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Critical phenomena associated with self-orthogonality in non-Hermitian quantum mechanics

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Abstract. – The delocalization phenomenon was discovered by Hatano *et al.* and Miller *et al.* for a class of non-Hermitian quantum-mechanical problems. We show that the delocalization is only one example of many possible critical phenomena which are associated with the self-orthogonality of an eigenstate of the non-Hermitian Hamiltonian. It is shown that in this class of problems the self-orthogonality occurs at the series of branch points in the complex energy plane that serve as gates for the "particle" to hop from one Bloch energy band to another one.

In conventional quantum mechanics the Hamiltonians must be Hermitian. Non-Hermitian Hamiltonians do appear however, in the study of the resonance phenomena [1,2] and in other physical contexts [3–8] which are described below.

There are many different reasons for using non-Hermitian quantum mechanics. One is to simplify the calculations. There are problems that are quite difficult and sometimes impossible to solve even numerically, for example, when studying the dynamics of molecular systems where the electronic and the nuclear coordinates are strongly coupled to one another and the Born-Oppenheimer approach is not applicable. In such cases, the non-Hermitian quantum mechanics enables us to take into consideration the coupling between the channels that are open for dissociation and ionization in a simple way [9,10]. Another example is studying the dynamics of a system which is coupled to a bath. Often the solution of the full problem is impossible due to the current available computational sources and technology. The calculations become possible by including complex absorbing potential terms (*i.e.*, non-Hermitian operators) into the Hamiltonian which introduce the environmental dynamical effects on the studied system [11,12]. Another obvious reason to use non-Hermitian quantum mechanics is when effects which cannot be described by Hermitian Hamiltonians are to be considered, such as diffusion effects, spatial fluctuations in inhomogeneous systems and effects induced by extended defects in type-II superconductors subjected to a tilted external magnetic field [3,13].

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In this letter we will show that the self-orthogonality property of eigenstates of non-Hermitian Hamiltonians is responsible for the appearance of critical phenomena (*e.g.*, sudden delocalization) in different fields of physics. The self-orthogonality of eigenstates is only possible in non-Hermitian quantum mechanics. In the Hermitian QM the definition of the inner product as the scalar product of two eigenvectors does not allow the self-orthogonality feature to appear. In non-Hermitian quantum mechanics we use the general definition of the inner product $(f \mid g) \equiv \langle f^* \mid g\rangle$ rather than the usual definition of scalar product $\langle f \mid g\rangle$. See, for example, refs. [14, 15] about the different possible definitions of a general inner product. It is convenient to define the inner product using the matrix representation of different operators. The matrices representing operators have right (column) eigenvectors, $|i)$, and left (row) eigenvectors, $(j|$. The left eigenvectors are obtained by taking the transpose of right eigenvectors of the transposed matrices. Therefore, when a matrix is complex and symmetric (associated with non-Hermitian Hamiltonian) the left eigenvectors are equal (no complex conjugation) to the right ones, $(f \mid g) \equiv \langle f^* \mid g\rangle$. The bi-orthogonality condition implies that $(j \mid i) = \delta_{i,j}$. However, it may happen that one of the eigenvectors is orthogonal to itself, *i.e.*, self-orthogonal, in the sense that $(j \mid j) = 0$ (take, for example, the case where the vector j consists of 2 non-zero components, 1 and i). When a finite-dimensional matrix has a self-orthogonal eigenvector, then the number of the linearly independent eigenvectors is smaller than the rank of the matrix and the spectrum is incomplete. Moiseyev and Friedland have proved that if $\hat{A}$ and $\hat{B}$ are two Hermitian operators, then one can always find at least one value for the complex parameter λ for which $\hat{A} + \lambda\hat{B}$ does have a self-orthogonal eigenvector [16]. Moiseyev and Friedland assumed that the incomplete spectrum phenomenon which goes along with the formation of a self-orthogonal state is a rare phenomenon and is not associated with any physical measurable quantity. However, recent theoretical studies of the appearance of relatively sharp peaks in the cross-section measured in scattering experiments of low-energy electrons from hydrogen molecule have shown that the self-orthogonality phenomenon is neither accidental nor rare [9, 10]. Moreover, it has been shown that there is a large set of physical phenomena that happen due to the appearance of self-orthogonal states such as excess noise in unstable lasers [17, 18], propagation near the optic axes of absorbing anisotropic crystals [19], and the diffraction of atomic beams by crystals of light [20].

In this letter the non-Hermitian Hamiltonian which is subject of our studies is given in dimensionless units by

$$\hat{\mathcal{H}} = -\frac{1}{2}\left(\frac{\partial}{\partial x} - g\right)^2 + V(x). \tag{1}$$

We have chosen the potential term, $V(x)$, to be a finite potential well (width equal to 1 and depth equal to -1).

The real parameter g is a drift velocity in studies of water flow [21–23] in aqueous media, winds, etc., or a non-Hermitian external field originating in the transverse magnetic field [13]. Note that for $g = 0$ the Hamiltonian presented above is Hermitian and possesses only one bound state. Nelson and co-workers have shown that a bound state localized inside the potential well turns to be an extended delocalized state as the vector potential parameter g gets a critical value, $g_c = \sqrt{-2E_{\text{bound}}(g = 0)}$, where $E_{\text{bound}}(g = 0)$ is the ground state eigenvalue of the Hermitian Hamiltonian $H = \hat{\mathcal{H}}(g = 0)$ [13, 24]. In our paper we will not study the problem with disorder as was done by Nelson *et al.* [13, 24] but rather concentrate on the model of a particle localized in a potential well. However, as we will show below, the same sudden delocalization phenomenon has been observed in this model Hamiltonian.

We have chosen here to impose one-dimensional periodic boundary conditions on the Hamiltonian given above. That is, $-\infty \leq x \leq +\infty$, where $V(x) = V(x + L)$. In our studied case even at $g = 0$ all states are delocalized in the sense that they are Bloch states, $\Psi_\alpha = \exp[ikx]\phi_{\alpha,k}(x)$, where $-\pi/2 \le k \le +\pi/2$ and $\phi_{\alpha,k}(x) = \phi_{\alpha,k}(x+L)$. However, the $\alpha = 1$ band is constructed from *multiple bound states* which are *localized* inside the periodic potential wells. The amplitudes of $\phi_{\alpha=1,k}(x)$ in between two adjacent potential wells are exponentially small as $L \to \infty$. The second band labeled by $\alpha = 2$, is embedded in the continuum part of the spectrum. The delocalization discussed by Nelson and co-workers is different from the Bloch delocalization mentioned above. Nelson's delocalization implies that the amplitudes of $\phi_{\alpha=1,k}(x)$ in between two adjacent potential wells is as large as inside the periodic potential wells. As we will show below, Nelson's delocalization is associated with the merging of two different energy bands of the non-Hermitian Hamiltonian. For some critical value g_{c_j}, two different band edges coalesce at $k = (2j-1)\pi/L$, $j = 1, 2, \ldots$. At these branch points (bp) the Bloch wave functions, $\phi_{\alpha=1,k=(2j-1)\pi/L}(x) = \phi_{\alpha=2,k=(2j-1)\pi/L}(x) \equiv \phi_j^{\mathrm{bp}}$, are self-orthogonal.

Nelson's delocalization can be explained in terms of infinitely large value of the standard deviation Δx due to the self-orthogonality property of ϕ_j^{bp}. On the basis of this argument, it is clear that infinitely large standard variation would be obtained for any dynamical property which is represented by an operator that does not commute with the non-Hermitian Hamiltonian. As we will show, the delocalization of the confined first band persists for values of g exceeding the critical value g_{bp}. Both states emerging after the coalescence have the nature of the continuum state, *i.e.* they are delocalized in the coordinate space.

As was discussed in the introduction, the left eigenfunctions of non-Hermitian Hamiltonians are not equal to the right eigenfunctions. The right Bloch states, $\phi^{\mathrm{R}}_{\alpha,k}$ were obtained by calculating the eigenfunctions of the Bloch Hamiltonian, $\hat{\mathcal{H}}_{\mathrm{B}} = \frac{1}{2}(-\frac{i\partial}{\partial x} + ig + k)^2 + V(x)$. The left Bloch states are eigenstates of $(\hat{\mathcal{H}}_{\mathrm{B}}^\dagger)^* = (\hat{\mathcal{H}}_{\mathrm{B}}(-g))^*$. Consequently, the left eigenfunctions are defined as

$$\phi^{\mathrm{L}}_{\alpha,k} = \phi^{\mathrm{R}*}_{\alpha,k}(-g). \tag{2}$$

Bi-orthogonality implies that

$$\left(\phi^{\mathrm{L}}_{\alpha'\neq\alpha,k}(g) \mid \phi^{\mathrm{R}}_{\alpha,k}(g)\right) \equiv \int_{-\infty}^{+\infty} \phi^{\mathrm{L}}_{\alpha'\neq\alpha,k}(x;g)\phi^{\mathrm{R}}_{\alpha,k}(x;g)\mathrm{d}x = 0. \tag{3}$$

However, following the general proof of Moiseyev and Friedland, by varying one complex parameter or two real parameters one can find values such that the above equality holds also when $\alpha' = \alpha$. Namely, one should find critical values of k (Bloch wave vector) and g (imaginary vector potential parameter) for which a branch point is obtained, $E_{\alpha=1}(g = g_{\mathrm{bp}}, k_{\mathrm{bp}}) = E_{\alpha=2}(g = g_{\mathrm{bp}}, k_{\mathrm{bp}})$. In the vicinity of a branch point the eigenvalue of the non-Hermitian Hamiltonian varies as

$$E \sim \left[(k - k_{\mathrm{bp}}) - i(g - g_{\mathrm{bp}})\right]^{\frac{1}{2}}. \tag{4}$$

The square root results from the fact that the branch point is obtained from coalescence of two eigenvalues. A branch point does not only imply degenerate eigenvalues but also coalescence of the corresponding eigenfunctions, $\phi^{\mathrm{R,L}}_{\alpha=1,k_{\mathrm{bp}}} - \phi^{\mathrm{R,L}}_{\alpha=2,k_{\mathrm{bp}}} \to 0$ as $g \to g_{\mathrm{bp}}$. Due to the bi-orthogonality property at the branch point, $\phi^{\mathrm{R,L}}_{\alpha=1,k_{\mathrm{bp}}} = \phi^{\mathrm{R,L}}_{\alpha=2,k_{\mathrm{bp}}}$ is a self-orthogonal function. That is, $(\phi^{\mathrm{L}}_{\alpha'=\alpha,k_{\mathrm{bp}}}(g_{\mathrm{bp}}) \mid \phi^{\mathrm{R}}_{\alpha,k_{\mathrm{bp}}}(g_{\mathrm{bp}})) = 0$. The results presented in fig. 1 show that the self-orthogonality is obtained for $g = g_{\mathrm{bp}} = 0.485$ and $k = k_{\mathrm{bp}} = \pi/L$, where $L = 10$ is the "lattice" constant in our model Hamiltonian. As $L \to \infty$, the branch point value of g, g_{bp}, approaches the critical value obtained by Nelson for the sudden appearance of delocalization when x is

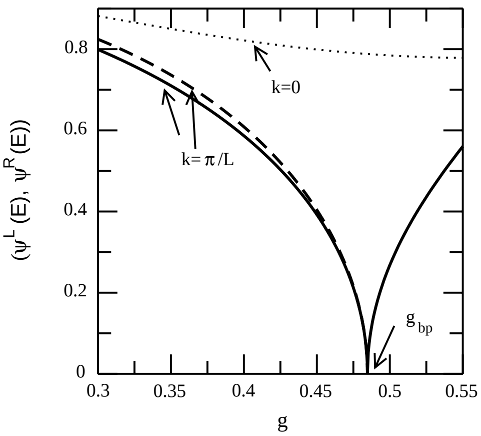

Fig. 1 – Coalescence of two complex eigenstates at $g = g_{\rm bp}$ when $k = \pi/2$. At the branch point $g = g_{\rm bp}$ the eigenfunction becomes self-orthogonal and $(\Psi \mid \Psi) = 0$.

an angle variable. As one can see from our results, the periodical boundary conditions are crucial to get the self-orthogonality phenomenon. To obtain a branch point in the spectrum of non-Hermitian Hamiltonian we need to have two real parameters. The first parameter, g, is the drift velocity and the second parameter, the Bloch wave vector k, is provided by the periodic boundary conditions.

In order to show that the self-orthogonality is associated with a branch point which results from the coalescence of the "ground bound" Bloch band with the continuum Bloch band, we carried out k-trajectory calculations (from $k = 0$ to $k = 2\pi/L$). From the results presented in fig. 2 one can see that when $g \neq g_{\rm bp}$ the Bloch bands are separated in the complex energy plane. The non-Hermitian "ground bound" Bloch band is a circle in the complex energy plane, whereas the non-Hermitian continuum Bloch band is a line. At the critical value of g, $g_{\rm bp}$, the two bands touch at the branch point obtained when $k = \pi/L$. At this point we obtained the self-orthogonality as shown in fig. 1.

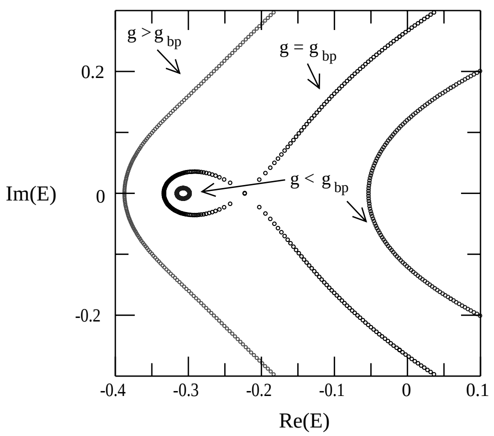

Fig. 2 – The complex eigenvalue band structure for three different values of g. The Bloch wave vector is varied within $0 \leq k \leq 2\pi/L$.

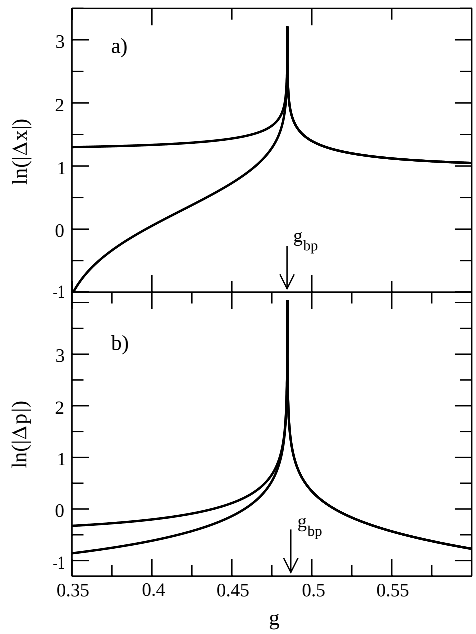

Fig. 3 – The standard deviations of position (a) and momentum (b) as a function of the drift velocity parameter g. The standard deviations diverge at $g = g_{\mathrm{bp}}$.

Calculation of the real and imaginary parts of the eigenvalues of the Hamiltonian as a function of the wave vector k shows a series of branch points obtained at $k_{\mathrm{bp}} = \pi/L, 3\pi/L, \ldots$. At each one of these branch points (associated with a sudden transition from one Bloch band to another) the eigenstate is self-orthogonal and therefore the expectation value of an operator $\hat{O}$ for which $[\hat{O}, \hat{\mathcal{H}}_{\mathrm{B}}] \neq 0$,

$$\left(\phi^{\mathrm{L}}_{\alpha,k_{\mathrm{bp}}} \middle| \hat{O} \middle| \phi^{\mathrm{R}}_{\alpha,k_{\mathrm{bp}}}\right) = \frac{\int_{-\infty}^{+\infty} \phi^{\mathrm{L}}_{\alpha,k_{\mathrm{bp}}} \hat{O} \phi^{\mathrm{R}}_{\alpha,k_{\mathrm{bp}}} \mathrm{d}x}{\int_{-\infty}^{+\infty} \phi^{\mathrm{L}}_{\alpha,k_{\mathrm{bp}}} \phi^{\mathrm{R}}_{\alpha,k_{\mathrm{bp}}} \mathrm{d}x} = \infty. \tag{5}$$

The results presented in fig. 3 illustrate the sudden delocalization phenomenon when $\hat{O} = \Delta x$ and $\hat{O} = \Delta \hat{p}_x$. As one can see from fig. 3a, below the branch point $g < g_{\mathrm{bp}}$, there is a clear distinction between the two states: one being a localized bound state and the other an extended continuum state. At the branch point both states coalesce and the standard deviation diverges at that point. After increasing the value of g beyond the critical value, $g > g_{\mathrm{bp}}$, both states emerging from the branch point have the standard deviation of the delocalized continuum state. This is in full contrast to the level crossing situation, where the nature of two states is exchanged after the crossing point.

In a way this non-Hermitian quantum behavior resembles the classical chaotic dynamics. The standard deviations of position and momentum diverge exponentially when the initial conditions are defined as a Gaussian ensemble distribution of particles localized in the chaotic region of the classical phase space.

In this letter we addressed a class of problems which are studied by non-Hermitian quantum mechanics. We have shown that in the case where periodic boundary conditions can be employed, the ground eigenstate becomes self-orthogonal when a physical parameter in the

Hamiltonian approaches a critical value. At this critical point the expectation value of *any* operator which does not commute with the Hamiltonian (*e.g.*, position; momentum) gets infinitely large value. Hence, the delocalization discovered by Nelson *et al.* is only one example of many possible critical phenomena.

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