TOPICAL REVIEW

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Topical Review

Shared symmetries of the hydrogen atom and the two-bit system

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Abstract

The hydrogen atom is the simplest system of atomic and molecular physics, while a two-qubit system is the simplest of quantum information. Remarkably, they share common symmetry aspects which are described in this paper, based on a correspondence between the four-dimensional unitary group and the six-dimensional rotational group with its non-compact extensions. Both systems involve 15 basic operators. Reductions to Lorentz and Poincare space–time group symmetries of a free particle are also discussed.

Keywords: symmetry of hydrogen, two-qubit pair, unitary and orthogonal groups, dynamical symmetry group, 15-parameter algebra/group

(Some figures may appear in colour only in the online journal)

1. Introduction

Our understanding of the structure and stability of the hydrogen atom grew alongside the development of quantum mechanics from its beginnings 100 years ago. As the simplest atomic system, the non-relativistic hydrogen atom also lent the language and notation for all larger atoms and molecules. With bound state energy levels having a larger degenerate manifold of states than expected from the spherical symmetry of the Coulomb interaction, it also became a paradigm throughout physics for systems with such larger symmetry. Most physicists are familiar with this symmetry under four-dimensional rotations called the SO(4) group, larger than that under SO(3) expected on the basis of the spherical symmetry of the $1/r$ potential between the proton and the electron [1]. Incidentally, yet another general context and extension of this basic system is that it applies to any other 'hydrogen-like' system of a positive $(+Ze)$ and a negative $(-e)$ particle bound together as in positron-electron (positronium), proton–anti-proton, positron-antiproton (anti-hydrogen), proton-muon, etc. The latest realization of such variants are exotic combinations such as a kaon and a pion [2]. Apart from a change in scale of lengths and energies because of differing reduced mass μ of the pair, they share a common physics. And, very recently, a spectroscopic transition, between the ground and first excited state, has been directly observed in the anti-hydrogen atom [3].

Somewhat less familiar are even higher symmetry groups such as the non-compact Lorentz group SO(3, 1), the five-dimensional SO(5) and non-compact counterpart SO(4, 1), and the six-dimensional non-compact SO(4, 2) that provide the full symmetry of the system, embracing all energy states of hydrogen, including also the continuum states, and further, also transitions between the states [4–6]. The dimension of these groups, which is also the number of basic generators, is six for four-dimensional, ten for five-dimensional and fifteen for the six-dimensional groups involved.

Turning to a spin-$1/2$ system, also a two-level system of quantum optics and the basic 'qubit' of the field of quantum information (cryptography, computation, teleportation) [7], it has the well-known symmetry group SU(2), also with three generators (the Pauli spin operators). Also well known is that

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Table 1. Generators of rotation group SO(3).

0	ℓ_z	$-\ell_y$
$-\ell_z$	0	ℓ_x
ℓ_y	$-\ell_x$	0

Table 2. Generators of rotation group SO(4).

0	ℓ_z	$-\ell_y$	A_x
$-\ell_z$	0	ℓ_x	A_y
ℓ_y	$-\ell_x$	0	A_z
$-A_x$	$-A_y$	$-A_z$	0

this group is isomorphic to the rotation group SO(3) of the spherically symmetric Coulomb system of the hydrogen atom, apart from a technical point of SU(2) being a double 'covering' group of SO(3). This feature has also been exploited from the start in the fields of nuclear magnetic and electron spin resonance to view evolution of a quantum spin in terms of rotations of a real vector on a 'Bloch sphere,' unitary evolution of a complex two-column vector captured in more immediate geometrical terms as rotations of a radial vector on a two-sphere (ordinary globe with two angles, latitude and longitude) [7, 8].

The basic element of the field of quantum information requires two qubits, that being the minimum required for handling quantum entanglement or other quantum correlations such as quantum discord or for building quantum gates needed in quantum computation [7]. This is a four-level system with symmetry group SU(4), much larger now, 15-dimensional, than for a single qubit. There is a similar correspondence now as in the previous paragraph between this symmetry and the one of six-dimensional rotations SO(6) and its non-compact variants [4–6]. This is at the heart of our considerations in this paper of the parallels between the hydrogen atom and the two-qubit system. Remarkably, no such close correspondence extends to higher numbers of qubits, there being no similar mapping between the SU(2^n) of n-qubits and a larger SO(N) orthogonal group [9], a result that rests on a number-theoretic conjecture of pure mathematics made also 100 years ago [10, 11] completely independent of either quantum structure of atoms or qubits.

The arrangement of this paper is as follows. Section 2 presents the various symmetry groups of the hydrogen atom, how they nest within one another and describe states and their degeneracies. Section 3 considers similarly the one- and two-qubit symmetry groups, especially to bring out the parallels to section 2. Section 4 considers other sub-groups and also a connection to the free particle and its 'Poincare' symmetries [6]. A maximal group of 15 generators and important sub-groups of six, seven and ten generators, provide a common platform for this wide variety of physical systems and phenomena.

2. The hydrogen atom, states and symmetries

We begin with a feature common to all isotropic potentials in three dimensions, invariance of the Hamiltonian under rotations. The generators of angular momentum with respect to the three independent, orthogonal axes (more properly viewed as three planes orthogonal to those axes), ℓ_i, $i = 1, 2, 3$: $\ell_x = yp_z - zp_y$, $\ell_y = zp_x - xp_z$, $\ell_z = xp_y - yp_x$, obey the commutation rules

$$[\ell_i, \ell_j] = \mathrm{i}\hbar\epsilon_{ijk}\ell_k, \tag{1}$$

and are displayed as an anti-symmetric array in table 1.

This group SO(3) has one quadratic Casimir invariant $\vec{\ell}^{\,2}$ with eigenvalue $\ell(\ell+1)\hbar^2$, and a sub-group SO(2) of the first 2×2 block of rotations in just the xy plane. With the usual azimuthal quantum number m of this ℓ_z rotation, each ℓ value has the well-known $(2\ell+1)$ degeneracy of $m = -\ell, \ldots, \ell$ of all spherically symmetric potentials including the hydrogen atom's Coulomb potential $1/r$. Note in table 1 how the extension from SO(2) to SO(3) involves the addition of a row and column, also in an anti-symmetric arrangement with a zero in the diagonal entry and the other two entries transforming as a two-dimensional vector under SO(2). This will be a useful perspective for other extensions that follow later in this paper with groups of larger dimension. The linear combinations $\ell_\pm = \ell_x \pm \mathrm{i}\ell_y$ change the m value by ± 1 while leaving the ℓ unchanged.

As is well known, bound state energy values with principal quantum number n and energies $E_n = -13.6\,\mathrm{eV}/n^2$ have a larger degeneracy, of n^2, all $\ell = 0, 1, \ldots, n-1$ sharing a common energy. This is a clear pointer to a higher symmetry that has long been associated with another vector, the Laplace–Runge–Lenz vector $\vec{A}$ [1],

$$\vec{A} = (-\mu e^4/2E_n)^{1/2}[(1/2\mu e^2)(\vec{\ell} \times \vec{p} - \vec{p} \times \vec{\ell}) + \vec{r}/r], \tag{2}$$

where μ is the reduced mass. Besides the axial $\vec{\ell}$, this polar vector, also of dimensions of angular momentum, also commutes with the Hamiltonian and has commutation relations appropriate to that of any three-dimensional vector:

$$[\ell_i, A_j] = \mathrm{i}\hbar\epsilon_{ijk}A_k. \tag{3}$$

Further $\vec{\ell} \cdot \vec{A} = 0$. In the classical Coulomb–Kepler ellipse, this vector lies in the orbital plane, points in the direction of the major axis, and has magnitude proportional to the eccentricity. While spherical symmetry and associated conservation of angular momentum would require only orbits confined to the plane perpendicular to $\vec{\ell}$, that the elliptic orbits are closed means both magnitude and direction of $\vec{A}$ are fixed and speaks to this higher symmetry of inverse square law forces. This result, already in classical mechanics, carries over into quantum physics as the extension from SO(3) in table 1 to SO(4) in table 2.

Table 3. Generators of rotation group SO(4) = SO(3) × SO(3).

0	$\frac{1}{2}(\ell_z + A_z)$	$-\frac{1}{2}(\ell_y + A_y)$	$\frac{1}{2}(\ell_x - A_x)$
$-\frac{1}{2}(\ell_z + A_z)$	0	$\frac{1}{2}(\ell_x + A_x)$	$\frac{1}{2}(\ell_y - A_y)$
$\frac{1}{2}(\ell_y + A_y)$	$-\frac{1}{2}(\ell_x + A_x)$	0	$\frac{1}{2}(\ell_z - A_z)$
$-\frac{1}{2}(\ell_x - A_x)$	$-\frac{1}{2}(\ell_y - A_y)$	$-\frac{1}{2}(\ell_z - A_z)$	0

Table 4. Generators of rotation group SO(4).

0	ℓ_z	$-\ell_y$	A'_x
$-\ell_z$	0	ℓ_x	A'_y
ℓ_y	$-\ell_x$	0	A'_z
A'_x	A'_y	A'_z	0

The quantum operators $\vec{A}$ obey commutation relations

$$[A_i, A_j] = \mathrm{i}\hbar\epsilon_{ijk}\ell_k, \tag{4}$$

so that the set of six operators $(\vec{\ell}, \vec{A})$ close, forming the Lie algebra of the four-dimensional group SO(4), thereby making this a higher symmetry of the hydrogen atom [1, 12, 13]. As per earlier remarks, table 1 is extended now by adding a fourth row and column in anti-symmetric arrangement with the vector $\vec{A}$ as shown in table 2.

Although the hydrogen Hamiltonian H commutes with all six $(\vec{\ell}, \vec{A})$, since they themselves do not as per equation (3) and equation (4), the maximal set of mutually commuting operators is only three, but with alternative choices $(H, \vec{\ell}^{\,2}, \ell_z)$ and (H, ℓ_z, A_z). These provide the spherical polar and parabolic representations [1], respectively, and with states $|n, \ell, m\rangle$ and $|n, m, n_1 - n_2\rangle$ labeled by corresponding quantum numbers, with $n = n_1 + n_2 + |m| + 1$. The group SO(4) has two quadratic Casimir invariants, $\vec{\ell} \cdot \vec{A}$ which is identically zero because the two vectors lie perpendicular to each other, and

$$\vec{\ell}^{\,2} + \vec{A}^2 = (n^2 - 1)\hbar^2. \tag{5}$$

This latter expression is a recasting of the Bohr energy levels, that the Hamiltonian in units of the Rydberg, $Ry = 13.6\,\mathrm{eV}$, can be written as $(H/Ry) = -(\vec{\ell}^{\,2} + \vec{A}^2 + \hbar^2)^{-1}$.

The asymmetry between the operators $\vec{\ell}$ and $\vec{A}$, the former closing under commutation as in equation (1) but not the latter in equation (4) can be removed in the linear combinations

$$\vec{j}_1 = \frac{1}{2}(\vec{\ell} + \vec{A}), \vec{j}_2 = \frac{1}{2}(\vec{\ell} - \vec{A}), \tag{6}$$

that behave like two independent angular momenta with commutations as in equation (1) and of equal magnitude $j_1 = j_2 = (n - 1)/2$. This view of the hydrogen atom in terms of such a pair of 'half-angular' momenta casts the parabolic representation as that corresponding to these j's and their m_j values, passage to the spherical representation then seen as the addition $\vec{j}_1 + \vec{j}_2 = \vec{\ell}$, such an addition of the two equal values spanning precisely the $\ell = 0, 1, \ldots, n - 1$ of a n-manifold. And, the unitary transformation between the states in the two representations reduces to the familiar angular momentum addition with Clebsch–Gordan or Wigner $3j$ coefficients: $|n\ell m\rangle = \Sigma_{n_1}|n_1 n_2 m\rangle\langle n_1 n_2 m|n\ell m\rangle$ [1, 12].

Correspondingly, table 2 may be re-arranged in terms of the two angular momenta j_1, j_2 as in table 3. Note this SO(4) = SO(3) × SO(3) arrangement as two independent angular momenta, one in the anti-symmetric 3 × 3 block and another in the fourth column and row. All these orthogonal groups with their anti-symmetric tabular forms of the generators are 'compact' with finite-dimensional representations and thus finite degeneracies such as $(2\ell + 1)$ and n^2. The latter pertains to the degeneracy of the negative energy bound states of hydrogen. Turning to states of positive energy, the continuum states, each energy E now is infinitely degenerate, accommodating all values of ℓ from 0 to ∞. n is now pure imaginary, and the j_1 and j_2 values given below equation (6) complex, $-\frac{1}{2} \pm \frac{1}{2\sqrt{-E}}$, with energy again in units of 13.6 eV. Such infinite-dimensional representations belong to the 'non-compact' group SO(3, 1) that replaces SO(4) in table 2 by table 4 where the operators $\vec{A}'$ differ from $\vec{A}$ again because of the sign change in E involved in their definition (equation (2)) that results in a sign change on the right-hand side of their commutation relationship in equation (4).

Whereas the $\vec{A}'$ in the fourth column and row of table 4 again transforms as a vector according to equation (3) under three-dimensional rotations of the SO(3) sub-block, the fourth row/column is now no longer anti-symmetric and reflects the comma in SO(3, 1). This is, of course, also the four-dimensional Lorentz group of space–time and special relativity [6, 13]. The electric $\vec{E}$ and magnetic $\vec{B}$ fields of electromagnetic waves have a similar 4 × 4 arrangement as in table 4 with the magnetic field components in an anti-symmetric 3 × 3 block and the electric field components arrayed in the fourth row/column. In the language of special relativity, the same sign change is referred to as rotations involving the fourth component being actually Lorentz boosts to be thought of as rotation through an imaginary angle with corresponding replacement of trigonometric sines and cosines by their hyperbolic counterparts. The two Casimir invariants are $\vec{E} \cdot \vec{B}$ which is again zero, and $\vec{E}^2 - \vec{B}^2$. We will return to these connections in section 4. Note again the change in sign of the Casimir invariant relative to equation (5).

A further interesting and little appreciated result of this view of the continuum states of hydrogen at an energy E is that the two j values in equation (6) are complex with real part equal to $(-1/2)$ so that their sum now not only yields an infinity of real ℓ values but the analytic continuation of the Clebsch–Gordan coefficients into the complex plane now gives the Coulomb phase shift involved in expanding a plane wave into Coulomb spherical waves [14].

Table 5. Generators of the non-invariance group SO(4, 1).

0	ℓ_z	$-\ell_y$	A_x	M_x
$-\ell_z$	0	ℓ_x	A_y	M_y
ℓ_y	$-\ell_x$	0	A_z	M_z
$-A_x$	$-A_y$	$-A_z$	0	$\tilde{T}$
M_x	M_y	M_z	$\tilde{T}$	0

Table 6. Generators of the non-invariance group SO(4, 2).

0	ℓ_z	$-\ell_y$	A_x	M_x	Γ_x
$-\ell_z$	0	ℓ_x	A_y	M_y	Γ_y
ℓ_y	$-\ell_x$	0	A_z	M_z	Γ_z
$-A_x$	$-A_y$	$-A_z$	0	$\tilde{T}$	Γ_4
M_x	M_y	M_z	$\tilde{T}$	0	Γ_0
Γ_x	Γ_y	Γ_z	Γ_4	$-\Gamma_0$	0

The group symmetries discussed so far are 'invariance' groups of the hydrogen Hamiltonian with all generators commuting with H so that the degenerate manifolds contain states of the same energy, n^2 in number. Somewhat less familiar are the non-invariance groups of hydrogen that put into a single manifold states of different energy [4–6, 13]. Thus, as a first step, one could put all bound states with $1 \leqslant n \leqslant N$, that is, $N(N+1)(2N+1)/6$ states into a single representation. This requires, of course, operators other than $\vec{\ell}$ and $\vec{A}$, ones with non-zero matrix elements between different n. In essence, an operator such as $\vec{r}$, the electric dipole operator that causes such transitions needs to be introduced. A linear combination of this with $\vec{A}$ called $\vec{M}$ defined exactly as its companion in equation (2) but with a minus sign in the last term with $\hat{r}$ proves convenient [6]. In addition, a fourth, scalar, operator

$$\tilde{T} = \vec{r} \cdot \vec{p} - \mathrm{i}\hbar, \tag{7}$$

is necessary to close the Lie algebra of the five-dimensional SO(5) with ten generators.

A single representation of this larger SO(5) group can accommodate all the $N(N+1)(2N+1)/6$ states of $1 \leqslant n \leqslant N$. As befits a compact group, its representations are also finite-dimensional but with a faster cubic N^3 growth compared to the quadratic n^2 growth of SO(4). At the same time, all remaining states of hydrogen from N upward and into the continuum can be incorporated in an infinite-dimensional representation, just as before in the complex continuation at fixed energy, but now of the non-compact SO(4, 1), also with ten generators [6, 12, 13]. This is illustrated in the array in table 5.

Once again, a hierarchy of nesting of these orthogonal groups and their non-compact versions is illustrated in that the four entries in the fifth column and row transform as a four-dimensional vector under the 4×4 block of table 2. Further, the four entries sub-divide into a vector under SO(3) of the 3×3 block of table 1 and a scalar $\tilde{T}$. The quadratic Casimir invariant is $\vec{\ell}^{\,2} + \vec{A}^{\,2} - \vec{M}^{\,2} - \tilde{T}^2$. With the previous result in equation (5) for the first two terms, and $\vec{M}^{\,2} + \tilde{T}^2 = (n^2+1)\hbar^2$, this quadratic invariant takes the value $-2\hbar^2$. A higher, fourth-order invariant is zero. In the counterpart compact group SO(5), the fifth row/column in table 5 would have also an anti-symmetric aspect as do the first four, an example to be encountered in section 3.

The next and final step towards a non-invariance group that gives a complete description of the hydrogen atom, of all its bound and continuum states and all possible transition matrix elements between them, involves the addition of five more generators to the ten of SO(4, 1) through a sixth column and row to table 5 [4, 6] to give the larger, also non-invariance, group SO(4, 2). A physical, as against a purely group-theoretical, argument for adding five more operators follows by considering the basic objects $\vec{r}$ and $\vec{p}$ and their scalar and vector combinations.

The ten operators so far in SO(4, 1) are the three vectors $\vec{\ell}$, $\vec{A}$, and $\vec{M}$, and scalar $\tilde{T}$. Alternatively, by recognizing that terms such as $\vec{\ell} \times \vec{p}$ in equation (2) can also be written in terms of $\vec{r}p^2$ and $\vec{p}\,(\vec{r} \cdot \vec{p}\,)$, the essential argument is that from the basic physical operators of the hydrogen atom such as $\vec{r}$, $\vec{p}$, and scalars r, p^2, combinations so as to form a closed algebra under commutation along with the Hamiltonian also bring in the vectors $\vec{\ell}$ and $\vec{r}p^2$ and scalar $\vec{r} \cdot \vec{p}$, and it is this set of four vector and three scalar (which means they commute with $\vec{\ell}$) operators that form the full basis of elements to describe the physics of hydrogen. Linear combinations of them with physical meaning are the ten introduced so far in table 5 plus one more vector operator [6, 12, 13]

$$\vec{\Gamma} = r\vec{p}\,,$$

and two scalars

$$\Gamma_0 = \frac{1}{2}[(\hbar/\mu e^2)rp^2 + (\mu e^2/\hbar)r]$$
$$\Gamma_4 = \frac{1}{2}[(\hbar/\mu e^2)rp^2 - (\mu e^2/\hbar)r], \tag{8}$$

all with dimensions of angular momentum. As with $\vec{A}$ and $\vec{M}$, $\vec{\Gamma}$ is also orthogonal to $\vec{\ell}$.

Arrayed as a sixth column and row in table 6, we now have the full set of 15 generators of the 'dynamical group' SO(4, 2) of hydrogen [6], a non-compact version of the six-dimensional rotation group SO(6). A quadratic Casimir invariant is $\vec{\ell}^{\,2} + \vec{A}^{\,2} - \vec{M}^{\,2} - \tilde{T}^2 + \Gamma_0^2 - \Gamma_4^2 - \vec{\Gamma}^2$. As with the counterpart SO(4, 1), it takes the value $-3\hbar^2$ for the physical states of interest, and two higher Casimir invariants, of fourth and sixth order, vanish [6]. Note the structure of the 4×4 anti-symmetric SO(4) plus two rows and columns for the comma-2 describing the doubly infinite representation of continuum states, one at fixed E with ℓ values running from 0 to ∞ and the other with E itself running from the ground state

through all possible negative and positive values all the way to infinity.

But other sub-groups and physically meaningful decompositions of the table are also interesting [6, 12, 13]. One is to view as four equal 3×3 blocks, the upper diagonal block being of $\vec{\ell}$ and SO(3). The lower diagonal box is somewhat similar with the three scalar operators obeying the commutation relations

$$[\Gamma_0, \Gamma_4] = \mathrm{i}\hbar\tilde{T}, [\Gamma_4, \tilde{T}] = -\mathrm{i}\hbar\Gamma_0, [\tilde{T}, \Gamma_0] = \mathrm{i}\hbar\Gamma_4, \quad (9)$$

similar to an angular momentum triad but, crucially, with one different sign. As can be seen from equation (8), rH can be written as a linear combination of the operators in equation (9) which accounts for why all the energy levels and radial wave functions can be obtained from them. The role played by multiplying the Hamiltonian by r is related to the so-called 'regularization' of the Coulomb problem, known also in the classical Kepler problem [15].

The anti-symmetry of Γ_0 in the lower corner is analogous to that of ℓ_z in the upper 2×2 corner of table 6, but there is now a symmetric arrangement of the row/column involving Γ_4 and $\tilde{T}$. A quadratic Casimir invariant is $\tilde{T}^2 + \Gamma_4^2 - \Gamma_0^2 = -\vec{\ell}^2$. This set describes the group SO(2, 1), another non-compact group and highlights another remarkable structure of hydrogen, that the purely radial aspects of the problem have this group symmetry [16, 17]. All three operators involve only radial elements as is clear from an alternative rendering of this triplet in terms of the radial momentum operator $p_r = (\hbar/\mathrm{i})(\partial/\partial r + 1/r)$, which is the Hermitian form for radial integrals with the volume element $r^2\mathrm{d}r$. The three operators form a closed algebra [13]

$$[rp_r, rp_r^2] = \mathrm{i}\hbar rp_r^2, [rp_r, r] = -\mathrm{i}\hbar r, [rp_r^2, r] = -2\mathrm{i}\hbar rp_r. \quad (10)$$

Thus, table 6 can be alternatively viewed as a direct product of two 3×3 sets, an upper 3×3 SO(3) block and a lower 3×3 SO(2, 1). This view of SO(4, 2) as SO(3) $\otimes$ SO (2, 1) with a separation of the angular and radial behavior of the hydrogen atom allows an algebraic handling of radial functions and of matrix elements of powers of r between them much as in the familiar algebra of angular momentum for the θ, ϕ part. For these aspects as well as other sub-group decompositions of SO(4, 2), a similar treatment of the parabolic representation in terms of two SO(2, 1)s, and connections to an oscillator in four-dimensional semi-parabolic coordinates, see [6, 13].

An interesting sub-group, for correspondence with a similar one in section 3, is to consider the top 4×4 block of table 6 with the lower corner 2×2 block of the single element Γ_0 that commutes with all in the upper block. This SO(3) $\otimes$ SO(3) $\otimes$ SO(2) seven-operator group has been little discussed in atomic physics but its counterpart in section 3 plays a crucial role in quantum information.

Comparisons with the isotropic harmonic oscillator are also worth noting. The three-dimensional oscillator also has extra degeneracies beyond the SO(3) expected from spherical symmetry. In that case, unlike the Laplace–Runge–Lenz vector, it is a symmetric second-rank tensor with five additional generators that expands to the larger symmetry of SU(3) as the invariance group [6]. Degenerate energy states within a manifold now run over all either even or odd ℓ, parity still conserved here unlike in hydrogen where the mixing of axial $\vec{\ell}$ and polar $\vec{A}$ puts states of all parity into the same manifold. The larger non-invariance group that embraces all (bound) energy states is Sp(6, R) with 21 generators so that this whole sequence is unlike that for the hydrogen atom [6]. However, the two-dimensional isotropic oscillator is equivalent to the hydrogen atom, the SO(2) of isotropy expanded to SU(1, 1) (expanded from one to three generators) within an energy manifold and SO(3, 2) with ten generators for the non-invariance group embracing all states in an infinite-dimensional representation [5]. This is the counterpart of hydrogen's SO(4, 1), smaller by one dimension than the complete group for hydrogen, reflecting that the oscillator spectrum has no (infinite) continuum. Other aspects of the oscillator, such as the isomorphism of SO(3, 2) with Sp(4, R), another group with ten generators, are outside the purview of our paper's focus on the hydrogen atom and a pair of qubits.

We end this section with the behavior under parity $\mathcal{P}$ and time reversal $\mathcal{T}$ transformations of the various operators of the hydrogen atom and the electromagnetic field. The operators (r, Γ_0, Γ_4, scalar potential) are even under both, whereas ($\vec{p}$, $r\vec{p}$, $\vec{\Gamma}$, vector potential) are odd under both. ($\vec{r}$, $\vec{A}$, $\vec{M}$, electric field) are odd under parity and even under time reversal, while ($\vec{\ell}$, $\vec{r} \cdot \vec{p}$, $\tilde{T}$, magnetic field) are of even parity and odd under time reversal.

3. Symmetries of one- and two-qubit systems

A spin-1/2 or two-level quantum system, a qubit, has only two base states. The unit operator and the three Pauli operators $\vec{\sigma}$ act on them and obey the commutation relations that follow from equation (1):

$$[\sigma_i, \sigma_j] = 2\mathrm{i}\epsilon_{ijk}\sigma_k, \quad (11)$$

appropriate to $\vec{j} = \frac{1}{2}\hbar\vec{\sigma}$. Exactly as in table 1, the three Pauli operators may be arranged in a 3×3 anti-symmetric array and the symmetry group, SU(2), differs from the previous SO(3) only in having a doubling of the representations. Squares of all Pauli operators, and the Casimir invariant also trivially, are the unit operator, the only one that commutes with all the $\vec{\sigma}$.

Besides the Lie algebra of commutators shared with all angular momenta, the spin-1/2 operators have a further structure of a Clifford algebra, closing under multiplication itself as

$$\sigma_i\sigma_j = \mathrm{i}\epsilon_{ijk}\sigma_k. \quad (12)$$

A matrix representation as 2×2 traceless matrices, one diagonal and the other two off-diagonal, all with eigenvalues ± 1 is very familiar, as also a representation of a general state by a two-column vector parametrized by two Bloch angles,

Table 7. Generators of group SU(2) X SU(2) of disjoint spins.

0	$\sigma_z^{(2)}$	$-\sigma_y^{(2)}$	$\sigma_x^{(1)}$
$-\sigma_z^{(2)}$	0	$\sigma_x^{(2)}$	$\sigma_y^{(1)}$
$\sigma_y^{(2)}$	$-\sigma_x^{(2)}$	0	$\sigma_z^{(1)}$
$-\sigma_x^{(1)}$	$-\sigma_y^{(1)}$	$-\sigma_z^{(1)}$	0

θ, ϕ, angles locating a point on a two-sphere called the Bloch sphere [7].

Quantum correlations such as entanglement, and quantum gates, require a minimum of two qubits, $\vec{\sigma}^{(1)}$ and $\vec{\sigma}^{(2)}$ [7]. Such a four-level system can be represented by 4×4 matrices with the unit operator and 15 others now forming a complete set of generators of the symmetry SU(4). Another physical context is provided by spin and isotopic spin in nuclear physics ever since Wigner's supermultiplet scheme [18]. See also the general discussion of symmetries of pairs of two-level systems with connections to the Liouville Representation in physics [19, 20].

Our aim in this paper is not to discuss the very rich group theory of SU(4) but rather to build up to the full SU(4) through smaller sub-groups of it to illuminate the parallels to the discussion in section 2 of the 15-operator algebra of the hydrogen atom. The immediate first sub-group, SU(2) $\otimes$ SU(2), of two disjoint spins with no couplings or interactions between them, a 4×4 block-diagonal matrix with two independent diagonal SU(2) blocks, places the six operators involved in an array such as table 3 with one spin in an anti-symmetric upper block and the other in an anti-symmetric arrangement in fourth row and column (table 7).

Indeed, this array is identical to that in table 3 of the two'half-angular momenta,' $\vec{j}_1$ and $\vec{j}_2$, of equation (6) for the $n = 2$ states of hydrogen when $j_1 = j_2 = \frac{1}{2}$ and the entries in that table reduce to the Pauli matrices as in table 7. The four degenerate parabolic states of that manifold are in one-to-one correspondence with the four states of two uncoupled qubits. In the spherical representation as 2s and 2p states of the atom, orthogonal linear combinations of the $m = 0$ states are two of the 'Bell basis' states [7]. Similarly, the two orthogonal linear combinations of the $|m| = 1$ 2p states provide the other two Bell states of quantum information [7]. Once again, as with a single qubit, the unit operator is the only invariant that commutes with all the operators in this table.

The next step is to consider a sub-group of SU(4) of seven generators with symmetry SU(2) $\otimes$ U(1) $\otimes$ SU(2). There are many independent such choices of seven out of the full fifteen. One convenient one with physical meaning attached describes two spin magnetic moments in an external magnetic field and with complete spin–spin Heisenberg interaction between them as well as 'cross-coherences' [21] :

$$\sigma_z^{(1)},\ \sigma_z^{(2)},\ \sigma_x^{(1)}\sigma_x^{(2)},\ \sigma_y^{(1)}\sigma_y^{(2)},\ \sigma_z^{(1)}\sigma_z^{(2)},\ \sigma_x^{(1)}\sigma_y^{(2)},\ \sigma_y^{(1)}\sigma_x^{(2)}. \quad (13)$$

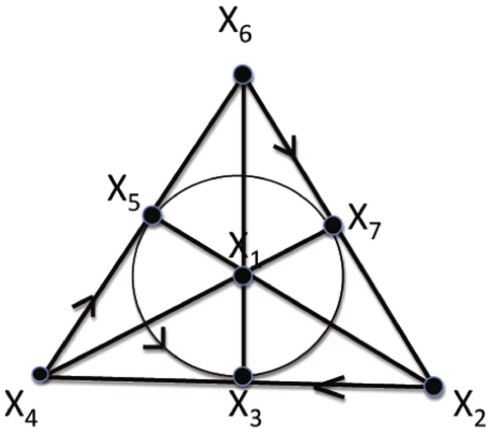

Figure 1. The multiplication diagram for the seven operators that underlie *X*-states with SU(2) $\otimes$ U(1) $\otimes$ SU(2) symmetry. Resembling the Fano plane and the multiplication diagram for octonions, each operator stands on three lines, and each line, including the inscribed circle, has on it three operators. On the interior medians, the product of any two operators gives the third, these objects commuting. On the remaining four lines, the operators anticommute, and the product of any two gives the third with a multiplicative $\pm$i, the plus (minus) depending on the direction of (along/against) the arrow [23].The choice in equation (13) is $X_1 = \sigma_z^{(1)}\sigma_z^{(2)}$, $X_2 = \mathrm{i}\sigma_y^{(1)}\sigma_x^{(2)}$, $X_3 = \mathrm{i}\sigma_z^{(2)}$, $X_4 = \mathrm{i}\sigma_y^{(1)}\sigma_y^{(2)}$, $X_5 = \mathrm{i}\sigma_x^{(1)}\sigma_y^{(2)}$, $X_6 = \mathrm{i}\sigma_z^{(1)}$, $X_7 = -\mathrm{i}\sigma_x^{(1)}\sigma_x^{(2)}$.

Figure 1 is a convenient rendering of the seven operators and the Clifford algebraic multiplication rules between them. A central element, $\sigma_z^{(1)}\sigma_z^{(2)}$, commutes with all the other six, whereas multiplication among themselves have the rule of equation (12) in an arrow notation with plus (minus) sign attached along (against) the arrow for the product of any two as the third element of that line [22, 23]. Note that the 'line' includes also the inscribed circle, this diagram being one of discrete projective geometry where it is called the Fano Plane [24], points and lines at infinity considered on par with those at finite values.

The six elements also group into two sets of three denoted by $\vec{S}$, $\vec{s}$ [21]:

$$\begin{aligned} S_x &= \frac{1}{2}[\sigma_z^{(1)} + \sigma_z^{(2)}],\ S_y = \frac{1}{2}[\sigma_x^{(1)}\sigma_x^{(2)} - \sigma_y^{(1)}\sigma_y^{(2)}], \\ S_z &= \frac{\mathrm{i}}{2}[\sigma_y^{(1)}\sigma_x^{(2)} + \sigma_x^{(1)}\sigma_y^{(2)}], \\ s_x &= \frac{1}{2}[\sigma_z^{(1)} - \sigma_z^{(2)}],\ s_y = \frac{1}{2}[\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_y^{(1)}\sigma_y^{(2)}], \\ s_z &= \frac{\mathrm{i}}{2}[\sigma_y^{(1)}\sigma_x^{(2)} - \sigma_x^{(1)}\sigma_y^{(2)}], \end{aligned} \quad (14)$$

in terms of two triplets with the same commutation relations as in equation (11) and each component of $\vec{S}$ commuting with every one of $\vec{s}$, so that they behave like independent spins and can be arranged as in table 7. However, they differ in that unlike Pauli matrices, their squares are not the unit operator but non-trivial in involving the commuting element $\sigma_z^{(1)}\sigma_z^{(2)}$:

$$S_i^2 = \frac{1}{2}(I + \sigma_z^{(1)}\sigma_z^{(2)}),\ s_i^2 = \frac{1}{2}(I - \sigma_z^{(1)}\sigma_z^{(2)}), \quad (15)$$

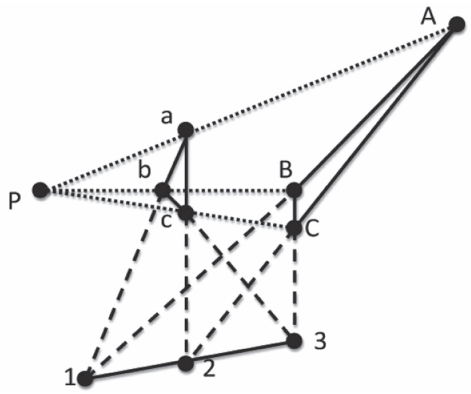

Figure 2. The Desargues diagram of projective geometry [22]. The two triangles, the rays from point P, and the line (123) constitute ten points on ten lines, with each point on three lines and vice versa. The two triangles are said to be in perspective with respect to P and to (123). The choice of ten operators in equation (16) and table 8 is $P = \sigma_z^{(1)}$, (123) $= \vec{\sigma}^{(2)}$, (cab) $= \sigma_x^{(1)}\vec{\sigma}^{(2)}$, (CAB) $= \sigma_y^{(1)}\vec{\sigma}^{(2)}$.

that is, $\sigma_z^{(1)}\sigma_z^{(2)}$ enters as a quadratic invariant [21]. This is analogous to the hydrogen atom's Γ_0 discussed at the end of section 2 but has been much more consequential in quantum information. This U(1) symmetry introduced by this common commuting element and resulting symmetry SU(2) $\otimes$ U(1) $\otimes$ SU(2) is the symmetry group of what are called X-states of a two-qubit system with wide applications [23]. They also extend through an iterative repetition to generate analogous X-states of n-qubit systems [25]. It should also be noted that any of the 15 operators of SU(4) can be chosen as the commuting element X_1 in figure 1 to give different SU(2) $\otimes$ U(1) $\otimes$ SU(2) choices, a table in [26] providing a convenient way of picking them.

Another extension beyond six operators is to drop the $\sigma_z^{(1)}\sigma_z^{(2)}$ element in equation (13) and add instead four to form a set of ten:

$$\sigma_z^{(1)},\ \vec{\sigma}^{(2)},\ \sigma_x^{(1)}\vec{\sigma}^{(2)},\ \sigma_y^{(1)}\vec{\sigma}^{(2)}. \tag{16}$$

This set of ten operators generates the five-dimensional orthogonal group SO(5) and can be represented by another diagram of projective geometry in figure 2 [22]. Again, there are many alternative sets of ten out of the 15 operators of SU(4) with this symmetry. Ten lines of triads, all arrowed now, with Clifford algebraic structure as per equation (12) connecting the ten operators may be viewed as six operators on two triangles put in perspective with respect to a point $\sigma_z^{(1)}$ or alternatively the line $\vec{\sigma}^{(2)}$. They can also be put into an SO(5) anti-symmetric form in table 8 analogous to table 5.

Note the SU(2) of the upper diagonal block and the U(1) element in the lower diagonal that are the line and point, respectively, in figure 2 with respect to which the two triangles are in perspective [22]. The operators forming those triangles stand as the anti-symmetric fourth and fifth row/columns that transform as the spinor $\vec{\sigma}^{(2)}$ under the upper block's SU(2). As per the caption in figure 2, the two triangles carry as a multiplicative factor of this spinor $\vec{\sigma}^{(2)}$ the components $\sigma_x^{(1)}$ and $\sigma_y^{(1)}$ of the first spinor, those being the companions of the $\sigma_z^{(1)}$ chosen for the U(1). Clearly, from this perspective, there are three different choices for that U(1) element (see discussion below on table 9).

Table 8. Generators of group SO(5) of two spins.

0	$\sigma_z^{(2)}$	$-\sigma_y^{(2)}$	$\sigma_x^{(1)}\sigma_x^{(2)}$	$\sigma_y^{(1)}\sigma_x^{(2)}$
$-\sigma_z^{(2)}$	0	$\sigma_x^{(2)}$	$\sigma_x^{(1)}\sigma_y^{(2)}$	$\sigma_y^{(1)}\sigma_y^{(2)}$
$\sigma_y^{(2)}$	$-\sigma_x^{(2)}$	0	$\sigma_x^{(1)}\sigma_z^{(2)}$	$\sigma_y^{(1)}\sigma_z^{(2)}$
$-\sigma_x^{(1)}\sigma_x^{(2)}$	$-\sigma_x^{(1)}\sigma_y^{(2)}$	$-\sigma_x^{(1)}\sigma_z^{(2)}$	0	$\sigma_z^{(1)}$
$-\sigma_y^{(1)}\sigma_x^{(2)}$	$-\sigma_y^{(1)}\sigma_y^{(2)}$	$-\sigma_y^{(1)}\sigma_z^{(2)}$	$-\sigma_z^{(1)}$	0

Table 9. Generators of group SU(4) of two spins.

0	$\sigma_z^{(2)}$	$-\sigma_y^{(2)}$	$\sigma_x^{(1)}\sigma_x^{(2)}$	$\sigma_y^{(1)}\sigma_x^{(2)}$	$\sigma_z^{(1)}\sigma_x^{(2)}$
$-\sigma_z^{(2)}$	0	$\sigma_x^{(2)}$	$\sigma_x^{(1)}\sigma_y^{(2)}$	$\sigma_y^{(1)}\sigma_y^{(2)}$	$\sigma_z^{(1)}\sigma_y^{(2)}$
$\sigma_y^{(2)}$	$-\sigma_x^{(2)}$	0	$\sigma_x^{(1)}\sigma_z^{(2)}$	$\sigma_y^{(1)}\sigma_z^{(2)}$	$\sigma_z^{(1)}\sigma_z^{(2)}$
$-\sigma_x^{(1)}\sigma_x^{(2)}$	$-\sigma_x^{(1)}\sigma_y^{(2)}$	$-\sigma_x^{(1)}\sigma_z^{(2)}$	0	$\sigma_z^{(1)}$	$-\sigma_y^{(1)}$
$-\sigma_y^{(1)}\sigma_x^{(2)}$	$-\sigma_y^{(1)}\sigma_y^{(2)}$	$-\sigma_y^{(1)}\sigma_z^{(2)}$	$-\sigma_z^{(1)}$	0	$\sigma_x^{(1)}$
$-\sigma_z^{(1)}\sigma_x^{(2)}$	$-\sigma_z^{(1)}\sigma_y^{(2)}$	$-\sigma_z^{(1)}\sigma_z^{(2)}$	$\sigma_y^{(1)}$	$-\sigma_x^{(1)}$	0

That the entries in the fourth and fifth row/column of table 8 do not close under commutation but result in the $\vec{\sigma}^{(2)}$ of the upper diagonal block is as in section 2 for the hydrogen atom where elements of $\vec{A}$ under commutation involve $\vec{\ell}$ as in table 2 and other tables such as 4–6 or equation (3). The four operators added in equation (16) to those in equation (13) stand as the third row and column of table 8 and provide the connection between the sub-groups SU(2) $\otimes$ U(1) $\otimes$ SU(2) and SO(5) of SU(4), along with that U(1) element $\sigma_z^{(1)}\sigma_z^{(2)}$. The SO(5) symmetry appears in many atomic, molecular, and quantum optical four-level systems, with two each of even and odd parity [26–28]. Because of selection rules for allowed electric dipole transitions, four complex coupling matrix elements between them plus two energy differences make for a ten-parameter symmetry.

The final step into the full two-qubit or general four-level problem involving 15 parameters, counted as three energy differences along the diagonal and six pairs of off-diagonal complex coupling matrix elements in a 4×4 matrix involves all 15 operators $I \otimes \vec{\sigma}^{(2)}$, $\vec{\sigma}^{(1)} \otimes I$, $\vec{\sigma}^{(1)} \otimes \vec{\sigma}^{(2)}$ and adds a sixth row and column to table 8 to give table 9. This is the entire su(4) algebra or SU(4) symmetry of the two-qubit system.

Table 9 is an arrangement of the two spin operators, completely symmetric in them with the diagonal SU(2) blocks of each spinor and an anti-symmetric off-diagonal block of the nine products of Pauli spinors [29]. It is analogous to table 6 of the hydrogen atom except that it describes now a completely anti-symmetric and compact group, the qubits' system being always finite-dimensional. Dropping any of the fourth, fifth, or sixth row and column gives an SO(5) of table 8. Each row and

Table 10. Generators of the Poincare group SO(3, 2).

0	ℓ_z	$-\ell_y$	V_x	P_x
$-\ell_z$	0	ℓ_x	V_y	P_y
ℓ_y	$-\ell_x$	0	V_z	P_z
V_x	V_y	V_z	0	H
P_x	P_y	P_z	H	0

column of these off-diagonal blocks behaves like a vector under both SU(2) of spins 1 and 2. The quadratic invariants are again trivial, every element in the table squaring to unity. In its 3×3 block aspect, table 9 differs crucially from its counterpart table 6 for the hydrogen atom where the upper and lower 3×3 blocks describe angular and radial behavior, respectively, with very different physics.

4. Reduction to the symmetries of the free particle

Yet another parallel of the group symmetries of the hydrogen atom in section 2, especially the four-dimensional invariance and five- and six-dimensional non-invariance groups, is to the Lorentz, Poincare, and conformal group symmetries of a particle of mass m in space–time [6, 13, 30–32]. This is to be expected, both on the grounds that we are again dealing with 4×4 matrices and that switching off the electric charge in the hydrogen Hamiltonian reduces it to that of a free particle.

With four vectors x_μ, $\mu = 1 - 4$, of space–time, the conformal group consists of the 15 operations: four translations $P_\mu = \mathrm{i}\frac{\partial}{\partial x_\mu}$, six Lorentz transformations described by the anti-symmetric $L_{\mu\nu} = \mathrm{i}\left(x_\mu \frac{\partial}{\partial x_\nu} - x_\nu \frac{\partial}{\partial x_\mu}\right)$ that includes rotations in space and Lorentz boosts, a scalar dilatation $D = \mathrm{i}x_\nu \frac{\partial}{\partial x_\nu}$, and a 'special conformal' $K_\mu = \mathrm{i}\left(2x_\mu x^\nu \frac{\partial}{\partial x_\nu} - x^2 \frac{\partial}{\partial x_\mu}\right)$. This set of 15 operators closes under commutation [6]. The four-dimensional manifold of coordinate position and time specifies a basic state, all others reached by operator action with this set.

An important sub-group of the ten generators that remain on dropping K_μ and D is the Poincare group SO(3, 2) shown in table 10 which is similar to hydrogen's SO(4, 1) in table 5 except that the fourth row and column are now also not anti-symmetric as are the fifth, with only the first three describing an anti-symmetric compact orthogonal group of three-dimensional rotations. Note the difference in double lines between the tables. We have indicated the fourth row/column entries by V for velocity boosts and they are like the A' in table 4. This first 4×4 block of table 10 of rotations and Lorentz boosts, six generators in all, gives the SO(3,1) sub-group just as the one in table 4 and is in the present context the familiar Lorentz group of space–time transformations [6, 13].

The correspondence between the operators of hydrogen and free particle is instructive. Orbital angular momentum $\vec{\ell}$ of SO(3) is common to both. The Laplace–Runge–Lenz vector or, better, the counterpart $\vec{A}'$ of section 2 (a sign difference involved in equation (4)) correspond to the Lorentz boosts, the $\vec{M}$ has as counterpart the $\vec{P}$, and the $\tilde{T}$ in equation (6) is replaced by the Hamiltonian. Explicitly, with reference to figure 3 for a free particle moving with constant $\vec{p}$ along a straight line and a general point not necessarily lying on that line, dropping a perpendicular from the point to the line defines a $\vec{r}_0$ with magnitude r_0, the impact parameter, constant. Also constant is the angular momentum, $\vec{\ell}$, pointing normal to the plane defined by the point and the line of motion and of magnitude $r_0 p$.

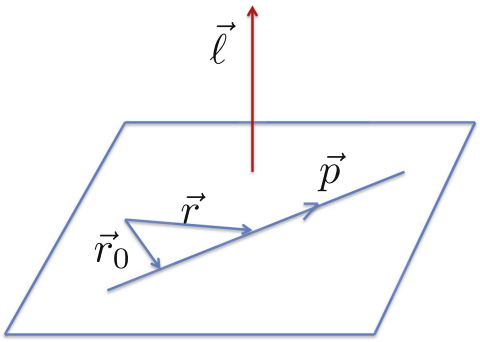

Figure 3. A free particle of energy E, momentum $\vec{p}$, angular momentum $\vec{\ell}$, and impact parameter $\vec{r}_0$, all constant, and instantaneous position $\vec{r}$. The Laplace–Runge–Lenz vector reduces to $\vec{\ell} \times \vec{p}$ and is also constant, $-2mE\vec{r}_0$.

Taking the origin of time as the closest position of the particle to the point, its instantaneous position is given by $\vec{r}(t) = \vec{r}_0 + (\vec{p}t/m)$. The Laplace–Runge–Lenz vector in equation (2) reduces to $\vec{\ell} \times \vec{p}$ and, indeed, with the second term in that definition vanishing for $e^2 = 0$, so does the counterpart $\vec{M}$ which differs only in the sign of that term. Thereby, both reduce to $(-2mE\vec{r}_0)$, again a constant. $\tilde{T}$ in equation (7) becomes $(2Et - \mathrm{i}\hbar)$, essentially therefore the Hamiltonian of the free particle as shown in table 10. Correspondence of the remaining five operators in the last row and column of table 6 to the similar five of the conformal group is also immediate. $\vec{\Gamma}$ is the constant $\vec{p}$ multiplied by r and the Γ_0 and Γ_4 in equation (8) become equal, again with the second term vanishing, and equal to $2mEr$.

Further clarification of the reduction of the hydrogen atom to a free particle can be seen by starting with the product of rH of the former written as $r\left(\frac{p^2}{2m} - E\right) = Ze^2$, which can be cast in terms of Γ_0 and Γ_4 in equation (8) alone [12, 16]. For hydrogen, using only the three operators in the lower 3×3 block of table 6 and rotating with respect to $\tilde{T}$ of this SO(2, 1) casts H in terms of Γ_0 alone, and with quantization $\Gamma_0 = n\hbar$, the Bohr energy values follow [6, 12, 13]. On the other hand, setting $e^2 = 0$ above yields the free particle's energy–momentum relation trivially. The step of multiplication by r that was previously noted as a crucial regularization is also emphasized by the argument.

It is also interesting to note that while we have discussed the usual three-dimensional systems, the results extend immediately to the hydrogen atom or free particle in n-dimensions. The same tables 5 and 6 apply except that the top rotation block is now an anti-symmetric $n \times n$ of SO(n) and the vectors in the other rows and columns are n-dimensional as well, so that the relevant symmetries are SO(n + 1,2) and SO(n, 2). Yet one more perspective brought out by the comparison of these systems is on the manifolds on which the operators act. For the free particle, it is the four-dimensional manifold of space–time, the three coordinates locating a point in space plus time. For the hydrogen atom, the various Kepler conics for the same energy extend this to a five-dimensional manifold. Besides the location of the focus, and time, an additional degree of freedom is the eccentricity needed to distinguish between the states of the same energy and other labels. Conics with differing orientation, velocity, and size are connected by the Γ operators, adding an 'extra dimension' to hydrogen.

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