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An extended hydrogen atom with Yangian $Y(sl(2))$

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Abstract. The hydrogen atom is extended by deforming the loop algebra $L(sl(2))$, which is shown to be the symmetrical algebra of the hydrogen atom, to the case with Yangian $Y(sl(2))$. A realization of $Y(sl(2))$ is proposed. Using this Yangian $Y(sl(2))$, the energy spectrum of the extended hydrogen atom is calculated.

Recently, considerable attention has been drawn to the Yangian in mathematics and physics. This quantum algebra was first introduced by Drinfeld [1]. Many new developments on Yangian symmetry in physical models have been reported, such as long-range interaction models [2], the one-dimensional Hubbard model [3], the two-dimensional sigma model [4], the two-dimensional chiral model with or without topological terms [5] and the Heisenberg model [6]. In order to explore the significance of the Yangian, it becomes more important to study whether simple physics systems have the Yangian and to find these systems and corresponding Yangian structures.

In this paper, an extended hydrogen atom (EHA) with $Y(sl(2))$ structure will be proposed from the point of view of quantum mechanics. It is well known that hydrogen atom possesses the dynamical group $SO(4,2)$ [7]. However, the $SO(4)$ group is looked upon as the conservation symmetry of the hydrogen atom [8]. Generators of $SO(4)$ are realized in terms of the angular momentum operator $\boldsymbol{L}$ and the so-called Runge–Lenz vector $\boldsymbol{R}$ for the fixed energy level. If one just considered $\boldsymbol{L}$ and $\boldsymbol{R}$, they are not closed to construct the algebra $so(4)$. However, we find that $\boldsymbol{L}$ and $\boldsymbol{R}$ obey the commutation relation of the loop algebra $L(sl(2))$ (more precisely, the subalgebra of $L(sl(2))$, which is just the corresponding classical algebra of $Y(sl(2))$ in the limit of the quantum deformation parameter tending to zero [6]. Therefore, it is interesting to study the hydrogen atom when it is extended to the case that the above-mentioned loop algebra is quantized. This can be achieved by deforming the angular momentum and Runge–Lenz vector directly. In this paper, the deformed angular momentum and Runge–Lenz vector will be constructed. Correspondingly, through deforming the so-called Pauli equation [8], the Hamiltonian of the EHA will be determined. Its energy spectrum will also be calculated.

It is well known that the Hamiltonian of the usual hydrogen atom reads

$$H_0 = \frac{\boldsymbol{p}^2}{2\mu} - \frac{e^2}{|\boldsymbol{r}|} \tag{1}$$

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where μ and e stand for the mass and electric charge of the electron, respectively. It has been pointed out [7] that the angular momentum $\boldsymbol{L}$ and Runge–Lenz vector

$$\boldsymbol{R} = \frac{1}{2\mu e^2}(\boldsymbol{p} \times \boldsymbol{L} - \boldsymbol{L} \times \boldsymbol{p}) - \frac{\boldsymbol{r}}{r} \tag{2}$$

are conserved quantities. They commute with the Hamiltonian (1). Since

$$[R_3, R_\pm] = \pm\frac{-2H_0}{\mu e^4}L_\pm \qquad [R_+, R_-] = \frac{4H_0}{\mu e^4}L_3 \tag{3}$$

where $R_\pm = R_1 + \mathrm{i}R_2$ we see that the commutation relation of the Runge–Lenz vector is not closed due to the Hamiltonian H_0 appearing on the right-hand side of (3). As we have pointed out, $\boldsymbol{L}$ and $\boldsymbol{R}$ cannot be looked upon as the generators of $SO(4)$ precisely.

However, after deriving them directly, we find that the angular momentum $\boldsymbol{L}$ and Runge–Lenz vector $\boldsymbol{R}$ satisfy the following commutation relations

$$\begin{aligned} &[L_3, L_\pm] = \pm L_\pm \qquad [L_+, L_-] = 2L_3 \\ &[L_3, R_\pm] = [R_3, L_\pm] = \pm R_\pm \qquad [L_\pm, R_\mp] = 2R_3 \\ &[L_3, R_3] = [L_\pm, R_\pm] = 0 \end{aligned} \tag{4}$$

in which $L_\pm = L_1 + \mathrm{i}L_2$ and

$$\begin{aligned} &[R_3, [R_+, R_-]] = 0 \qquad [R_\pm, [R_3, R_\pm]] = 0 \\ &2[R_3, [R_3, R_\pm]] \pm [R_\pm, [R_\pm, R_\mp]] = 0. \end{aligned} \tag{5}$$

This means that $\boldsymbol{L}$ and $\boldsymbol{R}$ form a subalgebra of the loop algebra $L(sl(2))$, i.e. the classical limitation of $Y(sl(2))$. It is interesting to 'quantize' the hydrogen atom so that the $L(sl(2))$ subalgebra determined by (4) and (5) become the Yangian $Y(sl(2))$.

According to Drinfeld [1], the Yangian $Y(sl(2))$ is generated by the generators $\{I_\pm, I_3\}$ and $\{J_\pm, J_3\}$ with the commutation relation as follows

$$\begin{aligned} &[I_3, I_\pm] = \pm I_\pm \qquad [I_+, I_-] = 2I_3 \\ &[I_3, J_\pm] = [J_3, I_\pm] = \pm J_\pm \qquad [I_\pm, J_\mp] = \pm 2J_3 \\ &[I_3, J_3] = [I_\pm, J_\pm] = 0 \end{aligned} \tag{6}$$

and

$$\begin{aligned} &[J_3, [J_+, J_-]] = \frac{\alpha^2}{4}I_3(J_-I_+ - I_-J_+) \\ &[J_\pm, [J_3, J_\pm]] = \frac{\alpha^2}{4}I_\pm(J_\pm I_3 - I_\pm J_3) \\ &2[J_3, [J_3, J_\pm]] \pm [J_\pm, [J_\pm, J_\mp]] = \frac{\alpha^2}{4}\{2I_3(J_\pm I_3 - I_\pm J_3) + I_\pm(I_-J_+ - J_-I_+)\} \end{aligned} \tag{7}$$

where α is the quantum deformation parameter. In order to 'quantize' the hydrogen atom, we must deform the angular momentum and Runge–Lenz vector so that they obey the above communication relations (6) and (7). We denote them as $\boldsymbol{L}^Y$ and $\boldsymbol{R}^Y$, which are called the Yangian angular momentum and the Yangian Runge–Lenz vector, respectively.

From the commutation relations (6), we can directly assign

$$L_3^Y = L_3 \qquad L_\pm^Y = L_\pm = L_1 \pm \mathrm{i}L_2. \tag{8}$$

In other words, the angular momentum remains unchanged in the deformation. Since the usual Runge–Lenz vector is the limitation of the Yangian Runge–Lenz vector when the quantum deformation parameter reduces to zero and equations (6) show that the communication relations of J_3 and $J_\pm$ with I_3 and $I_\pm$ are similar to those of I_3 and $I_\pm$ itself, it is believable that the Yangian Runge–Lenz vector should have the form

$$\boldsymbol{R}^Y = \boldsymbol{R} + \beta \boldsymbol{Q} \tag{9}$$

in which β is a parameter that should vanish when the quantum deformation parameter α reduces to zero and $\boldsymbol{Q}$ is a vector operator to be found. Through analysing equations (6) and (7), we find that the generators $\{Q_3, Q_\pm\}$ can be chosen as

$$\begin{aligned} Q_3 &= \frac{1}{\sqrt{H_0}}[\boldsymbol{L}^2, R_3] = \frac{1}{2\sqrt{H_0}}(L_+R_- - R_+L_-) \\ Q_\pm &= \frac{1}{\sqrt{H_0}}[\boldsymbol{L}^2, R_\pm] = \pm\frac{1}{\sqrt{H_0}}(L_3R_\pm - R_3L_\pm). \end{aligned} \tag{10}$$

From (9) and (10), the Yangian Runge–Lenz vector can be realized as follows:

$$\boldsymbol{R}^Y = \boldsymbol{R} + \beta \frac{1}{\sqrt{H_0}}[\boldsymbol{L}^2, \boldsymbol{R}]. \tag{11}$$

It can be verified that our Yangian angular momentum $\boldsymbol{L}^Y$ and Yangian Runge–Lenz vector $\boldsymbol{R}^Y$ satisfy

$$\begin{aligned} &[L_3^Y, L_\pm^Y] = \pm L_\pm^Y \qquad [L_+^Y, L_-^Y] = 2L_3^Y \\ &[L_3^Y, R_\pm^Y] = [R_3^Y, L_\pm^Y] = \pm R_\pm^Y \qquad [L_\pm^Y, R_\mp^Y] = \pm 2R_3^Y \\ &[L_3^Y, R_3^Y] = [L_\pm^Y, R_\pm^Y] = 0 \end{aligned} \tag{12}$$

and

$$\begin{aligned} &[R_3^Y, [R_+^Y, R_-^Y]] = \frac{8\beta^2}{\mu e^4} L_3^Y (R_-^Y L_+^Y - L_-^Y R_+^Y) \\ &[R_\pm^Y, [R_3^Y, R_\pm^Y]] = \frac{8\beta^2}{\mu e^4} L_\pm^Y (R_\pm^Y L_3^Y - L_\pm^Y R_3^Y) \\ &2[R_3^Y, [R_3^Y, R_\pm^Y]] \pm [R_\pm^Y, [R_\pm^Y, R_\mp^Y]] = \frac{8\beta^2}{\mu e^4}\{2L_3^Y(R_\pm^Y L_3^Y - L_\pm^Y R_3^Y) + L_\pm^Y(L_-^Y R_+^Y - R_-^Y L_+^Y)\}. \end{aligned} \tag{13}$$

We see that equations (12) and (13) are just the commutation relations of $Y(sl(2))$ with quantum deformation parameter $\alpha = 32\beta^2/\mu e^4$. Therefore, our Yangian angular momentum and Yangian Runge–Lenz vector indeed construct the Yangian $Y(sl(2))$. It must be pointed out that the generators (11) are different from the Yangian $Y(sl(2))$ realization in [9]. Equations (8) and (11) give a new realization of $Y(sl(2))$.

Now, let us deform the hydrogen atom (1). It is well known that the usual angular momentum and Runge–Lenz vector obey the Pauli equation,

$$\boldsymbol{R}^2 = \frac{2H_0}{\mu e^4}(\boldsymbol{L}^2 + 1) + 1. \tag{14}$$

Using the Pauli equation, the energy spectrum of the hydrogen atom can be determined algebraically [7]. The hydrogen atom was deformed by deforming Lie algebra SO(4) to the quantum algebra $SO_q(4)$ case in terms of deforming the Pauli equation [10]. Following this line, one can obtain an EHA with Yangian $Y(sl(2))$ structure. We have determined the Yangian angular momentum and Yangian Runge–Lenz vector as (8) and (11), respectively. Naturally, the Pauli equation (14) can be deformed in the form

$$\boldsymbol{R}^{Y_2} = \frac{2H}{\mu e^4}(\boldsymbol{L}^{Y2} + 1) + 1 \tag{15}$$

where H stands for the Hamiltonian of the EHA. Substituting (8) and (11) into (15), through tedious calculations, we have

$$H = \frac{\boldsymbol{p}^2}{2\mu} - \frac{e^2}{|\boldsymbol{r}|} - 4\beta^2 \left(\boldsymbol{L}^2 + 1 + \frac{\boldsymbol{L}^2}{\boldsymbol{L}^2 + 1} + \frac{\boldsymbol{L}^2 + 1}{\boldsymbol{R}^2 - 1} \right). \tag{16}$$

In (16), the Hamiltonian of the EHA has been expressed in terms of the usual angular momentum and Runge–Lenz vector to calculate the energy spectrum of the EHA conveniently. From (16), we see that the Hamiltonian H reduces to the Hamiltonian (1) when the quantum parameter β vanishes. The extension changes the Coulomb potential to a complicated expression, in which the extended potential depends on the usual angular momentum and the Runge–Lenz vector respectively. It must be pointed out that there is no operator order problem in equation (16) since $\boldsymbol{L}^2$ commuted with $\boldsymbol{R}^2$, which can be deduced from the Pauli equation (14) directly.

Because the angular momentum is the conservative quantity of the usual hydrogen atom (1), we can show that it is also conservative for the EHA (16). In fact, it is due to the Pauli equation (14) that the angular momentum is commutative with $\boldsymbol{R}^2$. This conclusion is apparent. On the other hand, $\boldsymbol{R}^2$ is also the conservative quantity of the EHA (16). Since

$$\boldsymbol{R}^{Y2} = \boldsymbol{R}^2 - 4\beta^2 \left(H_0^{-1}\boldsymbol{R}^2 - \frac{2\boldsymbol{L}^2}{\mu e^4} - H_0^{-1}\boldsymbol{R}^2\boldsymbol{L}^2 \right)$$

we have

$$[\boldsymbol{R}^{Y2}, \boldsymbol{R}^2] = [\boldsymbol{R}^{Y2}, \boldsymbol{L}^2] = [\boldsymbol{R}^{Y2}, H_0] = 0. \tag{17}$$

Therefore, we can conclude that $\boldsymbol{R}^{Y2}$ is commutative with the Hamiltonian of the EHA (16), i.e. it is another conservative quantity. From the Hamiltonian (16), we see that the Hamiltonian of the usual hydrogen atom (1) may also be regarded as being conservative for the EHA.

The energy spectrum of the EHA can be derived algebraically. As for the usual hydrogen atom, it is determined from the deformed Pauli equation (15) according to our realization (8) and (11). We prefer to obtain it in terms of the eigenstate of the usual hydrogen atom. This is due to the fact that the Hamiltonian of the EHA (16), the angular momentum operator $\boldsymbol{L}^2$ and L_z, and the Hamiltonian of the usual hydrogen atom (1) are commutative with each other. It is well known that the Hilbert space of the usual atom is given by the wavefunction

$$|nlm\rangle = R_{nl}(r)Y_{lm}(\theta, \phi)$$

where

$$R_{nl}(r) = -\left\{ \left(\frac{2}{na_0} \right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right\}^{1/2} \mathrm{e}^{-r/na_0} \left(\frac{2r}{na_0} \right)^l L_{n+l}^{2l+1} \left(\frac{2r}{na_0} \right)$$

and L_{n+l}^{2l+1} stands for the associated Laguerre polynomial. Using the Pauli equation (14) and the Hamiltonian (16), we derive the energy eigenvalue of the EHA as follows:

$$E_{nl} = -\frac{\mu e^4}{2n^2} - 4\beta^2 \left[l(l+1) + 1 + \frac{l^2 + l}{l^2 + l + 1} - n^2 \right] \tag{18}$$

$$n = 1, 2, 3, \ldots \qquad l = 0, 1, 2, \ldots, n-1.$$

It is easy to see that the energy spectrum of the EHA is determined in terms of the principle quantum number n and the angular quantum number l together. For the above-mentioned Hilbert space, the degeneration degree of the energy spectrum is $2l + 1$. Therefore, our extension has changed the symmetry of the system in the usual sense. Equation (18) shows that the deformation adds three terms to the energy spectrum of the usual hydrogen atom, which is decided by the principle quantum number and angular quantum number. The energy spectrum does not deal with the magnetic quantum number m. This is due to the fact that the angular momentum is still conservative in the EHA. When the quantum deformation parameter β vanishes, the energy spectrum of the extended hydrogen atom becomes that of the usual hydrogen atom exactly.

From (8), we see that the so-called Yangian angular momentum keeps the angular momentum character in the above-mentioned Hilbert space. Let us consider the properties of the Yangian Runge–Lenz vector. After tedious calculations, we obtain

$$\langle n'l'm+1|R_+^Y|nlm\rangle = \delta_{nn'}\delta_{ll'}\left\{\frac{2\beta^2}{\mu e^4}[2l(l+1)+1-n^2]+\frac{1}{n^2}\right\}^{1/2}\sqrt{(l-m)(l+m+1)} \tag{19}$$

and

$$\langle n'l'm-1|R_-^Y|nlm\rangle = \delta_{nn'}\delta_{ll'}\left\{\frac{2\beta^2}{\mu e^4}[2l(l+1)+1-n^2]+\frac{1}{n^2}\right\}^{1/2}\sqrt{(l+m)(l-m+1)}. \tag{20}$$

Furthermore, we have

$$\langle nlm|R_3^Y|n'l'm\rangle = \delta_{nn'}\delta_{ll'}m\left\{\frac{2\beta^2}{\mu e^4}[2l(l+1)+1-n^2]+\frac{1}{n^2}\right\}^{1/2}. \tag{21}$$

This means that the $Y(sl(2))$ generators realized by (8) and (11) represent the transition within the states with the same reciprocal quantum number n and angular quantum number l. In the derivation of (19)–(21), we applied the commutation relations of the Yangian Runge–Lenz vector

$$[R_+^Y, R_-^Y] = \frac{4\beta^2}{\mu e^4}L_3(2\boldsymbol{L}^2+1)+2\left(\frac{\beta^2}{H_0}-\frac{2H_0}{\mu e^4}\right)L_3 \tag{22}$$

and

$$[R_3^Y, R_\pm^Y] = \mp\frac{2H_0}{\mu e^4}L_\pm \pm \frac{2\beta^2}{\mu e^4}L_\pm(2\boldsymbol{L}^2+1)\pm\frac{\beta^2 L_\pm}{H_0}. \tag{23}$$

Furthermore, we can derive

$$\boldsymbol{R}^{Y2}|nlm\rangle = \left\{-\frac{l^2+l+1}{n^2}-\frac{8\beta^2}{\mu e^4}[(l^2+l+1)^2+l^2+l]\right\}|nlm\rangle. \tag{24}$$

In this paper, we deform the usual hydrogen atom to the so-called extended hydrogen atom (EHA). The angular momentum and Runge–Lenz vector that are shown to construct the subalgebra of the loop algebra $L(sl(2))$ are extended to the Yangian angular momentum and Yangian Runge–Lenz vector, which satisfy the commutation relations of the Yangian $Y(sl(2))$. A realization of the $Y(sl(2))$ generators is found. The Hamiltonian of the EHA is determined by deformation of the Pauli equation. The energy spectrum of the EHA is calculated. The selection rule and matrix elements of the $Y(sl(2))$ generators for the eigenstates of the usual atom are also studied.

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