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Minimal length uncertainty relation and the hydrogen atom

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Abstract. We propose a new approach to calculate perturbatively the effects of a particular deformed Heisenberg algebra on an energy spectrum. We use this method to calculate the harmonic oscillator spectrum and find that the corrections are in agreement with a previous calculation. Then, we apply this approach to obtain the hydrogen atom spectrum and we find that splittings of degenerate energy levels appear. Comparison with experimental data yields an interesting upper bound for the deformation parameter of the Heisenberg algebra.

1. Introduction

The study of modified Heisenberg algebra, by adding certain small corrections to the canonical commutation relations, has aroused a great interest for some years (see, for example, [1–5]). These modifications yield new short-distance structure characterized by a finite minimal uncertainty Δx_0 in position measurements. The existence of this minimal observable length has been suggested by quantum gravity and string theory [6–10]. In this context, the new short-distance behaviour would arise at the Planck scale and Δx_0 would correspond to a fundamental quantity closely linked with the structure of spacetime [11]. This feature constitutes a part of the motivation to study the effects of this modified algebra on various observables.

Recently, it has been suggested that this formalism could also be used to describe, as an effective theory, non-pointlike particles, e.g. hadrons, quasi-particles or collective excitations [3]. In this case, Δx_0 is interpreted as a parameter linked with the structure of particles and their finite size. In the work [3] the d -dimensional isotropic harmonic oscillator was solved, in the context of a non-vanishing Δx_0 , with particular interest in the three-dimensional case. This calculation shows that splittings of the usual degenerate energy levels appear, leaving only the degeneracy due to the independence of the energy on the azimuthal quantum number, m . It has also been indicated that application to the hydrogen atom should yield the relation between the scale of a non-pointlikeness of the electron and the scale of the effects caused on the hydrogen spectrum. Indeed, the high precision of the experimental data for the transition 1S–2S [12], for example, can yield an interesting upper bound for the possible, in the sense studied here, finite size of the electron.

The purpose of this work is to continue to investigate whether the ansatz concerning the deformation of the Heisenberg algebra, with a suitably adjusted scale, may also serve for an effective low-energy description of non-pointlike particles. In this way, we calculate corrections to the hydrogen spectrum using the minimally modified Heisenberg algebra, i.e. which preserves the commutation relations between position operators. To perform this calculation we propose a new approach which allows us to solve the Schrödinger equation

in the position representation. This method leads to the correct harmonic oscillator spectrum found in [3]. Application to the hydrogen atom shows that splittings of the usual degenerate energy levels are also present and that these corrections cannot be seen experimentally if Δx_0 is smaller than 0.01 fm.

2. Method

The modified Heisenberg algebra studied here, as in [3], is defined by the following commutation relations ($\hbar = c = 1$):

$$\begin{aligned} [\hat{X}_i, \hat{P}_j] &= i(\delta_{ij} + \beta\delta_{ij}\hat{P}^2 + \beta'\hat{P}_i\hat{P}_j) \\ [\hat{P}_i, \hat{P}_j] &= 0 \end{aligned} \quad (1)$$

where $\hat{P}^2 = \sum_{i=1}^3 \hat{P}_i\hat{P}_i$ and where $\beta, \beta' > 0$ are considered as small quantities of the first order. In this paper, we study only the case $\beta' = 2\beta$, which leaves the commutation relations between the operators \hat{X}_i unchanged [3], i.e. $[\hat{X}_i, \hat{X}_j] = 0$. This constitutes the minimal extension of the Heisenberg algebra and is thus of special interest.

To calculate a spectrum for a given potential we must find a representation of the operators \hat{X}_i and \hat{P}_i , involving position variables x_i and partial derivatives with respect to these position variables, which satisfies equations (1), and solve the corresponding Schrödinger equation

$$\left[\frac{\hat{P}^2}{2m} + V(\vec{X}) \right] \Psi(\vec{x}) = E\Psi(\vec{x}). \quad (2)$$

It is straightforward to verify that the following representations fulfil the relations (1), to first order in β :

$$\begin{aligned} \hat{X}_i\Psi(\vec{x}) &= x_i\Psi(\vec{x}) \\ \hat{P}_i\Psi(\vec{x}) &= p_i(1 + \beta\vec{p}^2)\Psi(\vec{x}) \quad \text{with} \quad p_i = \frac{1}{i} \frac{\partial}{\partial x_i}. \end{aligned} \quad (3)$$

Neglecting terms of order β^2 , the Schrödinger equation (2) takes the form

$$\left[\frac{\vec{p}^2}{2m} + \frac{\beta}{m}\vec{p}^4 + V(\vec{x}) \right] \Psi(\vec{x}) = E\Psi(\vec{x}). \quad (4)$$

This is the ordinary Schrödinger equation with an additional term proportional to \vec{p}^4 . As this correction is assumed to be small, we calculate its effects on energy spectra in the first order of perturbations. The evaluation of the spectrum to the first order in the deformation parameter β leads to

$$E_k = E_k^0 + \Delta E_k \quad (5)$$

where k denotes the set of quantum numbers which labels the energy level and where ΔE_k are the eigenvalues of the matrix

$$\frac{\beta}{m} \langle \Psi_k^0(\vec{x}) | \vec{p}^4 | \Psi_{k'}^0(\vec{x}) \rangle \equiv \frac{\beta}{m} \langle k | \vec{p}^4 | k' \rangle \quad (6)$$

where $\Psi_k^0(\vec{x})$ are solutions of (4) with $\beta = 0$. This matrix is computed with all the wavefunctions corresponding to the unperturbed energy level E_k^0 . This is a $g \times g$ matrix where g is the multiplicity of the state E_k^0 considered. In general, ΔE_k takes f ($f \leq g$) different values which removes the degeneracy of some energy levels. For an arbitrary interaction $V(\vec{x})$

used in the Schrödinger equation, the matrix (6) is non-diagonal. However, since we know the action of \vec{p}^2 (from equation (4)) on the unperturbed wavefunctions, the expression of the matrix elements, for a central potential, can be written as

$$4\beta m \left((E_{n,\ell}^0)^2 \delta_{nn'} - (E_{n,\ell}^0 + E_{n',\ell}^0) \langle n\ell m | V(r) | n'\ell m \rangle + \langle n\ell m | V(r)^2 | n'\ell m \rangle \right) \delta_{\ell\ell'} \delta_{mm'} \quad (7)$$

and, in the cases studied here, there are no degenerate states with equal values of angular momentum ℓ and azimuthal quantum number m which have different values of radial quantum number n . Thus the matrix (6) is diagonal and the correction to the spectrum can be written as

$$\Delta E_{n,\ell} = 4\beta m \left((E_{n,\ell}^0)^2 - 2E_{n,\ell}^0 \langle n\ell m | V(r) | n\ell m \rangle + \langle n\ell m | V(r)^2 | n\ell m \rangle \right). \quad (8)$$

This nice relation can be simplified if one considers the power-law central potential, $V(r) \sim r^p$. In this case, the virial theorem gives

$$\langle n\ell m | V(r) | n\ell m \rangle = \frac{2}{p+2} E_{n,\ell}^0 \quad (9)$$

which leads to the following form for the expression of the energy level shift in the first order in β :

$$\Delta E_{n,\ell} = 4\beta m \left((E_{n,\ell}^0)^2 \left(\frac{p-2}{p+2} \right) + \langle n\ell m | V(r)^2 | n\ell m \rangle \right). \quad (10)$$

This simple expression will allow us to find the correction of the harmonic oscillator and hydrogen spectra just by calculating the mean value of the square of the potential.

3. Harmonic oscillator

For this potential, the energy level shift is only given by the mean value of the square of the potential. The normalized unperturbed wavefunction of the harmonic oscillator reads

$$\Psi_{n\ell m}^0(\vec{r}) = \lambda^{3/2} \sqrt{\frac{2n!}{\Gamma(n+\ell+\frac{3}{2})}} (\lambda r)^\ell e^{-(\lambda r)^2/2} L_n^{\ell+1/2}((\lambda r)^2) Y_{\ell m}(\theta, \varphi) \quad (11)$$

where $\lambda = \sqrt{m\omega}$ and $L_n^\alpha(x)$ are Laguerre polynomials [13] (p 1037). n is the radial quantum number. Using the change of variable $x = (\lambda r)^2$, the energy shift is found to be

$$\Delta E_{n,\ell} = \frac{4\beta m (n!) k^2}{\lambda^4 \Gamma(n+\ell+\frac{3}{2})} \int_0^\infty x^{\ell+5/2} e^{-x} [L_n^{\ell+1/2}(x)]^2 dx \quad (12)$$

where $2k = m\omega^2$ is the strength of the oscillator force. The calculation of the remaining integral is straightforward. Knowing the following relations concerning the Laguerre polynomials [13] (p 1037, p 844)

$$L_n^{\alpha-1}(x) = L_n^\alpha(x) - L_{n-1}^\alpha(x) \quad (13)$$

$$\int_0^\infty e^{-x} x^\alpha L_n^\alpha(x) L_m^\alpha(x) dx = \frac{\Gamma(\alpha+n+1)}{n!} \delta_{nm} \quad (14)$$

we obtain the expression of the harmonic oscillator spectrum for the modified Heisenberg algebra (1)

$$E_{n,\ell} = \omega \left(2n + \ell + \frac{3}{2} \right) + (\Delta x_0)^2 \frac{1}{5} m \omega^2 \left(6n^2 + 9n + 6n\ell + \ell^2 + 4\ell + \frac{15}{4} \right) \quad (15)$$

where $\Delta x_0 = \sqrt{5\beta}$. This formula reproduces exactly the splittings calculated in [3] using another approach. Because the dependence on quantum numbers of the correction term is not

of the form $f(2n + \ell)$, we obtain splittings of degenerate levels. However, the energy does not depend on the azimuthal quantum number m and each level remains $(2\ell + 1)$ -fold degenerate.

This example shows the usefulness of this approach which provides, with simple calculations, an analytical expression of the energy shift. The main interest of this method is that it can easily be used to solve other problems analytically or numerically, such as the Coulomb problem which is solved in the next section.

4. Hydrogen atom

As we mentioned in the introduction, the evaluation of corrections of the energy spectrum can provide information concerning, in the sense studied here, an assumed finite size of electrons. The method used here to describe non-pointlike particles neglects the internal structure degree of freedom. However, obviously these effects have a much smaller order of magnitude and thus can be omitted.

The normalized unperturbed wavefunction of the hydrogen atom reads

$$\Psi_{n\ell m}^0(\vec{r}) = (2\gamma_n)^{3/2} \sqrt{\frac{(n - \ell - 1)!}{2n(n + \ell)!}} (2\gamma_n r)^\ell e^{-\gamma_n r} L_{n-\ell-1}^{2\ell+1}(2\gamma_n r) Y_{\ell m}(\theta, \varphi) \quad (16)$$

where $\gamma_n = m\alpha/n$ and α is the fine structure constant. n is the principal quantum number and ℓ varies between 0 and $n - 1$. The change of variable $x = 2\gamma_n r$ allows us to write the energy shift as

$$\Delta E_{n,\ell} = -12\beta m (E_{n,\ell}^0)^2 + 8\beta m \gamma_n^2 \alpha^2 \frac{(n - \ell - 1)!}{n(n + \ell)!} \int_0^\infty x^{2\ell} e^{-x} [L_{n-\ell-1}^{2\ell+1}(x)]^2 dx. \quad (17)$$

As for the harmonic oscillator problem, the evaluation of this integral is quite simple. Indeed, using the following relation for Laguerre polynomials [13] (p 1038)

$$\sum_{m=0}^n L_m^\alpha(x) = L_n^{\alpha+1}(x) \quad (18)$$

with the relation (14) and the following summation formula

$$\sum_{p=0}^b \frac{(p+a)!}{p!} = \frac{(a+b+1)!}{(1+a)b!} \quad (19)$$

the expression of the hydrogen spectrum, in the first order in the deformation parameter β , reads

$$E_{n,\ell} = -\frac{m\alpha^2}{2n^2} + (\Delta x_0)^2 \frac{m^3 \alpha^4}{5} \frac{(4n - 3(\ell + \frac{1}{2}))}{n^4(\ell + \frac{1}{2})}. \quad (20)$$

This formula shows that the corrections to the spectrum are always positive. The value of this additional term is maximum for the ground state and for each value of n , the maximal contribution is obtained for $\ell = 0$ levels. As for the harmonic oscillator case, the correction term, which depends explicitly on ℓ , lifts the degeneracy of energy levels which remain, however, $(2\ell + 1)$ -fold degenerate.

The accuracy concerning the measurement of the frequency of the radiation emitted during the transition 1S–2S is about 1 kHz [12]. Thus the energy difference between this two levels is determined with a precision of about 10^{-12} eV. Then, if we assume that the effects of electrons of finite size cannot yet be seen experimentally, we find

$$\Delta x_0 \leq 0.01 \text{ fm}. \quad (21)$$

However, corrections calculated here could already play a role in the theoretical description of the hydrogen atom, since the accuracy of theoretical calculations is less than the precision of experimental data. The main theoretical error is the determination of the proton charge radius. Thus, at the moment, comparison between experimental data and standard theoretical calculations cannot exclude the effects studied in this paper.

Nevertheless, the upper bound (21) seems to be reasonable. Moreover, a naive argument can give an order of magnitude of an ‘experimental’ upper bound for the finite size of the electron. Indeed, a lower bound for the mass of an excited state of the electron is about 85 GeV [14]. Thus a photon with an energy of about 85 GeV cannot excite an electron. In a first approximation, this means that the resolution obtained with this photon is not sufficient to detect finite-sized electrons. The wavelength of such a photon could constitute an upper bound for the size of electrons,

$$\Delta x_0 \leq \lambda \sim 0.015 \text{ fm.} \quad (22)$$

This naive argument applied to the nucleon and its first radial excitation N(1440) yields a size of about 2.5 fm which is the correct order of magnitude.

Thus in the (very?) near future, with an improvement of the accuracy of experimental data and, above all, an improvement of the precision of standard theoretical calculations, it could be possible either to lower the upper bound (21) or to detect the existence of a non-vanishing Δx_0 .

5. Summary

We have proposed a new formulation of the Schrödinger equation which takes into account the deformation of the Heisenberg algebra in the first order in the deformation parameter β . This modified algebra introduces a minimal observable length in the uncertainty relations. It has been proposed in [3] that this framework could be used to describe non-pointlike particles as an effective low-energy theory, neglecting their internal structure degree of freedom. The minimal length Δx_0 would then be linked with the non-pointlikeness of particles.

In section 3, we have calculated, with the new approach, the corrections to the harmonic oscillator spectrum which are in agreement with those derived in a previous calculation using another approach [3]. Note that this method can be generalized to other dimensions. In particular, we have verified that the spectrum of the one-dimensional harmonic oscillator is in agreement with that found in [1]. Moreover, the wavefunction in position space can also be calculated, in the first order in β , just as various observables associated to the systems studied.

In section 4, we have used this method to obtain the corrections to the hydrogen atom spectrum. Comparison with the experimental data for the transition 1S–2S [12] yields a plausible upper bound for the non-pointlikeness Δx_0 of the electron which is about 0.01 fm.

The formulation of the Schrödinger equation proposed here could prove to be very useful for studying properties of some systems and their various associated observables in the context of the deformed Heisenberg algebra studied here.

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