Comment on 'Numerical estimates of the spectrum for anharmonic PT symmetric potentials'

2013 Phys. Scr. 87 047001

(http://iopscience.iop.org/1402-4896/87/4/047001)

IOP Publishing | Physica Scripta
Phys. Scr. **87** (2013) 047001 (3pp) doi:10.1088/0031-8949/87/04/047001

COMMENT

Comment on 'Numerical estimates of the spectrum for anharmonic PT symmetric potentials'

Paolo Amore[1] **and Francisco M Fernández**[2]

[1] Facultad de Ciencias, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Colima, Mexico
[2] INIFTA (UNLP, CCT La Plata-CONICET), División Química Teórica, Boulevard 113 S/N, Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina

E-mail: paolo.amore@gmail.com and fernande@quimica.unlp.edu.ar

Received 26 September 2012
Accepted for publication 20 February 2013
Published 8 March 2013
Online at stacks.iop.org/PhysScr/87/047001

Abstract
We show that the authors of the commented paper (Bowen *et al* 2012 *Phys. Scr.* **85** 065005) draw their conclusions from the eigenvalues of truncated Hamiltonian matrices that do not converge as the matrix dimension increases. In some of the studied examples, the authors missed the real positive eigenvalues that already converge towards the exact eigenvalues of the non-Hermitian operators and focused their attention on the complex ones that do not. We also show that the authors misread Bender's argument about the eigenvalues of the harmonic oscillator with boundary conditions in the complex-x plane (Bender 2007 *Rep. Prog. Phys.* **70** 947).

PACS numbers: 03.65.Ge, 03.65.−w, 11.30.Er

1. Introduction

In a recent paper, Bowen *et al* [1] discussed the spectra of a class of non-Hermitian Hamiltonians having parity–time (PT) symmetry. They calculated the eigenvalues of truncated matrices for the non-Hermitian Hamiltonian operators in the basis set of the eigenfunctions of the harmonic oscillator and argued that their results did not agree with those of Bender and Boettcher [2]. They concluded that the discrepancy may be due to the fact that the Wentzel–Kramers–Brillouin (WKB) method used by the latter authors is unsuitable for such problems. For example, they stated, 'It is certainly not obvious that the physical conditions of the Bohr–Sommerfeld procedure should be valid for this non-physical path. The significant differences in the spectrum studied in this paper suggests that it is not valid' and also stated, 'It is not clear whether the motion along paths in the complex plane has any physical significance for quantization'. Curiously, the authors did not appear to pay attention to other methods for the calculation of the eigenvalues of those PT-symmetric Hamiltonians. For example, the WKB results were confirmed by numerical integration based on the Runge–Kutta (RK) algorithm [2, 3] as well as by diagonalization of a truncated Hamiltonian matrix in the basis set of harmonic-oscillator eigenfunctions [2] (a more detailed description of this approach was given in an earlier version of the paper [4]). In addition, Handy [5] and Handy and Wang [6] obtained accurate upper and lower bounds from the moments equations.

The results, conclusions and criticisms of Bowen *et al* [1] are at variance with all that has been established after several years of study in the field of non-Hermitian PT-symmetric Hamiltonians [3]. The purpose of this comment is to analyse their calculations to verify if such criticisms are well founded. In section 2, we briefly review the diagonalization method (DM) used by the authors, and in section 3, we analyse some of the models used by the authors to draw their conclusions; finally, in section 4, we summarize the main results and draw our own conclusions.

2. The method

Bowen *et al* [1] calculated the eigenvalues of the class of Hamiltonian operators

$$H = p^2 + sx^N \tag{1}$$

for $s = 1, -1, \mathrm{i}$ and $N = 2, 3, 4, 6, 8$. They resorted to matrix representations of the operators in the basis set of eigenfunctions $\{|n\rangle, n = 0, 1, \ldots\}$ of the harmonic oscillator ($s = 1$, $N = 2$) and diagonalized truncated Hamiltonian matrices $\mathbf{H}^{(M)} = (H_{mn})_{m,n=0}^{M-1}$, where $H_{mn} = \langle m|\, H\, |n\rangle$, for each of those cases. If the eigenvalues of the truncated matrices converge as M increases, then the limits of those sequences approach the eigenvalues of the operator (1).

The characteristic polynomial for the matrix $\mathbf{H}^{(M)}$ will exhibit M roots $W_n^{(M)}$, $n = 0, 1, \ldots, M-1$. In the case of Hermitian operators (for example, $s = 1$ and N even) all those roots are real because the matrix is Hermitian. This is not the case with the non-Hermitian operators. Furthermore, in the case of the Hermitian operators we know that the eigenvalues of the matrix approach the eigenvalues E_n of the operator from above $W_n^{(M)} > W_n^{(M+1)} > E_n$. On the other hand, there is no such variational principle in the case of non-Hermitian operators. Obviously, one has to be very careful when applying the DM to non-Hermitian operators. Bender and Weir [7] recently discussed an efficient application of the DM to one-, two- and three-dimensional PT-symmetric oscillators. The calculation of a great number of eigenvalues for such models is facilitated by the fact that the Hamiltonian matrices in the basis set of harmonic-oscillator eigenfunctions are sparse. In what follows, we discuss some of the examples chosen by Bowen *et al* [1].

3. Examples

3.1. Case $N = 2$

When $s = 1$ the matrix $\mathbf{H}$ is diagonal and yields the eigenvalues of the harmonic oscillator exactly: $E_n = 2n + 1$, $n = 0, 1, \ldots$. On the other hand, for $s = -1$ the eigenvalues of the matrix do not converge as M increases. Therefore, they are meaningless and bear no relation to the eigenvalues of the Hamiltonian $H = p^2 - x^2$. Surprisingly, the authors argued, 'This Hamiltonian has a spectrum with odd symmetry about zero energy'. If one solves the eigenvalue equation with the appropriate boundary conditions in the complex-x plane, one obtains purely imaginary eigenvalues: $E_n = \pm(2n+1)\mathrm{i}$.

The authors went even further and stated, 'Bender has also asserted that the spectrum of the simple harmonic oscillator (SHO) ($r = 0$) with a negative force constant has a discrete negative spectrum that is the negative of the positive force constant SHO; that is, $E_n = -\hbar\omega(n + 1/2)$'. However, Bender [3] never drew such a wrong conclusion. He discussed the harmonic oscillator $H = p^2 + \omega^2 x^2$ with eigenvalues $E_n(\omega) = (2n+1)\omega$ and eigenfunctions $\psi_n(\omega, x)$. The eigenfunctions behave asymptotically as $\psi_n(\omega, x) \sim \mathrm{e}^{-\omega x^2/2}$ when $|x| \to \infty$. If we substitute $-\omega$ for ω the eigenvalues change sign but the eigenfunctions are no longer square integrable. However, if we rotate the variable $\pi/2$ counterclockwise, then the resulting eigenfunction $\varphi_n(\omega, q) = \psi_n(-\omega, \mathrm{i}q)$ is square integrable. It is quite obvious that the substitution of $-\omega$ for ω changes the sign of the eigenvalues, but the force constant ($\propto \omega^2$) does not change. In fact, Bender [3] states, 'Notice that under the rotation that replaces ω by $-\omega$ the Hamiltonian remains invariant, and yet the signs of the eigenvalues are reversed!'. Therefore, it seems that Bowen *et al* [1] misread Bender's argument.

3.2. Case $N = 3$

When $s = 1$ the eigenvalues of the truncated matrices do not converge as M increases. However, the authors state, 'Here the spectrum was almost symmetric about zero…', in spite of the fact that the roots of the secular determinants are not valid approximations to the eigenvalues of the differential operator.

The only interesting case is undoubtedly the PT-symmetric Hamiltonian operator for $s = \mathrm{i}$. According to the authors, 'The calculation of the spectrum for the potential $V = \mathrm{i}\,x^3$ yielded a complex spectrum'. In this case the wedges in the complex-x plane where $\psi(x)$ vanishes exponentially as $|x| \to \infty$ contain the real axis [2]. Therefore, one expects the DM to yield meaningful results. Our calculation shows that the complex eigenvalues of the truncated matrices do not converge as M increases, but there are real ones that certainly converge towards the results obtained by Bender and Boettcher [2] by means of the WKB method and numerical integration. In fact, Bender and Boettcher [2, 4] discussed the calculation of the eigenvalues by means of the DM (see also [7]). They concluded that the method is only useful when $1 < N < 4$ and that the convergence to the exact eigenvalues is slow and not monotonic because the Hamiltonians are not Hermitian. Table 1 shows the convergence of the lowest eigenvalues of the truncated matrices towards those obtained by means of the RK method and the WKB approach; they are real and positive as argued by Bender and Boettcher [4].

An interesting feature of the DM for non-Hermitian operators is that the characteristic polynomial of degree M does not exhibit M real roots as in the case of the Hermitian matrices. In the present case, the truncated matrices also exhibit many complex eigenvalues but they do not converge as M increases. Another interesting feature is the behaviour of the approximate eigenvalues with respect to a scaling factor. Instead of using the eigenfunctions $\psi_n(x) = \langle x|\, n\rangle$ of the harmonic oscillator $p^2 + x^2$, we can try an alternative calculation with the scaled eigenfunctions $\alpha^{1/2}\psi_n(\alpha x)$, where α is an adjustable scaling factor. In the case of Hermitian operators, $W_n^{(M)}(\alpha)$ exhibits a minimum because of the variational principle. On the other hand, in the case of the complex potential $V = \mathrm{i}\,x^3$ the approximate eigenvalue oscillates and exhibits a kind of plateau with oscillations of smaller amplitude. The optimal value of α is somewhere in this region. For example, we find that $\alpha \approx 1.4$ is more convenient than the scaling parameter $\alpha = 1$ used in the calculation shown in table 1. However, it is our purpose to show here only the results for the same basis set chosen by Bowen *et al* [1].

3.3. Case $N \geqslant 4$

Obviously, the DM yields real positive eigenvalues for $s = 1$ and N even; that is to say: for the trivial Hermitian

Table 1. First eigenvalues of the truncated matrices of dimension M for $V(x) = \mathrm{i}\,x^3$.

M	E_0	E_1	E_2	E_3
10	1.156 101 684	3.730 834 96	–	–
15	1.156 038 818	4.149 429 07	–	–
20	1.156 383 056	4.109 441 589	–	–
25	1.156 258 544	4.109 537 412	7.553 497 517	–
30	1.156 267 013	4.109 170 441	7.562 399 797	11.248 840 01
35	1.156 266 986	4.109 228 991	7.562 011 977	11.314 522 25
40	1.156 267 082	4.109 228 365	7.562 284 307	11.313 721 88
45	1.156 267 072	4.109 228 831	7.562 273 020	11.314 523 60
50	1.156 267 072	4.109 228 753	7.562 274 330	11.314 421 88
55	–	4.109 228 754	7.562 273 854	11.314 424 13
60	–	4.109 228 753	7.562 273 860	11.314 421 76
65	–	4.109 228 753	7.562 273 854	11.314 421 84
70	–	4.109 228 753	7.562 273 855	11.314 421 82
75	–	–	7.562 273 855	11.314 421 82
80	–	–	–	11.314 421 82
RK	1.156 267 072	4.109 228 752	7.562 273 854	11.314 421 818
WKB	1.0943	4.0895	7.5489	11.3043

operators. When $s = -1$ the eigenvalues of the truncated Hamiltonian matrices do not converge and, consequently, they are not eigenvalues of the Hamiltonian operator. The DM is not expected to yield the eigenvalues of the PT-symmetric oscillators when $s = \mathrm{i}$ and N is odd because the wedges in the complex-x plane where $\psi(x)$ vanishes exponentially as $|x| \to \infty$ do not contain the real axis [2]. However, the characteristic polynomials do exhibit real positive roots that converge as M increases. They are related to the complex resonances of the oscillators with $s = 1$ [8].

The PT-symmetric Hamiltonian operator $H = p^2 - x^4$ deserves special attention because it is isospectral to the Hermitian one $H = p^2 + 4x^4 - 2x$ [9, 10]. Apparently, Bowen *et al* [1] were not aware of this relationship which could have convinced them that the former Hamiltonian does already have a positive spectrum.

4. Conclusion

It is clear that the discrepancy between the results of Bowen *et al* [1] and Bender and Boettcher [2] is merely due to the fact that the DM used by the former authors does not apply to some of the problems studied. Their conclusions were based on eigenvalues of the Hamiltonian matrices that do not converge. They only obtained meaningful results for the trivial cases of Hermitian Hamiltonians given by $s = 1$ and N even. In the only other selected case where the DM is expected to yield reasonable results, namely $V(x) = \mathrm{i}\,x^3$ (and we may also add greater odd values of N), the authors failed to find the converging real positive roots and have simply focused on the complex ones that do not converge.

References

[1] Bowen S P, Mancini J D, Fessatidis V and Murawski R K 2012 *Phys. Scr.* **85** 065005

[2] Bender C M and Boeftcher S 1998 *Phys. Rev. Lett.* **80** 5243

[3] Bender C M 2007 *Rep. Prog. Phys.* **70** 947

[4] Bender C M and Boettcher S 1997 Real spectra in non-Hermitian Hamiltonians having PT symmetry arXiv:physics/9712001v1 [math-ph]

[5] Handy C R 2001 *J. Phys. A: Math. Gen.* **34** L271

[6] Handy C R and Wang X Q 2001 *J. Phys. A: Math. Gen.* **34** 8297

[7] Bender C M and Weir D J 2012 *J. Phys. A: Math. Theor.* **45** 425303

[8] Fernández F M and Garcia J 2013 On the eigenvalues of some non-Hermitian oscillators arXiv:1301.1676 [math-ph]

[9] Jones H F and Mateo J 2006 *Phys. Rev.* D **73** 085002

[10] Bender C M, Brody D C, Chen J-H, Jones H F, Milton K A and Ogilvie C M 2006 *Phys. Rev.* D **74** 025016