Algebraic treatment of the Pais-Uhlenbeck oscillator and its PT-variant

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Abstract

The algebraic method enables one to study the properties of the spectrum of a quadratic Hamiltonian through the mathematical properties of a matrix representation called regular or adjoint. This matrix exhibits exceptional points where it becomes defective and can be written in canonical Jordan form. It is shown that any quadratic function of $K$ coordinates and $K$ momenta leads to a $2K$ differential equation for those dynamical variables. We illustrate all these features of the algebraic method by means of the Pais-Uhlenbeck oscillator and its PT-variant. We also consider a trivial quantization of the fourth-order differential equation for the quantum-mechanical dynamical variables.

1 Introduction

Since the seminal paper on generalizations of the field equations to equations of higher order by Pais and Uhlenbeck [1] there has been several attempts at a suitable quantization of fourth-order dynamical differential equations [2-4]. Most of the papers are based on the Pais-Uhlenbeck oscillator [1,3,7,9] but there are also other model candidates [8,10]. All these oscillators are quadratic

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functions of the coordinates and their conjugate momenta. In principle, any such Hamiltonian leads to a fourth-order dynamical differential equation \[11\]. In the discussion of the just mentioned quantization, concepts like exceptional points \[7\] (see \[12–15\] for a detailed discussion), breaking of commutation relations in the equal-frequency case \[2\], apparent reduction of the number of degrees of freedom \[2,8\] and Jordan matrices \[2–4,6,7\] appear over and over again.

The algebraic method is extremely useful for the analysis of the mathematical properties of quadratic Hamiltonians \[11,16,17\]. It consists of associating each quadratic function of \(K\) coordinates and their \(K\) conjugate momenta with a \(2K \times 2K\) matrix. The main features of the spectrum of the Hamiltonian emerge from the mathematical properties of its adjoint or regular matrix representation \[18,19\].

The purpose of this paper is to apply the algebraic method to the Pais-Uhlenbeck oscillator \[2–9\] and its complex-PT variant \[5–7\] and show that exceptional points, breaking of commutation relations, apparent reduction of degrees of freedom and Jordan matrices appear in a quite natural and straightforward way. At the same time we show the advantage of using the algebraic method for the analysis of this kind of oscillators.

In section 2 we review the main equations of the algebraic method for Hamiltonians that are quadratic functions of \(K\) coordinates and their conjugate momenta and show that any such operator leads to a differential equation of order \(2K\) for each dynamical variable. In section 3 we apply the algebraic method to the Pais-Uhlenbeck oscillator and its PT-symmetric variant. In section 4 we consider a trivial quantization of the fourth-order differential equation. Finally, in section 5 we summarize the main results of the paper and draw conclusions.

2 The algebraic method

The algebraic method is particularly useful for the analysis of the spectrum of quantum-mechanical Hamiltonians that are quadratic functions of the coordi-
nates and their conjugate momenta:

\[
H = \sum_{i=1}^{2K} \sum_{j=1}^{2K} \gamma_{ij} O_i O_j,
\]

(1)

where \( S_{2K} = \{O_1, O_2, \ldots, O_{2K}\} = \{x_1, x_2, \ldots, x_K, p_1, p_2, \ldots, p_K\} \), \([x_m, p_n] = i\delta_{mn}\), and \([x_m, x_n] = [p_m, p_n] = 0\). The method may also be applied to classical problems [20] but we do not discuss this case here. Since the Hamiltonian \( H \) satisfies the closure commutation relations

\[
[H, O_i] = \sum_{j=1}^{2K} H_{ji} O_j, \quad i = 1, 2, \ldots, 2K,
\]

(2)

we can define a \( 2K \times 2K \) matrix \( H \) with elements \( H_{ij} \) that is commonly known as the adjoint or regular matrix representation of \( H \) in the operator basis set \( S_{2K} \) [18,19]. In order to make this paper sufficiently self-contained, in this section we review the main results of our earlier papers [11,17].

Because of equation (2) it is possible to find an operator of the form

\[
Z = \sum_{i=1}^{N} c_i O_i,
\]

(3)

such that

\[
[H, Z] = \lambda Z,
\]

(4)

where \( \lambda \) is a complex number. If \( |\psi\rangle \) is an eigenvector of \( H \) with eigenvalue \( E \) then

\[
HZ |\psi\rangle = ZH |\psi\rangle + \lambda Z |\psi\rangle = (E + \lambda)Z |\psi\rangle;
\]

(5)

that is to say, \( Z |\psi\rangle \) is an eigenvector of \( H \) with eigenvalue \( E + \lambda \). It follows from equations (2), (3) and (4) that the coefficients \( c_i \) are solutions to

\[
(H - \lambda I)C = 0,
\]

(6)

where \( I \) is the \( 2K \times 2K \) identity matrix and \( C \) is a \( 2K \times 1 \) column matrix with elements \( c_i \). Equation (6) admits nontrivial solutions for those values of \( \lambda \) that are roots of

\[
P(\lambda) = \det(H - \lambda I) = 0.
\]

(7)
Clearly, the eigenvalues $\lambda_i, i = 1, 2, \ldots, 2K$ are the natural frequencies of $H$ (differences between pairs of eigenvalues of this operator). This matrix representation is not normal
\[
HH^\dagger \neq H^\dagger H, \tag{8}
\]
and for this reason it may be defective or non-diagonalizable (it may not have a complete basis set of eigenvectors).

We can also define the matrix $U$ with elements $U_{ij}$ given by
\[
[O_i, O_j] = U_{ij}\hat{1}, \tag{9}
\]
where $\hat{1}$ is the identity operator that we will omit from now on. This matrix can be written as
\[
U = i \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{10}
\]
where $0$ and $I$ are the $K \times K$ zero and identity matrices, respectively. Note that $U^\dagger = U^{-1} = U$. The matrices $H$ and $U$ are related by
\[
H = (\gamma + \gamma^t)U, \tag{11}
\]
where $\gamma$ is the $2K \times 2K$ matrix with elements $\gamma_{ij}$.

The well known Jacobi identity $[O_k, [H, O_i]] + [O_i, [O_k, H]] + [H, [O_i, O_k]] = 0$ leads to $[O_k, [H, O_i]] = [O_i, [H, O_k]]$. Therefore, it follows from the latter equation, (2) and (9) that $(UH)^t = H^tU^t = -H^tU = UH$, which leads to $UH^tU = -H$. We can thus prove that $\det(H + \lambda I) = P(-\lambda) = 0$; that is to say: if $\lambda$ is an eigenvalue then $-\lambda$ is also an eigenvalue. In other words, $P(\lambda)$ is a polynomial function of $\lambda^2$. We also have
\[
H^tUC = -\lambda UC, \\
H^tUC^* = -\lambda^* UC^*. \tag{12}
\]

If $\gamma^t = \gamma$ the quadratic Hamiltonian is Hermitian and $H$ is $U$-pseudo Hermitian
\[
H^\dagger = UHU, \tag{13}
\]
(for a more detailed discussion of quasi-Hermiticity or pseudo-Hermiticity see [21–25]). In this case $\gamma + \gamma^t = \gamma + \gamma^* = 2\Re\gamma$. Besides, it follows from $[H, Z]^\dagger = [Z^\dagger, H] = \lambda^* Z^\dagger$ that if $Z$ is solution to equation (11), then $Z^\dagger$ is solution to

$$[H, Z]^\dagger = -\lambda^* Z^\dagger. \quad (14)$$

In other words: both $\lambda$ and $-\lambda^*$ are roots of $P(\lambda) = 0$.

For every eigenvalue $\lambda_i$ we construct the operator

$$Z_i = \sum_{j=1}^{2K} c_{ij} O_j. \quad (15)$$

For convenience we label the eigenvalues in such a way that $\lambda_j = -\lambda_{2K-j+1}$, $j = 1, 2, \ldots, K$, and when they are real we organize them in the following way:

$$\lambda_1 < \lambda_2 < \ldots < \lambda_K < 0 < \lambda_{K+1} < \ldots < \lambda_{2K}. \quad (16)$$

If we take into account that $[H, Z_i Z_j] = (\lambda_i + \lambda_j) Z_i Z_j$ then we conclude that

$$[H, [Z_i, Z_j]] = (\lambda_i + \lambda_j) [Z_i, Z_j] = 0, \quad (17)$$

which tells us that $Z_i$ and $Z_j$ commute when $\lambda_i + \lambda_j \neq 0$. If $[Z_j, Z_{2K-j+1}] = \sigma_j \neq 0$ for all $j = 1, 2, \ldots, K$ then we can write $H$ in the following way

$$H = -\sum_{j=1}^{K} \frac{\lambda_j}{\sigma_j} Z_{2K-j+1} Z_j + E_0. \quad (18)$$

If $\psi_0$ is a vector in the Hilbert space where $H$ is defined that satisfies

$$Z_j \psi_0 = 0, \quad j = 1, 2, \ldots, K, \quad (19)$$

then $H \psi_0 = E_0 \psi_0$.

Consider the time-evolution of the dynamical variables

$$O_j(t) = e^{itH} O_j e^{-itH}, \quad (20)$$

and their equations of motion

$$\dot{O}_j(t) = i e^{itH} [H, O_j] e^{-itH} = i \sum_{k=1}^{2K} H_{kj} O_k(t). \quad (21)$$
If we define the row vector \( O(t) = (O_1(t) \ O_2(t) \ldots \ O_{2K}(t)) \) then we have the matrix differential equation \( \dot{O}(t) = iO(t)H \) with solution

\[
O(t) = O e^{itH}, \quad O = O(0).
\]  

Since \( P(H) = 0 \) then

\[
P \left( -i \frac{d}{dt} \right) O(t) = OP(H)e^{itH} = 0,
\]

gives us a differential equation of order \( 2K \) for the dynamical variables. Obviously, \( Z_j(t) = e^{it\lambda_j} Z_j, \ j = 1, 2, \ldots, 2K, \) satisfies this equation. It clearly tells us that any Hamiltonian that is a quadratic function of \( K \) coordinates and their conjugate momenta leads to a differential equation of order \( 2K \) for any such dynamical variable. In particular, for \( K = 2 \) we have \( P(\lambda) = (\lambda_1^2 - \lambda_2^2) (\lambda_2^2 - \lambda_1^2) = 0 \) and the fourth-order differential equation

\[
\frac{d^4}{dt^4} q + (\lambda_1^2 + \lambda_2^2) \frac{d^2}{dt^2} q + \lambda_1^2 \lambda_2^2 q = 0,
\]

where \( q \in \mathcal{S}_4 \). In principle, any pair of coupled oscillators may be a candidate for the quantization of a fourth-order differential equation like (24). Some of them have already been discussed and analysed [3–10], and many more can be proposed.

### 3 The Pais-Uhlenbeck oscillator

In this section we consider the standard Pais-Uhlenbeck oscillator [1,3–7,9]

\[
H = \frac{1}{2} p_x^2 + x p_y + \frac{\omega_1^2 + \omega_2^2}{2} x^2 - \frac{\omega_1^2 \omega_2^2}{2} y^2,
\]  

as well as its PT-symmetric modification [5,6]

\[
H = \frac{1}{2} p_x^2 - i x p_y + \frac{\omega_1^2 + \omega_2^2}{2} x^2 + \frac{\omega_1^2 \omega_2^2}{2} y^2.
\]

The latter exhibits two antiunitary symmetries [26] given by \( A_1 : (x, y, p_x, p_y) \rightarrow (-x, -y, p_x, p_y) \), \( A_2 : (x, y, p_x, p_y) \rightarrow (x, y, -p_x, -p_y) \) that satisfy \( A_q = A_q^{-1}, q = 1, 2, \) and \( A_q i A_q^{-1} = -i \). Since \( A_q H A_q^{-1} = H \) we have \( H A_q |\psi\rangle = A_q H |\psi\rangle = \ldots \).
\[ A_q E |\psi\rangle = E^* |\psi\rangle. \] If the antiunitary symmetry is exact \( A_q |\psi\rangle = a_q |\psi\rangle \) (with \( a_q \) being a complex number) then the eigenvalue \( E \) is real. The antiunitary symmetry \( A_1 \) was chosen by Bender and Manheim [6] in their analysis of the quantization of the fourth-order differential equation.

In what follows we consider the somewhat more general oscillator

\[ H = \frac{1}{2} p_x^2 + ax p_y + \frac{\omega_1^2 + \omega_2^2}{2} x^2 + b \frac{\omega_1^2 \omega_2^2}{2} y^2, \quad (27) \]

where \( a \) and \( b \) are complex numbers. The adjoint or regular matrix representation of this operator is

\[
H = \begin{pmatrix}
0 & -ai (\omega_1^2 + \omega_2^2) i & 0 \\
0 & 0 & b \omega_1^2 \omega_2^2 i \\
-i & 0 & 0 \\
0 & a i & 0
\end{pmatrix}. \quad (28)
\]

Its eigenvalues are the square roots of

\[ \xi_{\pm} = \frac{\omega_1^2 + \omega_2^2 \pm \sqrt{4a^2 b \omega_1^2 \omega_2^2 + (\omega_1^2 + \omega_2^2)^2}}{2}, \quad (29) \]

and are real provided that

\[ - \frac{(\omega_1^2 + \omega_2^2)^2}{4 \omega_1^2 \omega_2^2} < a^2 b < 0. \quad (30) \]

The two possibilities \( a^2 > 0, b < 0 \) or \( a^2 < 0, b > 0 \) lead to the Hamiltonians (25) or (26), respectively. If we choose \( a^2 b = -1 \) and \( \omega_1 > \omega_2 \) the resulting frequencies \( \lambda_1^2 = \omega_1^2 \) and \( \lambda_2^2 = \omega_2^2 \) are related to the corresponding ladder operators

\[
Z_1 = c_1 \left[ \frac{\omega_2 y}{a} + p_x - i \frac{(\omega_1^2 x + ap_y)}{\omega_1} \right], \\
Z_2 = c_2 \left[ \frac{\omega_2 y}{a} + p_x - i \frac{(\omega_1^2 x + ap_y)}{\omega_2} \right], \\
Z_3 = c_3 \left[ \frac{\omega_1 y}{a} + p_x + i \left( \omega_2 x + \frac{ap_y}{\omega_2} \right) \right], \\
Z_4 = c_4 \left[ \frac{\omega_1 y}{a} + p_x + i \left( \omega_1 x + \frac{ap_y}{\omega_1} \right) \right]. \quad (31)
\]
where $c_i$, $i = 1, 2, 3, 4$ are arbitrary real numbers. The only nonvanishing commutators are

$$[Z_1, Z_4] = \sigma_1 = 2c_1c_4 \frac{\omega_1^2 - \omega_2^2}{\omega_1},$$

$$[Z_2, Z_3] = \sigma_2 = 2c_2c_3 \frac{\omega_2^2 - \omega_1^2}{\omega_2}. \quad (32)$$

Note that even these commutators vanish (breaking of the commutator relation) in the case of equal frequencies which leads to an apparent reduction of the number of degrees of freedom [2, 3]. By means of equation (18) we obtain

$$H = \frac{\omega_1}{\sigma_1} Z_4 Z_1 + \frac{\omega_2}{\sigma_2} Z_3 Z_2 + \frac{\omega_2 - \omega_1}{2} \left( \frac{\omega_1^2}{\omega_1^2 - \omega_2^2} Z_4 Z_1 + \frac{\omega_2^2}{\omega_2^2 - \omega_1^2} Z_3 Z_2 + \omega_2 - \omega_1 \right). \quad (33)$$

The different signs of the coefficients of $Z_4 Z_1$ and $Z_3 Z_2$ reveal the well known fact that the spectrum of this oscillator is unbounded from above and below.

In the case of equal frequencies ($\omega_1 = \omega_2 = \omega$) the matrix representation can be written in canonical Jordan form. Consider, for example, the Hermitian version of the Pais-Uhlenbeck Hamiltonian (25) ($a = 1$, $b = -1$) for which

$$H = \begin{pmatrix} 0 & -i & 2\omega^2 i & 0 \\ 0 & 0 & 0 & -\omega^4 i \\ -i & 0 & 0 & 0 \\ 0 & 0 & i & 0 \end{pmatrix}. \quad (34)$$

The matrix

$$P = \begin{pmatrix} -\omega^2 i & 0 & \omega^2 i & 0 \\ \omega^3 & 3\omega^2 & \omega^3 & -3\omega^2 \\ \omega & 1 & \omega^3 & -1 \\ -i & -\frac{2i}{\omega} & i & -\frac{2i}{\omega} \end{pmatrix}, \quad (35)$$

enables us to bring $H$ into a canonical Jordan form by means of the similarity transformation

$$P^{-1}HP = \begin{pmatrix} -\omega & 1 & 0 & 0 \\ 0 & -\omega & 0 & 0 \\ 0 & 0 & \omega & 1 \\ 0 & 0 & 0 & \omega \end{pmatrix}, \quad (36)$$

8
that exhibits two Jordan blocks of dimension 2. In other words, the case of equal frequencies \( \omega_1 = \omega_2 = \omega \) corresponds to an exceptional point where two pairs of eigenvectors of the matrix \( H \) coalesce and, consequently, only two eigenvectors remain linearly independent. At this point the regular or adjoint matrix becomes defective and can be transformed into a canonical Jordan form.

4 Trivial quantization

The problem consists of obtaining a suitable quantum-mechanical Hamiltonian that leads to the following fourth-order differential equation of motion for the dynamical variables:

\[
\frac{d^4}{dt^4} q + (\omega_1^2 + \omega_2^2) \frac{d^2}{dt^2} q + \omega_1^2 \omega_2^2 q = 0.
\]

The solution is simple if we take into account that any quadratic function of two coordinates and momenta already yields this differential equation as shown in the preceding section and in an earlier communication [11]. Therefore, we only have to choose a suitable model from the large family of such Hamiltonians.

A well known textbook example will serve the purpose. Consider two identical masses fixed to two opposite walls with two springs with the same force constant \( k \). Then we join the masses each other with a third spring with a different force constant, say \( k_1 \). If the particles move in only one dimension then the system will oscillate with two different frequencies related to the two normal modes of vibration. Obviously, there is no problem in quantizing this model and we will obtain a Hamiltonian operator with a spectrum bounded from below. The case of equal frequencies is obtained when \( k_1 = 0 \) so that the system becomes a pair of two identical uncoupled harmonic oscillators. There is no problem in quantizing this classical model either and we again obtain a spectrum that is bounded from below. In both cases (different or equal frequencies) the eigenfunctions will be square integrable.

For simplicity we consider a dimensionless equation. If we express the force constants \( k \) and \( k_1 \) in terms of the frequencies \( \omega_1 \) and \( \omega_2 \) of the two normal
modes the Hamiltonian becomes
\[
H = \frac{1}{2} (p_1^2 + p_2^2) + \frac{\omega_1^2}{4} (x_1 - x_2)^2 + \frac{\omega_2^2}{4} (x_1 + x_2)^2.
\] (38)

Note that
\[
P(\lambda) = \lambda^4 - (\omega_1^2 + \omega_2^2) + \omega_1^2\omega_2^2,
\] (39)
that is consistent with equation (37). This Hamiltonian is separable
\[
H = \frac{1}{2} (p_x^2 + p_y^2) + \frac{\omega_1^2}{2} x^2 + \frac{\omega_2^2}{2} y^2,
\] (40)
in terms of the coordinates
\[
x = \frac{1}{\sqrt{2}} (x_1 - x_2), \quad y = \frac{1}{\sqrt{2}} (x_1 + x_2).
\] (41)

Therefore, the spectrum is bounded from below
\[
E_{n_1 n_2} = \omega_1 \left( n_1 + \frac{1}{2} \right) + \omega_2 \left( n_2 + \frac{1}{2} \right), \quad n_1, n_2 = 0, 1, \ldots,
\] (42)
and the eigenfunctions \( \psi_{n_1 n_2} (x_1, x_2) = \varphi_{n_1} (\omega_1, x_1) \varphi_{n_2} (\omega_2, x_2) \), where \( \varphi_n (\omega, x) \) is a Harmonic-oscillator eigenfunction, are square integrable.

The annihilation operators are
\[
a_1 = \frac{\sqrt{\omega_1}}{2} (x_1 - x_2) + \frac{i}{2\sqrt{\omega_1}} (p_1 - p_2),
\]
\[
a_2 = \frac{\sqrt{\omega_2}}{2} (x_1 + x_2) - \frac{i}{2\sqrt{\omega_2}} (p_1 + p_2),
\] (43)
and the creation ones their adjoints. In terms of these operators the Hamiltonian reads
\[
H = \omega_1 a_1^\dagger a_1 + \omega_2 a_2^\dagger a_2 + \frac{1}{2} (\omega_1 + \omega_2).
\] (44)

Obviously, the case of equal frequencies does not offer any difficulty because by construction the problem reduces to two uncoupled oscillators
\[
H = \frac{1}{2} (p_1^2 + p_2^2) + \frac{\omega_1^2}{2} (x_1^2 + x_2^2),
\] (45)
with spectrum
\[
E_{n_1 n_2} = \omega (n_1 + n_2 + 1).
\] (46)
We call this solution to the problem of the quantization of the fourth-order differential equation (37) trivial because it can be reduced to two dynamical differential equations of second order that are known to offer no difficulty. More precisely, the coordinates $x$ and $y$ satisfy

$$\ddot{x} + \omega_1^2 x = 0, \quad \ddot{y} + \omega_2^2 y = 0. \quad (47)$$

5 Further comments and conclusions

The algebraic method enables us to reduce the discussion of a quadratic Hamiltonian to the analysis of its regular or adjoint matrix representation. In this way we can easily elucidate several features of the spectrum of the operator without solving its eigenvalue equation explicitly. It is, for example, quite straightforward to determine whether the spectrum is real or not. In this paper, in particular, we have stressed and exploited the fact that any quadratic function of $K$ coordinates and their conjugate momenta leads to a differential equation of order $2K$ for any of those dynamical variables [11]. As far as we are aware, this feature of the quadratic Hamiltonians has not been taken into consideration in earlier studies of the subject.

The regular or adjoint matrix representation of the operator also reveals that at an exceptional point the matrix becomes defective (that is to say, it has less than $2K$ linearly independent eigenvectors). At such point there is a commutator breaking; that is to say, a pair of creation and annihilation operators for the same degree of freedom commute. The reason is that there is a one-to-one correspondence between the eigenvectors of the adjoint or regular matrix representation and the creation and annihilation (or ladder) operators. When two eigenvectors coalesce at an exceptional point, the corresponding creation and annihilation operators are found to commute.

At the exceptional point the defective matrix can be converted, by means of a similarity transformation, into a canonical Jordan form (a matrix that exhibits Jordan blocks). In the case of the Pais-Uhlenbeck oscillator this phenomenon
takes place at the equal-frequency limit. Although some of these results are well known and have been discussed earlier, it has been our purpose to show that the algebraic method enables us to study them in a simple and unified way.

With respect to the problem posed by the quantization of the fourth-order differential equation for the dynamical variables we have also shown that it is possible to obtain a quantum-mechanical quadratic Hamiltonian with a bounded-from-below spectrum and square-integrable eigenfunctions in the cases of different as well as equal frequencies.

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