Analytic approximation for eigenvalues of a class of $\mathcal{PT}$ symmetric Hamiltonians

O. D. Skoromnik[1, *] and I. D. Feranchuk[2, 3, 4, †]

[1] *Max Planck Institute for Nuclear Physics, Saupfercheckweg 1, 69117 Heidelberg, Germany*
[2] *Atomic Molecular and Optical Physics Research Group, Ton Duc Thang University, 19 Nguyen Huu Tho Str., Tan Phong Ward, District 7, Ho Chi Minh City, Vietnam*
[3] *Faculty of Applied Sciences, Ton Duc Thang University, 19 Nguyen Huu Tho Str., Tan Phong Ward, District 7, Ho Chi Minh City, Vietnam*
[4] *Belarusian State University, 4 Nezavisimosty Ave., 220030, Minsk, Belarus*

An analytical approximation for the eigenvalues of $\mathcal{PT}$ symmetric Hamiltonian $\mathsf{H} = -d^2/dx^2 - (\mathrm{i}x)^{\epsilon+2}$, $\epsilon > -1$ is developed via simple basis sets of harmonic-oscillator wave functions with variable frequencies and equilibrium positions. We demonstrate that our approximation provides high accuracy for any given energy level for all values of $\epsilon > -1$.

Introduction. — Bender and Boettcher introduced [1] a family of $\mathcal{PT}$ symmetric Hamiltonians

$$\mathsf{H} = -\frac{d^2}{dx^2} - (\mathrm{i}x)^{\epsilon+2}, \quad \epsilon > -1, \tag{1}$$

which, despite being non-Hermitian, can nevertheless possess real and discrete eigenvalues, if one considers the solution of the corresponding Schrödinger equation on the complex plane instead of the real axis [2, 3]. This remarkable discovery triggered theoretical investigations [4–32] and experimental activities towards the realization of systems that can be effectively described by $\mathcal{PT}$ symmetric Hamiltonians [33–50].

Usually, the numerical solution of the Schrödinger equation with the Hamiltonian (1) is performed either via the shooting method [1, 51], basis expansion [51], by discretizing the Schrödinger equation and applying the Arnoldi iteration [52], or via the solution of an integral equation [5].

On the other hand, analytical approximations can provide qualitative peculiarities of the system in a broad range of quantum numbers and parameters of the Hamiltonian and can serve as a basis for further numerical solutions. Moreover, the applicability of the known approximations for the Hermitian systems can be investigated in the non-Hermitian case. As such, an analytical approximation for the Hamiltonian (1) when $\epsilon \geq 0$ was derived through the modified quasi-classical WKB approximation [1], when the turning points are located on the complex plane.

In addition, the energy levels were determined by employing the variational method [53] for the three-parameter functional $\langle \mathsf{H}(a,b,c)\rangle = \int_C dx\psi(x)\mathsf{H}\psi(x) / \int_C \psi^2(x)dx$, where the path C on the complex plane is chosen in such a way that the trial function $\psi(x) = (\mathrm{i}x)^c \exp(a(\mathrm{i}x)^b)$ is exponentially decaying at infinity. While this procedure straightforwardly applies to the ground state, the calculation of the energies of the excited states is difficult due to the necessity of introducing the supersymmetric partner for the Hamiltonian. This requires the evaluation of an increasing number of derivatives, which in turns demands the knowledge of the ground state wave function with very high accuracy.

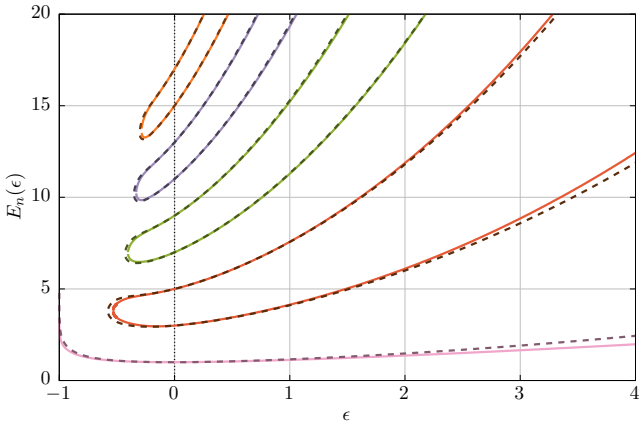

Figure 1. (Color online) The dependence of the eigenvalues E_n on the parameter ϵ. The dashed lines are the exact numerical solutions via the Arnoldi iteration. The solid lines are the analytic approximation.

In our work we propose a simple approach for the evaluation of an energy level for any given quantum number n and all values of the parameter $\epsilon > -1$ with high accuracy.

The idea is based on the method [54, 55] which was employed for the nonperturbative description of various Hermitian quantum systems. Consequently, we firstly illustrate the idea in the Hermitian case.

Method description. — Let us introduce sets $\nu_\alpha^i \equiv \nu_\alpha^1, \nu_\alpha^2, \ldots, \nu_\alpha^s$, $\alpha = 0, 1, \ldots$ of s parameters and a complete basis $|\psi_n(\nu_\alpha^i)\rangle$, which depends on these parameters. The index n here numerates the state vectors. For any given set of s parameters ν_α^i the basis functions are orthonormal $\langle\psi_n(\nu_\alpha^i)|\psi_k(\nu_\alpha^i)\rangle = \delta_{nk}$. However, for two different sets of parameters ν_α^i and $\nu_{\alpha'}^i$, $\alpha \neq \alpha'$ the basis functions are not orthogonal $\langle\psi_n(\nu_\alpha^i)|\psi_k(\nu_{\alpha'}^i)\rangle = S_{nk}^{\alpha\alpha'}$,

* olegskor@gmail.com
† Corresponding author: ilya.feranchuk@tdt.edu.vn

i.e. the overlapping integral $S_{nk}^{\alpha\alpha'}$ is non-vanishing.

For example, let us consider harmonic oscillator wave functions $y_n(x)$. Then the notations $y_n(\{\omega_1, u_1\}, x+u_1)$ and $y_n(\{\omega_2, u_2\}, x+u_2)$ mean that we have two sets of harmonic oscillator wave functions, numbered by the same index $n = 0, 1, 2, \ldots$ which, however, have two different frequencies and two different equilibrium positions. Therefore in this case a set of parameters $\{\nu_1^1, \nu_1^2\}$ ($\{\nu_2^1, \nu_2^2\}$) is given by the set $\{\omega_1, u_1\}$ ($\{\omega_2, u_2\}$) correspondingly. Consequently, the basis functions with the same $\{\omega, u\}$ are orthogonal to each other

$$\int_{-\infty}^{\infty} y_n(\{\omega_1, u_1\}, x+u_1) y_k(\{\omega_1, u_1\}, x+u_1) dx = \delta_{nk},$$

while for different $\{\omega, u\}$ the functions $y_n(\{\omega_1, u_1\}, x+u_1)$ and $y_k(\{\omega_2, u_2\}, x+u_2)$ are not orthogonal and define an overlapping integral S_{nk}^{12}. Another example can include hydrogen like basis sets with different charges and localization of nuclei.

Suppose that the eigenvalues E_n and eigenvectors $|\Psi_n\rangle$ of the stationary Schrödinger equation need to be found: $\mathsf{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$, $n = 0, 1, \ldots$. Let us take the state vector $|\Psi_n\rangle$ with the corresponding eigenvalue E_n and expand this state vector in a complete basis $|\psi_k(\nu_n^i)\rangle$

$$|\Psi_n\rangle = |\psi_n(\nu_n^i)\rangle + \sum_{k\neq n} C_{nk}|\psi_k(\nu_n^i)\rangle. \tag{2}$$

Here we set the index $\alpha = n$ in order to highlight that for different state vectors $|\Psi_n\rangle$ the parameters can be different. In addition, the state vector $|\Psi_n\rangle$ is normalized as $\langle\Psi_n|\psi_n(\nu_n^i)\rangle = 1$. By plugging Eq. (2) into the Schödinger equation and projecting on the state vector $|\psi_n(\nu_n^i)\rangle$ and $|\psi_l(\nu_n^i)\rangle$, $l \neq n$ one obtains the system of nonlinear equations for the determination of the energy E_n and coefficients C_{nk}, $k \neq n$:

$$E_n = H_{nn}(\nu_n^i) + \sum_{k\neq n} C_{nk} H_{nk}(\nu_n^i), \tag{3}$$

$$C_{nk} = \left[E_n - H_{kk}(\nu_n^i)\right]^{-1} \left[H_{kn}(\nu_n^i) + \sum_{l\neq n\neq k} C_{nl} H_{kl}(\nu_n^i)\right], \quad k \neq n, \tag{4}$$

where $H_{nk}(\nu_n^i) \equiv \langle\psi_n(\nu_n^i)|\mathsf{H}|\psi_k(\nu_n^i)\rangle$.

We stress here that the system of equations (3), (4) is completely equivalent to the original Schrödinger equation. Moreover, the system of equations for the determination of the energy level E_n is completely decoupled from the system of equations for the energy level $E_{n'}$, $n \neq n'$. This should not be confused with the Galerkin method [56], where the Hamiltonian of the system is written in a certain basis and the energy levels are determined as all eigenvalues of the system of N linear equations $\sum_k (H_{nk} - E_n\delta_{nk})C_{nk} = 0$. Instead in our case we have the system of nonlinear equations for any given energy level and in order to determine N eigenvalues one needs to solve N nonlinear systems of equations.

By construction of the system of equations (3), (4) we can employ the different parameters ν_n^i and $\nu_{n'}^i$ when seeking different eigenvalues E_n and $E_{n'}$. This of course requires the recalculation of the matrix elements. For example, imagine that the Hamiltonian in a certain single-parametric basis is represented as a 3×3 matrix. In order to determine the energy level E_0 one employs parameter ν_0 for the calculation of the matrix elements and obtains the system of equations for three unknowns, namely E_0, C_{01} and C_{02}. However, in order to calculate the energy level E_1 one can employ a different parameter $\nu_1 \neq \nu_0$ and obtain a system of equations for E_1, C_{10} and C_{12} in which the matrix element $H_{10}(\nu_1) \neq H_{01}^*(\nu_0)$, since $\nu_1 \neq \nu_0$.

In addition, we mention here that if one can solve the system of Eqs. (3), (4) exactly then the choice of the parameters is not important. In practice, however, it is either very complicated or impossible to solve the system of Eqs. (3), (4) exactly. Consequently, one seeks for an approximate solution. It is exactly here, when the different values of parameters come to hand and become very effective. The idea of our approach consists in adjusting the parameters in a way that the diagonal element of the Hamiltonian $H_{nn}(\nu_n^i)$ becomes the best possible approximation for the eigenvalue E_n. As an example, let us examine the case when the Hamiltonian is represented as 3×3 matrix in a basis which depends on two parameters ν_n^1 and ν_n^2, $n = 0, 1, 2$. If one fixes the parameters ν_0^1 and ν_0^2 from the system of equations

$$H_{01}(\nu_0^1, \nu_0^2) = 0, \quad H_{02}(\nu_0^1, \nu_0^2) = 0,$$

then the energy E_0 is simply given as the diagonal matrix element $H_{00}(\nu_0^1, \nu_0^2)$. Consequently, one can repeat this procedure for E_1 and E_2 and obtain these energy levels as the corresponding diagonal entities of the Hamiltonian $H_{11}(\nu_1^1, \nu_1^2)$, $H_{22}(\nu_2^1, \nu_2^2)$ calculated with the corresponding parameters, found from the vanishing matrix elements.

In reality, the Hamiltonian of the system in an s-parametric basis is represented via an infinitely dimen-

sional matrix and consequently one can make equal to zero only s matrix elements. The remaining contributions due to the non-vanishing matrix elements should be taken into account via Eqs. (3), (4). However, if the diagonal entity of the Hamiltonian $H_{nn}(\nu_n^i)$ with this choice of parameters provides a good approximation for the exact eigenvalue E_n, then the corrections due to the off-diagonal elements can be taken into account perturbatively, via the iteration scheme (see Refs. [54, 55]).

The main advantage of the above described approach is in fact that if the matrix elements can be evaluated analytically, then instead of the solution of the differential equation one employs a root search algorithm for the determination of the values of the parameters. This procedure was successfully applied to a variety of problems with Hermitian Hamiltonians, for example, one dimensional problems [54] including the anharmonic oscillator [55], the quantum Rabi model [57], the polaron problem [58] and scalar quantum field theory [59]. In addition it was recently employed for multi-electron atoms [60], which provided an analytic approximation for their energy levels with a relative accuracy of 5% for the whole periodic table.

The quantum anharmonic oscillator example. — For example, for the quantum anharmonic oscillator with the Hamiltonian:

$$\mathsf{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + \lambda x^4, \quad \lambda > 0, \tag{5}$$

the approximate solution can be found completely analytically. One employs the single-parametric harmonic oscillator wave functions $y_n(\omega_n, x)$ with the frequency ω_n and finds non-vanishing matrix elements

$$\begin{aligned} H_{nn}(\omega_n) &= \frac{1}{4\omega_n}(\omega_n^2+1)(1+2n) + \frac{3\lambda}{4\omega_n^2}(1+2n+2n^2), \\ H_{nk}(\omega_n) &= H_{kn}(\omega_n) = \frac{1}{4}\sqrt{(n+1)(n+2)}\left(\frac{1-\omega_n^2}{\omega_n} + \frac{2\lambda}{\omega_n^2}(2n+3)\right)\delta_{n+2,k} + \frac{\lambda}{4\omega_n^2}\sqrt{\frac{(n+4)!}{n!}}\delta_{n+4,k}. \end{aligned} \tag{6}$$

Since we introduced the single-parametric basis, we can make equal to zero only a single matrix element. The closest matrix element for a given state n is $H_{n,n+2}$. Consequently, from the condition $H_{n,n+2} = 0$ one trivially finds the equation for ω_n

$$\omega_n^3 - \omega_n - 2\lambda(2n+3) = 0. \tag{7}$$

From here, the energy levels of the anharmonic oscillator are defined through $E_n = H_{nn}(\omega_n)$, where ω_n is defined by Eq. (7). Interesting enough this provides a uniform approximation for different n and λ. Compare the exact solution with this simple analytical result (see Table I).

E_n^{Analytic} (E_n^{Exact})	λ 0.1	1	10	100
$n=0$	0.5603	0.8125	1.5313	3.1924
	(0.5591)	(0.8038)	(1.5050)	(3.1314)
$n=10$	17.3748	32.9931	68.9367	147.515
	(17.3519)	(32.9333)	(68.8037)	(147.227)
$n=40$	96.0745	195.865	416.735	895.387
	(95.5602)	(194.602)	(413.938)	(889.325)

Table I. Comparison of the eigenvalues for the anharmonic oscillator with the Hamiltonian (5) obtained through the analytic approximation with the ones calculated numerically via the Arnoldi iteration.

In addition, we mention here that the standard perturbation theory series for any $\lambda \neq 0$ has zero radius of convergence [3].

Application to the family of $\mathcal{PT}$-symmetric Hamiltonians (1). — Here, we apply this approach for the determination of an analytic approximation for the eigenvalues of non-Hermitian Hamiltonian (1), following the steps outlined below.

First, we introduce a basis. Since for $\epsilon = 0$ the exact solution of the problem is known, it is quite natural to employ a complete and orthogonal harmonic oscillator basis, which has a single quantum number n and frequency ω. It is well known that in order to perform the exact diagonalization of the Hamiltonian $\mathsf{H} = -d^2/dx^2 + x^2 + x$ one needs to shift the equilibrium position of the harmonic oscillator. In addition, for $\epsilon = 2$ the Hamiltonian (1) is equivalent [4] to $\mathsf{H} = -d^2/dx^2 + 4x^4 - 2x$, which has also linear x term. For this reason, we assume that our basis should have shifted equilibrium position. Moreover, as we are dealing with the non-Hermitian Hamiltonians the equilibrium position can be shifted into the complex plane, i.e., $x \to x + \mathrm{i}u$. This should not be confused with the complex scaling method [61, 62], when the rotation of the integration contour is performed, i.e., $x \to x\exp(\mathrm{i}\theta)$. Thus, we arrive to the two parametric harmonic oscillator basis

$$y_n(\omega_n, u_n, x) = \sqrt[4]{\frac{\omega_n}{\pi}}\frac{1}{\sqrt{2^n n!}}\exp\left(-\frac{\omega_n}{2}(x+\mathrm{i}u_n)^2\right) \times H_n(\sqrt{\omega_n}(x+\mathrm{i}u_n)). \tag{8}$$

Here $H_n(x)$ is the Hermitian polynomial and we have ω_n and u_n as parameters, which can be different for different states. For this reason, we denoted them with the index n. Consequently, the states with different n can have different ω_n or u_n and can be non-orthogonal.

Second, our basis functions contain only two free parameters and therefore, by adjusting them only two matrix elements, for a given energy level, can be made equal to zero. The remaining matrix elements should be taken into account by means of the iteration scheme of Refs. [54, 55]. However, since we are looking for simple analytical expressions for eigenvalues we limit ourselves only to the zeroth-order approximation and disregard the contributions due to the remaining off-diagonal elements. We consider that the final answer justifies this approximation.

Third, the scalar product for the calculation of the matrix elements in the harmonic oscillator basis, with u_n and ω_n fixed and real, is defined in a $\mathcal{PT}$ symmetric way

$$(y_n, y_m) = \int_{-\infty}^{\infty} y_n^\star(x) y_m(x) dx = (-1)^n \delta_{nm}, \qquad (9)$$

$$y_n^\star(x) = \mathcal{PT} y_n(x) = y_n^*(-x) = (-1)^n y_n(x). \qquad (10)$$

The relation (10) follows from the fact that under operation of $\mathcal{PT}$-symmetry the argument of the function changes into $-(x+\mathrm{i}u)$, that the exponent has quadratic argument and the property of the Hermitian polynomials $H_n(-x) = (-1)^n H_n(x)$. The relation (9) follows from Eq. (10) and the orthogonality of harmonic oscillator wave functions.

Fourth, a simple evaluation of the expectation value of the Hamiltonian and the matrix elements in the harmonic oscillator basis with u_n and ω_n fixed and real yields

$$H_{nn}(\omega_n, u_n) = \frac{(y_n, Hy_n)}{(y_n, y_n)} = \frac{1}{2}\omega_n(2n+1) - \frac{1}{\omega_n^{(\epsilon+2)/2}} \frac{1}{\sqrt{\pi} 2^n n!} \int_{-\infty}^{\infty} e^{-(x+\mathrm{i}u_n)^2} H_n^2(x+\mathrm{i}u_n)(\mathrm{i}x)^{\epsilon+2} dx, \qquad (11)$$

$$H_{nk}(\omega_n, u_n) = (-1)^n \Bigg(-\frac{\omega_n}{2}\sqrt{n(n-1)}\delta_{k,n-2} - \frac{\omega_n}{2}\sqrt{(n+1)(n+2)}\delta_{k,n+2} - \frac{1}{\omega_n^{(\epsilon+2)/2}} \frac{1}{\sqrt{\pi}\sqrt{2^n n! 2^k k!}} \int_{-\infty}^{\infty} e^{-(x+\mathrm{i}u_n)^2} H_n(x+\mathrm{i}u_n) H_k(x+\mathrm{i}u_n)(\mathrm{i}x)^{\epsilon+2} dx \Bigg), \quad k \neq n. \qquad (12)$$

Moreover, the integrals in Eqs. (11-12) can be evaluated analytically and are expressed through the parabolic cylinder special functions $D_\nu(x)$ [63]. This is achieved with the help of the following integral [64]

$$\int_{-\infty}^{\infty} (\mathrm{i}x)^\nu e^{-\beta^2 x^2 - \mathrm{i}qx} dx = 2^{-\frac{\nu}{2}} \sqrt{\pi} \beta^{-\nu-1} \exp\left(-\frac{q^2}{8\beta^2}\right) D_\nu\left(\frac{q}{\beta\sqrt{2}}\right), \qquad (13)$$

where $\mathrm{Re}\,\beta > 0$ and $\nu > -1$. For example, when $n = 0$ and $k = 1$ we get

$$H_{00}(\omega_0, u_0) = \frac{\omega_0}{2} - \frac{e^{u_0^2/2} 2^{-\frac{\epsilon+2}{2}}}{\omega_0^{(\epsilon+2)/2}} D_{\epsilon+2}(\sqrt{2}u_0) \qquad (14)$$

and

$$H_{01}(\omega_0, u_0) = \frac{\mathrm{i} e^{\frac{u_0^2}{2}} 2^{-\frac{\epsilon+4}{2}}}{\omega_0^{(\epsilon+2)/2}} \Big(D_{\epsilon+3}(\sqrt{2}u_0) - \sqrt{2}u_0 D_{\epsilon+2}(\sqrt{2}u_0) \Big). \qquad (15)$$

Fifth, according to the above described calculation scheme for the Hermitian case the parameters ω_n and u_n are determined from the condition that the nearest matrix elements are vanishing. Since we have only two parameters, only two matrix elements can be made equal to zero. In the case of Eqs. (11), (12) the nearest matrix elements are $H_{n,n+1}(\omega_n, u_n)$ and $H_{n,n+2}(\omega_n, u_n)$. The solution of the system of equations

$$\begin{cases} H_{n,n+1}(\omega_n, u_n) = 0 \\ H_{n,n+2}(\omega_n, u_n) = 0 \end{cases} \qquad (16)$$

gives ω_n and u_n. The equation for ω_n can be solved explicitly which yields

$$\omega_n = \left(-\frac{1}{\sqrt{\pi} 2^n n! (n+1)(n+2)} \int_{-\infty}^{\infty} e^{-(x+\mathrm{i}u_n)^2} H_n(x+\mathrm{i}u_n) H_{n+2}(x+\mathrm{i}u_n)(\mathrm{i}x)^{\epsilon+2} dx \right)^{\frac{2}{\epsilon+4}}, \qquad (17)$$

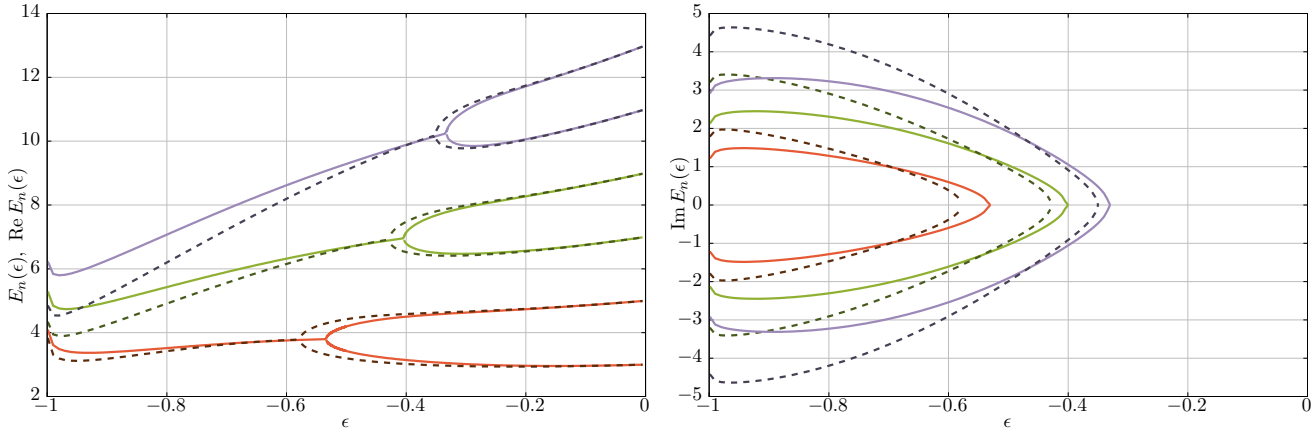

Figure 2. (Color online) The dependence of the eigenvalues E_n, their real and imaginary parts on the parameter ϵ, in the region $-1 < \epsilon \leq 0$. The dashed lines are the exact numerical solutions via the Arnoldi iteration. The solid lines are the analytic approximation via Eq. (19). After the point at $\epsilon = \epsilon_{\text{branching point}}$, where two energy level coalesce they appear as complex conjugate pairs, whose real parts together with the real energy levels are plotted on the left pane and imaginary parts on the right pane respectively.

while the values of u_n are determined as the roots of the function $g(u_n)$

$$g(u_n) = \frac{1}{\sqrt{\pi} 2^n n!} \frac{1}{\sqrt{2(n+1)}} \int_{-\infty}^{\infty} e^{-(x+\mathrm{i}u_n)^2} H_n(x+\mathrm{i}u_n) H_{n+1}(x+\mathrm{i}u_n)(\mathrm{i}x)^{\epsilon+2} dx, \quad \Rightarrow g(u_n) = 0 \quad \Rightarrow u_n, \tag{18}$$

We also add here that for integer values of ϵ the roots of the function $g(u_n)$ can be found exactly, as the parabolic cylinder functions are expressed through polynomials. This yields either quadratic or biquadratic equations for u_n. For other values of ϵ the numerical search for roots was employed.

Sixth, the previous analysis demonstrates [1] that when $\epsilon < -0.57793$ all energy levels except of the ground state coalesce. For this reason, in the vicinity of the exceptional points expression (3) in not applicable as is in the zeroth-order approximation and should be modified as in the perturbation theory case for the doubly degenerate levels [65]. An analogous linear combinations of multiple energy levels were also employed in magnetohydrodynamics [66], $\mathcal{PT}$-symmetric Bose-Hubbard model [67] and models of multiple coupled wave guides [68, 69].

Consequently, we form a linear combination of odd $n = 1, 3, 5, \ldots$ and even $n = 2, 4, 6, \ldots$ states instead. Being precise, we mixed $(1, 2)$, $(3, 4)$, $\ldots$ states. Then the energy levels are determined from the system of linear equations [65]

$$E_{1,2} = \frac{1}{2}(H_{11}(\omega_n, u_n) + H_{22}(\omega_n, u_n)) \pm \frac{1}{2}\sqrt{(H_{11}(\omega_n, u_n) - H_{22}(\omega_n, u_n))^2 + 4H_{12}^2(\omega_n, u_n)}. \tag{19}$$

Here H_{11} is the expectation value for the odd states, H_{22} for the even states and H_{12} is the matrix element between the odd and the even states. We pay attention here that due to the $\mathcal{PT}$-symmetric definition of the scalar product the square of the matrix element but not the square of the absolute value appears under the square root in Eq. (19). Since the matrix element between the odd and the even states in this case can not be equal to zero, we choose u_n and ω_n from the vanishing $H_{(2n+2),(2n+3)}$ and $H_{(2n+2),(2n+4)}$, $n = 0, 1, \ldots$ correspondingly.

In addition, Eq. (19) explains the appearances of square root singularities [3] for non-Hermitian Hamiltonians. In the non-Hermitian case the expression under the square root can vanish, thus leading to branching points at $\epsilon = \epsilon_{\text{branching point}}$. For $\epsilon < \epsilon_{\text{branching point}}$ the energy levels coalesce and become complex conjugate pairs (see also Ref. [52]).

Results and discussion. — In Fig. 1 we compare the

ϵ	n	E_{exact}	E_{analytic}	E_{WKB}	ϵ	n	E_{exact}	E_{analytic}	E_{WKB}
1	0	1.156	1.126	1.094	2	0	1.477	1.363	1.377
	1	4.109	4.138	4.089		1	6.003	6.104	5.956
	2	7.562	7.573	7.549		2	11.802	11.876	11.769
	3	11.314	11.290	11.304		3	18.459	18.417	18.432
	4	15.292	15.222	15.283		4	25.792	25.583	25.769
	5	19.452	19.332	19.444		5	33.694	33.284	33.675
	6	23.767	23.592	23.761		6	42.094	41.453	42.076
	7	28.176	27.985	28.212		7	50.937	50.044	50.921
	8	32.789	32.496	32.784		8	60.184	59.015	60.170

Table II. Comparison of the eigenvalues obtained through our analytic approximation E_{analytic} with the ones calculated numerically via the Arnoldi iteration E_{exact} and quasi-classical WKB approximation E_{WKB} [4].

exact numerical solution with the one obtained by the implementation of the above mentioned steps 1-6. As follows from the figure the agreement between analytical and numerical solutions is remarkable. In Table II we provide the numerical values of our analytic approximation, the exact numerical solution and the quasi-classical WKB approximation [4] for some selected values of ϵ. We also remind that the quasi-classical WKB approximation was found only for $\epsilon > 0$. In Fig. 2 we demonstrate that after the branching point the energy levels coalesce and become complex conjugate pairs.

The results of our paper demonstrate that the suggested algorithm based on the solution of the system of Eqs. (3), (4) is very effective for obtaining a good approximation for eigenvalues of $\mathcal{PT}$ symmetric Hamiltonians. Everything is reduced to the calculation of integrals, which define the matrix elements of the Hamiltonian operator. Consequently, our results could be especially important for quantum field theory and many-dimensional cases when the numerical solution of differential equations becomes problematic (in the Hermitian case please see Refs. [54] and [57–59]). It is also important to stress that the good approximation for the eigenvalues of localized states for the Hamiltonian (1) is mainly defined not by the exact asymptotic behavior of the wave functions $\sim \exp\left(-a|x|^{(\epsilon+4)/2}\right)$ but rather by the correct positions around which they are localized together with the widths of their maxima. In our case these are the parameters u and ω respectively.

Finally, since our zeroth-order approximation provides a very good accuracy we can assume that the iteration scheme of Refs. [54, 55] may be employed for the incorporation of corrections due to the off-diagonal matrix elements, thus offering a regular way to improve the zeroth-order approximation.

Outlook. — There is a current interest [52] in the determination of the eigenvalues when $\epsilon < -1$. Consequently, we have tested the suggested approach for $-1.05 \le \epsilon < -1$. For this we also applied Eq. (19), in which, however, we have mixed the odd and the even states in a different order. In this case we mixed $(0,1)$, $(2,3)$, ... states. The parameters ω_n and u_n were chosen from the condition that the matrix elements $H_{n+1,n+2}$ and $H_{n+1,n+3}$, $n = 0, 1, \ldots$ are vanishing.

In Fig. 3 we plot the dependence of the real and imaginary parts of eigenvalues on the parameter ϵ, in the region $-1.05 \le \epsilon < -0.95$. By observing the figure we can conclude that all qualitative peculiarities of the system behavior are reproduced, however the accuracy of the results is somewhat worse, than for $\epsilon > -1$. Consequently, we suggest to employ the iteration scheme of Ref. [54, 55] in this case. In addition, one can try to introduce the third parameter α_n in the state function. Indeed, the choice of the basis functions $y_n(\alpha_n, \omega_n, u_n, x) = \exp(\mathrm{i}\alpha_n x) y_n(\omega_n, u_n, x)$ still allows to evaluate all matrix elements analytically, however, Eqs. (3) and (4) should be generalized for the non-orthogonal basis [59]. The latter is motivated by the $\mathcal{PT}$-symmetric definition of the scalar product, since in this case the phase of the wave function becomes important.

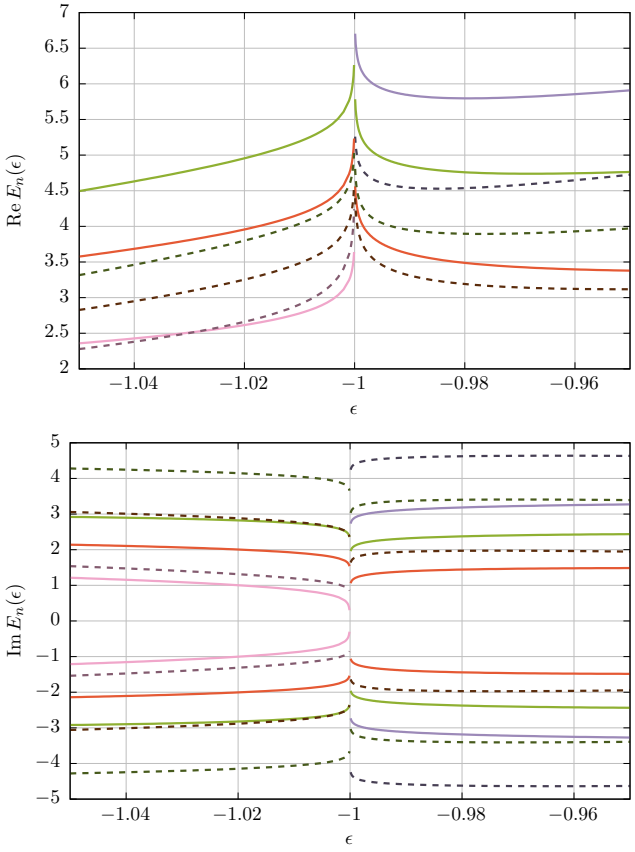

Figure 3. (Color online) The dependence of the real and imaginary parts of eigenvalues on the parameter ϵ, in the region $-1.05 \le \epsilon < -0.95$. The dashed lines are the exact numerical solutions via the Arnoldi iteration. The solid lines are the analytic approximation via Eq. (19) in which the states $(0,1)$, $(2,3)$, ... were mixed.

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