On a class of non-Hermitian Hamiltonians with
tridiagonal matrix representation

Francisco M. Fernández*
INIFTA, DQT, Sucursal 4, C. C. 16,
1900 La Plata, Argentina

Abstract
We show that some non-Hermitian Hamiltonian operators with tridiagonal matrix representation may be quasi Hermitian or similar to Hermitian operators. In the class of Hamiltonian operators discussed here the transformation is given by a Hermitian, positive-definite, diagonal operator. We show that there is an important difference between open boundary conditions and periodic ones. We illustrate the theoretical results by means of two simple, widely used, models.

1 Introduction
Non-Hermitian quantum mechanics has become quite popular in recent years because of its intrinsic mathematical interest and as a suitable tool for the interpretation of some physical phenomena [1-3] (and references therein). Some non-Hermitian Hamiltonians exhibit PT-symmetry [4] that is a particular case of antunitary symmetry [5] (some simple examples are discussed elsewhere [6]).

In particular, exactly-solvable models given in terms of tridiagonal matrices have proved useful for deriving and illustrating relevant properties of non-Hermitian systems [7-14]. Some non-Hermitian operators exhibit generalized
Hermiticity \[15\] or quasi Hermiticity \[16\] that provides the condition for a linear operator to be similar to a self-adjoint one \[17\].

The purpose of this paper is a discussion of a class of non-Hermitian operators with finite tridiagonal matrix representation somewhat more general than those discussed earlier \[7\]-\[14\]. In particular, we are interested in simple versions of the Hatano-Nelson model \[18\] that have recently proved useful in the study of the effect of the boundary conditions and the skin effect in non-Hermitian tight-binding models \[19\] and the exceptional degeneracy and topological phases in such systems \[20\]. More precisely, we study these models in the light of the above-mentioned generalized Hermiticity \[14\] or quasi Hermiticity \[16\] and the conditions under which the non-Hermitian Hamiltonians are similar to Hermitian ones \[17\].

In section 2 we derive the main results in the case of a Hatano-Nelson model with open boundary conditions (OBC); in section 3 we apply those results to a similar model with periodic boundary conditions (PBC); in section 4 we discuss quasi-Hermiticity, Hermiticity and PT-symmetry by means of a simple model; in section 5 we focus on the particular model discussed briefly by Roccati \[19\] with both OBC and PBC; in section 6 we analyze a model proposed by Yuce and Ramezani \[23\] that illustrates the concept of robust exceptional points (EPs); finally, in section 7 we summarize the main results of this paper and draw conclusions.

## 2 Open boundary conditions

We first consider a Hamiltonian operator with a tridiagonal matrix representation and OBC

\[
H = \sum_{j=1}^{N-1} (H_{j,j+1} |j\rangle \langle j+1| + H_{j+1,j} |j+1\rangle \langle j|) + \sum_{j=1}^{N} H_{j,j} |j\rangle \langle j|, \tag{1}
\]

where $H_{j,j}^* = H_{j,j}$. By means of a diagonal operator

\[
Q = \sum_{j=1}^{N} Q_j |j\rangle \langle j|, \quad Q_k \neq 0, \quad k = 1, 2, \ldots, N, \tag{2}
\]
we carry out the transformation

\[ \hat{H} = Q^{-1}HQ = \sum_{j=1}^{N-1} \left( \hat{H}_{j,j+1} |j\rangle \langle j+1| + \hat{H}_{j+1,j} |j+1\rangle \langle j| \right) + \sum_{j=1}^{N} H_{j,j} |j\rangle \langle j|, \]

\[ \hat{H}_{j,j+1} = \frac{Q_{j+1}}{Q_{j}} H_{j,j+1}, \quad \hat{H}_{j+1,j} = \frac{Q_{j}}{Q_{j+1}} H_{j+1,j}. \]  

(3)

If we require that \( \hat{H}^\dagger = \hat{H} \) then

\[ \frac{H_{j+1,j}^*}{H_{j,j+1}} = \left| \frac{Q_{j+1}}{Q_{j}} \right|^2 = R_j > 0. \]  

(4)

This equation is a sufficient condition for \( H \) to be similar to a Hermitian operator. Note that if \( R_j = 1 \) for all \( j \) the operator \( H \) is Hermitian. It is clear that if the nonzero off-diagonal matrix elements are of the form \( H_{j,j+1} = r_j e^{i\theta_j}, \ H_{j+1,j} = r_j e^{-i\theta_j}, \ r_j, \rho_j > 0 \), then the non-Hermitian Hamiltonian operator \( (\hat{H}) \) is similar to a Hermitian one and \( R_j = \rho_j/r_j \).

According to equation (4) it is sufficient for present purposes to choose \( Q_j = |Q_j| \) so that \( Q \) is both Hermitian \( (Q^\dagger = Q) \) and positive definite \( (\langle Q \rangle > 0) \). It follows from \( \hat{H}^\dagger = \hat{H} \) that \( Q^2 \hat{H} = \hat{H} Q^2 \) which is the condition required by Scholtz et al [16] for quasi Hermiticity and also by Williams’s theorems [17]. Besides, it follows from equation (4) that

\[ Q_j = \sqrt{R_{j-1}R_{j-2}...R_1} Q_1. \]  

(5)

Since \( (Q_1^{-1}Q)^{-1} H (Q_1^{-1}Q) = Q^{-1}HQ \) we can choose \( Q_1 = 1 \) without loss of generality.

The eigenvalue equation \( H\psi_n = E_n\psi_n \) becomes \( \hat{H}Q^{-1}\psi_n = E_nQ^{-1}\psi_n \) under the transformation (3). The eigenvectors \( \tilde{\psi}_n = Q^{-1}\psi_n \) of \( \hat{H} \) can be chosen to be orthonormal; therefore, \( \langle \tilde{\psi}_m | \tilde{\psi}_n \rangle = \langle \psi_m | Q^{-2} | \psi_n \rangle = \delta_{mn} \) suggests that we can choose the metric \( \eta = Q^{-2} \) as argued by Pauli [15] several years ago.

Since the dimensionless time-dependent equation [21]

\[ i \frac{\partial}{\partial t} \psi(t) = H\psi(t), \]  

(6)
can be transformed into
\[ i \frac{\partial}{\partial t} Q^{-1} \psi(t) = \tilde{H} Q^{-1} \psi(t), \] (7)
then its solution is given by
\[ Q^{-1} \psi(t) = \exp \left( -i t \tilde{H} \right) Q^{-1} \psi(0), \] (8)
where the time-evolution operator \( \exp \left( -i t \tilde{H} \right) \) is obviously unitary.

3 Periodic boundary conditions

In the case of PBC (\(|N + 1\rangle = |1\rangle\)) we write \( H_{N+1,N} = H_{1,N} \) and \( H_{N,N+1} = H_{N,1} \) so that the Hamiltonian operator reads
\[
H = \sum_{j=1}^{N-1} (H_{j,j+1} |j\rangle \langle j+1| + H_{j+1,j} |j+1\rangle \langle j|) \\
+ H_{1,N} |1\rangle \langle N| + H_{N,1} |N\rangle \langle 1| + \sum_{j=1}^{N} H_{j,j} |j\rangle \langle j|. \] (9)
In addition to the expressions given in equation (3) we have
\[
\tilde{H}_{1,N} = \frac{Q_{N}}{Q_{1}} H_{1,N} = \sqrt{R_{N-1} R_{N-2} \ldots R_{1}} H_{1,N}, \\
\tilde{H}_{N,1} = \frac{Q_{1}}{Q_{N}} H_{N,1} = \frac{H_{N,1}}{\sqrt{R_{N-1} R_{N-2} \ldots R_{1}}}. \] (10)
and the transformed Hamiltonian operator \( \tilde{H} \) is not Hermitian unless \( H_{1,N} \) and \( H_{N,1} \) are chosen conveniently. The additional requirement \( \tilde{H}_{N,1} = \tilde{H}_{1,N}^* \) leads to
\[ H_{N,1} = R_{N-1} R_{N-2} \ldots R_{1} H_{1,N}^*. \] (11)
Also in this case we have that \( H_{N,1} = r_{N} e^{i \theta_{N}} \) and \( H_{1,N} = \rho_{N} e^{-i \theta_{N}} \) but the ratio \( \rho_{N}/r_{N} \) depends on all the other ratios \( R_{j} \). If we define \( R_{N} = H_{1,N}^* / H_{N,1} \) then \( R_{N} R_{N-1} \ldots R_{1} = 1 \), where all the \( R_{j}, j = 1, 2, \ldots, N - 1 \), are arbitrary positive numbers.
Note that if we set \( H_{1,N} = 0 \) in equation (11) then \( H_{N,1} = 0 \) and we recover the open chain.
4 Simple model

In order to illustrate that there is no relevant connection between quasi-Hermiticity [16] and PT-symmetry [4] (or, more generally, antiunitary symmetry [5]), we choose the simplest non-Hermitian model given by

\[
H = \begin{pmatrix}
    a & re^{i\theta} \\
    \rho e^{-i\theta} & b
\end{pmatrix},
\] (12)

where \(a, b\) and \(\theta\) are real and \(r, \rho > 0\). This matrix is neither Hermitian or PT-symmetric but it is similar to the Hermitian one

\[
\tilde{H} = \begin{pmatrix}
    a & \sqrt{\rho} e^{i\theta} \\
    \sqrt{\rho} e^{-i\theta} & b
\end{pmatrix},
\] (13)

through the transformation given by

\[
Q = Q_1 \begin{pmatrix}
    1 & 0 \\
    0 & \sqrt{r}
\end{pmatrix}.
\] (14)

If \(r = \rho\) and \(a \neq b\) then the matrix (12) is not PT-symmetric but it is Hermitian, in which case \(Q = Q_1 I\), where \(I\) is the \(2 \times 2\) identity matrix.

If \(a = b\) and \(r = \rho\) the matrix (12) is PT-symmetric with the antiunitary symmetry based on the orthogonal matrix (parity)

\[
P = \begin{pmatrix}
    0 & 1 \\
    1 & 0
\end{pmatrix}.
\] (15)

However, this particular case is also Hermitian.

Finally, the matrix

\[
H^{PT} = \begin{pmatrix}
    \rho e^{i\beta} & re^{i\theta} \\
    re^{-i\theta} & \rho e^{-i\beta}
\end{pmatrix},
\] (16)

is neither Hermitian or quasi-Hermitian (in the sense discussed above) but it is PT-symmetric with parity given by (15). In this case, parity is broken when \(r^2 < \rho^2 \sin^2 \beta\). This model is discussed in Appendix A by means of a somewhat more general approach.
5 Simplified Hatano-Nelson model

In this section we apply the results developed above to a model outlined by Roccati [19] that is a simple version of the Hatano-Nelson model without disorder [18]. For clarity, we discuss the OBC and PBC separately in two short subsections.

5.1 Example with OBC

In this example $H_{j,j} = 0, H_{j,j+1} = J(1-\delta), H_{j+1,j} = J(1+\delta)$, where $J$ and $\delta$ are real model parameters. The condition $H^*_{j+1,j}/H_{j,j+1} = R_j = (1+\delta)/(1-\delta) > 0$ leads to $-1 < \delta < 1$ in agreement with Roccati’s choice [19]. The tridiagonal matrix representation of the transformed Hamiltonian $\tilde{H}$ is symmetric with $\tilde{H}_{j,j+1} = \tilde{H}_{j+1,j} = J\sqrt{1-\delta^2}$. We conclude that all the eigenvalues are proportional to $J\sqrt{1-\delta^2}$.

5.2 Example with PBC

Roccati [19] considered the PBC explicitly. If we take into account that $H_{N,N+1} = H_{N,1} = J(1-\delta)$ and $H_{N+1,N} = H_{1,N} = J(1+\delta)$ then the resulting non-Hermitian Hamiltonian exhibits real and complex eigenvalues. However, if we choose $H_{1,N}$ as before and

$$H_{N,1} = J\frac{(1+\delta)^N}{(1-\delta)^{N-1}},$$

(17) then the eigenvalues are real because

$$\tilde{H}_{N,1} = \tilde{H}_{1,N} = \frac{(1+\delta)^{N+1}}{(1-\delta)^{N+1}}.$$  

(18) Figure 1 shows the eigenvalues $E_n/J$ for this model when $N = 4$ as functions of $\delta$. There is a level crossing at $\delta = 0$ because of the higher symmetry of the resulting Hermitian operator with all nonzero matrix elements equal to $J$ (it resembles a Hückel matrix [22]).
The behaviour of the eigenvalues at $\delta = -1$ is

$$E_1 = -E_4 \sim -\left(\frac{\sqrt{10}}{2} + \frac{\sqrt{2}}{2}\right) \sqrt{\sigma} + O\left(\sigma^{3/2}\right),$$

$$E_2 = -E_3 \sim \left(\frac{\sqrt{2}}{2} - \frac{\sqrt{10}}{2}\right) \sqrt{\sigma} + O\left(\sigma^{3/2}\right), \sigma = \delta + 1. \quad (19)$$

On the other hand, at $\delta = 1$ we have

$$E_1 = -E_4 \sim -4\xi^{-1} + 4 - \xi - \frac{1}{2}\xi^2 - \frac{3}{8}\xi^3 + O\left(\xi^4\right),$$

$$E_2 = -E_3 \sim -\sqrt{2}\xi + \frac{\xi^{3/2}}{\sqrt{2}} + O\left(\xi^{5/2}\right), \xi = 1 - \delta. \quad (20)$$

We appreciate that there is a pole at $\delta = 1$ that comes from the pole in the matrix element $H_{N,1}$.

At $\delta = -1$ there is an EP of order four as shown in figures 2 and 3 for the real and imaginary parts of $E_n/J$, respectively. In fact, when $\delta = -1$ the $4 \times 4$ Hamiltonian matrix exhibits just one eigenvector.

### 6 Robust exceptional point

If an EP does not change much with respect to perturbations of the system, one commonly says that it is robust. In order to obtain robust EPs, Yuce and Ramezani (YR) \[23\] proposed a non-Hermitian tight binding Hamiltonian that is a particular case of

$$H = \sum_{j=1}^{N-1} (t_n |n\rangle \langle n + 1| + J_n |n + 1\rangle \langle n|) + \sum_{j=1}^{N} \beta_n |n\rangle \langle n|, \quad (21)$$

where $\beta_n$, $t_n$ and $J_n$ are real model parameters, $t_n$ and $J_n$ being the forward and backward tunnelings, respectively. If $t_nJ_n > 0$ for all $n$, this operator satisfies the conditions outlined in section 2 and, consequently, is similar to a Hermitian one. YR considered the particular case given by $\beta_n = \beta$ and $J_n = t_n - \gamma \delta_{n,N-1}$, $n = 1, 2, \ldots, N - 1$, with $t_n > 0$. Clearly, this operator is quasi-Hermitian and isospectral to a Hermitian one provided that $t_{N-1} (t_{N-1} - \gamma) > 0$, disregarding the values of the other model parameters because $t_nJ_n = t_n^2 > 0,$
\( n = 1, 2, \ldots, N - 2 \). Since \( t_{N-1} > 0 \), then the exceptional point \( \gamma_{EP} \) should appear at \( \gamma_{EP} \leq t_{N-1} \) because the condition just mentioned is sufficient but not necessary. Present argument shows that the random change of the parameters \( t_n \) (the disorder) will not affect the location of the EP indicated above as long as \( t_{N-1} \) is kept unchanged. We can easily generalize YR’s results. If we keep \( t_k > 0 \) unchanged and define \( J_n = t_n - \gamma \delta_{nk} \), then the arbitrary variation of the real model parameters \( t_n, n \neq k \), will not change the fact that \( \gamma_{EP} \leq t_k \).

Obviously, if \( t_k < 0 \) then \( \gamma_{EP} \geq t_k \). It is clear that the location of the EP is independent of \( \beta \) (it is only necessary to define \( \epsilon = E - \beta \) to realize that we may choose \( \beta = 0 \) without loss of generality).

In order to determine \( \gamma_{EP} \) we resort to the discriminant of the characteristic polynomial

\[
p_N(E, \gamma) = \det (H_N - E I_N),
\]

where \( H_N \) and \( I_N \) are the tridiagonal matrix representation of \( H \) and the \( N \times N \) identity matrix, respectively. The discriminant \( F_N(\gamma) = \text{Disc}_E(p_N(E, \gamma)) \) (see, for example, [24] and references therein) is a polynomial function of \( \gamma \) of degree \( 2N - 3 \) and the EPs are roots of \( F_N(\gamma) \).

For one of YR’s particular cases: \( t_n = 1, n = 1, 2, \ldots, N - 1 \), the argument
above predicts that $\gamma_{EP} \geq 1$. The following results:

\[
\begin{align*}
F_2 &= 4(1 - \gamma), \\
F_3 &= 4(2 - \gamma)^3, \\
F_4 &= 16 (1 - \gamma) \left( \gamma^2 - 2\gamma + 5 \right)^2, \\
F_5 &= 16 (3 - 2\gamma)^3 (\gamma^2 + 4)^2, \\
F_6 &= 64 (1 - \gamma) \left( 5\gamma^4 - 8\gamma^3 + 18\gamma^2 - 28\gamma + 49 \right)^2, \\
F_7 &= 64 (4 - 3\gamma)^3 (4\gamma^4 + 13\gamma^2 + 32)^2, \\
F_8 &= 256 (1 - \gamma) \left( 49\gamma^6 - 70\gamma^5 + 151\gamma^4 - 212\gamma^3 + 351\gamma^2 - 486\gamma + 729 \right)^2, \\
F_9 &= 256 (5 - 4\gamma)^3 (32\gamma^6 + 93\gamma^4 + 204\gamma^2 + 400)^2, \\
F_{10} &= 1024 (1 - \gamma) \times \left( 729\gamma^8 - 972\gamma^7 + 2052\gamma^6 - 2704\gamma^5 + 4350\gamma^4 - 5676\gamma^3 + 8228\gamma^2 - 10648\gamma + 14641 \right)^2, \\
F_{11} &= 1024 (6 - 5\gamma)^3 \left( 400\gamma^8 + 1084\gamma^6 + 2213\gamma^4 + 4032\gamma^2 + 6912 \right)^2,
\end{align*}
\] (23)

suggest that $\gamma_{EP} = 1$ when $N = 2K$, $K = 1, 2, \ldots$, and $\gamma_{EP} = (K + 1)/K$ when $N = 2K + 1$, in agreement with the theoretical prediction. We realize that $\gamma_{EP} = 1$ for all even values of $N$ but it changes when $N$ is odd in such a way that it approaches unity as $N$ increases. Note the multiplicity of the EPs for $N$ odd; for example, $p_5(E, 3/2) = E^3 (5 - 2E^2) / 2$ reveals an EP of order three (there is only one eigenvector with eigenvalue $E = 0$).

As a second example, we generated $t_n$, $n = 1, 2, \ldots, N - 1$, and $J_n$, $n = 1, 2, \ldots, N - 2$ randomly in the interval (0, 1) and kept $J_{N-1} = 1 - \gamma$ fixed. The results suggest that $\gamma_{EP} = 1$ for all $N = 2K$ while the value of $\gamma_{EP}$ changes, but remains greater than unity, for $N = 2K + 1$.

From numerical results for $\beta = 2$ and $N = 10$ YR [23] concluded that the EP at $\gamma = 1$ is robust. Present theoretical results and analytical calculations confirm this result that appears to be valid only for even values of $N$. Apparently, YR did not try odd values of $N$ and they even stated that “Without loss of generality we assume that $N$ is an even number.” Another YR’s wrong statement is “The Hamiltonian in eq. (4) becomes noninvertible when $\beta = 0$.” that only holds for
odd values of \( N \) because there is always an eigenvalue \( E = \beta \). For even values of \( N \), on the other hand, the Hamiltonian operator just mentioned is invertible for \( \beta = 0 \), except for some particular values of \( \gamma \).

7 Conclusions

Several authors have discussed features of non-Hermitian quantum mechanics by means of Hamiltonians with tridiagonal matrix representations \(^7\) \( \)\(^8\) \( \)\(^9\) \( \)\(^10\) \( \)\(^20\) \( \)\(^21\) (and references therein). In many of those cases the occurrence of real eigenvalues can be explained by the fact that the non-Hermitian Hamiltonians are quasi Hermitian or similar to Hermitian ones. Throughout this paper we have explored a class of such examples where the suitable transformation is given by a Hermitian, positive-definite, diagonal operator. Quasi Hermiticity appears more straightforwardly in the case of OBC, whereas for PBC one has to choose a pair of matrix elements with somewhat more care. Section 6 shows how present theoretical result may clarify, explain and even correct the conclusions drawn from numerical results on simple lattice models.

A More general approach

In this Appendix we will show that the matrix (16) is also similar to an Hermitian one. To this end, we resort to the more general results of Williams \(^17\) and Scholtz et al \(^18\).

Suppose that \( H \) is a non-Hermitian operator that satisfies

\[
H^\dagger G = GH,
\]  

(A.1)

where \( G \) is an Hermitian, positive-definite operator. Then, \( G^{-1} \) and \( G^{1/2} \) exist and equation (A.1) can be rewritten as \( G^{-1/2} H^\dagger G^{1/2} = G^{1/2} H G^{-1/2} \). Consequently,

\[
\tilde{H} = G^{1/2} H G^{-1/2},
\]  

(A.2)

is Hermitian.
As an example we consider the simple PT-symmetric $2 \times 2$ matrix representation

$$H = \begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix},$$  \hspace{1cm} (A.3)

that is identical to (16). In this case the matrix $G$ should be of the form

$$G = \begin{pmatrix} G_{11} & G_{12} \\ G_{12}^* & G_{22} \end{pmatrix},$$  \hspace{1cm} (A.1)

where $G_{11}$ and $G_{22}$ are real. It follows from equation (A.1) that $G_{11} = G_{22}$ and $G_{11} (a^* - a) - G_{12} b^* + b G_{12}^* = 0$. Besides, it is clear from equation (A.1) that we can choose $G_{11} = 1$ without loss of generality; therefore,

$$G = \begin{pmatrix} 1 & G_{12} \\ G_{12}^* & 1 \end{pmatrix},$$  \hspace{1cm} (A.4)

with the condition that

$$a^* - a - G_{12} b^* + b G_{12}^* = 0.$$  \hspace{1cm} (A.5)

Since the eigenvalues of $G$ are $g_1 = 1 - |G_{12}|$ and $g_2 = 1 + |G_{12}|$ we conclude that $G$ is positive-definite provided that $|G_{12}| < 1$.

As a particular example we consider

$$H = \begin{pmatrix} i \gamma & 1 \\ 1 & -i \gamma \end{pmatrix},$$  \hspace{1cm} (A.6)

According to equation (A.5) $G_{12} = -i \gamma$ and

$$G = \begin{pmatrix} 1 & -i \gamma \\ i \gamma & 1 \end{pmatrix},$$  \hspace{1cm} (A.7)

Note that $G$ is positive-definite provided that $|\gamma| < 1$, which is consistent with the fact that the eigenvalues of $H$, $E_1 = -\sqrt{1 - \gamma^2}$ and $E_2 = -\sqrt{1 - \gamma^2}$, are real under the same condition. By means of

$$G^{1/2} = \frac{1}{2} \begin{pmatrix} \sqrt{1 - \gamma} + \sqrt{\gamma + 1} & i (\sqrt{1 - \gamma} - \sqrt{\gamma + 1}) \\ -i (\sqrt{1 - \gamma} - \sqrt{\gamma + 1}) & \sqrt{1 - \gamma} + \sqrt{\gamma + 1} \end{pmatrix},$$  \hspace{1cm} (A.8)

we obtain

$$\tilde{H} = \begin{pmatrix} 0 & \sqrt{1 - \gamma^2} \\ \sqrt{1 - \gamma^2} & 0 \end{pmatrix},$$  \hspace{1cm} (A.9)
that is a real symmetric matrix when $|\gamma| < 1$.

The straightforward approach followed here appears to be simpler than the one based on the left and right eigenvectors of $H$. 

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Figure 1: Eigenvalues $E_n/J$ of the Roccati’s model [19] with PBC and $N = 4$

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Figure 2: Real part of the eigenvalues $E_n/J$ of the Roccati’s model \cite{19} with PBC and $N = 4$.

Figure 3: Imaginary part of the eigenvalues $E_n/J$ of the Roccati’s model \cite{19} with PBC and $N = 4$. 