J Math Chem (2011) 49:609–617
DOI 10.1007/s10910-010-9767-2

ORIGINAL PAPER

On the eigenvalues of a 3 by 3 non-Hermitian Hamiltonian

Ebru Ergun · Elgiz Bairamov

Received: 18 July 2010 / Accepted: 20 October 2010 / Published online: 4 November 2010

Abstract In this paper, we are concerned with a 3×3 complex matrix Jacobi (tri-diagonal matrix) arised from a non-Hermitian discrete quantum system. Necessary and sufficient conditions for reality of the eigenvalues of the matrix in question are established.

Keywords Discrete system · Non-Hermiticity · Jacobi matrix · Eigenvalue

1 Introduction

Some important problems of mathematical physics give rise to the consideration of non-Hermitian (non-selfadjoint) operators [1–3]. Especially non-Hermitian operators having real eigenvalues (spectrum) make sense for physical applications. This motivates construction and investigation of non-Hermitian operators with real spectrum. Recently one of the authors considered in [4] the following discrete non-Hermitian problem:

$$-\Delta^2 y_{n-1} + q_n y_n = \lambda \rho_n y_n, \quad n \in \Omega = \{-M, \ldots, -2, -1\} \cup \{2, 3, \ldots, N\}, \tag{1}$$

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

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

E. Ergun (✉)
Department of Physics, Ankara University, 06100 Tandogan, Ankara, Turkey
e-mail: ebruergun@mail.com

E. Bairamov
Department of Mathematics, Ankara University, 06100 Tandogan, Ankara, Turkey
e-mail: bairamov@science.ankara.edu.tr

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

$$\Delta y_n = y_{n+1} - y_n \quad (\text{so that } \Delta^2 y_{n-1} = y_{n-1} - 2y_n + y_{n+1}),$$

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

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

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 necessary and sufficient 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 [4]) and hence its eigenvalues are all real in this case. Further we will assume that $\delta \in (0, \pi/2)$. In [4] 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 [4], some necessary conditions for reality of the eigenvalues of problem (1)–(3) were obtained also in the case $M = 1$ and $N = 3$ (3×3 matrix case). In the present paper, we continue the work started in [4] and get necessary and sufficient conditions that ensure reality of the eigenvalues of problem (1)–(3) in the case $M = 1$ and $N = 3$.

2 Derivation of the 3 by 3 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

$$-y_{n-1} + v_n y_n - y_{n+1} = \lambda\rho_n y_n, \quad n \in \{-M, \ldots, -2, -1\} \cup \{2, 3, \ldots, N\}, \tag{5}$$
$$y_0 = (1 - e^{2i\delta})y_{-1} + e^{2i\delta}y_2, \quad y_1 = y_{-1}, \tag{6}$$
$$y_{-M-1} = y_{N+1} = 0, \tag{7}$$

where

$$v_n = 2 + q_n, \quad n \in \{-M, \ldots, -2, -1\} \cup \{2, 3, \ldots, N\}. \tag{8}$$

In the case $M = 1$ and $N = 3$, problem (5)–(7) takes the form

$$\left.\begin{array}{r} -y_{-2} + v_{-1}y_{-1} - y_0 = \lambda\rho_{-1}y_{-1} \\ -y_1 + v_2 y_2 - y_3 = \lambda\rho_2 y_2 \\ -y_2 + v_3 y_3 - y_4 = \lambda\rho_3 y_3 \end{array}\right\}, \tag{9}$$
$$y_0 = (1 - e^{2i\delta})y_{-1} + e^{2i\delta}y_2, \quad y_1 = y_{-1}, \tag{10}$$
$$y_{-2} = y_4 = 0. \tag{11}$$

Substituting (10) and (11) into (9) and using the explicit expression (4) for ρ_n, we get

$$\left.\begin{array}{r} [1 + (v_{-1} - 1)e^{-2i\delta}]y_{-1} - y_2 = \lambda y_{-1} \\ -e^{2i\delta}y_{-1} + v_2 e^{2i\delta}y_2 - e^{2i\delta}y_3 = \lambda y_2 \\ -e^{2i\delta}y_2 + v_3 e^{2i\delta}y_3 = \lambda y_3 \end{array}\right\}. \tag{12}$$

Putting

$$v_{-1} = a, \quad v_2 = b, \quad v_3 = c,$$
$$A = \begin{bmatrix} 1 + (a-1)e^{-2i\delta} & -1 & 0 \\ -e^{2i\delta} & be^{2i\delta} & -e^{2i\delta} \\ 0 & -e^{2i\delta} & ce^{2i\delta} \end{bmatrix}, \quad y = \begin{bmatrix} y_{-1} \\ y_2 \\ y_3 \end{bmatrix}, \tag{13}$$

we can write (12) in the form

$$Ay = \lambda y.$$

Consequently, 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 (13), where a, b, and c are real numbers defined by

$$a = v_{-1} = 2 + q_{-1}, \quad b = v_2 = 2 + q_2, \quad c = v_3 = 2 + q_3. \tag{14}$$

3 Necessary conditions for reality of the eigenvalues

The following theorem gives some necessary conditions for reality of the eigenvalues.

Theorem 1 *If the eigenvalues of the matrix A defined in (13) are all real, then necessarily*

$$a - 1 = b + c, \tag{15}$$
$$b + c - 1 + 2(bc - 1)\cos 2\delta = 0, \tag{16}$$
$$(b + c)(bc - 1) + 2(bc - c - 1)\cos 2\delta = 0. \tag{17}$$

Proof The eigenvalues of the matrix A coincide with the roots of the characteristic equation

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

that is

$$\begin{aligned} &\lambda^3 - [1 + (a-1)e^{-2i\delta} + (b+c)e^{2i\delta}]\lambda^2 \\ &\quad + [(a-1)(b+c) + (b+c-1)e^{2i\delta} + (bc-1)e^{4i\delta}]\lambda \\ &\quad - (a-1)(bc-1)e^{2i\delta} - (bc-c-1)e^{4i\delta} = 0. \end{aligned} \tag{18}$$

Denote the roots of Eq. 18 by λ_1, λ_2, and λ_3. By well-known relations between the roots and the coefficients of a polynomial, we have

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

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

$$(1 - a + b + c)\sin 2\delta = 0, \tag{19}$$
$$(b + c - 1)\sin 2\delta + (bc - 1)\sin 4\delta = 0, \tag{20}$$
$$(a - 1)(bc - 1)\sin 2\delta + (bc - c - 1)\sin 4\delta = 0. \tag{21}$$

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 (19)–(21),

$$\begin{aligned} &1 - a + b + c = 0, \\ &b + c - 1 + 2(bc - 1)\cos 2\delta = 0, \\ &(a - 1)(bc - 1) + 2(bc - c - 1)\cos 2\delta = 0. \end{aligned}$$

This completes the proof. □

It follows that, if at least one of the conditions (15)–(17) is not satisfied, then not all eigenvalues of the matrix A are real.

The following theorem gives more easy necessary conditions for reality of the eigenvalues.

Theorem 2 *If the eigenvalues of the matrix A are all real, then necessarily*

(i) $\delta \neq \frac{\pi}{4}$ $(\Leftrightarrow \cos 2\delta \neq 0)$;
(ii) $bc - 1 \neq 0$;
(iii) $bc - c - 1 \neq 0$;
(iv) $a \neq 1$ $(\Leftrightarrow b + c \neq 0)$;
(v) $a \neq 2$ $(\Leftrightarrow b + c \neq 1)$.

Proof (i) Assume that

$$\delta = \frac{\pi}{4}, \quad \text{that is,} \quad \cos 2\delta = 0. \tag{22}$$

We want to get then a contradiction. If (22) holds, then (16) and (17) give

$$b + c - 1 = 0 \quad \text{and} \quad (b + c)(bc - 1) = 0,$$

respectively. Hence

$$b + c = 1 \quad \text{and} \quad bc = 1.$$

Therefore b and c must be roots of the quadratic equation

$$x^2 - x + 1 = 0.$$

Since the roots of this equation,

$$x = \frac{1 \pm i\sqrt{3}}{2},$$

are nonreal, whereas a and b are real, we get a contradiction. Thus (i) is proved.

(ii) To show (ii) assume the contrary: Let

$$bc - 1 = 0, \quad \text{that is,} \quad bc = 1.$$

Then (16) gives

$$b + c - 1 = 0, \quad \text{that is,} \quad b + c = 1.$$

Therefore, as in the proof of (i), we get a contradiction from $bc = 1$ and $b+c = 1$.

(iii) To show (iii) assume the contrary:

$$bc - c - 1 = 0. \tag{23}$$

Then (17) gives

$$(b + c)(bc - 1) = 0.$$

Hence

$$b + c = 0 \quad \text{or} \quad bc = 1.$$

If $bc = 1$, then we get a contradiction by (ii). Therefore we should consider only the case

$$b + c = 0 \quad \text{and} \quad bc - 1 \neq 0. \tag{24}$$

From the first equation of (24), we have $b = -c$. Substituting this into (23), we get

$$c^2 + c + 1 = 0.$$

Hence

$$c = \frac{-1 \pm i\sqrt{3}}{2}$$

which is a contradiction because c was real. Thus (iii) is proved.

(iv) To show (iv) assume the contrary: $a = 1$. Then (15) gives $b + c = 0$, that is, $b = -c$. Substituting this into (17), we get

$$2(-c^2 - c - 1)\cos 2\delta = 0.$$

Next, by (i) we have $\cos 2\delta \neq 0$. Therefore $c^2+c+1 = 0$. But this is impossible since c is real.

(v) To show (v) assume the contrary: $a = 2$. Then (15) gives $b+c = 1$ and we get, from (16),

$$2(bc - 1)\cos 2\delta = 0.$$

But this is impossible by (i) and (ii). □

4 Necessary and sufficient conditions for reality of the eigenvalues

We will need the following known result (see, for example, [5]).

Proposition 3 *Consider the cubic equation*

$$\mu^3 + p\mu + q = 0 \tag{25}$$

with the real coefficients p *and* q. *Let us put*

$$D = -4p^3 - 27q^2 \tag{26}$$

that is called the discriminant of Eq. 25. Then:

(i) *If* $D < 0$, *then Eq. 25 has one real root and two nonreal complex conjugate roots.*
(ii) *If* $D = 0$, *then all three roots of Eq. 25 are real and at least two of them are equal to each other.*
(iii) *If* $D > 0$, *then Eq. 25 has three distinct real roots.*

Now we present the main result of this paper.

Theorem 4 *Let* a, b, c *be real numbers and* $\delta \in (0, \pi/2)$. *In order that the eigenvalues of the matrix* A *defined in (13) by using these numbers to be all real, it is necessary and sufficient that the following conditions be satisfied:*

$$a - 1 = b + c, \tag{27}$$
$$b + c - 1 + 2(bc - 1)\cos 2\delta = 0, \tag{28}$$
$$(b + c)(bc - 1) + 2(bc - c - 1)\cos 2\delta = 0, \tag{29}$$
$$\alpha^2\beta^2 - 4\beta^3 - 27\gamma^2 - 4\alpha^3\gamma + 18\alpha\beta\gamma \geq 0, \tag{30}$$

where

$$\alpha = -1 - 2(b + c)\cos 2\delta, \tag{31}$$
$$\beta = (b + c)^2 - bc + 1, \quad \gamma = bc - c - 1. \tag{32}$$

Proof If the eigenvalues of the matrix A are all real, then by Theorem 1 the conditions (15)–(17), that is (27)–(29), hold. Therefore, in this case the characteristic Eq. 18 takes the form

$$\begin{aligned}
&\lambda^3 - [1 + (a + b + c - 1)\cos 2\delta]\lambda^2 \\
&\quad + [(a - 1)(b + c) + (b + c - 1)\cos 2\delta + (bc - 1)\cos 4\delta]\lambda \\
&\quad - (a - 1)(bc - 1)\cos 2\delta - (bc - c - 1)\cos 4\delta = 0.
\end{aligned}$$

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

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

Hence, taking into account (27)–(29), we get

$$\lambda^3 - [1 + 2(b + c)\cos 2\delta]\lambda^2 + [(b + c)^2 - bc + 1]\lambda + bc - c - 1 = 0. \tag{33}$$

Thus, if the eigenvalues of the matrix A defined in (13) are all real, then a, b, c, and δ must satisfy the necessary conditions (27)–(29) and the eigenvalues of A coincide with the roots of Eq. 33. Now we define α, β, and γ by (31), (32) and rewrite (33) in the form

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

If we put

$$\lambda = \mu - \frac{\alpha}{3} \tag{35}$$

in (34), then we get the equation

$$\mu^3 + p\mu + q = 0 \tag{36}$$

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

$$p = -\tfrac{1}{3}\alpha^2 + \beta, \tag{37}$$

$$q = \tfrac{2}{27}\alpha^3 - \tfrac{1}{3}\alpha\beta + \gamma. \tag{38}$$

Note that since a, b, c, and $\cos 2\delta$ are real, the numbers α, β, and γ defined by (31), (32) and hence the numbers p and q defined by (37), (38) are real. The roots of Eqs. 34 and 36 are connected by Eq. 35. Therefore the reality of roots of Eq. 34 is equivalent to the reality of roots of Eq. 36. By Proposition 3, the roots of Eq. 36 are all real if and only if its discriminant D is non-negative. On the other hand, for this equation

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

Therefore the necessity of the condition (30) is also proved.

Now we prove the sufficiency of the conditions of the theorem. Thus assume that the conditions (27)–(30) 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 Eq. 18. Under the conditions (27)–(29) Eq. 18 reduces to the Eq. 33. Further, in virtue of Proposition 3, the roots of Eq. 33 are all real under the condition (30) in which α, β, and γ are defined by (31), (32) The proof is completed. □

Example 5 The conditions (27)–(29) 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 (27)–(29). Next, for these numbers we have, according to (31), (32),

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

and then according to (37), (38),

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

Therefore

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

and in virtue of Proposition 3 the roots of Eq. 36 and hence the eigenvalues of the matrix A are not all real.

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

References

1. C.I. Dolph, Recent developments in some non-selfadjoint problems of mathematical physics. Bull. Amer. Math. Soc. **67**, 1–69 (1961)
2. E.B. Davies, Non-selfadjoint differential operators. Bull. Lond. Math. Soc. **34**, 513–532 (2002)
3. 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, p. 28
4. E. Ergun, On the reality of the spectrum of a non-Hermitian discrete Hamiltonian. Rep. Math. Phys. **63**, 75–93 (2009)
5. A. Kurosh, *Higher Algebra* (Mir Publisher, Moscow, 1975)