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Connection between the hydrogen atom and the harmonic oscillator: The zero-energy case

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The connection between the three-dimensional hydrogen atom and a four-dimensional harmonic oscillator obtained in previous works, from a hybridization of the infinitesimal Pauli approach to the hydrogen system with the Schwinger approach to spherical and hyperbolical angular momenta, is worked out in the case of the zero-energy point of the hydrogen atom. This leads to the equivalence of the three-dimensional hydrogen problem with a four-dimensional free-particle problem involving a *constraint* condition. For completeness, the latter result is also derived by using the Kustaanheimo-Stiefel transformation introduced in celestial mechanics. Finally, it is shown how the Lie algebra of SO(4,2) quite naturally arises for the whole spectrum (discrete plus continuum plus zero-energy point) of the three-dimensional hydrogen atom from the introduction of the *constraint* condition into the Lie algebra of $Sp(8,\mathbb{R})$ associated with the four-dimensional harmonic oscillator.

I. INTRODUCTION

Since the landmark works on the O(4,2) dynamical symmetry of the nonrelativistic hydrogen atom,[1] a large amount of papers has been devoted to the quantum-mechanical Coulomb problem (cf., for example, Refs. 2–15 and references therein). In particular, the link between the three-dimensional hydrogen atom and the four-dimensional isotropic harmonic oscillator has been investigated more or less independently by several people in recent years.[3–7,9–15] In this regard, a word on the pioneer (though little-known) work by Ikeda and Miyachi[4] is in order. These authors use the following (well-known) Cartesian coordinates of $\mathbb{R}^4$

$$X_1=\sqrt{r}\,\cos\frac{\theta}{2}\cos\frac{\phi+\psi}{2},\quad X_2=\sqrt{r}\,\cos\frac{\theta}{2}\sin\frac{\phi+\psi}{2}\ ,$$
$$X_3=\sqrt{r}\,\sin\frac{\theta}{2}\cos\frac{\phi-\psi}{2},\quad X_4=\sqrt{r}\,\sin\frac{\theta}{2}\sin\frac{\phi-\psi}{2}\ , \tag{1}$$

and from the Schrödinger equation for the four-dimensional isotropic harmonic oscillator expressed in the coordinates (r,θ,ϕ,ψ), they derive the one for the three-dimensional hydrogen atom by imposing an *auxiliary condition.* Similar derivations of results equivalent to the just mentioned result have been recently achieved by Chen[10–12] and Iwai.[13] On the other hand, the connection between the three-dimensional hydrogen atom and a four-dimensional isotropic harmonic oscillator with a *constraint* has been elegantly derived by Boiteux[5–7] on the basis of the so-called Kustaanheimo-Stiefel (KS) transformation introduced (as a by-product of the theory of spinors) for regularizing the three-dimensional Kepler problem of classical mechanics.[16] Indeed, the original and apparently distant derivations by Boiteux[5] and Ikeda and Miyachi[4] are closely related in view of the fact that Eq. (1) leads to

$$X_1^2+X_2^2-X_3^2-X_4^2=r\cos\theta\ ,$$
$$2(X_1X_3-X_2X_4)=r\sin\theta\cos\phi\ ,$$
$$2(X_1X_4+X_2X_3)=r\sin\theta\sin\phi\ ,$$

which are nothing but a rewriting (up to an S_4 permutation) of the defining relations for the KS transformation [cf. Eq. (2) below].

Most of the papers on the connection between the $\mathbb{R}^3$ hydrogen atom and the $\mathbb{R}^4$ harmonic oscillator are concerned with the cases $E<0$ (discrete spectrum) and $E>0$ (continuous spectrum) of the hydrogen atom spectrum. The case $E=0$ (zero-energy point) has received little attention although, on one hand, the zero-energy Coulomb problem turns out to be of interest in atomic scatterings of the three-body Coulomb systems and, on the other hand, the related zero-energy Kepler problem may find applications in astrophysics (cf. Ref. 8). The zero-energy case has been briefly touched upon by Barut, Schneider, and Wilson[9] in their investigation of "lightlike states" solutions for a wave equation set up in the framework of the quantum theory of infinite component SO(4,2) fields. In fact, it appears from Ref. 9 that a three-dimensional Kepler motion with zero total energy and a free motion in four space are connected via the KS transformation. Furthermore, it has been noted by Chen[11] that the application to the three-dimensional hydrogen atom problem of a transformation of the type of Eq. (1) produces, in the case $E=0$, an equation that leads to Bessel functions. Finally, the topological equivalence between the hydrogenic system with $E=0$ and the free-particle system has been established by Chen[12] from a transformation of the type of Eq. (1).

It is one of the aims of this paper to fully explore the case $E=0$. This work constitutes the third part (cf. Refs. 14 and

15 for the first and second parts) of a series devoted to the hydrogen-oscillator connection and its implication regarding the SO(4,2) dynamical symmetry of the three-dimensional hydrogen atom. The guideline followed in Ref. 14 for $E<0$ and Ref. 15 for $E>0$ lies on a hybridization of the infinitesimal method developed by Pauli (cf. Ref. 2) for the $\mathbb{R}^3$ hydrogen atom with the boson calculus used by Schwinger for the $\mathbb{R}^3$ angular momentum theory. This line of thought is applied in Sec. III of the present paper to the case $E=0$. For the sake of completeness and comparison, the hydrogen-oscillator connection in the case $E=0$ is also treated in Sec. II by using the KS transformation. Finally, Sec. IV concerns the other aim of this work. It is shown in Sec. IV how the hydrogen-oscillator connection allows one to easily introduce the group SO(4,2) for the whole spectrum ($E<0$, $E>0$, and $E=0$) of the three-dimensional hydrogen atom.

II. APPROACH VIA THE KS TRANSFORMATION

The KS transformation $\{x_i:\ i=1,2,3\}\to\{u_\alpha:\ \alpha=1,2,3,4\}$ corresponds to the $\mathbb{R}^4\to\mathbb{R}^3$ surjection defined by[16]

$$x_1=u_1^2-u_2^2-u_3^2+u_4^2 \ ,$$
$$x_2=2(u_1u_2-u_3u_4),\quad x_3=2(u_1u_3+u_2u_4) \ . \tag{2}$$

As a preliminary result, it is a simple matter of straightforward but cumbersome calculation to use Eq. (2) for transforming the $\mathbb{R}^3$ Laplace operator according to

$$\Delta_x=(1/4r)\Delta_u-(1/4r^2)X^2 \ , \tag{3}$$

where

$$r=\left(\sum_{j=1}^{3}x_j^2\right)^{1/2}=\sum_{\alpha=1}^{4}u_\alpha^2 \ ,$$
$$\Delta_x=\sum_{j=1}^{3}\frac{\partial^2}{\partial x_j^2},\quad \Delta_u=\sum_{\alpha=1}^{4}\frac{\partial^2}{\partial u_\alpha^2} \ ,$$
$$X=u_4\frac{\partial}{\partial u_1}-u_3\frac{\partial}{\partial u_2}+u_2\frac{\partial}{\partial u_3}-u_1\frac{\partial}{\partial u_4} \ .$$

The operator X turns out to be the infinitesimal operator of a subgroup U(1) of a group O(4) that proves to be related to a group Sp(8,$\mathbb{R}$), cf. Sec. IV. [It should be realized that the term $-(1/4r^2)X^2$ in Eq. (3) has been overlooked in certain works dealing with the KS transformation.]

We are now in a position to transform the Schrödinger equation

$$[-(\hbar^2/2\mu)\Delta_x-Ze^2/r]\psi=E\psi \tag{4}$$

of a three-dimensional hydrogenlike atom with reduced mass μ and nucleus charge Ze. Equation (3) makes it possible to turn Eq. (4) into the $\mathbb{R}^4$ partial differential equation:

$$[-(\hbar^2/2\mu)\Delta_u+(\hbar^2/2\mu r)X^2-4Ze^2]\psi=4rE\psi \ . \tag{5}$$

By adopting the line of reasoning of Boiteux,[5] we take $X\psi=0$ in order to ensure the wave function ψ be univalued. Hence, Eq. (5) yields the system formed by the $\mathbb{R}^4$ Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu}\sum_{\alpha=1}^{4}\frac{\partial^2}{\partial u_\alpha^2}-4E\sum_{\alpha=1}^{4}u_\alpha^2\right)\psi=4Ze^2\psi \tag{6}$$

accompanied by the constraint relation (indeed a superselection rule, cf. Refs. 5-7)

$$\left(u_4\frac{\partial}{\partial u_1}-u_3\frac{\partial}{\partial u_2}+u_2\frac{\partial}{\partial u_3}-u_1\frac{\partial}{\partial u_4}\right)\psi=0 \ .$$

Equation (6) may be tackled for $E<0$, $E>0$, and $E=0$. In the case $E<0$, Eq. (6) identifies to the Schrödinger equation of a four-dimensional isotropic harmonic oscillator *with attractive potential* and this case has received a great deal of attention.[5-7,9] Less attention has been focused on the case where $E>0$ in Eq. (6) for which Eq. (6) can be regarded as the Schrödinger equation of a four-dimensional isotropic harmonic oscillator *with repulsive potential*.[9,15] The case when $E=0$ in Eq. (6) seems to have attracted little attention.[9]

In the case $E=0$, Eq. (6) reads

$$-\frac{\hbar^2}{2\mu}\sum_{\alpha=1}^{4}\frac{\partial^2\psi}{\partial u_\alpha^2}=4Ze^2\psi \ .$$

As a net result, the Schrödinger equation for a three-dimensional hydrogenlike atom with zero energy is equivalent to the Schrödinger equation for a four-dimensional free particle with energy $4Ze^2$:

$$(1/2\mu)(p_1^2+p_2^2+p_3^2+p_4^2)\psi=4Ze^2\psi \tag{7}$$

supplemented by the auxiliary condition:

$$(u_4p_1-u_3p_2+u_2p_3-u_1p_4)\psi=0 \ , \tag{8}$$

where p_α stands for $(\hbar/i)\partial/\partial u_\alpha$ with $\alpha=1,2,3,4$.

For the purpose of preparing an easy comparison of the preceding result with the corresponding one in Sec. III, we now introduce the canonical transformation $\{u_\alpha,p_\alpha:\ \alpha=1,2,3,4\}\to\{Q_\alpha,P_\alpha:\ \alpha=1,2,3,4\}$ defined by

$$p_1=-\sqrt{2}(\rho Q_3+P_2),\quad u_1=(\tfrac{1}{4}\sqrt{2})(-Q_2+P_3/\rho) \ ,$$
$$p_2=\sqrt{2}(\rho Q_1+P_4),\quad u_2=(\tfrac{1}{4}\sqrt{2})(Q_4-P_1/\rho) \ ,$$
$$p_3=-\sqrt{2}(\rho Q_4+P_1),\quad u_3=(\tfrac{1}{4}\sqrt{2})(-Q_1+P_4/\rho) \ ,$$
$$p_4=\sqrt{2}(\rho Q_2+P_3),\quad u_4=(\tfrac{1}{4}\sqrt{2})(Q_3-P_2/\rho) \ ,$$

where ρ is an arbitrary parameter we take in the form $\rho=\mu\omega$. This transformation enables us to rewrite Eqs. (7) and (8) as

$$[(1/2\mu)(P_1^2+P_2^2+P_3^2+P_4^2)+(\mu\omega^2/2)(Q_1^2+Q_2^2+Q_3^2+Q_4^2)+\omega(P_1Q_4+P_2Q_3+P_3Q_2+P_4Q_1)]\psi=2Ze^2\psi \tag{9}$$

and

$$[(1/2\mu)(P_1^2+P_2^2-P_3^2-P_4^2)+(\mu\omega^2/2)(Q_1^2+Q_2^2-Q_3^2-Q_4^2)]\psi=0 \ , \tag{10}$$

respectively. Clearly, Eq. (9) involves a four-dimensional isotropic harmonic oscillator part and Eq. (10) shows that this oscillator splits into a pair of coupled two-dimensional isotropic harmonic oscillators.

III. APPROACH VIA THE BOSON CALCULUS

We now consider the Pauli equations (published in 1926) in the situation where $E=0$. In the notation of Ref. 2, they write

$$[L_j,\ L_k]=i\hbar\epsilon_{jkl}L_l,\ [M_j,\ M_k]=0\ ,\quad [L_j,\ M_k]=i\hbar\epsilon_{jkl}M_l\ , \tag{11}$$

$$\vec{L}\cdot\vec{M}=\vec{M}\cdot\vec{L}=0\ , \tag{12}$$

$$\vec{M}^2-(Ze^2)^2=0\ , \tag{13}$$

where $\vec{L}\equiv(L_1,L_2,L_3)$ and $\vec{M}\equiv(M_1,M_2,M_3)$ denote the angular momentum operator and the Laplace-Runge-Lenz-Pauli operator corresponding to the three-dimensional hydrogenlike atom considered in Sec. II. As is well known, Eqs. (11) characterize the Lie algebra of $E(3)$. The cornerstone of the present approach is to find a boson realization of Eqs. (11). Following our previous works,[14,15] we construct the realization of $\vec{L}$ and $\vec{M}$ from the set $\{a_\alpha a_\beta, a_\alpha^\dagger a_\beta^\dagger, a_\alpha^\dagger a_\beta:\ \alpha,\beta=1,2,3,4\}$ of the elements of the Lie algebra of Sp(8,ℝ). From Ref. 9, it is an affair of combining a few relations to extract the following realization of $\vec{L}$ and $\vec{M}=\omega\vec{C}$:

$$\begin{aligned}
L_1&=\tfrac{1}{2}(a^\dagger\sigma_3 a+b^\dagger\sigma_3 b)\hbar\ ,\\
L_2&=\tfrac{1}{2}(a^\dagger\sigma_2 a-b^\dagger\sigma_2 b)\hbar\ ,\\
L_3&=-\tfrac{1}{2}(a^\dagger\sigma_1 a-b^\dagger\sigma_1 b)\hbar\ ,\\
C_1&=-\tfrac{1}{2}(a^\dagger\sigma_2\tilde{b}^\dagger-\tilde{a}\sigma_2 b-a^\dagger\sigma_3 a+b^\dagger\sigma_3 b)\hbar\ ,\\
C_2&=\tfrac{1}{2}(a^\dagger\sigma_3\tilde{b}^\dagger+\tilde{a}\sigma_3 b+a^\dagger\sigma_2 a+b^\dagger\sigma_2 b)\hbar\ ,\\
C_3&=-\tfrac{1}{2}(ia^\dagger\tilde{b}^\dagger-i\tilde{a}b+a^\dagger\sigma_1 a+b^\dagger\sigma_1 b)\hbar\ ,
\end{aligned} \tag{14}$$

where a, b, $a^\dagger$, $b^\dagger$, $\tilde{a}$, and $\tilde{b}^\dagger$ are defined from the row vectors $\tilde{a}=(a_1,\ a_2)$ and $\tilde{b}=(a_3,\ a_4)$ while σ_1, σ_2, and σ_3 stand for the Pauli matrices. It may be checked that Eq. (14) does satisfy the commutation relations (11). The realization afforded by Eq. (14) allows us to write Eqs. (12) and (13) in the enveloping algebra of the Lie algebra of Sp(8,ℝ). As a matter of fact, by introducing (14) into (12) and (13), we get

$$(a_1^\dagger a_1+a_2^\dagger a_2-a_3^\dagger a_3-a_4^\dagger a_4)(ia_1^\dagger a_4^\dagger-ia_1a_4+ia_2^\dagger a_3^\dagger-ia_2a_3+a_1^\dagger a_1+a_2^\dagger a_2+a_3^\dagger a_3+a_4^\dagger a_4+2)=0 \tag{15}$$

and

$$(ia_1^\dagger a_4^\dagger-ia_1a_4+ia_2^\dagger a_3^\dagger-ia_2a_3+a_1^\dagger a_1+a_2^\dagger a_2+a_3^\dagger a_3+a_4^\dagger a_4+2)^2-(2Ze^2/\hbar\omega)^2=0\ , \tag{16}$$

respectively. The system set up from Eqs. (15) and (16) admits as a solution

$$ia_1^\dagger a_4^\dagger-ia_1a_4+ia_2^\dagger a_3^\dagger-ia_2a_3+a_1^\dagger a_1+a_2^\dagger a_2+a_3^\dagger a_3+a_4^\dagger a_4+2=2Ze^2/\hbar\omega \tag{17}$$

and

$$a_1^\dagger a_1+a_2^\dagger a_2-a_3^\dagger a_3-a_4^\dagger a_4=0\ . \tag{18}$$

[Of course Eqs. (17) and (18) should be understood modulo their action on a state vector ψ.] Then, by passing from the a_α and $a_\alpha^\dagger$ to the Q_α and $P_\alpha(\alpha=1,2,3,4)$ with the help of the standard formulas

$$a_\alpha=(\mu\omega/2\hbar)^{1/2}Q_\alpha+i(1/2\hbar\mu\omega)^{1/2}P_\alpha\ ,$$
$$a_\alpha^\dagger=(\mu\omega/2\hbar)^{1/2}Q_\alpha-i(1/2\hbar\mu\omega)^{1/2}P_\alpha\ ,$$

we finally obtain that Eqs. (17) and (18) acting on ψ become identical to Eqs. (9) and (10), respectively.

IV. A NEW WAY TO INTRODUCE O(4,2)

We note that the constraint condition [Eq. (18)], obtained in the approach of Sec. III to the case $E=0$, coincides with the ones derived for the cases $E<0$ (cf. Ref. 14) and $E>0$ (cf. Ref. 15). It is appealing to examine the significance of such a condition from a group-theoretical point of view. As a result, it is straightforward to show that the introduction of Eq. (18) into the Lie algebra of Sp(8,ℝ) spanned by the 36 bilinears $a_\alpha a_\beta$, $a_\alpha^\dagger a_\beta^\dagger$, and $a_\alpha^\dagger a_\beta$ produces a Lie algebra *under constraint* which is isomorphic to the Lie algebra of SU(2,2), one of the covering groups of SO(4,2). This clearly shows the relevance of O(4,2) for the whole spectrum ($E<0$, $E>0$, and $E=0$) of the three-dimensional hydrogen atom. [We note that the original derivation of O(4,2), or more precisely O(6,ℂ), by Malkin and Man'ko[1] is concerned with the discrete spectrum of the hydrogen atom.]

We do not give the details of the derivation of the Lie algebra of SU(2,2) from the one of Sp(8,ℝ) under constraint. It is sufficient to understand the concept of a Lie algebra under constraint from the following trivial example. Let us consider the Lie algebra of SO(4) symbolized by $\vec{L}\times\vec{L}=i\vec{L}$, $\vec{L}\times\vec{A}=i\vec{A}$, and $\vec{A}\times\vec{A}=i\vec{L}$. The introduction of the constraint $\vec{A}=\vec{L}$ reduces the Lie algebra of SO(4) to the one of SO(3) and we hence say that the Lie algebra of SO(3) derives from the Lie algebra of SO(4) under constraint. From a mathematical viewpoint, the concept of a Lie algebra under constraint corresponds to the notion of quotient.

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