On coherent states for the hydrogen atom

1984 J. Phys. A: Math. Gen. 17 L737

(http://iopscience.iop.org/0305-4470/17/14/002)

J. Phys. A: Math. Gen. 17 (1984) L737–L740. Printed in Great Britain

LETTER TO THE EDITOR

On coherent states for the hydrogen atom

Christopher C Gerry

Physics Department, St Bonaventure University, St Bonaventure, New York 14778, USA

Received 3 May 1984

Abstract. Oscillator-like coherent states are introduced on the O(4) algebra of the H-atom dynamical symmetry group when given in terms of boson operators. It is shown that the correct classical frequencies may be obtained without the correspondence limit.

There have, over the years, been many discussions in the literature on the classical limit of the quantum Kepler problem—the hydrogen atom. These discussions consist of two different types of approaches to quasi-classical behaviour. There is of course the WKB approximation obtained in the limit that $\hbar \to 0$ (see Berry and Mount (1972) for a review). Then there are attempts to find wavepackets consisting of the right combinations of Coulomb wavefunctions to be concentrated on circular (Brown 1973) or elliptical orbits (Snieder 1983) of the corresponding classical Kepler problem. This second approach seems to be realised for high quantum numbers n and might therefore be said to be a reflection of the Bohr correspondence principle.

On the other hand Schrödinger (1926) discovered a set of gaussian states for the harmonic oscillator which do not spread in time and follow the classical motion of the oscillator. These states are now called coherent states. Schrödinger went on to speculate that a similar set of states for the H-atom could be constructed. That this was not realised is due to the fact that for the oscillator the energy eigenvalues are integer space while they are not for the H-atom (Nieto and Simmons 1979).

In this letter we give a preliminary account of an attempt to obtain a quasi-classical picture of the H-atom by introducing oscillator-like coherent states when the algebra of the dynamical symmetry group O(4) is realised in terms of boson operators. Here we shall limit our discussion to determination of the classical Kepler orbital frequencies while elsewhere we shall give a more detailed account including an attempt to obtain the classical elliptical orbits as well.

First we consider the harmonic oscillator of frequency ω where the Hamiltonian is

$$H_0 = \hbar\omega(a^\dagger a + \tfrac{1}{2}) \tag{1}$$

and where $[a, a^\dagger] = 1$. The eigenstates of (1) are of course the usual $|n\rangle$ where $a^\dagger a|n\rangle = n|n\rangle$. Coherent states $|z\rangle$ where z is a complex number may be introduced as linear combinations of the states $|n\rangle$ as either minimum uncertainty states, eigenstates of the operator a, or as states displaced from the ground state $|n=0\rangle$ via the operator $D(z) = \exp(za^\dagger - z^* a)$ (Glauber 1963). All definitions yield the same result namely

$$|z\rangle = \exp(-|z|^2/2) \sum_{n=0}^{\infty} z^n (n!)^{-1/2} |n\rangle. \tag{2}$$

Properties of these states are given in many places e.g. Klauder and Sudarshan (1968). From the Hamiltonian (1) we obtain the classical counterpart as

$$H_0^{\text{cl}} = \langle z|H_0|z\rangle = \hbar\omega(z^*z + \tfrac{1}{2}). \tag{3}$$

The variable z will satisfy the Hamiltonian equations

$$\mathrm{i}\hbar z = \partial H_0^{\text{cl}}/\partial z^* \tag{4a}$$

$$-\mathrm{i}\hbar z^* = \partial H_0^{\text{cl}}/\partial z. \tag{4b}$$

However, we may define the action variables $J = h(|z|^2 + \frac{1}{2})$ so that $H_0^{\text{cl}} = \nu J$ and $\nu = \text{-}\partial H_0^{\text{cl}}/\partial J$ as required for a periodic system (Goldstein 1980). In this case of course, the frequency is independent of the energy. The quantised energy levels are recovered via the Bohr–Sommerfeld rule $J = h(n + \frac{1}{2})$.

Now consider the H-atom (for a review of the O(4) formulation see Wulfman 1971). The Hamiltonian

$$H = p^2/2\mu - Ze^2/r \tag{5}$$

commutes with the angular momentum vector $\boldsymbol{L}$ and the Runge–Lenz vector

$$\boldsymbol{A}' = -\frac{Ze^2\boldsymbol{r}}{r} + \frac{1}{2\mu}(\boldsymbol{L}\times\boldsymbol{p} - \boldsymbol{p}\times\boldsymbol{L}). \tag{6}$$

As is well known $\boldsymbol{A}'$ is orthogonal to $\boldsymbol{L}$

$$\boldsymbol{A}'\cdot\boldsymbol{L} = \boldsymbol{L}\cdot\boldsymbol{A}' = 0 \tag{7}$$

and has the norm

$$A'^2 = (2/\mu)H(L^2 + \hbar^2) + (Ze^2)^2 \tag{8}$$

where H is from equation (5). If we define $\boldsymbol{A} = (-\mu/2E)^{1/2}\boldsymbol{A}'$ for $E < 0$ then the decomposition $\mathrm{O}(4) \sim \mathrm{SU}(2)_a \otimes \mathrm{SU}(2)_b$ emerges if we define the operators

$$\boldsymbol{S}_a = \tfrac{1}{2}(\boldsymbol{L} + \boldsymbol{A}), \qquad \boldsymbol{S}_b = \tfrac{1}{2}(\boldsymbol{L} - \boldsymbol{A}) \tag{9}$$

where $\boldsymbol{S}_a$ and $\boldsymbol{S}_b$ separately close on an SU(2) Lie algebra. The operators $\boldsymbol{S}_a$ and $\boldsymbol{S}_b$ may be realised in terms of four boson operators as

$$\boldsymbol{S}_a = \tfrac{1}{2}a^\dagger\boldsymbol{\sigma}a, \qquad \boldsymbol{S} = \tfrac{1}{2}b^\dagger\boldsymbol{\sigma}b \tag{10a, b}$$

where

$$a = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \qquad b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \tag{11}$$

and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices.

Now Kibler and Negadi (1983) have shown that in terms of these operators equations (7) and (8) become

$$(a_1^\dagger a_1 + a_2^\dagger a_2 + 1)^2 = (b_1^\dagger b_1 + b_2^\dagger b_2 + 1)^2 \tag{12}$$

and

$$-\mu Z^2 e^4/\hbar^2 E = (a_1^\dagger a_1 + a_2^\dagger a_2 + 1)^2 + (b_1^\dagger b_1 + b_2^\dagger b_2 + 1)^2 \tag{13}$$

respectively. Introducing the Fock space eigenstates† of $a_i^\dagger a_i$ as $|n_i\rangle$ and those of $b_i^\dagger b_i$ as $|m_i\rangle$ where $n_i, m_i = 0, 1, 2, \ldots$, one obtains from equation (12) the constraint condition

$$n_1 + n_2 = m_1 + m_2 \tag{14}$$

and from (13) (using equation (14)) the energy levels

$$E_n = -\mu Z^2 e^4 / 2n^2 \tag{15}$$

where $n = n_1 + n_2 + 1 = m_1 + m_2 + 1$.

We now introduce a set of ordinary coherent states for each of the sets of boson operators. That is let

$$|z_i^a\rangle = D(z_i^a)|n_i = 0\rangle, \qquad |z_i^b\rangle = D(z_i^b)|m_i = 0\rangle \tag{16a, b}$$

where $i = 1, 2$, are the set of four coherent states associated with a and b. Then equation (7) gives the condition

$$|z_1^a|^2 + |z_2^a|^2 = |z_1^b|^2 + |z_2^b|^2 \tag{17}$$

and one has the energy

$$H_{\text{cl}} = E = \frac{-2\pi^2 \mu k^2}{h^2(|z_1^a|^2 + |z_2^a|^2 + 1)^2} \tag{18}$$

where $k = Ze^2$. As in the case of the harmonic oscillator we may introduce the action variables

$$J_i^{a,b} = h(|z_i^{a,b}|^2 + \tfrac{1}{2}) \tag{19}$$

so that

$$H_{\text{cl}} = -2\pi^2 \mu k^2 / (J_1^a + J_2^a)^2 \tag{20a}$$

$$= -2\pi^2 \mu k^2 / (J_1^b + J_2^b)^2. \tag{20b}$$

From Hamilton's equation in action-angle variables one has

$$\begin{aligned} \nu_{\text{cl}} &= \partial H_{\text{cl}} / \partial J_1^{a,b} = \partial H / \partial J_2^{a,b} \\ &= 4\pi^2 \mu k^2 / (J_1^a + J_2^a)^3 \end{aligned} \tag{21}$$

which yields the correct relation for the period of Kepler orbits namely

$$\tau = 2\pi a^{3/2} (\mu / k)^{1/2} \tag{22}$$

where $a = -k/2E$. Quantisation may be regained by the application to the action variables of the Bohr–Sommerfeld rule stated earlier.

Finally we remark that our result in equation (21) is *not* dependent on taking n to be large but rather the coherent states are composed of a sum over all quantum numbers. Elsewhere we shall make use of the fact that the four-dimensional oscillators (i.e. the four operators of a and b) and the three-dimensional Kepler problems are related by the Kustaanheimo–Stiefel (1965) transformation first introduced in the context of celestial mechanics (see Barut *et al* (1979) for its quantum application). From this one may show that these coherent states do describe the expected elliptical orbits.

† These states are actually just relabelled SU(2) states of the Schwinger boson representation (Schwinger 1965).

References

Barut A O, Schneider C K E and Wilson R 1979 *J. Math. Phys.* **20** 2244–56

Berry M V and Mount K E 1972 *Rep. Prog. Phys.* **35** 315–97

Brown L S 1973 *Am. J. Phys.* **41** 525–3

Glauber R J 1963 *Phys. Rev.* **131** 2766

Goldstein H 1980 *Classical Mechanics* 2nd edn (Reading, Mass.: Addison-Wesley)

Kibler M and Negadi T 1983 *Lett. Nuovo Cimento* **37** 225–8

Klauder J R and Sudarshan E C G 1968 *Fundamentals of Quantum Optics* (New York: Benjamin) ch 7

Kustaanheimo P and Stiefel E 1965 *J. Reine angew. Math.* **218** 204

Nieto M M and Simmons L M 1979 *Phys. Rev.* **20** 1321–31

Schrödinger E 1926 *Naturwissenschaften* **14** 664

Schwinger J 1965 in *Quantum Theory of Angular Momentum* ed L C Biedenharn and H Van Dam (New York: Academic) p 229

Snieder D R 1983 *Am. J. Phys.* **51** 801–3

Wulfman C E 1971 in *Group Theory and its Applications* vol II, ed E M Loebl (New York: Academic) pp 145–97