

Non-Hermitian Hydrogen atom

Juan M. Romero · O. González-Gaxiola ·
R. Bernal-Jaquez

Received: 4 January 2013 / Accepted: 21 May 2013 / Published online: 4 June 2013
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Abstract We have constructed a set of non-Hermitian operators that satisfy the commutation relations of the $SO(3)$ -Lie algebra. Using these set of operators we have constructed a non-Hermitian Hamiltonian corresponding to the Hydrogen atom that includes a complex term but with the same spectra as in the Hermitian case. It is also found a non-Hermitian Runge–Lenz vector that represents a conserved quantity. In this way, we obtain a set of non-Hermitian operators that satisfy the commutation relations of the $SO(4)$ -Lie algebra.

Keywords Hydrogen atom · Lie algebra · \mathcal{PT} -symmetry Hamiltonians

1 Introduction

Quantum mechanics is considered as one the most solid and well established theories in physics. Different experiments have corroborated its predictions. However, at a theoretical level there are different facts that make us think that it could be necessary to modify or extend this theory. For example, it has not been possible to find a consistent quantum-mechanical formulation of general relativity, then quantum theory maybe modified in order to make it compatible with general relativity.

As it is well known, quantum mechanics has been formulated in terms of Hermitian operators in order to obtain real spectra. However, it has become clear that Hermiticity is not a necessary condition to obtain real spectra. This opens the possibility for quantum mechanics to be extended using non-Hermitian operators, this is the so called \mathcal{PT} -symmetry theory, see review [1] and its references.

J. M. Romero · O. González-Gaxiola · R. Bernal-Jaquez (✉)
Departamento de Matemáticas Aplicadas y Sistemas, Universidad Autónoma
Metropolitana-Cuajimalpa, Artificios 40. Col. Hidalgo, Mexico, D.F. 01120, Mexico
e-mail: r.bernal.jaquez@gmail.com; rbernal@correo.cua.uam.mx

The \mathcal{PT} -version of quantum mechanics has strongly attracted attention because it gives a way to deal with some problems that are out of the scope of conventional quantum mechanics. For example, we can solve certain kind of problems in which the potentials are given by complex-valued functions and whose spectra results to be real [2]. In the same way, using this formulation it has been possible to achieve a consistent quantization of a system with high order derivatives: the so called the Pais-Uhlenbeck oscillator model [3]. This opens the possibility to construct in a consistent way high order derivatives field theories. This fact is important because different theories with high order derivatives have been recently proposed, for example, in extensions of the standard model [4], in the noncommutative spaces [5] and gravity theories [6]. In this way, it becomes possible that an extension of \mathcal{PT} -symmetry theory applied to field theory can give a consistent description of these systems.

There is not a finished version of the theory, however, a growing number of themes are under study in the \mathcal{PT} -framework, some of them can be found [7–11]. An aspect that has been scarcely treated in the \mathcal{PT} -context is the study of symmetries and conserved quantities. In this work, we will study some aspects of this topic. We will obtain a non-Hermitian set of operators that satisfy the commutation relations of the Lie $SO(3)$ rotation group. It will be shown that these operators generate rotations in the configuration space x_i , and not in the momentum space $\vec{p} = -i\nabla$ but in a modified non-Hermitian momentum space $\vec{p}_f = \vec{p} + i\vec{\nabla}f$, originally considered by Dirac in his seminal book [12]. Also, we will show that the Casimir of the algebra has real spectra and that its eigenfunctions, under the \mathcal{PT} -inner product, form a complete basis. This eigenfunctions will be called \mathcal{PT} -spherical harmonics.

Additionally we will study a central potential Hamiltonian with an additional complex term. It will be shown that the conventional angular momentum is not a conserved quantity anymore and we will have a modified non-Hermitian angular momentum operator. As a particular case, we obtain the solutions of the corresponding \mathcal{PT} -Hydrogen atom that includes a complex term, and it will be found that a non-Hermitian Runge–Lenz vector is a conserved quantity. Then we will have the non-Hermitian generators of the $SO(4)$ -Lie algebra.

This work is organized as follows: Sect. 2 make a brief review of \mathcal{PT} -theory and of conventional spherical harmonics, in Sect. 3 we study the \mathcal{PT} -rotations, in Sect. 4 we study the completeness relation, Sect. 5 is devoted to the study of symmetry transformations, in Sect. 6 we deal with the central potential problem, in Sect. 7 we will study the Hydrogen atom and at last we conclude with a summary of our results.

2 \mathcal{PT} -symmetry and spherical harmonics

In this section, a review of some well known facts of \mathcal{PT} -symmetry theory and spherical harmonics is made before consider the \mathcal{PT} -transformed version of this functions

2.1 \mathcal{PT} -inner product

\mathcal{PT} -theory considers the transformations under the parity operator \mathcal{P} and the time reversal operator \mathcal{T} . Under the \mathcal{P} -operator we have the transformation

$$(x, y, z) \rightarrow (-x, -y, -z) \quad (1)$$

and under \mathcal{T}

$$i \rightarrow -i \quad (2)$$

In this way, any function $f(\vec{x})$ can be transform as

$$\mathcal{PT}(f(\vec{x})) = f^*(-\vec{x}). \quad (3)$$

Note that, in spherical coordinates \mathcal{P} produces the transformation

$$(r, \theta, \varphi) \rightarrow (r, \pi - \theta, \varphi + \pi), \quad (4)$$

under the operator \mathcal{P} a f function transforms as

$$\mathcal{P}(f(r, \theta, \varphi)) = f(r, \pi - \theta, \varphi + \pi), \quad (5)$$

therefore

$$\mathcal{PT}(f(r, \theta, \varphi)) = f^*(r, \pi - \theta, \varphi + \pi). \quad (6)$$

Now, the \mathcal{PT} -inner product induced by the operators \mathcal{P} and \mathcal{T}

$$\langle f|g \rangle = \int d\vec{x} [\mathcal{PT}f(x)]g(x). \quad (7)$$

This expressions will be used in sections bellow. An exhaustive study of the \mathcal{PT} -theory can be found in [1].

2.2 Spherical harmonics

The angular momentum components are given by the Hermitian operators [13]

$$L_x = -i \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right), \quad L_y = -i \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right), \quad L_z = -i \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right).$$

Its algebra is given by

$$[L_x, L_y] = iL_z, \quad [L_z, L_x] = iL_y, \quad [L_y, L_z] = iL_x. \quad (8)$$

Considering $L^2 = L_x^2 + L_y^2 + L_z^2$ and Eq. (8), we have

$$[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = 0. \quad (9)$$

An important equation in mathematical-physics is the eigenvalue equation $L^2 Y_{lm} = l(l + 1)Y_{lm}$, $l = 0, 1, 2 \dots$, that in spherical coordinates is written

$$L^2 Y_{lm}(\theta, \varphi) = - \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y_{lm}(\theta, \varphi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y_{lm}(\theta, \varphi)}{\partial \varphi^2} \right] = l(l + 1)Y_{lm}(\theta, \varphi). \tag{10}$$

If $\varphi \in (0, 2\pi)$ and $\theta \in (0, \pi)$, the solutions of this equation are given by the spherical harmonics [14]

$$Y_{lm}(\theta, \varphi) = \sqrt{\frac{(2l + 1)(l - m)!}{4\pi(l + m)!}} e^{im\varphi} P_l^m(\cos \theta), \quad -l \leq m \leq l, \tag{11}$$

with $l = 0, 1, 2, 3$

$$P_l^m(u) = (-1)^m (1 - u^2)^{\frac{m}{2}} \frac{d^m}{du^m} P_l(u), \quad P_l(u) = \frac{1}{2^l l!} \frac{d^l}{du^l} (u^2 - 1)^l \tag{12}$$

where $P_l^m(u)$ denoted the associated Legendre polynomials and $P_l(u)$ the Legendre polynomials respectively. The spherical harmonics satisfy the orthonormality relation

$$(Y_{l'm'}(\theta, \varphi) | Y_{lm}(\theta, \varphi)) = \int d\Omega Y_{l'm'}^*(\theta, \varphi) Y_{lm}(\theta, \varphi) = \delta_{mm'} \delta_{ll'}. \tag{13}$$

where δ_{kl} is the Kronecker delta function.

Given that the spherical harmonics constitute an orthonormal basis, we can write any function $F(\theta, \varphi)$ as a linear combination of them, that is

$$F(\theta, \varphi) = \sum_{l \geq 0} \sum_{m=-l}^l C_{lm} Y_{lm}(\theta, \varphi). \tag{14}$$

Using Eq. (13), we find

$$C_{lm} = \int d\Omega Y_{lm}^*(\theta, \varphi) F(\theta, \varphi). \tag{15}$$

Substituting C_{lm} in Eq. (14) and making the change of variables $u' = \cos \theta'$, $u = \cos \theta$ we obtain

$$F(\theta, \varphi) = \int_0^{2\pi} d\varphi \int_{-1}^1 du' F(u', \varphi') \left(\sum_{l \geq 0} \sum_{m=-l}^l Y_{lm}^*(u', \varphi') Y_{lm}(u, \varphi) \right).$$

Therefore, the expression inside the parenthesis must be equal to $\delta(\varphi - \varphi') \delta(u - u')$, that is

$$\sum_{l \geq 0} \sum_{m=-l}^l Y_{lm}^*(\theta', \phi') Y_{lm}(\theta, \phi) = \delta(\phi - \phi') \delta(\cos \theta - \cos \theta'), \quad (16)$$

this expression is called completeness relation.

Under the parity operator the spherical harmonics transform as

$$\mathcal{P}(Y_{lm}(\theta, \varphi)) = Y_{lm}(\pi - \theta, \varphi + \pi) = (-1)^l Y_{lm}(\theta, \varphi), \quad (17)$$

and under the \mathcal{PT} -operator, we have

$$\mathcal{PT}(Y_{lm}(\theta, \varphi)) = Y_{lm}^*(\pi - \theta, \varphi + \pi) = (-1)^l Y_{lm}^*(\theta, \varphi). \quad (18)$$

This results will be used below.

3 \mathcal{PT} -symmetry and rotations

Given any $f = f(r, \theta, \varphi)$, we can define the operators

$$L_{fi} = e^f L_i e^{-f}. \quad (19)$$

In general L_{fi} is a non-Hermitian operator, however

$$[L_{fx}, L_{fy}] = iL_{fz}, \quad [L_{fz}, L_{fx}] = iL_{fy}, \quad [L_{fy}, L_{fz}] = iL_{fx}, \quad (20)$$

that we can identify as the $SO(3)$ -Lie algebra commutation relations. Considering $L_f^2 = L_{fx}^2 + L_{fy}^2 + L_{fz}^2$ and Eq. (20), we have

$$[L_f^2, L_{fi}] = 0, \quad (21)$$

therefore, we have the same algebra as the one satisfied by L_i . Besides

$$L_f^2 Y_{flm}(\theta, \varphi) = l(l+1) Y_{flm}(\theta, \varphi), \quad Y_{flm}(\theta, \varphi) = e^f Y_{lm}(\theta, \varphi), \quad (22)$$

that will be called \mathcal{PT} -spherical harmonics. In this case, the \mathcal{PT} -inner product is given by

$$\langle Y_{f'l'm'}(\theta, \varphi) | Y_{flm}(\theta, \varphi) \rangle_f = \int d\Omega \mathcal{PT}(Y_{f'l'm'}(\theta, \varphi)) Y_{flm}(\theta, \varphi). \quad (23)$$

Under a \mathcal{PT} -transformation, we have

$$\mathcal{PT}(Y_{flm}) = e^{f^*(r, \pi - \theta, \varphi + \pi)} (-1)^l Y_{lm}^*(\theta, \varphi). \quad (24)$$

therefore we can write

$$\langle Y_{f'l'm'}(\theta, \varphi) | Y_{flm}(\theta, \varphi) \rangle_f = (-1)^l \int d\Omega e^{f^*(r, \pi - \theta, \varphi + \pi) + f(r, \theta, \varphi)} Y_{l'm'}^*(\theta, \varphi) Y_{lm}(\theta, \varphi).$$

It becomes clear that, under this inner product not any function f allows the set Y_{flm} to be an orthogonal set. However, if the following condition is fulfilled

$$e^{f^*(r, \pi - \theta, \varphi + \pi) + f(r, \theta, \varphi)} = \lambda, \quad \lambda = \text{const} \tag{25}$$

then we have

$$\langle Y_{f'l'm'}(\theta, \varphi) | Y_{flm}(\theta, \varphi) \rangle_f = (-1)^l \lambda \delta_{l'l} \delta_{m'm}. \tag{26}$$

In this way, the spherical harmonics $Y_{flm}(\theta, \varphi)$ are orthogonal under the \mathcal{PT} -inner product only if Eq. (25) is satisfy. It is worthy to mention that due to the parity of the wave functions, in some \mathcal{PT} -symmetry systems the following orthogonality relations

$$\langle \phi_m | \phi_n \rangle = (-1)^n \delta_{m,n}, \tag{27}$$

may be obtained [1].

4 Completeness relation

Using the \mathcal{PT} -spherical harmonics $Y_{flm}(\theta, \varphi)$, we can have the expansion

$$F(\theta, \varphi) = \sum_{l \geq 0} \sum_{m=-l}^l a_{lm} Y_{flm}(\theta, \varphi). \tag{28}$$

Appeling to the orthonormality relations Eq. (26), we find

$$a_{lm} = \frac{(-1)^l}{\lambda} \langle Y_{flm}(\theta, \varphi) | F(\theta, \varphi) \rangle_f = \frac{(-1)^l}{\lambda} \int d\Omega \mathcal{PT} (Y_{flm}(\theta, \varphi)) F(\theta, \varphi) \tag{29}$$

substituting this result into Eq. (28), we obtain

$$\begin{aligned} F(\theta, \varphi) &= \sum_{l \geq 0} \sum_{m=-l}^l \frac{(-1)^l}{\lambda} \int d\Omega' \mathcal{PT} (Y_{flm}(\theta', \varphi')) F(\theta', \varphi') Y_{flm}(\theta, \varphi) \\ &= \int d\Omega' F(\theta', \varphi') \left[\sum_{l \geq 0} \sum_{m=-l}^l \frac{(-1)^l}{\lambda} \mathcal{PT} (Y_{flm}(\theta', \varphi')) Y_{flm}(\theta, \varphi) \right] \\ &= \int d\Omega' F(\theta', \varphi') \left[\sum_{l \geq 0} \sum_{m=-l}^l \frac{e^{f^*(r, \pi - \theta', \varphi' + \pi) + f(r, \theta, \varphi)}}{\lambda} Y_{lm}^*(\theta', \varphi') Y_{lm}(\theta, \varphi) \right], \end{aligned}$$

therefore

$$\delta(\phi - \phi')\delta(\cos\theta - \cos\theta') = \sum_{l \geq 0} \sum_{m=-l}^l \frac{e^{f^*(r, \pi - \theta', \phi' + \pi) + f(r, \theta, \phi)}}{\lambda} Y_{lm}^*(\theta', \phi') Y_{lm}(\theta, \phi). \quad (30)$$

This is the completeness relation for the \mathcal{PT} -spherical harmonics. A similar completeness relation is found for different systems in \mathcal{PT} -quantum mechanics [1].

5 Symmetry transformations

Consider the operators A, B, C that satisfy the following commutation relations

$$[A, B] = C. \quad (31)$$

Transforming the A, B, C operators, we obtain $A_f = e^f A e^{-f}$, $B_f = e^f B e^{-f}$ y $C_f = e^f C e^{-f}$, then

$$[A_f, B_f] = C_f. \quad (32)$$

We know that $[L_i, x_j] = i\epsilon_{ijk}x_k$, where x_k is the position operator. If we consider the transformation $x_{fi} = e^f x_i e^{-f} = x_i$, we arrive to

$$[L_{fi}, x_j] = i\epsilon_{ijk}x_k, \quad (33)$$

therefore the operators L_{fi} generate infinitesimal rotations in the space x_i . However, as the momentum operator is given by $p_i = -i\frac{\partial}{\partial x^i}$, then

$$[L_{fi}, p_j] \neq i\epsilon_{ijk}p_k, \quad (34)$$

and we say that the operators L_{fi} does not generate infinitesimal rotations in the space p_i . Now, if p_{fi} is given by $p_{fi} = e^f p_i e^{-f}$, then we have

$$[L_{fi}, p_{fj}] = i\epsilon_{ijk}p_{fk}. \quad (35)$$

Note that

$$\vec{p}_f = e^f \vec{p} e^{-f} = \vec{p} + i\vec{\nabla}f. \quad (36)$$

this operator was studied by Dirac in his seminal book [12] and is also obtained by Andersen in his work about canonical transformations but without given the conditions under which the \mathcal{PT} symmetry is preserved. If the Hamiltonian operator is given by

$$H = \frac{\vec{p}^2}{2m} + V(r), \quad (37)$$

then

$$[L_i, H] = 0. \tag{38}$$

Defining H_f by

$$H_f = e^f H e^{-f}, \tag{39}$$

we have that, in general

$$[L_i, H_f] \neq 0, \tag{40}$$

therefore the angular momentum L_i is not a conserved quantity for Hamiltonians of the form H_f . However

$$[L_{fi}, H_f] = 0, \tag{41}$$

then the modified angular momentum L_{fi} is conserved. Note that the Hamiltonian H_f is given by

$$H_f = \frac{\vec{p}_f^2}{2m} + V(r) = \frac{m}{2} \left(\vec{p} + i\vec{\nabla}f \right)^2 + V(r) \tag{42}$$

In the next section we will consider one important example.

6 The central problem

Consider the Hamiltonian

$$H = \frac{m}{2} \vec{p}^2 + V(x, y, z), \tag{43}$$

then

$$\begin{aligned} H_f &= e^f H e^{-f} = \frac{m}{2} \left(\vec{p} + i\vec{\nabla}f \right)^2 + V(x, y, z) \\ &= \frac{m}{2} \left(\vec{p}^2 + 2i\vec{\nabla}f \cdot \vec{p} + (\nabla^2 f) - (\vec{\nabla}f)^2 \right) + V(x, y, z), \end{aligned} \tag{44}$$

that is a non-Hermitian Hamiltonian. If the potential is given by

$$V(x, y, z) = -\frac{m}{2} \left(\nabla^2 f - (\vec{\nabla}f)^2 \right) + U(x, y, z), \tag{45}$$

then we can write

$$H_f = \frac{m}{2} \left(\vec{p}^2 + 2i\vec{\nabla}f \cdot \vec{p} \right) + U(x, y, z). \tag{46}$$

This kind of Hamiltonians naturally arise in some statistical models [15].

Note that if ψ is an eigenfunction in the equation

$$H\psi = E\psi \quad (47)$$

then we can define the f -states $\psi_f = e^f \psi$ that satisfy

$$H_f \psi_f = E \psi_f. \quad (48)$$

It follows that although H_f is a non-Hermitian operator it does have a real spectrum.

As an example, let us consider the central potential problem $V(r)$ whose Schrodinger equation is given by [13]

$$H\psi = \left(\frac{m}{2} \vec{p}^2 + V(r) \right) \psi = E\psi \quad (49)$$

and whose solutions

$$\psi_E(r, \theta, \varphi) = \phi_E(r) Y_{lm}(\theta, \varphi) \quad (50)$$

satisfy the orthogonality relations

$$\langle \psi_{E'}(r, \theta, \varphi) | \psi_E(r, \theta, \varphi) \rangle = \int dr r^2 d\Omega \psi_{E'}^*(r, \theta, \varphi) \psi_E(r, \theta, \varphi) = \delta_{EE'}. \quad (51)$$

Then the solutions of the equation

$$\begin{aligned} H_f \psi_f &= \left[\frac{m}{2} \left(\vec{p}^2 + 2i \vec{\nabla} f \cdot \vec{p} + \nabla^2 f - (\vec{\nabla} f)^2 \right) + V(r) \right] \psi_f \\ &= E \psi_f \end{aligned} \quad (52)$$

are given by

$$\psi_{Ef}(r, \theta, \varphi) = e^{f(r, \theta, \varphi)} \phi_E(r) Y_{lm}(\theta, \varphi). \quad (53)$$

The \mathcal{PT} -inner product for the ψ_f -states is given by

$$\begin{aligned} \langle \psi_{E'f}(r, \theta, \varphi) | \psi_{Ef}(r, \theta, \varphi) \rangle_f &= \int dr d\Omega \mathcal{PT} (\psi_{E'f}(r, \theta, \varphi)) \psi_{Ef}(r, \theta, \varphi) \\ &= \int dr d\Omega (-1)^l e^{f^*(r, \pi - \theta, \varphi + \pi) + f(r, \theta, \varphi)} \phi_{E'}^*(r) \phi_E(r) Y_{l'm'}^*(\theta, \varphi) Y_{lm}(\theta, \varphi). \end{aligned}$$

Besides, if $f(r, \theta, \varphi)$ satisfies Eq. (25) and considering Eq. (51), we have

$$\begin{aligned} \langle \psi_{E'f}(r, \theta, \varphi) | \psi_{Ef}(r, \theta, \varphi) \rangle_f &= (-1)^l \lambda \int dr d\Omega \phi_{E'}^*(r) \phi_E(r) Y_{l'm'}^*(\theta, \varphi) Y_{lm}(\theta, \varphi) \\ &= \lambda (-1)^l \delta_{EE'}. \end{aligned} \quad (54)$$

Given that $[L_i, H_f] \neq 0$, it follows that L_i is not a conserved quantity. However, as

$$[L_{fi}, H_f] = 0, \tag{55}$$

then L_{fi} is conserved.

7 The Hydrogen atom

In the case of the Hydrogen atom, we have the potential

$$V(r) = -\frac{Ze^2}{r}, \tag{56}$$

where the solutions are given by

$$\begin{aligned} \psi_{Nlm}(\rho, \theta, \varphi) &= \frac{2}{N^2} \sqrt{\frac{Z^3}{a_{RB}^3} \frac{(N-l-1)!}{(N+l)!}} \rho^l L_{N-(l+1)}^{2l+1}(\rho) e^{-\frac{\rho}{2}} Y_{lm}(\theta, \varphi), \\ E_N &= -\frac{Ze^2}{a_{RB}N^2}, \quad N = n + l + 1, \quad n = 0, 1, 2 \dots, \end{aligned}$$

where a_{RB} is the Bohr radius and

$$\rho = \alpha r, \quad \alpha = 2\sqrt{\frac{-2mE}{\hbar^2}}. \tag{57}$$

Taking into account Eq. (52), we have the equation

$$H_f \psi_f = \left[\frac{m}{2} \left(\vec{p}^2 + 2i \vec{\nabla} f \cdot \vec{p} + \nabla^2 f - (\vec{\nabla} f)^2 \right) - \frac{Ze^2}{r} \right] \psi_f = E \psi_f \tag{58}$$

whose solutions are given by

$$\psi_{fNlm}(\rho, \theta, \varphi) = e^{f(r,\theta,\varphi)} \psi_{Nlm}(\rho, \theta, \varphi) \tag{59}$$

this are orthogonal functions if equation (25) is satisfied. A remarkable fact is that L_{fi} is a conserved quantity. In the conventional Hydrogen atom, the Runge–Lenz vector is also conserved [13]

$$R_i = \frac{1}{2} \left(\vec{L} \times \vec{p} - \vec{p} \times \vec{L} + \frac{Ze^2 \vec{r}}{r} \right)_i. \tag{60}$$

In the case of the Hamiltonian H_f , we have

$$[R_{fi}, H_f] = 0, \tag{61}$$

and we can say that the transformed non-Hermitian Runge–Lenz vector is conserved.

Note that in this case, we have obtained a set of conserved quantities L_{fi} , L_f^2 , R_{fi} , that are the non-Hermitian generators of the $SO(4)$ algebra.

8 Conclusions

In this work we have constructed a set of non-Hermitian operators L_{fi} that satisfy the commutation relations of the $SO(3)$ -Lie algebra. We have shown that this operators generate rotations in the configuration space and not in the conventional momentum space but in a modified non-Hermitian momentum space $\vec{p}_f = \vec{p} + i\nabla f$. It is worthy to mention that this operator was originally considered by Dirac in his seminal book and corresponds to a canonical transformation studied in [16]. Besides, the L_{if} generators are related with a new type of spherical harmonics that result to be \mathcal{PT} -orthonormal. Additionally, we have shown that this quantities are conserved for mechanical systems described by a central potential Hamiltonian with an additional complex term. As a particular case, we have obtained the solutions of the corresponding \mathcal{PT} -Hydrogen atom that includes a complex term, and we have found that a non-Hermitian Runge–Lenz vector is a conserved quantity. Considering this case, one remarkable result is that, as we have obtained the non-Hermitian generators of the $SO(3)$ -Lie algebra and also a non-Hermitian Runge–Lenz vector, then we have the non-Hermitian generators of the $SO(4)$ -Lie algebra.

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