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Brief Reports

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Connection between the hydrogen atom and the four-dimensional oscillator

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The connection between the three-dimensional hydrogen atom and a four-dimensional harmonic oscillator (or equivalently a coupled pair of two-dimensional harmonic oscillators) subjected to a constraint condition is further explored. In particular, the role the constraint condition plays in determining the phase relationship between the pair of two-dimensional oscillators is examined. Furthermore, the connection is discussed in a group-theoretical context involving the Lie algebras of SO(4), SO(3,1), E(3), SO(4,2), and Sp(8, $\mathbb{R}$).

I. INTRODUCTION

The connection between the (three-dimensional) hydrogen atom and the four-dimensional isotropic harmonic oscillator has been a subject of considerable interest in the last 15 years (cf. Refs. 1–6). Recently, a number of papers have appeared in the literature[7–11] in which the connection is further discussed. In Refs. 7–9, the connection is established directly without making use of what is now often referred to as the Kustaanheimo-Stiefel (KS) transformation by introducing boson realizations of the angular momentum operator **L** and the Laplace-Runge-Lenz-Pauli operator **A** and by using two basic conditions satisfied by **L** and **A**, and the Hamiltonian operator H of the hydrogen atom. The approach in Refs. 7–9 is particularly appropriate to generate the dynamical symmetry group SO(4,2) of the three-dimensional hydrogen atom from the dynamical symmetry group Sp(8, $\mathbb{R}$) of the four-dimensional harmonic oscillator. Furthermore, Cornish[10] derived the hydrogen-oscillator connection by defining two complex stereographic coordinates, which can be shown to be the complex version of the KS coordinates, and discussed the physical significance of the constraint imposed by the KS transformation. Finally, Gracia-Bondía[11] used the KS transformation to obtain the connection and proceeded to derive the Green's function for the hydrogen atom within the framework of the Weyl-Wigner-Moyal phase-space formulation of nonrelativistic quantum mechanics. In all the cited references, the theoretical and physical significance of the constraint (or annihilation) condition imposed by the KS transformation or by its equivalent, $\mathbf{L}\cdot\mathbf{A}=0$, is not fully discussed.

In this Brief Report, we will discuss in detail the role the constraint plays in determining the phase relationship between the pair of two-dimensional oscillators which arises when the space of the four-dimensional oscillator is broken in two parts, in eliminating the superfluous states, and in allowing for the separation of the hydrogenic system in parabolic coordinates. We will also show that the constraint is related to the fact that the SO(4) Lie algebra is the direct sum of two SO(3) Lie subalgebras spanned by two triads of operators. The relationship between the 15 infinitesimal generators of SO(4,2) and the 36 infinitesimal generators of Sp(8, $\mathbb{R}$) will also be discussed.

II. $\mathbb{R}^3-\mathbb{R}^2\otimes\mathbb{R}^2$ HYDROGEN-OSCILLATOR CONNECTION

We define the four-dimensional Cartesian coordinates by

$$y_1=y\cos\alpha\cos\beta\ , \tag{1}$$

$$y_2=y\cos\alpha\sin\beta\ , \tag{2}$$

$$y_3=y\sin\alpha\cos\gamma\ , \tag{3}$$

$$y_4=y\sin\alpha\sin\gamma\ . \tag{4}$$

They have been known for a long time (cf. Refs. 12 and 13) and can be related to the KS transformation $(y_1,y_2,y_3,y_4\rightarrow r,\theta,\phi)$, rewritten in the context of the discrete spectrum of the hydrogen atom, through the relationship $y^2=2r/n$, $\alpha=\theta/2$, and $\beta+\gamma=\phi$. (We work in a system such that $\hbar=Ze^2=m=1$ so that the discrete energy levels of hydrogen are $-1/n^2$.) The latter relationship is consistent with the constraint condition imposed by the KS transformation, which reads

$$y_2q_1-y_1q_2-y_4q_3+y_3q_4=0\ , \tag{5}$$

where $q_j = -i\partial/\partial y_j$. [Equation (5) and some similar relations in this paper are understood modulo their action on a wave function ψ of hydrogen.] Equation (5) is equivalent to $\mathbf{L}\cdot\mathbf{A}=0$ because[14]

$$\mathbf{L}\cdot\mathbf{A} = (a_1^\dagger a_1 + a_2^\dagger a_2 + a_3^\dagger a_3 + a_4^\dagger a_4 + 2) \times (a_2^\dagger a_1 - a_1^\dagger a_2 + a_3^\dagger a_4 - a_4^\dagger a_3) = 0 \ , \tag{6}$$

where

$$a_j = (y_j + iq_j)/\sqrt{2} \ , \tag{7}$$

$$a_j^\dagger = (y_j - iq_j)/\sqrt{2} \ . \tag{8}$$

It then follows that

$$a_2^\dagger a_1 - a_1^\dagger a_2 + a_3^\dagger a_4 - a_4^\dagger a_3 = i(y_2 q_1 - y_1 q_2 - y_4 q_3 + y_3 q_4) = 0 \ , \tag{9}$$

which agrees with Eq. (5). The determination of the relationship between the phase angles β and γ can be made if we express Eqs. (1)–(4) in the form

$$y_1 = \mu\cos\beta \ , \tag{10}$$

$$y_2 = \mu\sin\beta \ , \tag{11}$$

$$y_3 = \nu\cos\gamma \ , \tag{12}$$

$$y_4 = \nu\sin\gamma \ , \tag{13}$$

from which we obtain

$$\frac{\partial}{\partial y_1} = \cos\beta\frac{\partial}{\partial\mu} - \frac{\sin\beta}{\mu}\frac{\partial}{\partial\beta} \ , \tag{14}$$

$$\frac{\partial}{\partial y_2} = \sin\beta\frac{\partial}{\partial\mu} + \frac{\cos\beta}{\mu}\frac{\partial}{\partial\beta} \ , \tag{15}$$

$$\frac{\partial}{\partial y_3} = \cos\gamma\frac{\partial}{\partial\nu} - \frac{\sin\gamma}{\nu}\frac{\partial}{\partial\gamma} \ , \tag{16}$$

$$\frac{\partial}{\partial y_4} = \sin\gamma\frac{\partial}{\partial\nu} + \frac{\cos\gamma}{\nu}\frac{\partial}{\partial\gamma} \ . \tag{17}$$

Accordingly, Eq. (5) can be written out as [see Eq. (27) below]

$$N_3\psi = \frac{1}{2i}\left(\frac{\partial}{\partial\beta} - \frac{\partial}{\partial\gamma}\right)\psi = 0 \ . \tag{18}$$

Since the operator N_3 acts on the angular part $e^{im\phi}$ of the hydrogen wave function ψ, Eq. (18) can be satisfied only if $\phi = \beta + \gamma$. As a result, the transformation defined by Eqs. (10)–(13) allows converting the (quantum-mechanical) hydrogen atom problem into the one for a pair of *two-dimensional* isotropic harmonic oscillators which satisfy the following equations:

$$-\tfrac{1}{2}\left(\frac{\partial^2}{\partial\mu^2} + \frac{1}{\mu}\frac{\partial}{\partial\mu} + \frac{1}{\mu^2}\frac{\partial^2}{\partial\beta^2} - \mu^2\right)\psi = N_a\psi \ , \tag{19}$$

$$-\tfrac{1}{2}\left(\frac{\partial^2}{\partial\nu^2} + \frac{1}{\nu}\frac{\partial}{\partial\nu} + \frac{1}{\nu^2}\frac{\partial^2}{\partial\gamma^2} - \nu^2\right)\psi = N_b\psi \ , \tag{20}$$

$$L_3\psi = -\tfrac{1}{2}i\left(\frac{\partial}{\partial\beta} + \frac{\partial}{\partial\gamma}\right)\psi = m\psi \ , \tag{21}$$

with $N_a + N_b = 2n$. Equation (21) [cf. Eq. (24)] indicates that the two oscillators have the same angular momentum m. The replacement of the angular parts in Eqs. (19) and (20) by $-m^2$ yields the well-known equations for the hydrogen atom separated in the squared parabolic coordinates (cf. Ref. 15).

III. LIE ALGEBRAIC APPROACH

The operators L_3 and N_3 are members of two triads of operators (L_1, L_2, L_3) and (N_1, N_2, N_3) which are elements of two SO(3) Lie algebras, the direct sum of which forms the SO(4) Lie algebra. In terms of the KS coordinates, they are given by

$$L_1 = \tfrac{1}{2}(-y_2 q_3 + y_3 q_2 - y_1 q_4 + y_4 q_1) \ , \tag{22}$$

$$L_2 = \tfrac{1}{2}(y_1 q_3 - y_3 q_1 - y_2 q_4 + y_4 q_2) \ , \tag{23}$$

$$L_3 = \tfrac{1}{2}(y_1 q_2 - y_2 q_1 + y_3 q_4 - y_4 q_3) \ , \tag{24}$$

$$N_1 = \tfrac{1}{2}(-y_2 q_3 + y_3 q_2 + y_1 q_4 - y_4 q_1) \ , \tag{25}$$

$$N_2 = \tfrac{1}{2}(y_1 q_3 - y_3 q_1 + y_2 q_4 - y_4 q_2) \ , \tag{26}$$

$$N_3 = \tfrac{1}{2}(y_1 q_2 - y_2 q_1 - y_3 q_4 + y_4 q_3) \ . \tag{27}$$

It can be seen that the two sets of operators differ only in the sign of y_4 or, equivalently, the sign of γ. Thus, the hydrogenic wave functions are those associated with the right-handed oscillator[16] consisting of a pair of two-dimensional oscillators having the same angular momentum m. The constraint condition [Eq. (18)] then means that the operator N_3 annihilates the physical states of the hydrogen atom, for which L_3 is diagonal and $L_\pm = L_1 \pm iL_2$ are the raising and lowering operators. The roles of L_i and N_i are reversed when the sign of y_4 is reversed.

As a consequence, we can identify those generators of the group Sp(8, ℝ) that span the group SO(4,2). The 36 generators of Sp(8, ℝ) have been obtained in terms of four-dimensional Cartesian coordinates by Staunton.[17] The result of a comparison between the two sets of generators is given in Table I.

The group SO(4), a subgroup of both the special pseudo-orthogonal group SO(4,2) and the real symplectic group Sp(8, ℝ), is the degeneracy group of the hydrogenic bound states. The group SO(3,1) of the continuum states of the hydrogen atom is the analytic continuation of SO(4) when n is allowed to become $-i\eta$ while the Euclidean group E(3) for the zero-energy point is a contraction of SO(4). Since the angular momentum is energy independent, l and m remain good quantum numbers for all energies. The boson realizations of the Laplace-Runge-Lenz-Pauli vector $\mathbf{A}$ for positive energies and zero energy can be obtained by analytic continuation and group contraction, respectively. To obtain the vector $\mathbf{A}$ for $E>0$, we let n in $y_j = (2/n)^{1/2} s_j$, where $\sum_j s_j^2 = r$, be equal to $-i\eta$. For example (see Table I),

$$L_{14} = \tfrac{1}{2}\left(-\frac{n}{2}\frac{\partial^2}{\partial s_1 \partial s_3} + \frac{2}{n}s_1 s_3 + \frac{n}{2}\frac{\partial^2}{\partial s_2 \partial s_4} - \frac{2}{n}s_2 s_4\right)$$
$$\rightarrow \tfrac{1}{2}i\left(\frac{\eta}{2}\frac{\partial^2}{\partial s_1 \partial s_3} + \frac{2}{\eta}s_1 s_3 - \frac{\eta}{2}\frac{\partial^2}{\partial s_2 \partial s_4} - \frac{2}{\eta}s_2 s_4\right) \ . \tag{28}$$

The expression in the last set of parentheses is in the form

TABLE I. A comparison of the SO(4,2) generators and Sp(8,ℝ) generators. (See Ref. 17 for additional notations.)

SO(4,2)	Sp(8,ℝ)	$y_4 \to -y_4$
$L_{23}=L_1$	$-B_1$	$-F_{30}=N_1$
$L_{31}=L_2$	B_2	$T_2=N_2$
$L_{12}=L_3$	S_{12}	$E_{12}=N_3$
$L_{14}=\frac{1}{2}(q_1q_3+y_1y_3-q_2q_4-y_2y_4)$	$-F_{20}$	D_0
$L_{24}=\frac{1}{2}(q_2q_3+y_2y_3+q_1q_4+y_1y_4)$	$-F_{10}$	B_3
$L_{34}=\frac{1}{4}(q_1^2+q_2^2-q_3^2-q_4^2+y_1^2+y_2^2-y_3^2-y_4^2)$	C_0	C_0
$L_{15}=\frac{1}{2}(-q_1q_3+y_1y_3+q_2q_4-y_2y_4)$	$-F_{23}$	D_3
$L_{25}=\frac{1}{2}(-q_2q_3+y_2y_3-q_1q_4+y_1y_4)$	F_{31}	B_0
$L_{35}=\frac{1}{4}(-q_1^2-q_2^2+q_3^2+q_4^2+y_1^2+y_2^2-y_3^2-y_4^2)$	C_3	C_3
$L_{45}=\frac{1}{2}(-y_1q_1-y_2q_2-y_3q_3-y_4q_4+2i)$	$-S_{30}$	$-S_{30}$
$L_{36}=\frac{1}{2}(y_1q_1+y_2q_2-y_3q_3-y_4q_4)$	E_{30}	E_{30}
$L_{46}=\frac{1}{4}(-q_1^2-q_2^2-q_3^2-q_4^2+y_1^2+y_2^2+y_3^2+y_4^2)$	A_3	A_3
$L_{56}=\frac{1}{4}(q_1^2+q_2^2+q_3^2+q_4^2+y_1^2+y_2^2+y_3^2+y_4^2)$	A_0	A_0
$L_{16}=\frac{1}{2}(y_1q_3+y_3q_1-y_2q_4-y_4q_2)$	$-D_1$	F_{12}
$L_{26}=\frac{1}{2}(y_2q_3+y_3q_2+y_1q_4+y_4q_1)$	D_2	T_1

of the expression for L_{15} with the exception that n is replaced by η. Therefore, for $E>0$, we have $L_{j4}\to iL_{j5}$ and the Laplace-Runge-Lenz-Pauli vector is given by $i(L_{15},L_{25},L_{35})$ which is in agreement with the result in Ref. 8. For $E=0$, the vector $\mathbf{A}$ can be obtained by a group contraction process as follows:

$$A_j=\lim_{n\to\infty} L_{j4}/n=-\lim_{n\to\infty} L_{j5}/n=\frac{1}{2}\lim_{n\to\infty} \times(L_{j4}-L_{j5})/n=\frac{1}{2}(L_{j4}-L_{j5})/n \ . \tag{29}$$

This result again is in agreement with the result in Ref. 9 (see Appendix).

The group E(3) is the group of translations and rotations in three-dimensional space. The three-dimensional space for the group operations is the $\mathbf{u}$ space, which is the geometric inversion of the $\mathbf{p}$ space.[18] In the $\mathbf{u}$ space, we have $\mathbf{L}=\mathbf{u}\times\mathbf{A}=\mathbf{u}\times\mathbf{A}_0$, where $\mathbf{u}=2\mathbf{p}/p^2$, $\mathbf{A}=\mathbf{A}_0+\mathbf{u}/u^2$, $\mathbf{A}=-iu\nabla_u u^{-1}$, and $\mathbf{A}_0=-i\nabla_u$. It is interesting to note that $\mathbf{A}$ is a non-Hermitian operator and the zero-energy wave function is the eigenfunction of $\mathbf{A}$. The zero-energy wave function is not normalizable but can be shown to be orthogonal to all (non-zero-energy) bound state wave functions.

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APPENDIX

In this Appendix, we establish the agreement between the vector $\mathbf{A}$ and the vector $\mathbf{C}$ of Ref. 9. With $\mu=\hbar=1$ and $c=2\sqrt{\rho}$, we first let $s_1=cu_1$, $s_2=cu_4$, $s_3=cu_2$, $s_4=cu_3$, and $t_1=p_1/c$, $t_2=p_4/c$, $t_3=p_2/c$, $t_4=p_3/c$. Then, we obtain from Eqs. (13) and (27) of Ref. 9 the following boson operators:

$$a_1=\frac{1}{2}(t_3-s_4-it_4-is_3) \ , \tag{A1}$$

$$a_2=\frac{1}{2}(t_2-s_1-it_1-is_2) \ , \tag{A2}$$

$$a_3=\frac{1}{2}(-t_1+s_2+it_2+is_1) \ , \tag{A3}$$

$$a_4=\frac{1}{2}(-t_4+s_3+it_3+is_4) \ , \tag{A4}$$

with the operators $a_\alpha^\dagger$, $\alpha=1,2,3,4$, being the complex conjugate of a_α. According to the definition of $\mathbf{C}$ in Eq. (22) of Ref. 9, we have

$$C_1=\frac{1}{2}(ia_1^\dagger a_4^\dagger-ia_1a_4-ia_2^\dagger a_3^\dagger + ia_2a_3+a_1^\dagger a_1+a_4^\dagger a_4-a_2^\dagger a_2-a_3^\dagger a_3) \ .$$

Utilizing Eqs. (A1)–(A4), we can show that

$$\tfrac{1}{2}i(a_1^\dagger a_4^\dagger - a_1 a_4) = \tfrac{1}{4}(t_3^2 + t_4^2 - s_3^2 - s_4^2) \ ,$$

$$\tfrac{1}{2}i(a_2^\dagger a_3^\dagger - a_2 a_3) = \tfrac{1}{4}(t_1^2 + t_2^2 - s_1^2 - s_2^2) \ ,$$

$$\tfrac{1}{2}(a_1^\dagger a_1 + a_4^\dagger a_4) = \tfrac{1}{4}(t_3^2 + t_4^2 + s_3^2 + s_4^2) \ ,$$

$$\tfrac{1}{2}(a_2^\dagger a_2 + a_3^\dagger a_3) = \tfrac{1}{4}(t_1^2 + t_2^2 + s_1^2 + s_2^2) \ .$$

A substitution of these results yields

$$C_1 = \tfrac{1}{2}(-t_1^2 - t_2^2 + t_3^2 + t_4^2) \ .$$

On the other hand, since $y_\alpha = (2/n)^{1/2} s_\alpha$ and $q_\alpha = (n/2)^{1/2} t_\alpha$, with the use of L_{34} and L_{35} given in Table I we obtain from Eq. (29)

$$A_3 = (-t_1^2 - t_2^2 + t_3^2 + t_4^2)/8 \ .$$

Therefore, $C_1 = 4A_3$. In a similar manner, we can establish $L_1 = L_{12}$, $L_2 = L_{23}$, $L_3 = L_{31}$, $C_2 = 4A_1$, and $C_3 = 4A_2$. The factor of 4 does not affect the commutation relationship.

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