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On a q-analogue of the spin–orbit coupling

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Abstract. Based on the tensor method, a q-analogue of the spin–orbit coupling is introduced in a q-deformed Schrödinger equation, previously derived for a central potential. Analytic expressions for the matrix elements of the representations $j = \ell \pm \frac{1}{2}$ are derived. The spectra of the harmonic oscillator and the Coulomb potential are calculated numerically as a function of the deformation parameter, without and with the spin–orbit coupling. The harmonic oscillator spectrum presents strong analogies with the bound spectrum of a Woods–Saxon potential customarily used in nuclear physics. The Coulomb spectrum simulates relativistic effects. The addition of the spin–orbit coupling reinforces this picture.

1. Introduction

Particular interest has been devoted over the last decade to the quantum algebra $su_q(2)$ [1–5]. This algebra is generated by three operators L_+, L_0 and L_-, also called the q-angular momentum components. They have the following commutation relations:

$$\left[L_0, L_\pm\right] = \pm L_\pm \tag{1}$$

$$\left[L_+, L_-\right] = [2L_0] \tag{2}$$

where the quantity in square brackets is defined as

$$[n] = \frac{q^n - q^{-n}}{q - q^{-1}}. \tag{3}$$

In the most general case the deformation parameter q is an arbitrary complex number and physicists consider it as a phenomenological parameter [6]. When $q = 1$, the quantum algebra $su_q(2)$, which defines a q-analogue of the angular momentum, reduces to the Lie algebra $su(2)$ of the ordinary angular momentum.

It is therefore interesting to investigate q-analogues of dynamical systems and to look for new effects when $q \neq 1$. This has been first achieved for the harmonic oscillator by using algebraic methods, such as, for example, in [4, 5]. Taking, for example, $q = \exp(\mathrm{i}s)$ with s a real, positive quantity, one can find that the distance between subsequent levels of the q-harmonic oscillator decreases when the excitation increases. This is a desired property in describing rotational bands of deformed nuclei [6]. However, the accidental degeneracy of the harmonic oscillator persists in this treatment.

Another, more appealing way to introduce q-analogues of simple dynamical systems, is through deriving a q-deformed Schrödinger equation. In this vein several attempts have been made for the harmonic oscillator, such as, for example, in [7–9], for an attractive Coulomb potential [10, 11] or for both potentials [12, 13]. This procedure leads to the removal of the accidental degeneracy whenever it exists.

Here we follow the approach of [13] where a q-deformed Schrödinger equation has been derived for a general central potential and the exact solution for the particular cases of the Coulomb and the harmonic oscillator potentials have been obtained. The crucial starting point in [13] was the search for a Hermitian realization of the position, momentum and angular momentum operators, all behaving as *vectors* with respect to $su_q(2)$ algebra. This allowed the construction of an angular momentum operator entering the expression of the Hamiltonian. Its components are different from the generators of the $su_q(2)$ algebra. In the case of central potentials (spinless particles) the eigenfunctions of the q-deformed angular momentum have been derived as q-deformed spherical harmonics and then closed expressions for the eigenvalues of the q-deformed Schrödinger equation have obtained as a function of q.

This study is devoted to the derivation of a q-deformed spin–orbit coupling, consistent with the approach of [13]. There an angular momentum Λ_μ ($\mu = 0, \pm 1$) has been defined as a *q-vector* with respect to the $su_q(2)$ algebra (1) and (2). By analogy, here we introduce a spin operator σ_μ which is a *q-vector* in the algebra of S_μ analogous to (1) and (2). Next a Hermitian spin operator Σ_μ is constructed as a *q-vector* in the coproduct algebra of the total angular momentum J_μ by using a unitary version of the universal R-matrix. The spin–orbit interaction is defined as a q-scalar Hermitian operator in the space of J_μ and its matrix elements are calculated exactly for the representations $j = \ell \pm \frac{1}{2}$.

In previous applications of the q-deformed algebras to physical systems, such as, for example, [14], the spin–orbit coupling is derived in a different way, based on a boson realization of the $so_q(3)$ algebra [15]. There the spin operator does not form a vector in the coproduct algebra. Accordingly the eigenvalues of the spin–orbit operator are different from ours.

In the next section we summarize the findings of [13]. In section 3 a q-analogue of the spin–orbit coupling is derived. In section 4 we calculate numerically the spectra of the q-harmonic oscillator and the q-Coulomb potentials without and with a spin–orbit contribution. Physical implications are discussed. We stress that we do not aim at a particular fit of the deformation parameter to describe some particular system but at modelling physical systems through the $su_q(2)$ algebra. The final section is devoted to some closing remarks.

2. Spinless particles

In this section we follow closely [13]. The Hamiltonian entering the q-deformed Schrödinger equation is

$$H = \tfrac{1}{2}\vec{p}^2 + V(r). \tag{4}$$

Here and in the following we shall take

$$\hbar = c = e = m = 1. \tag{5}$$

The eigenfunctions of this Hamiltonian are

$$\Psi(r, x_0, \varphi) = r^L u_L(r) Y_{\ell m}(q, x_0, \varphi) \tag{6}$$

where $Y_{\ell m}(q, x_0, \varphi)$ are the normalized q-spherical harmonics (56) and (57) of [13], depending of the deformation parameter q and $x_0 = \cos\theta$. They are related to q-hypergeometric functions [16].

The function $r^L u_L(r)$ satisfies the following radial equation:

$$\left\{\frac{1}{2}\left[-\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{1}{r^2}L(L+1)\right] + V_0(r)\right\} r^L u_L(r) = E_{n\ell} r^L u_L(r) \tag{7}$$

where L is the non-negative solution of

$$L(L+1) = \frac{[2\ell]}{[2]}\frac{[2\ell+2]}{[2]} + c_\ell^2 - c_\ell \tag{8}$$

with

$$c_\ell = \frac{q^{2\ell+1} + q^{-2\ell-1}}{[2]}. \tag{9}$$

It then follows that for the Coulomb potential

$$V_0(r) = -\frac{1}{r} \tag{10}$$

the eigenvalue is

$$(E_{n\ell})_{Coulomb} = -\frac{1}{2(n+L+1)^2} \tag{11}$$

and for the harmonic oscillator potential

$$V_0(r) = \tfrac{1}{2}r^2 \tag{12}$$

the eigenvalue is

$$(E_{n\ell})_{oscillator} = (2n + L + \tfrac{3}{2}) \tag{13}$$

n being in both cases the radial quantum number.

The spectrum is degenerate with respect to the magnetic quantum number m but the accidental degeneracy typical for the undeformed equation is removed both for the Coulomb and the harmonic oscillator potentials when $q \neq 1$.

From equation (9) it follows that for $\ell = 0$ one has $c_\ell = 1$. Thus for $\ell = 0$ the only non-negative solution of (8) is $L = 0$, for all deformations. Consequently, the $\ell = 0$ levels are independent of the deformation parameter both for the harmonic oscillator and the Coulomb potentials. The centrifugal barrier disappears and taking $V_0(r) = 0$ one reobtains the free-particle case, as for undeformed equations.

For $\ell \neq 0$ it is useful to distinguish between two different types of deformation parameter:

(i) $$q = \mathrm{e}^s \qquad \text{with } s \text{ real.} \tag{14}$$

In this case one can easily prove that $c_\ell \geqslant 1$ so that equation (8) has real solutions. Therefore, to each non-zero ℓ corresponds a positive L which is no longer an integer. We found it interesting to use real q for the Coulomb potential, as shown in section 3. The other case is

(ii) $$q = \mathrm{e}^{\mathrm{i}s} \qquad \text{with } s \text{ real.} \tag{15}$$

In this case for small values of s one can find numerically that real positive values of L exist. This case is applicable to the harmonic oscillator potential, because it leads to interesting analogies of its spectrum with a known case in nuclear physics, as discussed in section 4.

3. Derivation of the spin–orbit coupling

Now the Hamiltonian (4) contains a potential of the form

$$V = V_0(r) + \alpha(r)V_{S\text{–}O} \tag{16}$$

where V_0 is the central potential from the previous section, $V_{S\text{–}O}$ is the spin–orbit operator and α is a function which vanishes when $r \to \infty$. In atomic or nuclear physics the spin–orbit operator is the ordinary scalar product between the spin and angular momentum. In the deformed case considered here we aim at introducing a similar definition. However, there are inherent differences due to the more complex nature of the q-deformed vector operators, as explained below.

By analogy to the q-angular momentum L_μ one can define a spin operator S_μ through relations similar to (1)–(3). The operators L_μ and S_μ satisfy the Hermiticity relations

$$L^\dagger_{\pm,0} = L_{\pm,0} \qquad S^\dagger_{\pm,0} = S_{\pm,0}. \tag{17}$$

However, the situation is different from the $su(2)$ case because neither L_μ nor S_μ form a vector with respect to their $su_q(2)$ algebra. In an $su_q(2)$ algebra a q-vector of components V_i ($i = 0, \pm 1$), is defined through the relations [13]

$$(L_\pm V_i - q^i V_i L_\pm) q^{L_0} = \sqrt{[2]} V_{i\pm 1} \qquad [L_0, V_i] = i V_i \tag{18}$$

where one takes $V_{\pm 2} = 0$ whenever it appears.

However, as in [13], instead of L_μ we have to use Λ_μ defined as

$$\Lambda_{\pm 1} = \mp \sqrt{\frac{1}{[2]}} q^{-L_0} L_\pm \tag{19}$$

$$\Lambda_0 = \frac{1}{[2]} \left(q L_+ L_- - q^{-1} L_- L_+ \right). \tag{20}$$

These quantities form a vector in the $su_q(2)$ algebra, i.e. satisfy the relations (18) as can easily be checked. By analogy to (19) and (20) we introduce a vector of components σ_μ in the $su_q(2)$ algebra having S_μ as generators

$$\sigma_{\pm 1} = \mp \sqrt{\frac{1}{[2]}} q^{-S_0} S_\pm \tag{21}$$

$$\sigma_0 = \frac{1}{[2]} \left(q S_+ S_- - q^{-1} S_- S_+ \right). \tag{22}$$

In the space generated by S_μ the quantities L_μ are scalars and vice versa, which implies that

$$[\sigma_\mu, \Lambda_{\mu'}] = 0. \tag{23}$$

In dealing with the spin–orbit operator we have to also introduce the coproduct algebra of L_μ and S_μ. The generators J_μ of this algebra are defined as

$$J_\pm = L_\pm q^{-S_0} + S_\pm q^{L_0} \tag{24}$$

$$J_0 = L_0 + S_0. \tag{25}$$

One can directly prove that they satisfy commutation relations of type (1) and (2). One can also prove that Λ_μ are the components of a vector in the coproduct algebra, which means that they satisfy relations analogous to (18) with J_μ instead of L_μ. On the other hand, σ_μ do not fulfil such relations. However, instead of σ_μ one can introduce another vector Σ_μ satisfying relations of type (18) with J_μ instead of L_μ. This can be achieved by using the universal R-matrix. In fact, we need both the R-matrix and its conjugate [17]. The latter is denoted here by $\mathcal{R}$.

The R-matrix or its conjugate has the property that it replaces q by q^{-1} in definition (24), i.e. one has

$$R\left(L_\pm q^{-S_0} + S_\pm q^{L_0}\right) = \left(L_\pm q^{S_0} + S_\pm q^{-L_0}\right) R \tag{26}$$

and

$$\mathcal{R}\big(L_\pm q^{-S_0} + S_\pm q^{L_0}\big) = \big(L_\pm q^{S_0} + S_\pm q^{-L_0}\big)\mathcal{R}. \tag{27}$$

The operator (25) remains unchanged or, in other words,

$$[R, J_0] = 0 \qquad [\mathcal{R}, J_0] = 0. \tag{28}$$

We found it convenient to use the R-matrix as defined in [18]. For $s = \frac{1}{2}$ it contains only two terms

$$R = q^{2L_0S_0} + \frac{\lambda}{\sqrt{q}} L_- S_+ \tag{29}$$

where

$$\lambda = q - 1/q. \tag{30}$$

One can check that the expression (29) satisfies (26). The conjugate $\mathcal{R}$ of R takes the form

$$\mathcal{R} = q^{-2L_0S_0} - \lambda\sqrt{q} L_+ S_- \tag{31}$$

and it satisfies equation (27). Using (29) and (31) one defines [19]

$$\Sigma_\mu(R) = R^{-1}\sigma_\mu R \tag{32}$$

and

$$\Sigma_\mu(\mathcal{R}) = \mathcal{R}^{-1}\sigma_\mu \mathcal{R}. \tag{33}$$

The operator (32) with $\mu = 0, \pm 1$ forms a vector in the space of the coproduct algebra. The proof is given in appendix A. In a similar way one can prove that the operator (33) is also a vector in the coproduct algebra.

Note that none of the above operators is Hermitian but each μ-component of one is related to the corresponding component of the other through the relation

$$\Sigma^+_\mu(R) = \left(-\frac{1}{q}\right)^\mu \Sigma_{-\mu}(\mathcal{R}) \tag{34}$$

relating operators associated with R and $\mathcal{R}$. To overcome the lack of Hermiticity one can make use of the unitary matrix R_u introduced in [17] as

$$R_u = \frac{1}{N}\left(\sqrt{q}R + \frac{1}{\sqrt{q}}\mathcal{R}\right) \tag{35}$$

where $N = q^{l+1/2} + q^{-l-1/2}$ is a normalization factor. With the help of R_u one can define the vector

$$\Sigma_\mu(R_u) = R_u^\dagger \sigma_\mu R_u \tag{36}$$

the components of which are Hermitian operators, i.e. satisfy the relation

$$\Sigma^\dagger_\mu(R_u) = \left(-\frac{1}{q}\right)^\mu \Sigma_{-\mu}(R_u). \tag{37}$$

Now we can define a Hermitian spin–orbit operator as

$$V_{S\text{–}O} = \tfrac{1}{2}\vec{\Sigma}(R_u)\vec{\Lambda} + \tfrac{1}{2}\vec{\Lambda}\vec{\Sigma}(R_u) \tag{38}$$

where the scalar product between the q-vectors $\vec{\Sigma}(R_u)$ and $\vec{\Lambda}$ is defined as in [13]

$$\vec{\Sigma}(R_u)\vec{\Lambda} = \left(-\frac{1}{q}\right)^\mu \Sigma_\mu(R_u)\Lambda_{-\mu} \tag{39}$$

with an implied summation over μ. Using (36) one can rewrite (38) as

$$V_{S\text{–}O} = \tfrac{1}{2}(R_u^+ \vec{\sigma} R_u \vec{\Lambda} + \text{Hermitian conjugate})$$
$$= \tfrac{1}{2}(R_u^+ \vec{\sigma} R_u \vec{\Lambda} + \vec{\Lambda} R_u^+ \vec{\sigma} R_u). \tag{40}$$

Let us consider the first term in the right-hand side of (40) where R_u is replaced by its definition (35)

$$\tfrac{1}{2} R_u^+ \vec{\sigma} R_u \vec{\Lambda} = \frac{1}{2N^2} \left(\sqrt{q} R^+ + \frac{1}{\sqrt{q}} \mathcal{R}^+ \right) \vec{\sigma} \left(\sqrt{q} R + \frac{1}{\sqrt{q}} \mathcal{R} \right) \vec{\Lambda}. \tag{41}$$

Here we look for example at the term $(\sqrt{q} R^+ + \frac{1}{\sqrt{q}} \mathcal{R}^+)\vec{\sigma}\sqrt{q}R$, which can be rewritten by inserting the identity $RR^{-1} = 1$ in front of $\vec{\sigma}$ and also using the property $\mathcal{R}^+ R = 1$. This gives

$$\left(\sqrt{q} R^+ + \frac{1}{\sqrt{q}} \mathcal{R}^+ \right) \vec{\sigma} \sqrt{q} R \vec{\Lambda} = q R^+ R \vec{\Sigma}(R) \vec{\Lambda} + \vec{\Sigma}(R) \vec{\Lambda} = (1 + q R^+ R) \vec{\Sigma}(R) \vec{\Lambda}. \tag{42}$$

In a similar way the other term of (41) becomes

$$\left(\sqrt{q} R^+ + \frac{1}{\sqrt{q}} \mathcal{R}^+ \right) \vec{\sigma} \frac{1}{\sqrt{q}} \mathcal{R} \vec{\Lambda} = \left(1 + \frac{1}{q} \mathcal{R}^+ \mathcal{R} \right) \vec{\Sigma}(\mathcal{R}) \vec{\Lambda} \tag{43}$$

where we have used $\mathcal{R}\mathcal{R}^{-1} = 1$ and $R^+ \mathcal{R} = 1$. Thus

$$\tfrac{1}{2} R_u^+ \vec{\sigma} R_u \vec{\Lambda} = \frac{1}{2N^2} \left[(1 + q R^+ R) \vec{\Sigma}(R) \vec{\Lambda} + \left(1 + \frac{1}{q} \mathcal{R}^+ \mathcal{R} \right) \vec{\Sigma}(\mathcal{R}) \vec{\Lambda} \right]. \tag{44}$$

One can see that in the above relation the vectors $\vec{\Sigma}$ and $\vec{\Lambda}$ are next to each other as they should be in a q-scalar product. For the second term of (40) we have

$$\tfrac{1}{2} \vec{\Lambda} R_u^+ \vec{\sigma} R_u = \frac{1}{2N^2} \vec{\Lambda} \left(\sqrt{q} R^+ + \frac{1}{\sqrt{q}} \mathcal{R}^+ \right) \vec{\sigma} \left(\sqrt{q} R + \frac{1}{\sqrt{q}} \mathcal{R} \right) \tag{45}$$

or using

$$\mathcal{R}^+ = R^{-1} \qquad R^+ = \mathcal{R}^{-1} \tag{46}$$

in the manner explained above, we obtain

$$\tfrac{1}{2} \vec{\Lambda} R_u^+ \vec{\sigma} R_u = \frac{1}{2N^2} \left[\vec{\Lambda} \vec{\Sigma}(\mathcal{R})(1 + q R^+ R) + \vec{\Lambda} \vec{\Sigma}(R) \left(1 + \frac{1}{q} \mathcal{R}^+ \mathcal{R} \right) \right]. \tag{47}$$

Thus the spin–orbit interaction takes the form

$$V_{S\text{–}O} = \frac{1}{2N^2} \left[(1 + q R^+ R) \vec{\Sigma}(R) \vec{\Lambda} + \left(1 + \frac{1}{q} \mathcal{R}^+ \mathcal{R} \right) \vec{\Sigma}(\mathcal{R}) \vec{\Lambda} \right.$$
$$\left. + \vec{\Lambda} \vec{\Sigma}(\mathcal{R})(1 + q R^+ R) + \vec{\Lambda} \vec{\Sigma}(R) \left(1 + \frac{1}{q} \mathcal{R}^+ \mathcal{R} \right) \right] \tag{48}$$

i.e. it contains the operators

$$\vec{\Sigma}(R)\vec{\Lambda} \quad \vec{\Sigma}(\mathcal{R})\vec{\Lambda} \quad \vec{\Lambda}\vec{\Sigma}(R) \quad \vec{\Lambda}\vec{\Sigma}(\mathcal{R}) \quad R^+ R \quad \mathcal{R}^+ \mathcal{R}. \tag{49}$$

These are scalars because they commute with J_i $(i = 0, \pm 1)$. In particular, for the last two operators, the commutation with J_0 follows directly from (28). To prove the commutation with $J_\pm$ we have to use equations (26) and (27). For example, in the case of $R^+ R$ we have

$$\begin{aligned} R^+ R \left(L_\pm q^{-S_0} + S_\pm q^{L_0} \right) &= R^+ \left(L_\pm q^{S_0} + S_\pm q^{-L_0} \right) R \\ &= R^+ \left(L_\pm q^{S_0} + S_\pm q^{-L_0} \right) \mathcal{R} R^+ R \\ &= R^+ \mathcal{R} \left(L_\pm q^{-S_0} + S_\pm q^{L_0} \right) R^+ R \\ &= \left(L_\pm q^{-S_0} + S_\pm q^{L_0} \right) R^+ R \end{aligned} \tag{50}$$

where after the second equality sign alternative forms of equations (46) have been used.

We can obtain the expectation value of $V_{S\text{–}O}$ for states of total angular momentum $j = \ell \pm \frac{1}{2}$ by calculating the expectation values of the scalars (49). The simplest way is to use the state of maximum weight with $m = j$. For $j = l + \frac{1}{2}$ this state reads

$$\psi_{\ell+1/2,\ell+1/2} = Y_{\ell\ell}\chi_{1/2} \tag{51}$$

where $Y_{\ell m}$ are defined by equations (56) and (57) of [13] and χ_{m_s}, with $m_s = \pm\frac{1}{2}$, is the $s = \frac{1}{2}$ spinor. In this case one can show that the last two operators of the list (49) have the following expectation values:

$$\langle R^+R\rangle_{\ell+1/2} = q^{2l} \qquad \langle \mathcal{R}^+\mathcal{R}\rangle_{\ell+1/2} = q^{-2l}. \tag{52}$$

For $j = \ell - \frac{1}{2}$ and $m = j$ the wavefunction is

$$\psi_{\ell-1/2,\ell-1/2} = \frac{1}{\sqrt{[2\ell+1]}}\left(\sqrt{\frac{[2\ell]}{q}}Y_{\ell\ell}\chi_{-1/2} - q^l Y_{\ell,\ell-1}\chi_{1/2}\right). \tag{53}$$

In this case the last two operators of (49) have the following expectation values:

$$\langle R^+R\rangle_{\ell-1/2} = q^{-2l-2} \qquad \langle \mathcal{R}^+\mathcal{R}\rangle_{\ell-1/2} = q^{2l+2}. \tag{54}$$

Both for $j = \ell + \frac{1}{2}$ and $j = \ell - \frac{1}{2}$ the proof is similar to that given in appendix B for the other scalars of (49). Using all of these expectation values in the case where $j = \ell + \frac{1}{2}$ one can easily show that the expectation value of $V_{S\text{–}O}$ is

$$E_{\ell+1/2} = \frac{[2\ell]}{[2]^2}\frac{q^{l+5/2} + q^{-l-5/2}}{q^{l+1/2} + q^{-l-1/2}}. \tag{55}$$

In a similar but somewhat longer way the following expectation value of $V_{S\text{–}O}$ is obtained for $j = \ell - \frac{1}{2}$:

$$E_{\ell-1/2} = -\frac{[2l+2]}{[2]^2}\frac{q^{l-3/2} + q^{-l+3/2}}{q^{l+1/2} + q^{-l-1/2}}. \tag{56}$$

The proof of equations (55) and (56) is given in appendix B. In the limit $q \to 1$ $E_{\ell+1/2}$ and $E_{\ell-1/2}$ recover the expectation values of the non-deformed spin–orbit coupling $\vec{s}\cdot\vec{\ell}$, namely $\ell/2$ for $j = \ell + \frac{1}{2}$ and $-(\ell+1)/2$ for $j = \ell - \frac{1}{2}$, respectively.

4. Numerical results

In figure 1 we represent the eigenvalues (11) of the Coulomb potential as a function of s (real), when $q = \mathrm{e}^s$ (equation (14)). One can see that every $E_{n\ell}$ increases with s when $\ell \neq 0$, the reason being that one has $L > \ell$ when one chooses q to be real. Therefore, at a given $q \neq 1$ one has

$$E_{2\mathrm{p}} > E_{2\mathrm{s}} \qquad E_{3\mathrm{d}} > E_{3\mathrm{p}} > E_{3\mathrm{s}} \qquad \text{etc.} \tag{57}$$

These inequalities are similar to those satisfied by the eigenvalues of the Klein–Gordon equation for which one has $E(n,\ell) < E(n-1,\ell+1)$ for fixed $n+\ell+1$ [20, 21]. One expects similar inequalities to also be satisfied by the eigenvalues of the spinless Bethe–Salpeter (or Herbst) equation for a particle in an attractive Coulomb potential [22]. In fact, as long as $Z\alpha < \pi/2$ where Z is the charge and α is the fine-structure constant, the expansion of the eigenvalues of the Herbst equation coincides with that of the Klein–Gordon equation [23]. Thus the results shown in figure 1 suggest that the splitting found for $q \neq 1$ can simulate a relativistic kinematic effect.

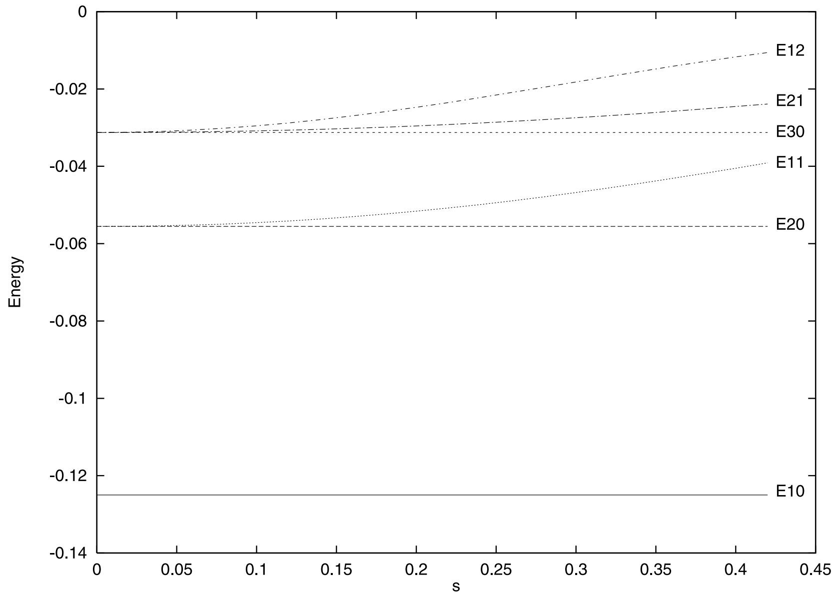

Figure 1. Eigenvalues $(E_{n\ell})_{Coulomb}$ of equation (11) as a function of s for a deformation parameter of type (14). The identification with the spectroscopic notation is $E_{10} = E_{1s}$, $E_{20} = E_{2s}$, $E_{11} = E_{2p}$, $E_{30} = E_{3s}$, $E_{21} = E_{3p}$ and $E_{12} = E_{3d}$.

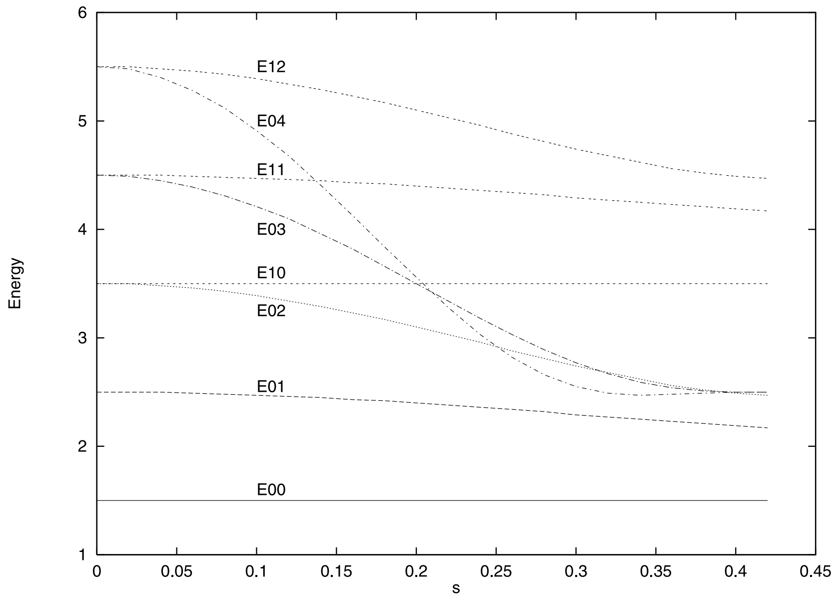

Figure 2. Eigenvalues $(E_{n\ell})_{oscillator}$ of equation (13) as a function of s for a deformation parameter of type (15). The identification with the spectroscopic notation is $E_{00} = E_{1s}$, $E_{01} = E_{1p}$, $E_{02} = E_{1d}$, $E_{10} = E_{2s}$, $E_{03} = E_{1f}$, $E_{11} = E_{2p}$, $E_{04} = E_{1g}$ and $E_{12} = E_{2d}$.

In figure 2 the eigenvalues (13) of the harmonic oscillator potential are plotted as a function of s, where s and the deformation parameter are related by equation (15). This choice is based

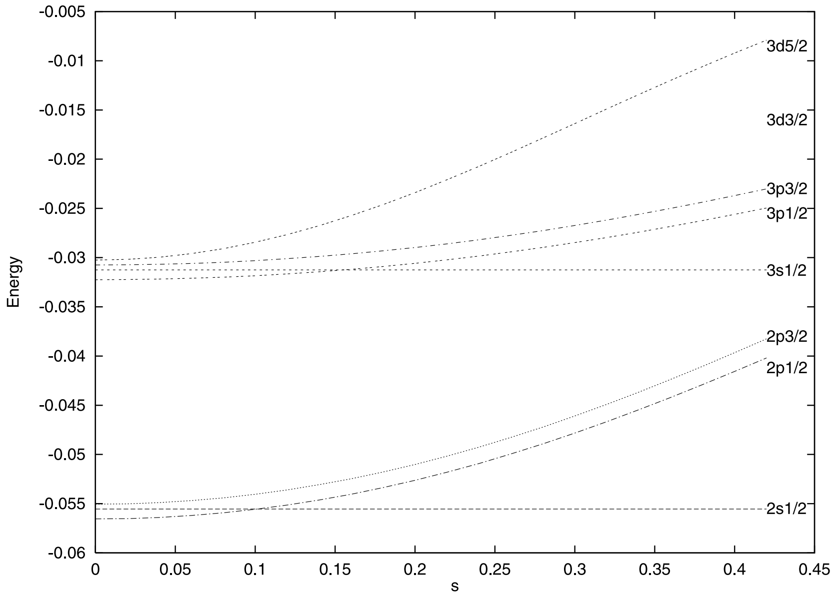

Figure 3. $(E_{n\ell})_{Coulomb} + \alpha E_{\ell\pm 1/2}$ with $\alpha = 0.001$ as a function of s for a deformation parameter of type (14).

on the fact that it implies $L < \ell$, so that in the interval $0 < s < 0.13$ the q-deformed spectrum satisfies inequalities as

$$E_{1\mathrm{d}} < E_{2\mathrm{s}} \qquad E_{1\mathrm{f}} < E_{2\mathrm{p}} \qquad E_{1\mathrm{g}} < E_{2\mathrm{d}} \qquad \text{etc} \tag{58}$$

which correspond to a potential with a form which is between a harmonic oscillator and a square-well potential. In nuclear physics [24] the standard form is the Woods–Saxon potential

$$V(r) = Vf(r) \qquad f(r) = \left[1 + \exp\left(\frac{r - R_0}{a}\right)\right]^{-1} \tag{59}$$

depending on three parameters V, R_0 and a. In the limit $a \to 0$ one approaches a square-well potential of radius R_0 and depth V. The bound spectrum of a potential of type (59) satisfies the inequalities (58) (see figures 2–23 of [24]).

Next we add the spin–orbit contribution. To single out the role of $V_{S\text{–}O}$ here we choose α to be a constant. In figure 3 we plot $(E_{n\ell})_{Coulomb} + \alpha E_{\ell\pm 1/2}$ as a function of s, where s is related to q by equation (14). The levels are labelled by $n\ell j$, where ℓ is the value of the angular momentum at $q = 1$ and $j = \ell \pm \frac{1}{2}$. With $\alpha > 0$ one always has $j = \ell + \frac{1}{2}$ levels above the $j = \ell - \frac{1}{2}$ levels due to equations (55) and (56). For convenience we choose $\alpha = 0.001$. We therefore see that the energies increase with increasing j for fixed ℓ and increasing n or ℓ for fixed j. Such a pattern corresponds to solutions of the Dirac equation for a Coulomb potential plus a perturbation which removes the twofold degeneracy of the eigenvalues for a Coulomb field. In [25] it has been shown that for a Dirac particle moving in a purely attractive potential the level sequence is

$$2\mathrm{p}_{3/2} > 2\mathrm{p}_{1/2} > 2\mathrm{s}_{1/2} \tag{60}$$

$$3\mathrm{d}_{5/2} > 3\mathrm{d}_{3/2} > 3\mathrm{p}_{3/2} > 3\mathrm{p}_{1/2} > 3\mathrm{s}_{1/2} \qquad \text{etc} \tag{61}$$

which here is the case when $s > 0.11$ for the first and when $s > 0.17$ for both rows of inequalities, respectively. Such sequences are expected for alkaline atoms.

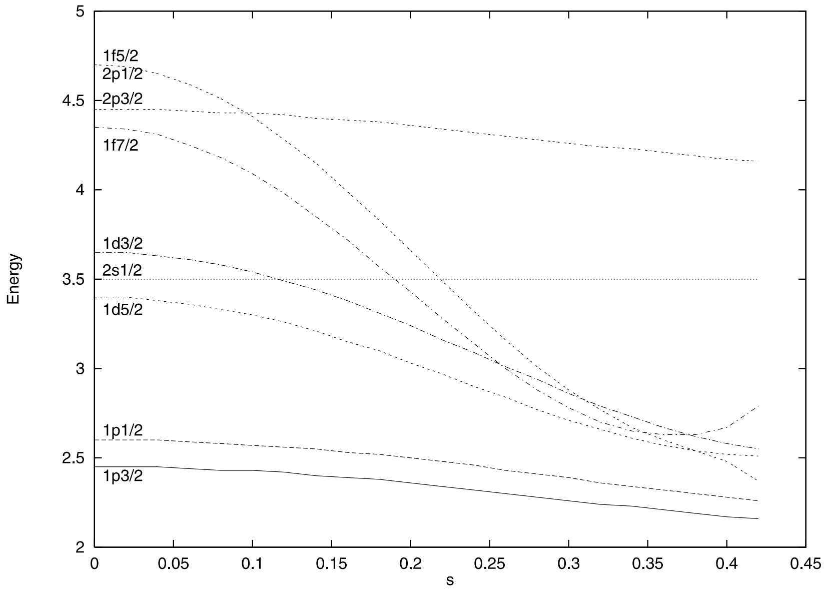

Figure 4. $(E_{n\ell})_{oscillator} + \alpha E_{\ell\pm 1/2}$ with $\alpha = -0.1$ as a function of s for a deformation parameter of type (15). The ground state energy $E_{1s_{1/2}} = 1.5$, which is independent of s, is not drawn.

In a similar way we add the spin–orbit coupling (55) and (56) to $(E_{n\ell})_{oscillator}$ of equation (13) and in figure 4 we plot $(E_{n\ell})_{oscillator} + \alpha E_{\ell\pm 1/2}$ as a function of s, where s is related to q via equation (15). For the sake of the discussion here we choose $\alpha = -0.1$. The addition of a spin–orbit coupling to $(E_{n\ell})_{oscillator}$ brings us a picture which is even closer to the single-particle spectra encountered in nuclear physics. Provided α is negative the level sequence of figure 4 is similar to that of the neutron single-particle spectrum (see, e.g., figures 2–30 of [24]). Also Hartree–Fock calculations based on effective density-dependent nucleon–nucleon interactions [26] give a similar spectrum.

5. Summary

We have constructed a q-analogue of the spin–orbit coupling used in a q-deformed Schrödinger equation previously derived for a central potential. The spin–orbit coupling is a q-scalar product between the angular momentum Λ_μ and the spin operator Σ_μ both defined a q-vectors in the coproduct algebra of the generators J_μ. The spin operator has been obtained with the help of a Hermitian form of the universal R-matrix. Accordingly, our result is new and entirely different from previous work on spin–orbit coupling.

Numerically, we have shown that the q-deformed Schrödinger equation for a spinless particle in a Coulomb field has a spectrum which simulates relativistic effects. The removal of the accidental degeneracy by a real deformation of the type $q = e^s$ with $s > 0$ leads to a level sequence similar to that of the Klein–Gordon or of the Herbst equations. With the addition of a spin–orbit coupling the level sequence is close to that of alkaline atoms.

The q-deformed Schrödinger equation for a spinless particle in a harmonic oscillator potential has a spectrum similar to that of the bound spectrum of a Woods–Saxon potential. The deformation is of type $q = e^{is}$, with s real and positive. The addition of a spin–orbit coupling leads to a spectrum similar to single-particle spectra of nuclei. It would be interesting to pursue this study in a more quantitative way.

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Appendix A

In this appendix we prove that the operators

$$\Sigma_\mu(R) = R^{-1}\sigma_\mu R \tag{A1}$$

with $\mu = 0, \pm 1$ form a q-vector in the coproduct algebra of J_μ defined by (24) and (25). A vector is an irreducible tensor of rank $\lambda = 1$. The proof given below is valid for any λ. Let us consider a q-tensor U^λ_μ which is irreducible in the space generated by S_μ. By definition it must obey the following relations [27]:

$$[S_0, U^\lambda_\mu] = \mu U^\lambda_\mu \tag{A2}$$

$$(S_\pm U^\lambda_\mu - q^\mu U^\lambda_\mu S_\pm)q^{S_0} = \sqrt{[\lambda \mp \mu][\lambda \pm \mu + 1]}U^\lambda_\mu. \tag{A3}$$

The operator σ_μ defined by (21) and (22) is an example of U^λ_μ with $\lambda = 1$. In the composite system of the coproduct algebra of J_μ a tensor W^λ_μ defined by

$$W^\lambda_\mu = R^{-1}U^\lambda_\mu R \tag{A4}$$

is irreducible if it satisfies relations analogous to (A2) and (A3) but with J_μ instead of S_μ. Suppose W^λ_μ satisfies such relations. Below we show that they are compatible with (A2) and (A3).

The validity of

$$[J_0, W^\lambda_\mu] = \mu W^\lambda_\mu \tag{A5}$$

is immediate due to the independence of J_0 of q, see equation (25). Using (24) the analogue of (A3) becomes

$$\begin{aligned}\big((L_\pm q^{-S_0} + S_\pm q^{L_0})R^{-1}U^\lambda_\mu R - q^\mu R^{-1}U^\lambda_\mu R(L_\pm q^{-S_0} + S_\pm q^{L_0})\big)\, q^{L_0+S_0}&\\ = \sqrt{[\lambda \mp \mu][\lambda \pm \mu + 1]}R^{-1}U^\lambda_{\mu\pm1}R&\end{aligned} \tag{A6}$$

for W^λ_μ defined by (A4). We multiply the above equation by R on the left and by R^{-1} on the right and use equation (26) to shift the R from the left to the right of $L_\pm q^{-S_0} + S_\pm q^{L_0}$. Using the identity $RR^{-1} = 1$ we obtain

$$\big((L_\pm q^{S_0} + S_\pm q^{-L_0})U^\lambda_\mu - q^\mu U^\lambda_\mu(L_\pm q^{S_0} + S_\pm q^{-L_0})\big)q^{L_0+S_0} = \sqrt{[\lambda \mp \mu][\lambda \pm \mu + 1]}U^\lambda_{\mu\pm1}. \tag{A7}$$

Next we use

$$q^{S_0}U^\lambda_\mu = q^\mu U^\lambda_\mu q^{S_0} \tag{A8}$$

which is a consequence of (A2) and

$$q^{-L_0}U^\lambda_\mu = U^\lambda_\mu q^{-L_0} \tag{A9}$$

which is a consequence of (23). These relations help to cancel out two of the four terms in the left-hand side of (A7). The resulting equation is (A3) which proves that (A6) is correct. Identifying W^λ_μ with Σ_μ, i.e. setting $\lambda = 1$ in (A5) and (A6) we obtain equations of type (18) for Σ_μ, i.e. we prove that Σ_μ is a q-vector in the coproduct algebra J_μ.

Appendix B

In this appendix we show how formulae (55) and (56) can be obtained. For this purpose we need the expectation values of the scalars (49). In order to calculate explicitly the expectation value of the first and third scalar products from the list (49) we need the operators $\Sigma_\mu(\mu = 0, \pm 1)$, which can be obtained by introducing equation (29) in (32). This gives

$$\begin{aligned}
\Sigma_1(R) &= q^{-2L_0}\sigma_1 \\
\Sigma_0(R) &= \sigma_0 - [2]\lambda\Lambda_{-1}\sigma_1 \\
\Sigma_{-1}(R) &= q^{2L_0}\sigma_{-1} - [2]\lambda q^{L_0}\Lambda_{-1}q^{L_0}\sigma_0 + [2]\lambda^2 q^{L_0}\Lambda_{-1}^2 q^{L_0}\sigma_1.
\end{aligned} \tag{B1}$$

To calculate the expectation value of the second and fourth scalar products (49) we need

$$\begin{aligned}
\Sigma_1(\mathcal{R}) &= q^{2L_0}\sigma_1 - [2]\lambda q^{L_0}\Lambda_1 q^{L_0}\sigma_0 + [2]\lambda^2 q^{L_0}\Lambda_1^2 q^{L_0}\sigma_{-1} \\
\Sigma_0(\mathcal{R}) &= \sigma_0 - [2]\lambda\Lambda_1\sigma_{-1} \\
\Sigma_{-1}(\mathcal{R}) &= q^{-2L_0}\sigma_{-1}
\end{aligned} \tag{B2}$$

which have been derived from the formulae (31) and (33).

For the purpose of this appendix, as an example, we first calculate the expectation value of the third scalar product from the list (49). This is

$$\vec{\Lambda}\,\vec{\Sigma}(R) = -\frac{1}{q}\Lambda_1\Sigma_{-1}(R) + \Lambda_0\Sigma_0(R) - q\Lambda_{-1}\Sigma_1(R). \tag{B3}$$

From this expression only the first and second terms bring a non-vanishing contribution to the expectation value when $j = \ell + \frac{1}{2}$. Looking at the expression of $\Sigma_{-1}(R)$ above we see that only the second term contributes so that $-1/q\Lambda_1\Sigma_{-1}(R)$ has a non-vanishing contribution due to

$$\frac{[2]}{q}\lambda\Lambda_1 q^{L_0}\Lambda_{-1}q^{L_0}\sigma_0. \tag{B4}$$

Using the definition (19) one can rewrite this operator as

$$-\frac{\lambda}{q}L_+L_-\sigma_0. \tag{B5}$$

At this stage we need the relation

$$L_+L_-Y_{\ell m}(q, x_0, \varphi) = [\ell + m][\ell - m + 1]Y_{\ell m}(q, x_0, \varphi). \tag{B6}$$

For the particular case of $m = \ell$ we have

$$L_+L_-Y_{\ell\ell}(q, x_0, \varphi) = [2\ell]Y_{\ell\ell}(q, x_0, \varphi). \tag{B7}$$

The relation (B6) has a spin counterpart

$$S_+S_-\chi_{m_s} = [s + m_s][s - m_s + 1]\chi_{m_s}. \tag{B8}$$

Together with (22) this gives

$$\Sigma_0\chi_{1/2} = \sigma_0\chi_{1/2} = \frac{q}{[2]}S_+S_-\chi_{1/2} = \frac{q}{[2]}\chi_{1/2}. \tag{B9}$$

Altogether we obtain

$$-\frac{1}{q}\Lambda_1\Sigma_{-1}(R)\psi_{\ell+1/2,\ell+1/2} = -\frac{\lambda[2\ell]}{[2]}\psi_{\ell+1/2,\ell+1/2}. \tag{B10}$$

According to (B1) the non-zero contribution of $\Lambda_0\Sigma_0(R)$ acting on $\psi_{\ell+1/2,\ell+1/2}$ comes from $\Lambda_0\sigma_0$. Using Λ_0 as defined by (20) and the relation (B6) we obtain

$$\Lambda_0 Y_{\ell\ell} = \frac{q}{[2]}[2\ell]Y_{\ell\ell}. \tag{B11}$$

Together with (B9) this gives

$$\Lambda_0\Sigma_0(R)\psi_{\ell+1/2,\ell+1/2} = \frac{q^2}{[2]^2}[2\ell]\psi_{\ell+1/2,\ell+1/2}. \tag{B12}$$

The addition of (B10) and (B12) leads to the following expectation value:

$$\langle\vec{\Lambda}\,\vec{\Sigma}(R)\rangle_{\ell+1/2} = \frac{q^{-2}}{[2]^2}[2l]. \tag{B13}$$

In the same representation, i.e. $j = \ell + \frac{1}{2}$ the expectation value of $\vec{\Sigma}(R)\vec{\Lambda}$ is even easier to obtain inasmuch as only the term $\Sigma_0(R)\Lambda_0$ contributes. Using the result (B12) one finds

$$\langle\vec{\Sigma}(R)\vec{\Lambda}\rangle_{\ell+1/2} = \frac{q^2}{[2]^2}[2l]. \tag{B14}$$

In a similar manner as above we obtain

$$\langle\vec{\Sigma}(\mathcal{R})\vec{\Lambda}\rangle_{\ell+1/2} = \frac{q^{-2}}{[2]^2}[2l] \tag{B15}$$

and

$$\langle\vec{\Lambda}\,\vec{\Sigma}(\mathcal{R})\rangle_{\ell+1/2} = \frac{q^2}{[2]^2}[2l]. \tag{B16}$$

By using the expectation values (B13)-(B16), together with (52) and (54) one can calculate the expectation value of (48) which leads straightforwardly to (55).

For the representation $j = \ell - \frac{1}{2}$, in a similar but longer way one obtains

$$\begin{aligned}\langle\vec{\Sigma}(R)\vec{\Lambda}\rangle_{\ell-1/2} &= \langle\vec{\Lambda}\,\vec{\Sigma}(\mathcal{R})\rangle_{\ell-1/2} = -\frac{q^2}{[2]^2}[2l+2]\\ \langle\vec{\Sigma}(\mathcal{R})\vec{\Lambda}\rangle_{\ell-1/2} &= \langle\vec{\Lambda}\,\vec{\Sigma}(R)\rangle_{\ell-1/2} = -\frac{q^{-2}}{[2]^2}[2l+2].\end{aligned} \tag{B17}$$

The relations (52), (54) and (B17) lead to the expectation value (56).

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