Effects of variation of hyperfine splitting (structure) in atomic physics.

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Abstract. The possible variation of the fundamental constants is currently a very popular research topic. Theories unifying gravity and other interactions suggest the possibility of spatial and temporal variation of physics constants in the universe. Current interest is high because in superstring theories which have additional dimensions compactified on tiny scales any variation of the size of the extra dimensions results in changes in the 3-dimensional coupling constants. String theory also suggest the space to be noncommutative i.e., the space coordinates do not commute with each other. In this paper we study the hyperfine splitting in the framework of the noncommutative quantum mechanics (NCQM) developed in the literature. We show that the energy difference between two excited states \( F = I + \frac{1}{2} \) and the ground state \( F = I - \frac{1}{2} \) states in a noncommutative space (NCS) is bigger than the one in commutative case, so the radiation wavelength in NCS must be shorter than the radiation wavelength in commutative spaces. We also find an upper bound for the non-commutativity parameter. Since in the very tiny string scale or at very high energy situation the effects of non-commutativity of space may appear so the hyperfine splitting is not constant and changes as energy changes (high energy situation). The results would be of interest both for theoretical and optical spectroscopists.

1. Introduction
Recently there have been much interest in the study of physics in noncommutative spaces (NCS). In the usual quantum mechanics, the coordinates and momenta have the following commutation relations:

\[
[x_i, x_j] = 0 \quad [x_i, p_j] = i\hbar \delta_{ij} \quad [p_i, p_j] = 0,
\]

(1)

At very short scales, say string scale, the coordinates may not commute and the commutation relations are as follows:

\[
[\hat{x}_i, \hat{x}_j] = i\theta_{ij} \quad [\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij} \quad [\hat{p}_i, \hat{p}_j] = 0,
\]

(2)

where \( \theta_{ij} \) is an antisymmetric tensor which can be defined as \( \theta_{ij} = \frac{1}{2} \epsilon_{ijk} \theta_k \). The hat symbol represents the operators in the NCS.

2. Hyperfine splitting in noncommutative quantum mechanics.
It is shown in [1] that for the Hamiltonian of the type \( H = \frac{\hat{p}^2}{2m} + V(\hat{x}) \), the noncommutative Hamiltonian \( H_{nc} = H_\theta \) can be obtained by a shift in the argument of the potential:

\[
x_i = \hat{x}_i + \frac{1}{2} \theta_{ij} \hat{p}_j \quad \hat{p}_i = p_i.
\]

(3)
which leads to $H_\theta = \frac{p^2}{2m} + V(x_i - \frac{i}{\hbar} \theta_i p_j)$. The variables $x_i$ and $p_i$ now, satisfy in the same commutation relations as the usual (commutative) case i.e. Eq.(1). The magnetic dipole moment of the nucleus is given by $\vec{M} = \frac{Ze_N}{2\hbar c} I$.

where $Ze$, $M_N$, $I$ and $g_N$ are its electric charge, mass, spin and gyromagnetic ratio respectively. In the commutative case, the vector potential due to a point-like magnetic dipole is given by $\vec{A}(\vec{r}) = -\frac{1}{4\pi}(\vec{M} \times \vec{\nabla})$.

As shown in [1], their proposal for the non commutative H-atom Hamiltonian can be generalized to other systems, i.e. taking the usual Hamiltonian that is now a function of noncommutative coordinates $(\hat{x}, \hat{p})$, so we take the usual expression for vector potential but now being a function of noncommutative coordinates, accordingly this leads to a expression for the noncommutative Hamiltonian which is the same as the usual Hamiltonian that is now a function of noncommutative coordinates, so $\hat{A}(\vec{r}) = -\frac{1}{4\pi}(\hat{M} \times \hat{\nabla})$ where the hat symbol represents the same variable in the NCS.

From Eq.(3), we observe that $\frac{\partial}{\partial x_i} = \frac{\partial}{\partial x_i}$, so $\nabla = \nabla$. This is because the noncommutativity of space has no effect on spin.

One can derive the magnetic field produced by the nucleus from the vector potential $\hat{B} = \nabla \times \hat{A}$. Then the perturbative Hamiltonian is given by :

$$H_I = -\hat{M}_e \cdot \hat{B} = \frac{e}{m_e c} \vec{S} \cdot \hat{B} = \frac{Ze^2 g_N}{2m_e M_N c^2} \frac{1}{4\pi} \vec{S} \cdot \left[ -\hat{I} \nabla^2 \frac{1}{r} + \nabla (\vec{I} \cdot \nabla) \frac{1}{r} \right]$$

where $\hat{M}_e = \frac{e}{m_e c} \vec{S}$ is the electron magnetic dipole and $m_e$ is its mass.

We first consider the second term in $H_I$:

$$\left\langle \left\langle (\vec{S} \cdot \nabla)(\vec{I} \cdot \nabla) \frac{1}{r} \right\rangle \right\rangle = S_i k_i \left\langle \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_k} \frac{1}{r} \right\rangle = S_i k_i \left\langle \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_k} \frac{1}{r} \right\rangle$$

Using Eq.(3), we have :

$$\frac{1}{\sqrt{rr}} = \frac{1}{\sqrt{\bar{r}}} = r^{-1} \left[ 1 + \frac{1}{r^2} \left( \frac{1}{4} \vec{L} \cdot \vec{\theta} - \frac{1}{8} \theta_{ij} \theta_{kl} p_j p_k + O(\theta^3) \right) \right]$$

One can show that for the states with $\ell = 0$ in Eq.(5), the contributions of the terms with $i \neq j$ will vanish and for the terms with $i = j$ it gives $\frac{1}{3} S_i k_i \left\langle \nabla^2 \frac{1}{r} \right\rangle$. We note that the first term in the brackets in Eq.(4) is $-S_i k_i \nabla^2 \frac{1}{r}$, so :

$$\langle H_I \rangle = -\hat{M}_e \cdot \hat{B} = \frac{e}{m_e c} \vec{S} \cdot \hat{B} = \frac{Ze^2 g_N}{2m_e M_N c^2} \frac{1}{4\pi} \left[ -\frac{2}{3} S_i k_i \left\langle \nabla^2 \frac{1}{r} \right\rangle \right]$$

Using perturbation theory we proceed as follows :

$$\langle \Psi + \theta \Delta^{(1)} \Psi \left| V(\vec{r}) + \theta H^{(1)}_I + \theta^2 H^{(2)}_I \right| \Psi + \theta \Delta^{(1)} \Psi \rangle$$

where :

$$\theta H^{(1)}_I = -\frac{Ze^2 g_N}{48\pi m_e M_N c^2} S_i k_i \nabla^2 \frac{1}{r^3} \vec{L} \cdot \vec{\theta}$$

$$\theta^2 H^{(2)}_I = \frac{Ze^2 g_N}{96\pi m_e M_N c^2} S_i k_i \nabla^2 \frac{1}{r^3} \theta_{ij} \theta_{kl} p_j p_k$$

and $V = -\frac{Ze^2}{r}$. We set $\theta_3 = 0$ and the rest of the $\theta$-components to zero, which can be done by a rotation or a redefinition of coordinates, so $\vec{L} \cdot \vec{\theta} = L_z \theta$. 


Using the first-order perturbation theory for the wave functions, we have:

\[ \Psi_n^\theta = \Psi_n + \sum_{k \neq n} \frac{k \ell j j' | \beta \theta L_z | n \ell j j'}{|E_n^\theta - E_k^\theta|} \Psi_k, \beta = -\frac{Ze^2 g_N}{48\pi m_e M_N c^2} S_i I_i \nabla^2 \frac{1}{r^3} \]  

(11)

This leads to:

\[ \Psi_n^\theta = \Psi_n + \beta \theta \sum_{k \neq n} \frac{j_2 \hbar \left(1 + \frac{1}{2\ell+1}\right) \delta_{\ell j} \delta_{j_j'}}{|E_n^\theta - E_k^\theta|} \Psi_k \quad j = \ell \pm \frac{1}{2} \]  

(12)

The first-order correction terms are:

\[ 2 \left\langle \Psi | V(r) \right| \theta \Delta^{(1)} \Psi + \left\langle \Psi \right| \theta H_1^{(1)} \right| \Psi \rangle. \]

We consider the \( \ell = 0 \) states, so it is obvious that the second term i.e. the correction to the Hamiltonian to the first order, vanishes: \( \theta H_1^{(1)} = 0 \).

we note that in the relation \( j = \ell \pm \frac{1}{2} \), for \( \ell = 0 \) states only the upper sign(plus) is acceptable which gives \( j = \frac{1}{2} \). But this corresponds to the upper sign(minus) in Eq.(12), which leads to \( \Psi_n^\theta = \Psi_n \), and this means that to the first order in \( \theta \), there is no corrections to the wave functions i.e. \( \theta \Delta^{(1)} \Psi = 0 \). One can show the same is true for the second-order term \( \theta \Delta^{(2)} \Psi = 0 \). Therefore, the noncommutativity of space to the first order has no effect on the hyperfine splitting, so we study the noncommutativity effects to the second order. The third term in Eq.(6), can be written as:

\[ \frac{1}{8\pi^3} \left( \theta_i \theta_{ik} p_j p_k \right) = \frac{1}{32\pi^3} (\epsilon_{ijk} \epsilon_{ikv} p_j p_k \theta \theta_v = \frac{1}{32\pi^3} (p^2 \theta^2 - (\vec{p} \cdot \vec{\theta})^2) \]  

(13)

Then we have:

\[ \left\langle \nabla^2 \left( \theta_i \theta_{ik} p_j p_k \right) \right\rangle = \frac{1}{8} \theta^2 \left\langle \left( p_x^2 + p_y^2 \right) \nabla^2 \frac{1}{r^3} \right\rangle. \]

By symmetry considerations we have:

\[ \left\langle p_x^2 \right\rangle = \left\langle p_y^2 \right\rangle = \left\langle p_z^2 \right\rangle = \frac{1}{3} \left\langle p^2 \right\rangle, \]  

so:

\[ \left\langle H_1^{(2)} \right\rangle = \frac{Z e^2 g_N}{96\pi m_e M_N c^2} \theta^2 \vec{S} \cdot \vec{I} \left\langle p_i^2 \right\rangle \]  

(14)

To calculate the expectation value of \( p_i^2 \), we note that \( \frac{p_i^2}{2m} + V = E \), where \( V = -\frac{Ze^2}{r} \), then we have \( p_i^2 = 2mH_0 + 2m \frac{Ze^2}{r} \). Therefore Eq.(10) reads:

\[ \theta^2 \left\langle H_1^{(2)} \right\rangle = \frac{Z e^2 g_N}{48\pi m_e M_N c^2} \theta^2 \vec{S} \cdot \vec{I} \left[ E_\alpha \left\langle \frac{1}{r^3} \right\rangle + Z e^2 \left\langle \frac{1}{r^6} \right\rangle \right] \]  

(15)

If \( F \) is the total spin of the electron and nucleus, then the value of \( \frac{S \vec{I}}{\hbar} \) is \( \frac{1}{2} I \) for \( F = I + \frac{1}{2} \) and \( \frac{1}{2} (I - 1) \) for \( F = I - \frac{1}{2} \). So the expectation value of the Hamiltonian \( \left\langle H_1 \right\rangle \) to the second order is given by:

\[ \left\langle H_1 \right\rangle = \Delta E_{NC} = \frac{(Ze^2)^2 \hbar^2 g_N}{48\pi m_e M_N c^2} \theta^2 \left( -\frac{1}{2} \mu \frac{Ze^2}{n^2 \hbar^2} f(5) + f(6) \right) \]  

(16)

where \( f(\alpha) = \left\langle \frac{1}{r^6} \right\rangle \) and \( \alpha = \frac{e^2}{\hbar^2} \).

for the ground state of hydrogen atom, \( n = 1; Z = 1 \), and by substituting the values of \( \mu, e, \hbar, f(5) \) and \( f(6) \) we found out that the term in the parentheses is positive and therefore the correction due to noncommutativity of space on \( \Delta E_{NC} (F = 1 \rightarrow F = 0) \) is positive. This leads
us to the fact that the energy difference between the two states in a NCS is bigger than the one in commutative case, so the radiation wavelength in NCS spaces must be shorter than the radiation wavelength in commutative spaces.

The magnitude of $\Delta E_{NC}$, for a H-atom can be obtained by substitution of the values of various quantities: $c = 3.0 \times 10^8 \text{ms}^{-1}$, $e = 1.602 \times 10^{-19} \text{C}$, $m_e = 9.109 \times 10^{-31} \text{kg}$, $M_N = 1.673 \times 10^{-27} \text{kg}$, $\hbar = 1.055 \times 10^{-34} \text{Js}$, $g_N \simeq 5.56$ and the Bohr radius $a_0 = 5.292 \times 10^{-11} \text{m}$, which leads us to the result $\Delta E_{NC} = 10^{-28} \theta^2$.

On the other hand one can use the data on the hyperfine splitting to impose some bounds on the value of noncommutativity parameter $\theta$. The best measurement of the hyperfine splitting is for Hydrogen and its relative accuracy is about $10^{-12}$[2]. Since the noncommutativity of space has not been detected so far, the value of $\Delta E_{NC}$, should be of the order of $10^{-12}$, so we have $\Delta E_{NC}(F = 1 \rightarrow F = 0) \leq 10^{-12}$, which gives $\theta \leq \left(10^3 \text{Gev}\right)^{-2}$. This is in agreement with other results presented in the literature, e.g.[1].

References
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[2] Essen L et.al., 1971 Nature 229 110.