). They are concentrated around the even integers, reflecting the slowly-varying nature of \( g \). Note that by convention the wave-function is taken to be \( cek(x) \) at positive integers \( k \) and \( sek(x) \) at negative integers.

When the sum of equation (21) is performed, the development of the intensity, shown in figure 3, shows no surprises: the beam, representing a Gaussian wave-front at normal incidence, essentially propagates straight ahead, with a small amount of lateral spreading.

3.2. Propagation in non-Hermitian case

The situation, however, is very different in the non-Hermitian case. We now need to fit the initial Gaussian \( g(x) \) to the transformed wave-functions \( \psi_k(x) \) rather than to the \( \varphi_k(x) \). That is,
\[
g(x) = \sum_r d_r \psi_k(x).
\] (22)

But from equation (3), which in terms of wave-functions reads \( \psi_k(x) = \varphi_k(x - \frac{1}{2}i\theta) \), this can be recast as
\[
g\left(x + \frac{1}{2}i\theta\right) = \sum_r d_r \varphi_k(x),
\] (23)

and then \( \psi(x, z) = \varphi(x - \frac{1}{2}i\theta, z) \).

In fact, for the parameters taken, the coefficients \( d_r \) differ very little from the \( c_r \). However, because we are plotting \( |\psi(x, z)|^2 \) rather than \( |\varphi(x, z)|^2 \), the intensity pattern is very different, showing the characteristic birefringence and power oscillations first noted in [8]. Figure 4 shows precisely the same features as figure 2(a) in that paper. It turns out that the asymmetry is primarily due to the contribution of the Bloch functions with \( |k| \approx 2 \).

4. Interpolating potential

One may ask whether the birefringence shown in figure 4 is a general feature of PT-symmetric potentials, or whether there is something special about the sinusoidal potential. In particular, does the feature persist for a periodic square-well potential (which in practice would be much easier to construct)? The answer seems to be in the negative, at least for a broad initial wave packet, and the transition from the sinusoidal case to the square-well case can be neatly studied by using Jacobi \( sn \) functions, whose \( m \) parameter allows one to interpolate between the two cases. That is, we replace
\[
V = \frac{1}{2} A \left( \cos 2x + 2i V_0 \sin 2x \right)
\] (24)

with
\[
W = \frac{1}{2} A \left[ \text{sn} \left( \frac{\pi - 4x}{\pi} K(m), m \right) + 2i V_0 \text{sn} \left( \frac{4x}{\pi} K(m), m \right) \right].
\] (25)

rescaling the argument so that the period remains \( \pi \). The imaginary part of the potential is shown in figure 5 for the two cases \( m = 0.5 \) and \( m = 0.99999 \).
For $m = 0$ we reproduce figure 4, but by the time $m$ reaches 0.5 the birefringence is much less prominent (see figure 6, upper panel), and for $m = 0.99999$, at which point the potential is essentially a periodic square-well, it has more or less disappeared (figure 6, lower panel). Since in intermediate cases the wave-functions are not well-known functions, these figures were produced using the original method of direct integration of the differential equation for the $z$-development. The occurrence of birefringence or otherwise depends not only on the shape of the potential, but also on the width of the initial distribution. For example, if the width is halved to $w = 3\pi$, so that larger $k$ values are excited, birefringence persists even up to $m = 0.99999$, although it is still considerably weaker than for $m = 0$. In all cases any additional beams go to the right, the left-right asymmetry being due to the fact that the potential is not $P$-symmetric, but rather $PT$ symmetric.
5. Conclusions

We have shown that it is a simple matter to derive the band structure and Bloch eigenfunctions of non-Hermitian sinusoidal potentials of the type occurring in equation (5) using the equivalent Hermitian Hamiltonian of equation (7) and the corresponding Mathieu and related functions built in to Mathematica. The dynamics (z-development in optics) can also be implemented using the method of stationary states. Although in practical terms the z-development of the original equation is more efficiently found by direct numerical integration using the split operator method and fast Fourier transform, it is hoped that the stationary state method helps...
to elucidate the difference between the Hermitian and non-Hermitian situations. In particular, it turned out for the parameters we used that the expansion coefficients did not differ significantly in the two cases: the difference between figures 3 and 4 was overwhelmingly due to the fact that in the Hermitian case one was plotting $|\psi(x, z)|^2$, whereas in the non-Hermitian case the relevant function was instead the continuation $|\phi(x - \frac{1}{2}i\theta, z)|^2$.

In our previous discussion we have limited our discussion to the case $V_0 < 1/2$, when the $PT$ symmetry is unbroken and the eigenvalues are real. In the symmetry-broken case $V_0 > \frac{1}{2}$, the corresponding identity is instead

$$\cos 2x + 2i V_0 \sin 2x = i\sqrt{4V_0^2 - 1} \sin(2x - i\zeta),$$

where $\zeta = \text{arccoth}(2V_0)$. However, in this case we have not gained a great deal from the similarity transformation, since the equivalent Hamiltonian $h$ is itself non-Hermitian. Indeed the second main result of [15], that no real eigenvalues at all remained above a second critical value of $V$, was obtained by numerical methods applied to the complex Mathieu equation.

At the critical value $V_0 = \frac{1}{2}$, the equivalent potential vanishes altogether, so that the equivalent theory is simply a free theory, with spectrum $\beta = -k^2$, as was also noted by Longhi [11]. Part of this spectrum can be observed, in the reduced zone scheme in figure 1(b) of [8]. The transformation in this case is a singular one, with $\theta \to \infty$, so the methods used below can not be implemented for this limiting case. Nonetheless it is true that in this case the eigenfunctions for the non-Hermitian $V$ are again known functions, in fact modified Bessel functions $I_k(\sqrt{2e^{i\pi}})$, so that one might hope that the stationary state method could here be used directly for the $V$ itself. However, as was pointed out by Longhi [11], this is not possible because of spectral singularities, or the non-completeness of the Bessel functions at the B-Z boundaries $k = \text{integer}$.

The last part of the paper was concerned with the potential of equation (25), which, with the use of the parameter $m$ interpolates between the sinusoidal and square-well potentials. We showed that such phenomena as birefringence are by no means universal, but depend sensitively on the shape of the non-Hermitian potential and also on that of the incoming wave packet.

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