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THE FLOQUET METHOD FOR PT-SYMMETRIC PERIODIC POTENTIALS

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Abstract. By the general theory of $\mathcal{PT}$-symmetric quantum systems, their energy levels are either real or occur in complex-conjugate pairs, which implies that the secular equation must be real. However, for periodic potentials it is by no means clear that the secular equation arising in the Floquet method is indeed real, since it involves two linearly independent solutions of the Schrödinger equation. In this brief note we elucidate how that reality can be established.

Keywords: band structure, PT symmetry, Floquet method.

The study of systems governed by Hamiltonians for which the standard requirement of Hermiticity is replaced by that of $\mathcal{PT}$-symmetry has undergone significant development in recent years [1–6]. Provided that the symmetry is not broken, that is, that the energy eigenfunctions respect the symmetry of the Hamiltonian, the energy eigenvalues are guaranteed to be real. In the case where the symmetry is broken energy levels may instead appear as complex-conjugate pairs. This phenomenon is particularly interesting for the case of periodic $\mathcal{PT}$-symmetric potentials, where unusual band structures may occur [7, 8].

An important physical realization of such systems arises in classical optics, because of the formal similarity of the time-dependent Schrödinger equation to the paraxial equation for the propagation of electromagnetic waves. This equation takes the form [9]

$$i\frac{\partial\psi}{\partial z} = -\left(\frac{\partial^2}{\partial x^2} + V(x)\right)\psi, \tag{1}$$

where $\psi(x,z)$ represents the envelope function of the amplitude of the electric field and z is a scaled propagation distance. The optical potential $V(x)$ is proportional to the variation in the refractive index of the material through which the wave is passing. In optics this potential may well be complex, with its imaginary part representing either loss or gain. If loss and gain are balanced in a $\mathcal{PT}$-symmetric way, so that $V^*(x) = V(-x)$. we have the situation described above. Optical systems of this type have a number of very interesting properties [9–14], particularly when they are periodic.

In such a case the potential $V(x)$, whose period we can take as π, without loss of generality, satisfies the two conditions $V^*(-x) = V(x) = V(x+\pi)$. For periodic potentials we are interested in finding the Bloch solutions, which are solutions of the time-independent Schrödinger equation

$$-\left(\frac{\partial^2}{\partial x^2} + V(x)\right)\psi_k(x) = E\psi_k(x) \tag{2}$$

with the periodicity property $\psi_k(x+\pi) = e^{ik\pi}\psi_k(x)$.

The standard way of obtaining such solutions is the Floquet method, whereby $\psi_k(x)$ is expressed in terms of two linearly-independent solutions, $u_1(x)$ and $u_2(x)$, of Eq. (2), with initial conditions

$$\begin{aligned} u_1(0) &= 1, \qquad u_1'(0) = 0,\\ u_2(0) &= 0, \qquad u_2'(0) = 1. \end{aligned} \tag{3}$$

Then $\psi_k(x)$ is written as the superposition

$$\psi_k(x) = c_k u_1(x) + d_k u_2(x). \tag{4}$$

Imposing the conditions $\psi_k(\pi) = e^{ik\pi}\psi(0)$ and $\psi_k'(\pi) = e^{ik\pi}\psi'(0)$ and exploiting the invariance of the Wronskian $W(u_1,u_2)$ one arrives at the secular equation

$$\cos k\pi = \Delta \equiv \frac{1}{2}\left(u_1(\pi) + u_2'(\pi)\right). \tag{5}$$

In the Hermitian situation both $u_1(\pi)$ and $u_2(\pi)$ are real, and the equation for E has real solutions (bands) when $|\Delta| \le 1$. However, in the non-Hermitian, $\mathcal{PT}$-symmetric, situation it is not at all obvious that Δ is real, since that implies a relation between $u_1(\pi)$ and $u_2'(\pi)$, even though $u_1(x)$ and $u_2(x)$ are linearly independent solutions of Eq. (2). It is that problem that we wish to address in the present note. In fact we will show that $u_2'(\pi) = u_1^*(\pi)$.

The clue to relating $u_1(\pi)$ and $u_2(\pi)$ comes from considering a half-period shift, namely $x = z + \pi/2$. We write $\varphi(z) = \psi(z+\pi/2)$ and $U(z) = V(z+\pi/2)$. Then $\varphi(z)$ satisfies the Schrödinger equation

$$-\left(\frac{\partial^2}{\partial z^2} + U(z)\right)\varphi_k(z) = E\varphi_k(z). \tag{6}$$

The crucial point is that because of the periodicity and $\mathcal{PT}$-symmetry of $V(x)$ the new potential $U(z)$ is also $\mathcal{PT}$-symmetric. Thus $U(-z) = V(-z+\pi/2) = V(-z-\pi/2) = V^*(z+\pi/2) = U^*(z)$.

Now we can express the Floquet functions $u_1(x)$, $u_2(x)$ in terms of Floquet functions $v_1(z)$, $v_2(z)$ of the transformed equation (6), satisfying

$$\begin{aligned} v_1(0) &= 1, \qquad v_1'(0) = 0, \\ v_2(0) &= 0, \qquad v_2'(0) = 1. \end{aligned} \tag{7}$$

It is easily seen that the relation is

$$\begin{aligned} u_1(x) &= v_2'(-\pi/2)v_1(z) - v_1'(-\pi/2)v_2(z), \\ u_2(x) &= -v_2(-\pi/2)v_1(z) + v_1(-\pi/2)v_2(z), \end{aligned} \tag{8}$$

in order to satisfy the initial conditions on $u_1(x)$, $u_2(x)$. So

$$\begin{aligned} u_1(\pi) &= v_2'(-\pi/2)v_1(\pi/2) - v_1'(-\pi/2)v_2(\pi/2), \\ u_1'(\pi) &= v_2'(-\pi/2)v_1'(\pi/2) - v_1'(-\pi/2)v_2'(\pi/2), \\ u_2(\pi) &= -v_2(-\pi/2)v_1(\pi/2) + v_1(-\pi/2)v_2(\pi/2), \\ u_2'(\pi) &= -v_2(-\pi/2)v_1'(\pi/2) + v_1(-\pi/2)v_2'(\pi/2). \end{aligned} \tag{9}$$

But, because of the $\mathcal{PT}$-symmetry of Eq. (6) and the initial conditions satisfied by $v_1(z)$, $v_2(z)$,

$$\begin{aligned} v_1(-\pi/2) &= (v_1(\pi/2))^*, \\ v_1'(-\pi/2) &= -(v_1'(\pi/2))^*, \\ v_2(-\pi/2) &= -(v_2(\pi/2))^*, \\ v_2'(-\pi/2) &= (v_2'(\pi/2))^*. \end{aligned} \tag{10}$$

Hence, indeed, $u_1(\pi) = (u_2'(\pi))^*$, so that Δ in Eq. (5) is real and the energy eigenvalues of the Bloch wavefunctions are either real or occur in complex conjugate pairs. From Eq. (10) we also see that $u_1'(\pi)$ and $u_2(\pi)$ are real. The statement $u_1(\pi) = (u_2'(\pi))^*$ is in fact the $\mathcal{PT}$-generalization of the relation $u_1(\pi) = u_2'(\pi)$ implied without proof by Eq. (20.3.10) of Ref. [16] for the Hermitian case of the Mathieu equation, where $V(x) = \cos(2x)$.

If we wish, we may express everything in terms of u_1, u_2 because from Eq. (8)

$$\begin{aligned} u_1(\pi/2) &= v_2'(-\pi/2), \\ u_1'(\pi/2) &= -v_1'(-\pi/2), \\ u_2(\pi/2) &= -v_2(-\pi/2), \\ u_2'(\pi/2) &= v_1(-\pi/2). \end{aligned} \tag{11}$$

Hence

$$\begin{aligned} u_1(\pi) &= (u_2'(\pi))^* \\ &= u_1(\pi/2)(u_2'(\pi/2))^* + u_1'(\pi/2)(u_2(\pi/2))^*, \end{aligned} \tag{12}$$

which is the $\mathcal{PT}$-generalization of a relation implied by Eq. (20.3.11) of Ref. [16] after the use of the invariance of the Wronskian.

Similarly

$$\begin{aligned} u_1'(\pi) &= 2\mathrm{Re}\left(u_1^*(\pi/2)u_1'(\pi/2)\right), \\ u_2(\pi) &= 2\mathrm{Re}\left(u_2^*(\pi/2)u_2'(\pi/2)\right). \end{aligned} \tag{13}$$

To conclude, we have shown that the secular equation for the band structure of $\mathcal{PT}$-symmetric periodic potentials is indeed real, even though in the Floquet method the discriminant involves the two ostensibly independent functions $u_1(x)$ and $u_2(x)$. The crucial point is that for such potentials there is also a PT symmetry about the midpoint of the Brillouin zone. The proof involves expressing $u_1(x)$ and $u_2(x)$ in terms of shifted functions $v_1(x)$ and $v_2(x)$, and shows that $u_1(\pi)$ and $u_2'(\pi)$ are actually complex conjugates of each other. The proof incidentally casts light on certain relations that hold for real symmetric potentials, such as $\cos(2x)$.

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