Spectral singularities and Bragg scattering in complex crystals

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Spectral singularities that spoil the completeness of Bloch-Floquet states may occur in non-Hermitian Hamiltonians with complex periodic potentials. Here an equivalence is established between spectral singularities in complex crystals and secularities that arise in Bragg diffraction patterns. Signatures of spectral singularities in a scattering process with wave packets are elucidated for a $\mathcal{PT}$-symmetric complex crystal.

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I. INTRODUCTION

The Dirac-von Neumann formulation of quantum mechanics prescribes that the Hamiltonian H of a physical system must be Hermitian. This requirement ensures a real-valued energy spectrum and a unitary (probability-preserving) temporal evolution. In the last decade, complex extensions of quantum mechanics which relax the Hermiticity constraint have been proposed (see, e.g., [1,2]). Indeed, a diagonalizable non-Hermitian Hamiltonian (NHH) having a real spectrum is enough to construct a unitary quantum system, provided that the inner product of the Hilbert space is properly modified [2]. In particular, Bender and collaborators showed that a NHH possessing parity-time ($\mathcal{PT}$) symmetry may serve to develop a complex extension of quantum mechanics below a phase transition (symmetry-breaking) point [3,4]. Experimental realizations of $\mathcal{PT}$ Hamiltonians have been recently proposed in optical media with a complex refractive index [5–8], and the first observation of $\mathcal{PT}$-symmetry breaking has been reported in a passive optical waveguide coupler [9].

For a NHH, the reality of the spectrum does not ensure diagonalizability, which may be prevented by the presence of exceptional points in the point spectrum of H [10], or of spectral singularities in the continuous part of the spectrum [11–13]. Exceptional points, also referred to as Hermitian degeneracies (see [10]), correspond to degeneracies where both eigenvalues and eigenvectors coalesce as a system parameter is varied. Other singular points may also occur in low-dimensional (e.g., matrix) non-Hermitian Hamiltonians, such as branch points in the complex plane in which eigenvalue degeneracy does not correspond to a lack of completeness of the spectrum [14]. Such singularities have various physical implications, which have been investigated in different physical fields (see, for instance, [7,9,10,15] and references therein). They play an important role in the study of open quantum systems, particularly in relation to the resonance states (for a recent review, see [16]). But they must not be confused with spectral singularities as defined in [11–13]. Unlike exceptional and branch points that can be present for non-Hermitian operators with a discrete spectrum, spectral singularities are exclusive features of certain non-Hermitian operators having a continuous part in their spectrum [13]. Following [11–13], spectral singularities refer to divergences (poles) of the resolvent on the continuous spectrum of H, which do not correspond to square integrable eigenfunctions. The physical implications of such spectral singularities have been investigated so far for wave scattering from complex potential barriers [12,13,17,18] and shown—notably by Mostafazadeh—to correspond to resonance states with vanishing spectral width [17,18]. Another physically relevant class of NHHs with continuous spectrum is provided by complex periodic potentials [19–21]. Complex crystals have been investigated in different areas of physics, ranging from matter waves [22–24] to optics [6,8,23–25]. Compared to ordinary crystals, complex crystals exhibit some unique properties, such as violation of the Friedel's law of Bragg scattering, double refraction, nonreciprocal diffraction, and anomalous transport [6,22–25], which make them a rather unique class of synthetic materials. Spectral singularities for periodic non-self-adjoint Schrödinger operators have been studied by mathematicians [26]; however, their physical implications in connection with complex crystals have not been explored yet.

It is the aim of this work to investigate the onset of spectral singularities in complex crystals and to show their physical impact in Bragg scattering processes. In particular, we prove rather generally that spectral singularities are associated with a secular growth of plane waves diffracted off the crystal when the incident angle is an integer multiple of the Bragg angle. With reference to a specific $\mathcal{PT}$-symmetric complex crystal, previously considered in Ref. [6], we show that spectral singularities occur at the $\mathcal{PT}$-symmetry-breaking point and can be revealed in a diffraction experiment using a spatially confined wave packet that excites the crystal at normal incidence. Unlike plane-wave excitation, broadening of the angular spectrum for a wave packet is shown to lead to a saturation of the secular growth of the wave amplitude.

II. SPECTRAL SINGULARITIES IN COMPLEX CRYSTALS AND BRAGG SCATTERING

A. Bloch-Floquet states and spectral singularities

Wave dynamics in a complex one-dimensional crystal is governed by a Schrödinger-type equation, which in dimensionless form can be written as

$$i\partial_t\psi(x,t) = -\partial_x^2\psi + V(x)\psi \equiv H\psi, \quad (1)$$

where $V(x+a) = V(x)$ is the complex potential of period a. Physically, Eq. (1) describes diffraction of matter or optical waves by a complex lattice [see Fig. 1(a)], where t is a fictitious time related to the propagation distance inside the crystal

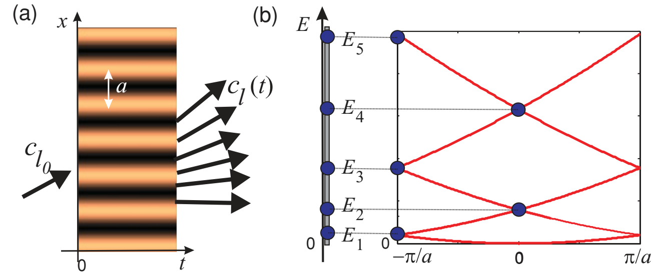

FIG. 1. (Color online) (a) Schematic of Bragg scattering of a plane wave off a complex crystal. (b) Band structure of the complex crystal $V(x) = V_0 \exp(ik_B x)$. The circles mark the spectral singularities inside the continuous spectrum.

[6,22,23,25]. The geometry of the spectrum of H is studied in, e.g., [21]; here we will assume an entirely real energy spectrum; however, at this stage no requirement about $\mathcal{PT}$ symmetry of H is needed. As in ordinary crystals, from the canonical form of the translation operator [27] it follows that any eigenfunction $\phi(x)$ of H ($H\phi = E\phi$) which is bounded at $x \to \pm\infty$ is a linear combination of Bloch-Floquet–type solutions satisfying the condition $\phi(x+a) = \phi(x)\exp(iqa)$, where $-\pi/a \leqslant q < \pi/a$ is an arbitrary real number that varies in the first Brillouin zone. The set of Bloch-Floquet eigenfunctions with energy $E_\alpha(q)$ can be expanded in series of plane-wave basis $|q,n\rangle = (2\pi)^{-1/2}\exp[i(q+nk_B)x]$ as

$$\phi_\alpha(x,q) = \sum_n w_n^{(\alpha)}(q)|q,n\rangle, \tag{2}$$

where $k_B = 2\pi/a$ is the Bragg wave number, α is the band index, and $n = 0, \pm 1, \pm 2, \ldots$. In Eq. (2), $\mathbf{w}^{(\alpha)}(q) \equiv \{w_n^{(\alpha)}(q)\}$ are the eigenvectors, with corresponding eigenvalues $E_\alpha(q)$, of the matrix $\mathcal{H}(q)$ defined by

$$\mathcal{H}_{n,m}(q) = (q+nk_B)^2\delta_{n,m} + V_{n-m}, \tag{3}$$

with $V(x) = \sum_n V_n \exp(ik_B n)$. Let $\mathcal{J}(q)$ be the Jordan canonical form of $\mathcal{H}(q)$, to which $\mathcal{H}(q)$ can be reduced by a similarity transformation, i.e., $\mathcal{H}(q) = \mathcal{T}(q)\mathcal{J}(q)\mathcal{T}^{-1}(q)$. In the band computation, degenerate eigenvalues of $\mathcal{H}(q)$ are counted by their geometric (and not algebraic) multiplicity, i.e., by the number of Jordan blocks that represent the eigenvalue, and the eigenvectors $\mathbf{w}^{(\alpha}(q)$ are thus linearly independent. Note that the matrix representation of H in the plane-wave basis is given by $\langle q',n'|Hq,n\rangle = \mathcal{H}_{n',n}(q)\delta(q-q')$.

As in ordinary crystals, the eigenvalues can be ordered such that $E_\alpha(-q) = E_\alpha(q)$, and for any fixed value of q, with $q \neq 0$ or $q \neq -\pi/a$, the energies $E_\alpha(q)$ are all distinct. At $q = 0$ or at $q = -\pi/a$, eigenvalue degeneracy, with algebraic multiplicity not larger than 2, is allowed (see, e.g., [27]). For the problem of spectral singularities, a key role is played by *defective* eigenvalues of $\mathcal{H}(q)$, at either $q = 0$ or $q = -\pi/a$, i.e., eigenvalues whose geometric multiplicity is smaller than their algebraic multiplicity.

More precisely, we will prove that the completeness of a periodic NHH admitting a purely continuous spectrum, i.e., the absence of spectral singularities in complex crystals, is equivalent to the issue of completeness (i.e., absence of defective eigenvalues) for the non-Hermitian matrix Hamiltonian $\mathcal{H}(q)$ at $q = 0$ and $q = -\pi/a$. Note that the discrete NHH problem defined by the matrix $\mathcal{H}(q)$ at $q = 0, -\pi/a$ can be obtained from the original problem (1) provided that the functional space is restricted to the space of functions satisfying the periodic boundary conditions $\psi(x+a,t) = \pm\psi(x,t)$. Moreover, the appearance of a defective eigenvalue of $\mathcal{H}(q)$ (when a control parameter is varied) corresponds to the occurrence of an exceptional point in the discrete spectrum of $\mathcal{H}(q)$. The correspondence between spectral singularities in the continuous spectrum of H and exceptional points (defective eigenvalues) in the point spectrum of the matrix $\mathcal{H}(q)$ is more precisely established by the following theorem.

Theorem 1. The set of Bloch-Floquet eigenfunctions (2) is complete, i.e., H is diagonalizable, if and only if the matrix $\mathcal{H}(q)$ does not have defective eigenvalues at $q = 0$ or $q = -\pi/a$. In other words, spectral singularities in the continuous spectrum of H correspond to exceptional points in the point spectrum of the matrix $\mathcal{H}(q)$ at the center ($q = 0$) or at the edge ($q = -\pi/a$) of the Brillouin zone.

Proof. Let us first prove that $\{\phi_\alpha(x,q)\}$ is a complete set of (improper) functions if and only if $\mathcal{H}(q)$ is diagonalizable for any arbitrary value of q inside the first Brillouin zone. Suppose that $\{\phi_\alpha(x,q)\}$ is a complete set. Then for any q in the first Brillouin zone and for any integer n, there exists a set of complex numbers $\{c_{n,\alpha}(q)\}$ such that $|q,n\rangle = \sum_\alpha c_{n,\alpha}(q)\phi_\alpha(x,q)$, i.e., $|q,n\rangle = \sum_m(\sum_\alpha c_{n,\alpha}(q)w_m^{(\alpha)}(q))|q,m\rangle$, where we used Eq. (2). Hence, $\sum_\alpha c_{n,\alpha}(q)w_m^{(\alpha)}(q) = \delta_{n,m}$. Since the previous relation holds for any integer value n, the set of eigenvectors $\{\mathbf{w}^{(\alpha)}(q)\}$ is complete, i.e., $\mathcal{H}(q)$ is diagonalizable. Suppose now that $\mathcal{H}(q)$ is diagonalizable, and let us show that $\{\phi_\alpha(q,x)\}$ is a complete set. In fact, for an arbitrarily assigned square integrable function $f(x)$, let $F(k)$ be the Fourier transform of $f(x)$ and $F_n(q) = F(q+nk_B)$, where q varies in the first Brillouin zone and $n = 0, \pm 1, \pm 2, \ldots$. Then $f(x) = \sum_n \int_{-\pi/a}^{\pi/a} dq\, F_n(q)|q,n\rangle$. Since $\mathcal{H}(q)$ is diagonalizable, the eigenvectors $\mathbf{w}^{(\alpha)}(q)$ form a complete set, and one can thus determine a set of functions $c_\alpha(q)$ such that $F_n(q) = \sum_\alpha c_\alpha(q)w_n^{(\alpha)}(q)$. Hence, $f(x) = \sum_\alpha \int_{-\pi/a}^{\pi/a} dq\, c_\alpha(q)\sum_n w_n^{(\alpha)}(q)|q,n\rangle = \sum_\alpha \int_{-\pi/a}^{\pi/a} dq\, c_\alpha(q)\phi_\alpha(x,q)$, i.e., $f(x)$ can be decomposed as a superposition of Bloch-Floquet eigenfunctions. Since $f(x)$ is arbitrary, it follows that $\{\phi_\alpha(x,q)\}$ is a complete set. The theorem is finally proved after observing that for $q \neq 0, -\pi/a$, the eigenvalues $E_\alpha(q)$ are distinct, and thus $\mathcal{H}(q)$ is diagonalizable.

Similar to that of spectral singularities found in scattering complex potentials [13], a physically relevant consequence of spectral singularities is to prevent the construction of a biorthogonal eigensystem for H, i.e., to resolve the identity in terms of the biorthogonal basis associated with H. By definition, H is diagonalizable if $\phi_\alpha(x,q)$, together with a set of (generalized) eigenfunctions $\phi_\alpha^\dagger(x,q)$ of the adjoint $H^\dagger$, form a complete biorthogonal system, i.e., they satisfy $\langle\phi_\alpha(x,q)|\phi_\beta^\dagger(x,q')\rangle = \delta_{\alpha,\beta}\delta(q-q')$ and $\sum_\alpha \int_{-\pi/a}^{\pi/a} dq |\phi_\alpha(x,q)\rangle\langle\phi_\alpha^\dagger(x,q)| = \mathcal{I}$. As $H^\dagger = -\partial_x^2 + V^*(x)$, it can be easily shown that one has $\phi_\alpha^\dagger(x,q) = \mathcal{N}_\alpha(q)\phi_\alpha^*(x,-q)$, where $\mathcal{N}_\alpha(q)$ is a multiplying term that needs to be determined. A direct computation of the scalar product $\langle\phi_\alpha(x,q)|\phi^\dagger_\beta(x,q')\rangle$ using expansion (2) yields $\langle\phi_\alpha(x,q)|\phi^\dagger_\beta(x,q')\rangle=\delta(q-q')\delta_{\alpha,\beta}\mathcal{N}_\alpha(q)\mathcal{D}_\alpha(q)$, where we have set $\mathcal{D}_\alpha(q)=\langle\mathbf{w}^{(\alpha)}(q)|\mathbf{w}^{(\alpha)\dagger}(q)\rangle$ and $\mathbf{w}^{(\alpha)\dagger}(q)=\mathbf{w}^{(\alpha)*}(-q)$. Therefore, completeness of the biorthogonal system is ensured by letting $\mathcal{N}_\alpha(q)=1/\mathcal{D}_\alpha(q)$ provided that $\mathcal{D}_\alpha(q)\neq 0$. Because $\mathcal{D}_\alpha(q)$ vanishes if and only if the energy $E_\alpha(q)$ is a defective eigenvalue of the matrix $\mathcal{H}(q)$, from Theorem 1 one concludes that a spectral singularity prevents the construction of a biorthogonal eigensystem for H.

Finally, it is also worth mentioning the following theorem, which shows that the defective eigenvalues of $\mathcal{H}$ correspond to the spectral singularities of H, defined as the divergence points of the resolvent $G(z)=(z-H)^{-1}$ on the continuous spectrum.

Theorem 2. Any defective eigenvalue of $\mathcal{H}$ is a divergence point for the resolvent $G(z)=(z-H)^{-1}$.

Proof. Let $|\chi\rangle$ and $|\varphi\rangle$ be two square integrable functions of the Hilbert space, and let us introduce the complex function of z, $G_{\chi,\varphi}(z)$, defined by $G_{\chi,\varphi}(z)\equiv\langle\chi|G(z)\varphi\rangle$. To prove the theorem, it is enough to show that there exists at least a couple of functions $|\chi\rangle$ and $|\varphi\rangle$ such that $G_{\chi,\varphi}(z)$ is unbounded as $z\to E_0$, E_0 being a defective eigenvalue of $\mathcal{H}$. To this end, after expanding $|\chi\rangle$ and $|\varphi\rangle$ on the plane-wave basis $|q,n\rangle$, one can readily show that

$$G_{\chi,\varphi}(z)=\sum_{n,m}\int_{-\pi/a}^{\pi/a}dq\,\chi_m^*(q)\varphi_n(q)\mathcal{R}_{m,n}(z,q), \qquad (4)$$

where $\chi_m(q)\equiv\langle q,m|\chi\rangle$, $\varphi_n(q)\equiv\langle q,n|\varphi\rangle$, and $\mathcal{R}(z,q)=[z-\mathcal{H}(q)]^{-1}=\mathcal{T}(q)[z-\mathcal{J}(q)]^{-1}\mathcal{T}^{-1}(q)$ is the resolvent of the matrix $\mathcal{H}(q)$. Note that the spectral functions $\chi_m(q)$ and $\varphi_n(q)$ are simply related to the Fourier transforms of $|\chi\rangle$ and $|\varphi\rangle$ as described in the proof of Theorem 1, and hence the inversion relations $|\chi(x)\rangle=\sum_n\int_{-\pi/a}^{\pi/a}dq\,\chi_n(q)|q,n\rangle$ and $|\varphi(x)\rangle=\sum_n\int_{-\pi/a}^{\pi/a}dq\,\varphi_n(q)|q,n\rangle$ hold. If E_0 is a defective eigenvalue of $\mathcal{H}(q)$, say at $q=0$, with algebraic multiplicity 2 and geometric multiplicity 1, then there exists one element of the matrix $\mathcal{R}(z,q)$, say $\mathcal{R}_{m_0,n_0}(z,q)$, which has a second-order pole at $z=E_0$ when $q=0$. This follows from the well-known form of the resolvent $[z-\mathcal{J}(q)]^{-1}$ of a Jordan matrix possessing a Jordan block with dimension 2. In the neighborhoods of $q=0$ and $z=E_0$, $\mathcal{R}_{m_0,n_0}(z,q)$ behaves like $\sim 1/[(z-E_0-\alpha q)(z-E_0+\alpha q)]$, where α is a constant and $E_0\pm\alpha q$ are the two eigenvalues that cross and become a defective eigenvalue at $q=0$. Let us now choose the spectral functions $\chi_m(q)$ to vanish for $m\neq m_0$, and $\varphi_n(q)$ to vanish for $n\neq n_0$; conversely, $\chi_{m_0}(q)$ and $\varphi_{n_0}(q)$ are assumed to be nonvanishing and bounded functions of q in the interval $(-\pi/a,\pi/a)$. The functions $|\chi\rangle$ and $|\varphi\rangle$ in direct space that yield such spectral functions are determined by the corresponding inversion relations given above. For instance, if $\chi_{m_0}(q)$ and $\varphi_{n_0}(q)$ assume a constant value in the interval $(-\pi/a,\pi/a)$, then $|\chi(x)\rangle=\mathcal{N}[\sin(\pi x/a)/(x)]\exp(ik_Bm_0x)$ and $|\varphi(x)\rangle=\mathcal{N}[\sin(\pi x/a)/(x)]\exp(ik_Bn_0x)$, where $\mathcal{N}$ is a normalization constant. Under such a choice, the sum in Eq. (4) reduces to the only term $m=m_0$ and $n=n_0$. Owing to the behavior of $\mathcal{R}(z,q)$ near $z=E_0$ and $q=0$, the corresponding integral on the right-hand side of Eq. (4) diverges as $z\to E_0\pm i0^+$, i.e., $G_{\chi,\varphi}(z)$ is unbounded in the neighborhood of $z=E_0$, which proves the theorem.

B. Spectral singularities and secular Bragg diffraction

An important physical implication of spectral singularities in complex crystals is the appearance of a secular growth of the amplitudes of waves scattered off the lattice when it is excited by a plane wave at special incident angles. Such an anomalous behavior has been previously noticed by Berry [23,24] for certain absorptive potentials; here we prove that this is a very general feature of complex crystals related to the existence of spectral singularities.

Theorem 3. Let $\psi(x,t)=\exp(-iHt)\psi_0(x)$ be the Bragg diffraction pattern corresponding to crystal excitation, at $t=0$, with a plane wave $\psi(x,0)=\exp(ikx)$ of wave number k. Then H has spectral singularities if and only if for some integer n and $k=nk_B/2$, the solution $\psi(x,t)$ contains secular (linearly growing) terms in t.

Proof. Let us set $k=q+l_0k_B$, where l_0 is an integer, and $-\pi/a\leqslant q<\pi/a$. Then the solution $\psi(x,t)$ of Eq. (1) with the initial condition $\psi(x,0)=\exp(ikx)$ is given by $\psi(x,t)=\sum_{l=-\infty}^{\infty}c_l(t)\exp[i(q+lk_B)x]$, where $c_l(t)$ satisfy the coupled equations $i(dc_l/dt)=\sum_m\mathcal{H}_{l,m}(q)c_m(t)$ with the initial conditions $c_l(0)=\delta_{l,l_0}$. Physically, the coefficients c_l are the amplitudes of diffracted waves at various orders at plane t [see Fig. 1(a)]. Hence $c_l(t)=\mathcal{M}_{l,l_0}(q,t)$, where $\mathcal{M}(q,t)=\exp[-it\mathcal{H}(q)]$. The exponential matrix $\mathcal{M}$ can be calculated from the Jordan decomposition of $\mathcal{H}$ as $\mathcal{M}=\mathcal{T}\exp(-it\mathcal{J})\mathcal{T}^{-1}$. Having in mind the form of the exponential of a Jordan matrix [28], it follows that secular growing terms in some of the coefficients $c_l(t)$ [and hence in $\psi(x,t)$] appear if and only if $\mathcal{H}(q)$ has at least one defective eigenvalue, the largest growing term being $\sim t^\rho$ where ρ is the (maximal) difference between the algebraic and geometric multiplicity of defective eigenvalues. In our case, $\rho=1$ because the maximal algebraic multiplicity of any eigenvalue of $\mathcal{H}(q)$ is 2; moreover, since $\mathcal{H}(q)$ may have defective eigenvalues only for $q=0$ or $q=-\pi/a$, secular growing terms may appear solely when the wave number k of the exciting plane wave is an integer multiple of $k_B/2$. The absence of secular growing terms in $c_l(t)$ for any excitation wave number $k=nk_B/2(n=0,\pm1,\pm2,\ldots)$ implies that the matrix $\mathcal{J}$ is diagonal, which ensures the lack of defective eigenvalues of $\mathcal{H}$ and thus of spectral singularities of H according to Theorem 1.

III. BRAGG SCATTERING IN $\mathcal{PT}$ COMPLEX CRYSTALS AND WAVE-PACKET DYNAMICS

Let us specialize the previous results to the case of a $\mathcal{PT}$-symmetric lattice, for which $V(-x)=V^*(x)$. Let $V_R(x)$ and $\lambda V_I(x)$ be the real and imaginary parts of the potential, respectively, where $\lambda\geqslant 0$ measures the anti-Hermitian strength of H. The spectrum of H is real for $\lambda\leqslant\lambda_c$, where $\lambda_c\geqslant 0$ defines the symmetry-breaking point. According to the previous analysis, complex-conjugate pairs of eigenvalues for $\mathcal{H}(q)$ should appear as λ is increased from below to above λ_c. The typical scenario that describes symmetry breaking in a finite-dimensional $\mathcal{PT}$ matrix is the appearance of an exceptional point via the merging of two real eigenvalues into a single real and defective eigenvalue at $\lambda = \lambda_c$ (see, for instance, [7,29]). We note that the existence of such a branching point for a certain class of non-Hermitian matrices as a control parameter is varied was proven in a rather general way in Ref. [30] (see also [7]). We may thus conjecture that for a $\mathcal{PT}$ complex crystal, symmetry breaking is accompanied by the appearance of spectral singularity, which arises from defective eigenvalues of $\mathcal{H}$ at $q = 0$ or $q = -\pi/a$. This scenario is in agreement with numerical or analytical results obtained from band computation of specific complex periodic potentials (see, for instance, [6,8]).

As an example, let us consider the $\mathcal{PT}$ crystal defined by

$$V_R(x) = V_0 \cos(2\pi x/a), \quad V_I(x) = V_0 \sin(2\pi x/a), \quad (5)$$

which has been recently considered to highlight unusual diffraction and transport properties of complex optical lattices [6,25]. In this case, $\lambda_c = 1$ [6], and at the symmetry-breaking point, one has $V(x) = V_0 \exp(ik_B x)$, a potential which is amenable for an analytical study [19,23]. For this potential, $\mathcal{H}$ has a block diagonal form, namely, $\mathcal{H}_{n,m} = (n + k_B q)^2 \delta_{n,m} + V_0 \delta_{m,n+1}$, and its eigenvalues are simply the elements on the main diagonal, i.e., $E_\alpha(q) = (q + \alpha k_B)^2 (\alpha = 0, \pm 1, \pm 2, \ldots)$. This means that, as previously noticed [6,19,25], the band structure of the $\mathcal{PT}$ potential $V = V_0 \exp(ik_B x)$ coincides with the free-particle energy dispersion curve $E = k^2$, periodically folded inside the first Brillouin zone [see Fig. 1(b)]. The eigenvalues are distinct for $q \neq 0, -\pi/a$. At the crossings of the folded parabolas of Fig. 1(b), i.e., at $q = 0$ and at $q = -\pi/a$, one has $E_{-\alpha}(q) = E_\alpha(q)$ and $E_{1-\alpha}(q) = E_\alpha(q)$, respectively, i.e., the eigenvalues coalesce in pairs and become defective. Therefore, the continuous spectrum of H, $E \geqslant 0$, contains a sequence of spectral singularities at $E_n = (nk_B/2)^2$, $n = 1, 2, 3, \ldots$ [see Fig. 1(b)], which spoils the completeness of the Bloch-Floquet eigenfunctions. The defective nature of degenerate eigenvalues at $q = 0$ and $q = -\pi/a$ can be readily proven by direct calculation of the eigenvectors $\mathbf{w}^{(\alpha)}$ of $\mathcal{H}$. Note that as wave scattering from complex potential *barriers* enables a finite number of spectral singularities in the continuous spectrum [12,17], in our example the number of spectral singularities is countable but infinite.

According to Theorem 3, a secular growth of Bragg diffraction pattern for a plane wave that excites the crystal at normal incidence (or tilted by an angle which is an integer multiple of the Bragg angle) provides a distinctive signature of the appearance of spectral singularities at the $\mathcal{PT}$-symmetry-breaking transition point $\lambda = \lambda_c = 1$. However, in any experimental setting aimed to observe such a secular growth, the wave that excites the crystal is always spatially limited or truncated, and it is thus of major relevance to investigate the impact of spectral singularities on the evolution of a wave packet with a broadened angular spectrum, an issue which was not considered in previous works by Berry.

Here we investigate the Bragg diffraction of a wave packet with a broadened momentum distribution, $\psi(x,0) = \int dk\, F(k) \exp(ikx)$, and show that spectral broadening leads to a *saturation* of the secular growth of scattered waves. Such a saturation behavior is basically due to the fact that spectral singularities are of measure zero (they are a countable set of points embedded in the continuous energy spectrum $E \geqslant 0$). For the sake of simplicity, we consider a shallow lattice and a wave packet with a narrow spectrum $F(k)$ centered at $k = -k_B/2$ of width $\Delta k \ll k_B$. Following the same lines detailed in the proof of Theorem 3, one can show that the diffraction pattern $\psi(x,t)$ can be written as the interference of different wave packets describing one-side diffraction at various orders, namely,

$$\psi(x,t) = \psi_0(x,t) + V_0 \psi_1(x,t) + V_0^2 \psi_2(x,t) + \cdots, \quad (6)$$

where $\psi_n(x,t) = \int dk\, F(k) c_n(k,t) \exp[i(k + nk_B)x]$, with $c_0(k,t) = \exp(-ik^2 t)$ and $c_n(k,t) = -i \int_0^t d\xi\, c_{n-1}(k,\xi) \exp[i(k + nk_B)^2(\xi - t)]$ for $n \geqslant 1$. For a shallow lattice, i.e., for $|V_0| \ll 1$, we can limit to consider the first two terms on the right-hand side of Eq. (6). The leading term, $\psi_0(x,t) = \int dk\, F(k) \exp(-ik^2 t + ikx)$, is simply the freely diffracting wave packet that one would observe in the absence of the crystal and that propagates with a constant speed $v = dx/dt = k_B$. The expression of $\psi_1(x,t)$ is more involved; however, its asymptotic behavior for $t \gg \pi/(k_B \Delta k)$ assumes a rather simple and physically interesting form, namely,

$$\psi_1 \sim -\frac{i\pi}{k_B} F\left(-\frac{k_B}{2}\right) \exp\left(i\frac{k_B x}{2} - i\frac{k_B^2 t}{4}\right) \Phi\left(\frac{x}{k_B t}\right), \quad (7)$$

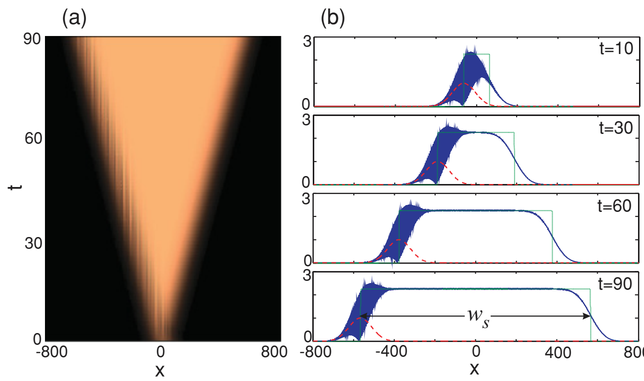

FIG. 2. (Color online) Evolution of a Gaussian wave packet in the complex lattice $V(x) = V_0 \exp(ik_B x)$ for $V_0 = 0.2$, $a = 1$, and $w = 80$. In (a) a snapshot of $|\psi(x,t)|$ is shown, whereas in (b) the profiles of $|\psi(x,t)|$ at a few values of t are reported. In (b), the dashed lines correspond to the wave-packet evolution in absence of the lattice, whereas the dotted curves correspond to $|\psi_1(x,t)|$ as predicted by Eq. (7).

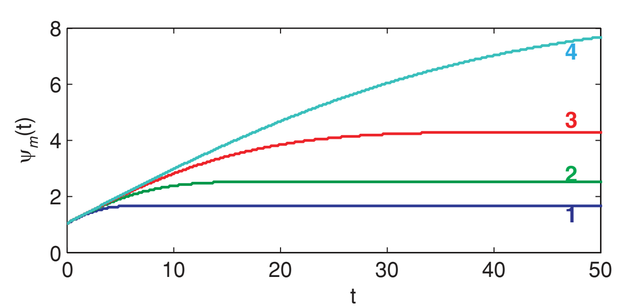

FIG. 3. (Color online) Saturation of secular Bragg scattering for a Gaussian wave packet that excites the complex lattice of Fig. 2 at normal incidence. The curves show the evolution of the maximum wave-packet amplitude $\psi_m(t)$ versus t for a few values of input wave-packet spot size w. Curve 1: $w = 40$; curve 2: $w = 80$; curve 3: $w = 150$; curve 4: $w = 300$.

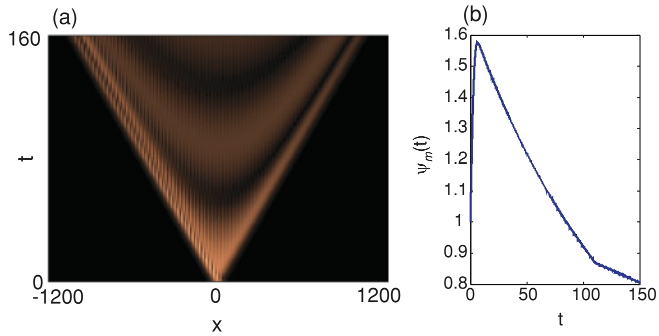

FIG. 4. (Color online) (a) Evolution of a Gaussian wave packet [modulus of $\psi(x,t)$] in the complex lattice (5) for $V_0 = 0.2$, $a = 1$, $w = 80$, and below the $\mathcal{PT}$-symmetry-breaking point ($\lambda = 0.9$). In (b), the corresponding evolution of the maximum wave-packet amplitude $\psi_m(t)$ is shown.

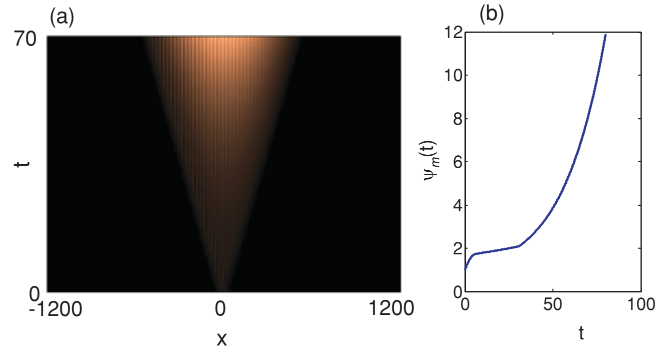

FIG. 5. (Color online) Same as Fig. 4, but above the $\mathcal{PT}$-symmetry-breaking point ($\lambda = 1.1$).

where $\Phi(\xi) = 1$ for $|\xi| < 1$ and $\Phi(\xi) = 0$ for $|\xi| > 1$. Equation (7) shows that, owing to wave packet broadening in momentum space, the secular growth with t of the diffracted beam saturates to the value $\sim (\pi/k_B)|F(-k_B/2)|$, while the beam assumes a square shape whose width w_s spreads in space with a constant speed $v = dw_s/dt = k_B$. Note that v equals the translation speed of the freely diffracting wave packet ψ_0.

This behavior is confirmed by direct numerical simulations of Eq. (1), as shown in Fig. 2. The figure depicts the evolution of $|\psi(x,t)|$ for a Gaussian wave packet $\psi(x,0) = \exp[-(x/w)^2 - ik_B x/2]$ with spectrum $F(k) = [w/(2\sqrt{\pi})]\exp[-(k+k_B/2)^2 w^2/4]$ that excites the crystal at $t = 0$. The evolution of the freely diffracting wave packet $|\psi_0|$ and of the asymptotic behavior of $|\psi_1|$ predicted by Eq. (6) are also shown for comparison. Note the formation of interference fringes on the left side of the wave packet, which arise from the interference of ψ_0 and ψ_1. The spectral-broadening-induced saturation of the secular growth of the wave packet is clearly shown in Fig. 3, where the behavior of the maximum amplitude $\psi_m(t)$ of the wave packet versus t, defined by

$$\psi_m(t) = \max_x |\psi(x,t)|, \tag{8}$$

is depicted for a few decreasing values of the wave-packet input spot size w. Note that in the early stage of the dynamics, the peak amplitude linearly increases with t, as expected for a plane wave according to Theorem 3. The linear growth then saturates to a steady-state value and, as Fig. 3 clearly shows, the saturation process occurs earlier for wave packets with smaller input size w.

It should be pointed out that saturation of $\psi_m(t)$ to a steady-state value, as predicted by Eq. (7) and confirmed by numerical simulations depicted in Figs. 2 and 3, is indeed a signature of spectral singularities of the underlying Hamiltonian that arise at $\lambda = \lambda_c = 1$. This is clearly shown in Figs. 4 and 5, where a typical wave-packet evolution is reported for the complex crystal defined by Eq. (5) either below ($\lambda = 0.9\lambda_c = 0.9$, Fig. 4) and above ($\lambda = 1.1\lambda_c = 1.1$, Fig. 5) the $\mathcal{PT}$-symmetry-breaking transition point. In both cases, H is diagonalizable, and there are not spectral singularities. Note that below the $\mathcal{PT}$-symmetry-breaking point, the energy spectrum is real-valued; and, after an initial increase, $\psi_m(t)$ does not settle down to a steady-state value, rather it tends to monotonically decay (Fig. 4) like in an ordinary (Hermitian) crystal. On the other hand, above the $\mathcal{PT}$-symmetry-breaking point ($\lambda = 1.1$), the energy spectrum contains pairs of complex-conjugate eigenvalues, and $\psi_m(t)$ monotonically increases, as shown in Fig. 5. Therefore, the scattering process with wave packets can be used to highlight the appearance of spectral singularities at the $\mathcal{PT}$-symmetric-breaking point, which are revealed as the saturation of the wave-packet amplitude growth to a steady-state (nondecaying) value.

If the lattice is realized in a periodic dielectric medium as discussed in [6], at light wavelength $\lambda = 1.5\ \mu$m, assuming a bulk refractive index $n_s = 1.5$ and a maximum refractive index change (both real and imaginary parts) of $\Delta n = 2 \times 10^{-4}$, the simulations of Fig. 2 correspond, as an example, to an optical lattice with spatial period $a \simeq 6.2\mu$m excited by a Gaussian beam of size $w \simeq 493\ \mu$m; the spatial units along the x and t axes are $l_x \simeq 6.2\ \mu$m and $l_t \simeq 477\ \mu$m, respectively. The same scales hold for the simulations shown in Figs. 4 and 5.

IV. CONCLUSIONS

In this work, it has been shown that Bragg scattering in complex crystals provides a physically important process to visualize the appearance of spectral singularities in non-Hermitian Hamiltonians with complex periodic potentials. In particular, clear signatures of spectral singularities could be gained in a diffraction experiment with wave packets. These results may suggest the investigation of possible experimental systems to observe spectral singularities in complex lattices, such as photonic systems [6,9].

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