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LETTER TO THE EDITOR

Coherent states for the hydrogen atom

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Abstract. We construct a system of coherent states for the hydrogen atom that is expressed in terms of elementary functions. Unlike the previous attempts in this direction, this system possesses properties equivalent to most of those for the harmonic oscillator, with modifications due to the character of the problem.

1. Introduction

In 1926 Schrödinger constructed the superposition of states for the harmonic oscillator, afterwards called the system of coherent states (CS). It is parametrized by complex numbers and possesses a number of remarkable properties: (a) in configuration space it may be expressed in the closed form; (b) the evolution operator $e^{-i\mathcal{H}t}$ transforms an arbitrary state of the system into a state also belonging to the system; (c) each state returns to its initial value after a lapse of time $T = 2\pi/\omega$, i.e. the operator $e^{-i\mathcal{H}T}$ maps each state onto itself; (d) each state of the system moves classically, i.e. the expectation values of coordinates and momenta for an arbitrary state have the same temporal dependence as those for the corresponding classical problem; (e) the system of CS yields the resolution of the identity; (f) for each state of the system the uncertainty $\Delta p \Delta x$ attains its minimum possible value; (g) the system is invariant under the action of the Heisenberg–Weyl group; (h) each state of the system is well localized in the configuration space. These properties are considered in detail, for example, in [1]. The problem of the generalization of this construction to other potentials appears naturally. One example of its successful solution is a recent construction of the CS system for the one-dimensional Morse potential [2]. Similar to the case of the harmonic oscillator, this CS system is parametrized by the complex numbers, and the expectation values of coordinates and momenta are expressed in terms of this parameter. This CS system obeys the conditions (a), (e), (h) and an analogue of the condition (g) with some solvable group different from the Heizenberg–Weyl one. Meanwhile, the problem of construction of CS for the hydrogen atom stated by Schrödinger is of significant interest on its own. In this case we should justify the set of properties, the validity of which we demand. For example, as the symmetry group of the hydrogen atom is $SO(4, 2)$ [3], it is natural to replace (g) by the condition (g′) invariance under the action of the $SO(4, 2)$ group or certain of its subgroups. Validity of the properties (b), (c) and (d) for the harmonic oscillator is a consequence of the fact that its energy levels are multiples of the ground-state level. Then, during the time taken to return the ground state to its initial value, all other states do so too. For the hydrogen atom it is correct in some fictitious time variable rather than t [4]. This suggests replacing the properties (b), (c) and (d) by: (b′) stability of the system under the evolution with respect to the mentioned fictitious time variable; (c′) if the fictitious time variable changes for the fixed (independent of the state) value, then all states of the system return to their initial values; (d′) during evolution with respect to the fictitious time variable the expectation value of $\boldsymbol{x}$ circumscribes an ellipse. The property (f) also needs modification since the dispersions $\Delta x \Delta p_x$ and $\Delta r \Delta p_r$ are nonminimal, even for the ground state of the hydrogen atom. Instead of (f), we can introduce the following criterion for extracting the states which are closest to the classical ones [1]: (f′) the value of

$$\Delta C_2 = \langle\psi|C_2|\psi\rangle - g^{mn}\langle\psi|X_m|\psi\rangle\langle\psi|X_n|\psi\rangle$$

is minimal for all the states of our system. Here X_m, g^{mn} and $C_2 = g^{mn}X_mX_n$ are the generators of the symmetry group of our CS system, the Cartan tensor of this group and its Casimir operator, respectively. Starting from the Mostowski (1977) paper [5], many authors proposed various systems of states obeying different sets of the above properties. Here we shall enumerate only exact results without pretending to completeness. Klauder [6] constructed the CS system possessing the properties (b) and (e). In [7] it was shown that, for these systems, one can satisfy the property (g′) for the $SO(4)$ group. This approach was criticized by Bellomo and Stroud [8], who showed that the properties (c), (d) and (h) fail to be satisfied. Following the general Perelomov method [1], Mostowski [5] constructed the CS system satisfying the property (g′) for the group $SO(4,2)$. De Prunele [9] considered the properties of this system and showed that the property (a) is satisfied for circular orbits only and the property (h) fails to be satisfied. Let us point out that this CS system is a particular case of that for the space $SU(N,N)/S(U(N)\otimes U(N))$ introduced by Perelomov to describe the pair creation of bosonic particles of nonzero spin in the external field [1]. Starting from the correspondence between the three-dimensional hydrogen atom and the four-dimensional harmonic oscillator (see also [10] and references therein), Gerry [4] constructed the CS system for the hydrogen atom as a direct product of two CS systems for the $SO(3)$ group. For this CS system the properties (b′), (c′), (d′) and (g′) for the $SO(4)$ group are satisfied. The mentioned correspondence naturally suggests to us using the basis numerated by ‘number operators’ [4]. Using the coordinate realization of this basis given in [3], in this letter we construct the CS system obeying the properties (a), (b′), (c′), (d′), (f′), (g′) (for the $SO(3,2)$ group) and (h). In the quasiclassical limit (i.e. for large $\langle r\rangle$) it passes into the usual plane wave, as it should for the potential tending to zero at infinity.

2. Construction

It is well known [3] that the wavefunction of a hydrogen atom in parabolic coordinates

$$x + \mathrm{i}y = \xi\eta\mathrm{e}^{\mathrm{i}\phi} \qquad z = \tfrac{1}{2}(\xi^2 - \eta^2) \qquad r = \tfrac{1}{2}(\xi^2 + \eta^2)$$

is

$$\langle\boldsymbol{x}|n_1n_2m\rangle = (-1)^{n_1+\frac{1}{2}(m-|m|)}\frac{\mathrm{e}^{\mathrm{i}m\phi}}{\sqrt{\pi}}\mathrm{e}^{-\frac{1}{2}(\xi^2+\eta^2)} \times(\xi\eta)^{|m|}\left(\frac{(n_1+|m|)!(n_2+|m|)!}{n_1!n_2!}\right)^{-1/2} L_{n_1}^{|m|}(\xi^2)L_{n_2}^{|m|}(\eta^2).$$

In comparison with equation (2.4) of [3] we have redenoted $\xi \to \xi^2$, $\eta \to \eta^2$ and corrected a misprint in the normalization factor. Let us consider the states

$$|\lambda_1\lambda_2\rangle = c_0\sum_{n=0}^{\infty}\sum_{m=-\infty}^{\infty}(\lambda_1\lambda_2)^{\frac{1}{2}(2n+|m|+1)}\left(\frac{\lambda_1}{\lambda_2}\right)^{m/2}|nnm\rangle \qquad (1)$$

where λ_1, λ_2 are the complex numbers and $|\lambda_1\lambda_2| < 1$. Using the formulae [11]

$$\sum_{n=0}^{\infty} \frac{n!}{\Gamma(n+\alpha+1)} L_n^\alpha(x) L_n^\alpha(y) z^n = (1-z)^{-1} \exp\left(-z\frac{x+y}{1-z}\right)(-xyz)^{-\alpha/2} J_\alpha\left(2\frac{(-xyz)^{1/2}}{1-z}\right) \qquad |z| < 1$$

$$\sum_{n=-\infty}^{\infty} t^n J_n(z) = \exp[(t-t^{-1})z/2]$$

we obtain

$$\langle \boldsymbol{x}|\lambda_1\lambda_2\rangle = \frac{c_0}{\sqrt{\pi}} \frac{(\boldsymbol{u}^2)^{1/2}}{1+\boldsymbol{u}^2} \exp\left(\frac{r(\boldsymbol{u}^2-1)+2\mathrm{i}\boldsymbol{u}\boldsymbol{x}}{\boldsymbol{u}^2+1}\right) \tag{2}$$

where $\boldsymbol{u}$ is the vector with components

$$\boldsymbol{u} = \left(\frac{\mathrm{i}}{2}(\lambda_2-\lambda_1), \frac{1}{2}(\lambda_1+\lambda_2), 0\right). \tag{3}$$

It is well known that the $SO(3)$ transformations acting in the space of vectors $|n_1n_2m\rangle$ correspond to the usual rotations in configuration space. Then, acting on the vector $|\lambda_1\lambda_2\rangle$ by the rotation which transforms the vector (3) into the arbitrary complex 3-vector of the same length, we obtain the resulting state as a series of vectors $|n_1n_2m\rangle$ too; however, this series will have a much more complicated form than (1). Then we shall consider $\boldsymbol{u}$ as an arbitrary complex 3-vector obeying the condition $\boldsymbol{u}^2 < 1$; we denote the corresponding state as $|\boldsymbol{u}\rangle$ rather than $|\lambda_1\lambda_2\rangle$. To represent (2) in a more compact form, we introduce the complex space-like unit 4-vector

$$l_{\boldsymbol{u}}^\mu = \left(\mathrm{i}\frac{1-\boldsymbol{u}^2}{1+\boldsymbol{u}^2}, \frac{-2\boldsymbol{u}}{1+\boldsymbol{u}^2}\right).$$

Then $l_{\boldsymbol{u}} \cdot l_{\boldsymbol{u}} = -1$ (the analogous transformation takes place for the CS for the $SO(4,1)$ group too [12]), and the light-like forward 4-vector

$$n_{\boldsymbol{x}}^\mu = (r, \boldsymbol{x}) \qquad n_{\boldsymbol{x}} \cdot n_{\boldsymbol{x}} = 0 \qquad n_{\boldsymbol{x}}^0 \geqslant 0. \tag{4}$$

Then we can rewrite (2) in the form

$$\langle \boldsymbol{x}|\boldsymbol{u}\rangle = \frac{c_0}{2\sqrt{\pi}} (\boldsymbol{l}_{\boldsymbol{u}}^2)^{1/2} \exp(\mathrm{i} l_{\boldsymbol{u}} \cdot n_{\boldsymbol{x}}).$$

From (4) it follows that the measure $r^{-1}\,\mathrm{d}V = \frac{1}{2}\,\mathrm{d}(\xi^2)\,\mathrm{d}(\eta^2)\,\mathrm{d}\phi$ for the scalar product of wavefunctions of the hydrogen atom [3] coincides with the Lorentz-invariant measure over the light cone. Then it is easily seen that, for finiteness of the norm of the vector $|\boldsymbol{u}\rangle$, the inequality

$$w_{\boldsymbol{u}} \cdot w_{\boldsymbol{u}} = \frac{1 - 2\boldsymbol{u}\boldsymbol{u}^* + \boldsymbol{u}^2\boldsymbol{u}^{*2}}{|1+\boldsymbol{u}^2|^2} > 0 \qquad w_{\boldsymbol{u}}^\mu = \operatorname{Im} l_{\boldsymbol{u}}^\mu \tag{5}$$

should be satisfied. The vectors obeying this inequality compose the symmetric space [13]

$$SO(3,2)/(SO(3) \otimes SO(2)) \simeq \mathrm{Sp}\,(2,\mathbb{R})/U(2).$$

This space is that of the CS for the bosonic system of two degrees of freedom [1]. To clarify their connection with those of the hydrogen atom, let us introduce two mutually commuting sets of creation–destruction operators:

$$[a_\alpha, a_\beta^\dagger] = [b_\alpha, b_\beta^\dagger] = \delta_{\alpha\beta} \qquad \alpha, \beta = 1, 2$$

such as $a_\alpha|0\rangle = b_\alpha|0\rangle = 0$ at $\alpha = 1, 2$, where $|0\rangle \equiv |\boldsymbol{u} = \boldsymbol{0}\rangle = |n_1 = n_2 = m = 0\rangle$. Then the arbitrary vector $|n_1n_2m\rangle$ may be obtained by some combination of the operators $a_\alpha^\dagger, b_\alpha^\dagger$ acting on the vector $|0\rangle$. Then we can define the representation of the $SO(3,2)$ group acting in the space of vectors $|n_1 n_2 m\rangle$ in the following way [3]:

$$\begin{aligned} L_{ij} &= \tfrac{1}{2}(a^\dagger\sigma_k a + b^\dagger\sigma_k b) \qquad & L_{i5} &= -\tfrac{1}{2}(a^\dagger\sigma_i C b^\dagger - aC\sigma_i b) \\ L_{i0} &= \frac{1}{2\mathrm{i}}(a^\dagger\sigma_i C b^\dagger + aC\sigma_i b) \qquad & L_{50} &= \tfrac{1}{2}(a^\dagger a + b^\dagger b + 2) \end{aligned} \tag{6}$$

where $C = \mathrm{i}\sigma_2$. These generators obey the commutation relations

$$[L_{AB}, L_{CD}] = \mathrm{i}(\eta_{AD}L_{BC} + \eta_{BC}L_{AD} - \eta_{AC}L_{BD} - \eta_{BD}L_{AC}) \tag{7}$$

where $A, B, \ldots = 0, \ldots, 3, 5$ and $\eta_{AB} = (+1, -1, -1, -1, +1)$. In comparison with the notation of Barut and Rasmussen [3] we suppressed the fourth coordinate, and the sixth coordinate has traded places with the zeroth one. Let us introduce the new set of operators

$$A_\alpha = \frac{1}{\sqrt{2}}(a_\alpha + b_\alpha) \qquad B_\alpha = \frac{1}{\sqrt{2}}(a_\alpha - b_\alpha)$$
$$[A_\alpha, A^\dagger_\beta] = [B_\alpha, B^\dagger_\beta] = \delta_{\alpha\beta}.$$

All other commutators vanish. Since the matrices $C\sigma_i$ and $\sigma_i C$ are symmetric then the generators (6) are the linear combination of generators of the $\mathrm{Sp}(2,\mathbb{R}) \simeq SO(3,2)$ group:

$$X_{\alpha\beta} = A_\alpha A_\beta \qquad X^\dagger_{\alpha\beta} = A^\dagger_\alpha A^\dagger_\beta \qquad Y_{\alpha\beta} = \tfrac{1}{2}(A_\alpha A^\dagger_\beta + A^\dagger_\beta A_\alpha)$$

and of those obtained from the ones above by replacing A with B. Then the $SO(3,2)$ group acts as a group of canonical $\mathrm{Sp}(2,\mathbb{R})$ transformations of each set $(A_\alpha, A^\dagger_\alpha)$ and $(B_\alpha, B^\dagger_\alpha)$ separately. Putting $\boldsymbol{w}_u = \boldsymbol{0}$ by virtue of the Lorentz invariance for the normalization factor we obtain

$$|c_0|^2 = \frac{1 - 2\boldsymbol{u}\boldsymbol{u}^* + \boldsymbol{u}^2\boldsymbol{u}^{*2}}{|\boldsymbol{u}^2|}. \tag{8}$$

Then the normalized CS system is

$$\langle \boldsymbol{x}|\boldsymbol{u}\rangle = \frac{1}{\pi^{1/2}}(w_{\boldsymbol{u}} \cdot w_{\boldsymbol{u}})^{1/2} \exp(\mathrm{i}l_{\boldsymbol{u}} \cdot n_{\boldsymbol{x}}).$$

3. Properties

It is well known that the generator L_{50} possesses the property [3]

$$L_{50}|n_1 n_2 m\rangle = (n_1 + n_2 + |m| + 1)|n_1 n_2 m\rangle.$$

Then, using (1) and (8) we obtain

$$\mathrm{e}^{\mathrm{i}\varepsilon L_{50}}|\boldsymbol{u}\rangle = \mathrm{e}^{\mathrm{i}\varphi(\varepsilon)}|\boldsymbol{u}\mathrm{e}^{\mathrm{i}\varepsilon}\rangle. \tag{9}$$

Then, due to the Lorentz invariance of our CS system, it follows from the commutation relations (7) that this system is invariant under the action of the full $SO(3,2)$ group. The generator L_{50} corresponds to evolution with respect to the fictitious time variable [4]. Then the CS system we have constructed obeys the properties (b′) and (c′). Let us consider the spatial distribution of the probability density of our CS. Denoting

$$w^\perp_{\boldsymbol{u}} = [(w^1_{\boldsymbol{u}})^2 + (w^2_{\boldsymbol{u}})^2]^{1/2} \qquad w^1_{\boldsymbol{u}} = w^\perp_{\boldsymbol{u}} \cos\alpha_{\boldsymbol{u}} \qquad w^2_{\boldsymbol{u}} = w^\perp_{\boldsymbol{u}} \sin\alpha_{\boldsymbol{u}}$$

we obtain

$$|\langle \boldsymbol{x}|\boldsymbol{u}\rangle| = \frac{1}{\pi^{1/2}}(w \cdot w)^{1/2} \exp[-(w^0_{\boldsymbol{u}} - w^3_{\boldsymbol{u}})\xi^2 - (w^0_{\boldsymbol{u}} + w^3_{\boldsymbol{u}})\eta^2 + 2\xi\eta w^\perp_{\boldsymbol{u}} \cos(\phi - \alpha_{\boldsymbol{u}})].$$

It is Gaussian with respect to the variables ξ and η separately and then the property (h) is satisfied. Using the Lorentz invariance, it is easy to show that the equalities

$$\begin{aligned} \langle \boldsymbol{u}|n_x^\mu|\boldsymbol{u}\rangle &= \frac{w_{\boldsymbol{u}}^\mu}{w_{\boldsymbol{u}}\cdot w_{\boldsymbol{u}}} \\ \langle \boldsymbol{u}|n_x^\mu n_x^\nu|\boldsymbol{u}\rangle &= \frac{4w_{\boldsymbol{u}}^\mu w_{\boldsymbol{u}}^\nu - \eta^{\mu\nu}(w_{\boldsymbol{u}}\cdot w_{\boldsymbol{u}})}{2(w_{\boldsymbol{u}}\cdot w_{\boldsymbol{u}})} \end{aligned} \tag{10}$$

hold. We define the expectation value of the variable f as

$$\langle f\rangle = \frac{\langle \boldsymbol{u}|rf|\boldsymbol{u}\rangle}{\langle \boldsymbol{u}|r|\boldsymbol{u}\rangle}.$$

Here and in (10) we take the scalar product with the measure $r^{-1}\,\mathrm{d}V$. Without loss of generality we can consider $\boldsymbol{u} = (\boldsymbol{k} + \mathrm{i}\boldsymbol{m})\mathrm{e}^{\mathrm{i}\theta}$, where $\boldsymbol{k}, \boldsymbol{m} \in \mathbb{R}^3$ and $\boldsymbol{km} = 0$. Then using (10) and (5) we obtain

$$\langle \boldsymbol{x}\rangle = \frac{2\boldsymbol{w}_{\boldsymbol{u}}}{w_{\boldsymbol{u}}\cdot w_{\boldsymbol{u}}} = -4\frac{(1+\boldsymbol{k}^2-\boldsymbol{m}^2)\boldsymbol{m}\cos\theta + (1+\boldsymbol{m}^2-\boldsymbol{k}^2)\boldsymbol{k}\sin\theta}{1-2(\boldsymbol{k}^2+\boldsymbol{m}^2)+(\boldsymbol{k}^2-\boldsymbol{m}^2)^2}.$$

In view of (9) from the above expression the property (d′) follows immediately. Let us emphasize that, unlike the case of the harmonic oscillator, changing $\langle \boldsymbol{x}\rangle$ does not mean changing the position of the probability density maximum. With arbitrary $\boldsymbol{u}$ this maximum is situated at the point $\boldsymbol{x} = \mathbf{0}$—at the centre of the ellipse. This is a result of the fact that, for arbitrary $\boldsymbol{u}$, the states with $n_1 = n_2 = 0$ dominate. For our CS system the property (f′) is satisfied. Indeed, we can consider our CS system as that constructed using the general Perelomov method [1] acting by the $SO(3,2)$ transformations onto the fiducial vector $|0\rangle$, since this vector has the stationary subgroup $SO(3)\otimes SO(2)$. Let us consider the stationary (up to multiplication by the real constant) subalgebra $\mathcal{B}$ of this vector in the complexified Lie algebra $\mathcal{G}^c$ of the $SO(3,2)$ group. The subalgebra $\mathcal{B}$ is composed of the generators L_{ij}, $L_{i5}+\mathrm{i}L_{i6}$ and L_{56}; together with its conjugated subalgebra $\overline{\mathcal{B}}$ the subalgebra $\mathcal{B}$ exhausts the full algebra $\mathcal{G}^c$, i.e. the subalgebra $\mathcal{B}$ possesses the so-called maximality property (in the case of the full conformal group this was pointed out in [9]). On the other hand, for an arbitrary Lie group the property (f′) is satisfied if we construct our CS system starting from the fiducial vector which has the maximal stationary subalgebra in the Lie algebra $\mathcal{G}^c$ [1]. It is well known that the Shilov boundary of the space $\mathrm{Sp}(2,\mathbb{R})/U(2)$ is $S^1\times S^2$ [13]; the passage to it may be performed by putting $\boldsymbol{u}\to\boldsymbol{q}\mathrm{e}^{\mathrm{i}\beta}$, where $\boldsymbol{q}$ is real and $\boldsymbol{q}^2 = 1$. Then it is readily seen that $w_{\boldsymbol{u}}^\mu \to 0$ and from (10) we obtain

$$\langle r\rangle = \frac{2w_{\boldsymbol{u}}^0}{w_{\boldsymbol{u}}\cdot w_{\boldsymbol{u}}} \to \infty.$$

Then passage to the Shilov boundary corresponds to the quasiclassical limit. In such a case the particle motion should become free; indeed, putting $c_0 = 1$ and $\beta = 0$ we obtain $|\boldsymbol{u}\rangle \to \mathrm{e}^{\mathrm{i}\boldsymbol{qx}}$, i.e. the plane wave for a particle of unit mass.

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References

[1] Perelomov A M 1986 *Generalized Coherent States and Their Applications* (Berlin: Springer)
[2] Benedict M and Molnar B 1999 *Phys. Rev.* A **60** 1737
[3] Barut A O and Rasmussen W 1973 *J. Phys. B: At. Mol. Phys.* **6** 1695
[4] Gerry C 1986 *Phys. Rev.* A **33** 6
[5] Mostowski J 1977 *Lett. Math. Phys.* **2** 1

[6] Klauder J R 1996 *J. Phys. A: Math. Gen.* **29** L293
[7] Majumdar P and Sharatchandra H S 1997 *Phys. Rev.* A **56** R3322
[8] Bellomo P and Stroud C R Jr 1999 *Phys. Rev.* A **59** 900
[9] de Prunele E 1990 *Phys. Rev.* A **42** 2542
[10] Nouri S 1999 *Phys. Rev.* A **60** 1702
[11] Bateman H 1953 *Higher Transcendental Functions* vol 2 (New York: McGraw-Hill)
[12] Pol'shin S A 2000 *J. Phys. A: Math. Gen.* **33** 5077
[13] Piatetsky-Chapiro I I 1966 *Géometrie des Domaines Classiques et Theorie des Fonctions Automorphes* (Paris: Dunod)