On the Eigenvalues of a Non-Hermitian Hamiltonian

Ebru Ergun

Department of Physics, Ankara University, 06100 Tandogan, Ankara, Turkey (e-mail: eergun@science.ankara.edu.tr)

Abstract: We study a 4 by 4 complex matrix Jacobi (tri-diagonal matrix) arised from a non-Hermitian discrete quantum system. Reality of the eigenvalues of the matrix in question is investigated.

Keywords: Discrete system, non-Hermitian, Jacobi matrix, eigenvalue.

1. INTRODUCTION

Some important problems of mathematical physics give rise to the consideration of non-Hermitian (non-selfadjoint) operators [3, 4, 8]. For the past ten years non-Hermitian Hamiltonians and complex extension of quantum mechanics have received a lot of attention, see review papers [2, 11]. It turned out that non-Hermitian operators having real eigenvalues (spectrum) can also be used in quantum mechanics. This motivates construction and investigation of non-Hermitian operators with real spectrum. Recently the author considered in [5] the following discrete non-Hermitian problem:

$$-\Delta^2 y_{n-1} + q_n y_n = \lambda \rho_n y_n, \tag{1}$$

$$n \in \Omega = \{-M, \dots, -2, -1\} \cup \{2, 3, \dots, N\},$$

$$y_{-1} = y_1, \quad \Delta y_{-1} = e^{2i\delta} \Delta y_1, \tag{2}$$

$$y_{-M-1} = y_{N+1} = 0, \tag{3}$$

where $M \geq 1$ and $N \geq 2$ are some fixed integers, $(y_n)_{n=-M-1}^{N+1}$ is a desired solution, Δ is the forward difference operator defined by

$$\Delta y_n = y_{n+1} - y_n$$

(so that $\Delta^2 y_{n-1} = y_{n-1} - 2y_n + y_{n+1}$), the coefficients q_n are real numbers given for $n \in \Omega$, $\delta \in [0, \pi/2)$, and ρ_n are given for $n \in \Omega$ by

$$\rho_n = \begin{cases} e^{2i\delta} & \text{if} \quad n \leq -1, \\ e^{-2i\delta} & \text{if} \quad n \geq 2. \end{cases} \tag{4}$$

The problem (1)–(3) can be viewed as a discrete analogue of the real line equivalent of some continuous quantum systems on a complex contour examined in [1, 10]. The main distinguishing features of problem (1)–(3) are that it involves a complex-valued coefficient ρ_n of the form (4) and that transition conditions (impulse conditions) of the form (2) are presented which also involve a complex coefficient. Such a problem is non-Hermitian with respect to the usual inner product. In spite of this fact, the eigenvalues (spectrum) of problem (1)–(3) may be real.

The eigenvalue problem (1)–(3) can be reduced to investigation of the eigenvalues and eigenvectors of a complex Jacobi matrix (tri-diagonal matrix) and this matrix plays the role of a Hamiltonian.

The main question related to the problem (1)–(3), in which we are interested, is to find the conditions on q_n and δ under which the eigenvalues of this problem are all real. Solution of this problem for arbitrary M and N turns out to be rather complicated.

If $\delta = 0$, then the problem (1)–(3) is selfadjoint (see [5]) and hence its eigenvalues are all real in this case. Further we will assume that $\delta \in (0, \pi/2)$. In [5] it is shown that if $M = 1$, $N = 2$ (2×2 matrix case), and $\delta \in (0, \pi/2)$, then the eigenvalues of problem (1)–(3) are all real if and only if

$$q_{-1} = 0, \; q_2 = -1, \; \text{and } \delta \in \left(0, \frac{\pi}{6}\right].$$

Moreover, under these conditions the eigenvalues are positive, distinct for $\delta \in (0, \pi/6)$ and equal to each other for $\delta = \pi/6$.

In [6], it is proved that if $M = 1$, $N = 3$ (3×3 matrix case), then the eigenvalues of problem (1)–(3) are all real if and only if

$$a - 1 = b + c, \tag{5}$$

$$b + c - 1 + 2(bc - 1)\cos 2\delta = 0, \tag{6}$$

$$(b + c)(bc - 1) + 2(bc - c - 1)\cos 2\delta = 0, \tag{7}$$

$$\alpha^2\beta^2 - 4\beta^3 - 27\gamma^2 - 4\alpha^3\gamma + 18\alpha\beta\gamma \geq 0, \tag{8}$$

where

$$\alpha = -1 - 2(b + c)\cos 2\delta, \tag{9}$$

$$\beta = (b + c)^2 - bc + 1, \quad \gamma = bc - c - 1, \tag{10}$$

$$a = 2 + q_{-1}, \quad b = 2 + q_2, \quad c = 2 + q_3. \tag{11}$$

In the present paper, we investigate reality of the eigenvalues of problem (1)–(3) in the case $M = 2$ and $N = 3$ (4×4 matrix case).

2. THE 3 BY 3 CASE

For the completeness, in this section following [6] we prove that conditions (5)–(8) are necessary and sufficient for the reality of all eigenvalues of the matrix

$$A = \begin{bmatrix} 1 + (a-1)e^{-2i\delta} & -1 & 0 \\ -e^{2i\delta} & be^{2i\delta} & -e^{2i\delta} \\ 0 & -e^{2i\delta} & ce^{2i\delta} \end{bmatrix}. \tag{12}$$

Note that the eigenvalues of problem (1)–(3) in the case $M = 1$ and $N = 3$ coincide with the eigenvalues of the

3×3 matrix A given in (12), where a, b, and c are real numbers defined by (11).

First we prove the necessity of conditions (5)–(8). Assume that the eigenvalues of the matrix A are all real. The eigenvalues of the matrix A coincide with the roots of the characteristic equation

$$\det(A - \lambda I_3) = 0$$

that is

$$\lambda^3 - [1 + (a-1)e^{-2i\delta} + (b+c)e^{2i\delta}]\lambda^2$$
$$+[(a-1)(b+c) + (b+c-1)e^{2i\delta} + (bc-1)e^{4i\delta}]\lambda$$
$$-(a-1)(bc-1)e^{2i\delta} - (bc-c-1)e^{4i\delta} = 0. \tag{13}$$

Denote the roots of equation (13) by λ_1, λ_2, and λ_3. By well-known relations between the roots and the coefficients of a polynomial, we have

$$\lambda_1 + \lambda_2 + \lambda_3 = 1 + (a-1)e^{-2i\delta} + (b+c)e^{2i\delta},$$
$$\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 = (a-1)(b+c)$$
$$+(b+c-1)e^{2i\delta} + (bc-1)e^{4i\delta},$$
$$\lambda_1\lambda_2\lambda_3 = (a-1)(bc-1)e^{2i\delta} + (bc-c-1)e^{4i\delta}.$$

If the roots λ_1, λ_2, and λ_3 are all real, then left-hand sides in the last three equations are real. Then the right-hand sides must also be real. This yields

$$(1-a+b+c)\sin 2\delta = 0, \tag{14}$$
$$(b+c-1)\sin 2\delta + (bc-1)\sin 4\delta = 0, \tag{15}$$
$$(a-1)(bc-1)\sin 2\delta + (bc-c-1)\sin 4\delta = 0. \tag{16}$$

Since $\sin 2\delta \neq 0$ for $\delta \in (0, \pi/2)$ and $\sin 4\delta = 2\sin 2\delta \cos 2\delta$, we get from (14)–(16),

$$1 - a + b + c = 0,$$
$$b + c - 1 + 2(bc-1)\cos 2\delta = 0,$$
$$(a-1)(bc-1) + 2(bc-c-1)\cos 2\delta = 0.$$

Therefore the necessity of conditions (5)–(7) is proved.

We will need the following known result (see, for example, [9]).

Proposition 1. Consider the cubic equation

$$\mu^3 + p\mu + q = 0 \tag{17}$$

with the real coefficients p and q. Let us put

$$D = -4p^3 - 27q^2 \tag{18}$$

that is called the discriminant of equation (17). Then:

(i) If $D < 0$, then equation (17) has one real root and two nonreal complex conjugate roots.
(ii) If $D = 0$, then all three roots of equation (17) are real and at least two of them are equal to each other.
(iii) If $D > 0$, then equation (17) has three distinct real roots.

If the eigenvalues of the matrix A are all real, then as we have shown the conditions (5)–(7) hold. Therefore, in this case the characteristic equation (13) takes the form

$$\lambda^3 - [1 + (a+b+c-1)\cos 2\delta]\lambda^2$$
$$+[(a-1)(b+c) + (b+c-1)\cos 2\delta + (bc-1)\cos 4\delta]\lambda$$
$$-(a-1)(bc-1)\cos 2\delta - (bc-c-1)\cos 4\delta = 0.$$

Using the identity $\cos 4\delta = 2\cos^2 2\delta - 1$ we can rewrite the last equation in the form

$$\lambda^3 - [1 + (a+b+c-1)\cos 2\delta]\lambda^2$$
$$+\{(a-1)(b+c) - bc + 1$$
$$+[b + c - 1 + 2(bc-1)\cos 2\delta]\cos 2\delta\}\lambda + bc - c - 1$$
$$-[(a-1)(bc-1) + 2(bc-c-1)\cos 2\delta]\cos 2\delta = 0.$$

Hence, taking into account (5)–(7), we get

$$\lambda^3 - [1 + 2(b+c)\cos 2\delta]\lambda^2$$
$$+[(b+c)^2 - bc + 1]\lambda + bc - c - 1 = 0. \tag{19}$$

Thus, if the eigenvalues of the matrix A defined in (12) are all real, then a, b, c, and δ must satisfy the necessary conditions (5)–(7) and the eigenvalues of A coincide with the roots of equation (19). Now we define α, β, and γ by (9), (10) and rewrite (19) in the form

$$\lambda^3 + \alpha\lambda^2 + \beta\lambda + \gamma = 0. \tag{20}$$

If we put

$$\lambda = \mu - \frac{\alpha}{3} \tag{21}$$

in (20), then we get the equation

$$\mu^3 + p\mu + q = 0 \tag{22}$$

which does not contain the term with μ^2, where

$$p = -\frac{1}{3}\alpha^2 + \beta, \tag{23}$$
$$q = \frac{2}{27}\alpha^3 - \frac{1}{3}\alpha\beta + \gamma. \tag{24}$$

Note that since a, b, c, and $\cos 2\delta$ are real, the numbers α, β, and γ defined by (9), (10) and hence the numbers p and q defined by (23), (24) are real. The roots of equations (20) and (22) are connected by equation (21). Therefore the reality of roots of equation (20) is equivalent to the reality of roots of equation (22). By Proposition 1, the roots of equation (22) are all real if and only if its discriminant D is non-negative. On the other hand, for this equation

$$D = -4p^3 - 27q^2$$
$$= -4\left(-\frac{1}{3}\alpha^2 + \beta\right)^3 - 27\left(\frac{2}{27}\alpha^3 - \frac{1}{3}\alpha\beta + \gamma\right)^2$$
$$= \alpha^2\beta^2 - 4\beta^3 - 27\gamma^2 - 4\alpha^3\gamma + 18\alpha\beta\gamma.$$

Therefore the necessity of the condition (8) is also proved.

Now we prove the sufficiency of the conditions (5)–(8). Thus assume that the conditions (5)–(8) are satisfied. We have to show that then the eigenvalues of the matrix A are all real. The eigenvalues of A coincide with the roots of equation (13). Under the conditions (5)–(7) equation (13) reduces to the equation (19). Further, in virtue of Proposition 1, the roots of equation (19) are all real under the condition (8) in which α, β, and γ are defined by (9), (10) The proof is completed.

Example 2. The conditions (5)–(7) in general are not sufficient for reality of the eigenvalues of A. Indeed, the numbers

$$a = \frac{3}{2}, \quad b = \frac{1}{2}, \quad c = 0, \quad \cos 2\delta = -\frac{1}{4}$$

satisfy the conditions (5)–(7). Next, for these numbers we have, according to (9), (10),

$$\alpha = -\frac{3}{4}, \quad \beta = \frac{5}{4}, \quad \gamma = -1,$$

and then according to (23), (24),

$$p = \frac{17}{16}, \quad q = -\frac{23}{32}.$$

Therefore

$$D = -4p^3 - 27q^2 < 0$$

and in virtue of Proposition 1 the roots of equation (22) and hence the eigenvalues of the matrix A are not all real.

It follows that, if at least one of the conditions (5)–(8) is not satisfied, then not all eigenvalues of the matrix A are real.

3. DERIVATION OF THE 4 BY 4 NON-HERMITIAN HAMILTONIAN

Since $\Delta^2 y_{n-1} = y_{n-1} - 2y_n + y_{n+1}$ and from the second condition in (2) we have

$$y_0 - y_{-1} = e^{2i\delta}(y_2 - y_1)$$

so that (taking into account $y_1 = y_{-1}$)

$$y_0 = y_{-1} + e^{2i\delta}(y_2 - y_1) = (1 - e^{2i\delta})y_{-1} + e^{2i\delta}y_2,$$

problem (1)–(3) can be written as

$$-y_{n-1} + v_n y_n - y_{n+1} = \lambda\rho_n y_n, \tag{25}$$
$$n \in \{-M, \dots, -2, -1\} \cup \{2, 3, \dots, N\},$$
$$y_0 = (1 - e^{2i\delta})y_{-1} + e^{2i\delta}y_2, \quad y_1 = y_{-1}, \tag{26}$$
$$y_{-M-1} = y_{N+1} = 0, \tag{27}$$

where

$$v_n = 2 + q_n, \tag{28}$$
$$n \in \{-M, \dots, -2, -1\} \cup \{2, 3, \dots, N\}.$$

In the case $M = 2$ and $N = 3$, problem (25)–(27) takes the form

$$-y_{n-1} + v_n y_n - y_{n+1} = \lambda\rho_n y_n, \ n \in \{-2, -1, 2, 3\},$$
$$y_0 = (1 - e^{2i\delta})y_{-1} + e^{2i\delta}y_2, \quad y_1 = y_{-1},$$
$$y_{-3} = y_4 = 0.$$

Hence

$$\left.\begin{array}{c} -y_{-3} + v_{-2}y_{-2} - y_{-1} = \lambda\rho_{-2}y_{-2} \\ -y_{-2} + v_{-1}y_{-1} - y_0 = \lambda\rho_{-1}y_{-1} \\ -y_1 + v_2 y_2 - y_3 = \lambda\rho_2 y_2 \\ -y_2 + v_3 y_3 - y_4 = \lambda\rho_3 y_3 \end{array}\right\}, \tag{29}$$

$$y_0 = (1 - e^{2i\delta})y_{-1} + e^{2i\delta}y_2, \quad y_1 = y_{-1}, \tag{30}$$
$$y_{-3} = y_4 = 0. \tag{31}$$

Substituting (30) and (31) into (29) and using the explicit expression (4) for ρ_n, we get

$$\left.\begin{array}{c} v_{-2}e^{-2i\delta}y_{-2} - e^{-2i\delta}y_{-1} = \lambda y_{-2} \\ -e^{-2i\delta}y_{-2} + [1 + (v_{-1} - 1)e^{-2i\delta}]y_{-1} - y_2 \\ = \lambda y_{-1} \\ -e^{2i\delta}y_{-1} + v_2 e^{2i\delta}y_2 - e^{2i\delta}y_3 = \lambda y_2 \\ -e^{2i\delta}y_2 + v_3 e^{2i\delta}y_3 = \lambda y_3. \end{array}\right\}. \tag{32}$$

Setting

$$v_{-2} = d, \quad v_{-1} = a, \quad v_2 = b, \quad v_3 = c,$$

$$A = \begin{bmatrix} de^{-2i\delta} & -e^{-2i\delta} & 0 & 0 \\ -e^{-2i\delta} & 1 + (a-1)e^{-2i\delta} & -1 & 0 \\ 0 & -e^{2i\delta} & be^{2i\delta} & -e^{2i\delta} \\ 0 & 0 & -e^{2i\delta} & ce^{2i\delta} \end{bmatrix}, \tag{33}$$

$$y = \begin{bmatrix} y_{-2} \\ y_{-1} \\ y_2 \\ y_3 \end{bmatrix},$$

we can write (32) in the form

$$Ay = \lambda y.$$

Thus, the eigenvalues of problem (1)–(3) in the case $M = 2$ and $N = 3$ coincide with the eigenvalues of the matrix A given in (33), where

$$d = v_{-2} = 2 + q_{-2}, \quad a = v_{-1} = 2 + q_{-1},$$
$$b = v_2 = 2 + q_2, \quad c = v_3 = 2 + q_3.$$

4. REALITY OF THE EIGENVALUES

Now we investigate conditions for reality of the eigenvalues of the matrix A defined in (33). The eigenvalues of the matrix A coincide with the roots of the characteristic equation

$$\det(A - \lambda I_4) = 0$$

that is

$$\lambda^4 + \alpha\lambda^3 + \beta\lambda^2 + \gamma\lambda + \theta = 0, \tag{34}$$

where

$$\alpha = -1 - (a - d - 1)e^{-2i\delta} - (b + c)e^{2i\delta},$$
$$\beta = de^{-2i\delta} + (ad - d - 1)e^{-4i\delta} + d(b + c)$$
$$+(a - 1)(b + c) + (b + c - 1)e^{2i\delta} + (bc - 1)e^{4i\delta},$$

$$\gamma = [-d(a - 1)(bc - 1) + b + c]e^{-2i\delta} - d(b + c - 1)$$
$$-(a + d - 1)(bc - 1)e^{2i\delta} - (bc - c - 1)e^{4i\delta},$$
$$\theta = (ad - d - 1)(bc - 1) + d(bc - c - 1)e^{2i\delta}.$$

If the roots of equation (34) are all real, then by well-known relations between the roots and the coefficents of a polynomial we get that the coefficients must be real. This gives the necessary conditions (for reality of the eigenvalues of A)

$$(a - b - c - d - 1)\sin 2\delta = 0,$$
$$(b + c - d - 1)\sin 2\delta + (bc - ad + d)\sin 4\delta = 0,$$
$$[-d(a - 1)(bc - 1) + b + c + (a + d - 1)(bc - 1)]\sin 2\delta$$
$$+(bc - c - 1)\sin 4\delta = 0,$$
$$d(bc - c - 1)\sin 2\delta = 0.$$

Since $\sin 2\delta \neq 0$ for $\delta \in (0, \pi/2)$ and $\sin 4\delta = 2\sin 2\delta\cos 2\delta$, we get from the last conditions that

$$a - b - c - d - 1 = 0,$$
$$b + c - d - 1 + 2(bc - ad + d)\cos 2\delta = 0,$$
$$-d(a - 1)(bc - 1) + b + c + (a + d - 1)(bc - 1)$$
$$+2(bc - c - 1)\cos 2\delta = 0,$$
$$d(bc - c - 1) = 0.$$

Then the coefficients α, β, γ, θ take the form

$$\alpha = -1 - (a + b + c - d - 1)\cos 2\delta, \tag{35}$$
$$\beta = d(b + c) + (a - 1)(b + c)$$
$$+(b + c + d - 1)\cos 2\delta + (ad + bc - d - 2)\cos 4\delta, \tag{36}$$
$$\gamma = -d(b + c - 1) - [d(a - 1)(bc - 1)$$
$$+(a + d - 1)(bc - 1) - b - c]\cos 2\delta - (bc - c - 1)\cos 4\delta, \tag{37}$$
$$\theta = (ad - d - 1)(bc - 1). \tag{38}$$

Thus, we have to investigate conditions for reality of roots of the fourth order polynomial equation (34) with the real coefficients given by formulas (35)–(38). This problem can be reduced to the case of third order polynomial equation (investigated in [6]; see also Section 2 above) as follows. First, if we make in (34) the change of variable

$$\lambda = \mu - \frac{\alpha}{4},$$

then we get an equation of the form

$$\mu^4 + p\mu^2 + q\mu + r = 0 \tag{39}$$

with the real coefficients p, q, r, which does not contain the term with μ^3. Next, using an auxiliary parameter t we can transform the left-hand side of this equation as follows:

$$\mu^4 + p\mu^2 + q\mu + r$$

$$= \left(\mu^2 + \frac{p}{2} + t\right)^2 + q\mu + r - \frac{p^2}{4} - t^2 - 2t\mu^2 - pt$$

$$= \left(\mu^2 + \frac{p}{2} + t\right)^2 - \left[2t\mu^2 - q\mu + \left(t^2 + pt - r + \frac{p^2}{4}\right)\right]. \qquad (40)$$

Choose now t so that the polynomial in μ standing in the brackets is a complete square. For this it must have a single double root, that is, the equality

$$q^2 - 4 \cdot 2t\left(t^2 + pt - r + \frac{p^2}{4}\right) = 0 \qquad (41)$$

must be held. The equality (41) is a cubic equation in t with real coefficients. Let t_0 be a real root of this equation. For $t = t_0$ the polynomial standing in the brackets in (40) has double root $q/(4t_0)$ and therefore equation (39) takes the form

$$\left(\mu^2 + \frac{p}{2} + t_0\right)^2 - 2t_0\left(\mu - \frac{q}{4t_0}\right)^2 = 0$$

which is splited into the two equations

$$\mu^2 - \sqrt{2t_0}\mu + \left(\frac{p}{2} + t_0 + \frac{q}{2\sqrt{2t_0}}\right) = 0, \qquad (42)$$

$$\mu^2 + \sqrt{2t_0}\mu + \left(\frac{p}{2} + t_0 - \frac{q}{2\sqrt{2t_0}}\right) = 0. \qquad (43)$$

Therefore the roots of equation (39) coincide with the roots of quadratic equations (42), (43).

ACKNOWLEDGEMENTS

This work was supported by Grant 109T032 from the Scientific and Technological Research Council of Turkey (TUBITAK).

REFERENCES

[1] C. M. Bender, S. Boettcher, Real spectra in non-Hermitian Hamiltonians having PT-symmetry, *Phys. Rev. Lett.* 80 (1998) 5243–5246.

[2] C. M. Bender, Making sense of non-Hermitian Hamiltonians, *Rep. Progr. Phys.* 70 (2007) 947–1018.

[3] E. B. Davies, Non-selfadjoint differential operators, *Bull. London Math. Soc.* 34 (2002) 513–532.

[4] C. I. Dolph, Recent developments in some non-selfadjoint problems of mathematical physics, *Bull. Amer. Math. Soc.* 67 (1961) 1–69.

[5] E. Ergun, On the reality of the spectrum of a non-Hermitian discrete Hamiltonian, *Rep. Math. Phys.* 63 (2009) 75–93.

[6] E. Ergun, E. Bairamov, On the eigenvalues of a 3 by 3 non-Hermitian Hamiltonian, *J. Math. Chem.* (2010). To appear.

[7] E. Ergun, On the spectrum of a discrete non-Hermitian quantum system, *Symmetry, Integrability and Geometry: Methods and Applications (SIGMA)*, 5 (2009), Paper 007, 24 pages.

[8] G. Sh. Guseinov, Inverse spectral problems for tridiagonal N by N complex Hamiltonians, *Symmetry, Integrability and Geometry: Methods and Applications (SIGMA)*, 5 (2009), Paper 018, 28 pages.

[9] A. Kurosh. *Higher Algebra*, Mir Publisher, Moscow, 1975.

[10] A. Mostafazadeh, Pseudo-Hermitian description of PT-symmetric systems defined on a complex contour, *J. Phys. A: Math. Gen.* 38 (2005) 3213–3234.

[11] A. Mostafazadeh, Pseudo-Hermitian quantum mechanics, *preprint ArXiv:* quant-ph/0810.5643 (2008).

[12] A. Mostafazadeh and A. Batal, Physical aspects of pseudo-Hermitian and PT-symmetric quantum mechanics, *J. Phys A: Math. Gen.* 37 (2004) 11645–11679.

[13] K. C. Shin, On the reality of the eigenvalues for a class of PT-symmetric oscillators, *Commun. Math. Phys.* 229 (2002) 543–564.

[14] M. Znojil, Matching method and exact solvability of discrete PT-symmetric square wells, *J. Phys. A: Math. Gen.* 39 (2006) 10247–10261.

[15] M. Znojil, Maximal couplings in PT-symmetric chain models with the real spectrum of energies, *J. Phys. A: Math. Theor.* 40 (2007) 4863–4875.

[16] M. Znojil, Tridiagonal PT-symmetric N by N Hamiltonians and fine-tuning of their observability domains in the strongly non-Hermitian regime, *J. Phys. A: Math. Theor.* 40 (2007) 13131–13148.

[17] M. Znojil, Complete set of inner products for a discrete PT-symmetric square-well Hamiltonian, *J. Math. Phys.* 50, 122105 (2009).