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The noncommutative quadratic Stark effect for the H-atom

Noureddine Chair[1,2] **and Mohammad A Dalabeeh**[1]

[1] Physics Department, Al al-bayt University, Mafraq, Jordan
[2] The Abdus Salam International Centre For Theoretical Physics, 1-34014 Trieste, Italy

E-mail: n.chair@rocketmail.com, nchair@alalbayt.aabu.edu.jo and chairn@ictp.trieste.it

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Abstract
Using both the second-order correction of perturbation theory and the exact computation due to Dalgarno–Lewis, we compute the second-order noncommutative Stark effect, i.e., shifts in the ground-state energy of the hydrogen atom in the noncommutative space in an external electric field. As a side result we also obtain a sum rule for the mean oscillator strength. The energy shift at the lowest order is quadratic in both the electric field and the noncommutative parameter θ. As a result of noncommutative effects the total polarizability of the ground state is no longer diagonal.

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1. Introduction

When an atom is subjected to an external electric field in a given direction the energy levels of the atom shift; this is the Stark effect (see, e.g., Bethe and Salpeter (1957)). If the electric field is weak the shift in the energy level is linear in the electric field, by parity arguments there will be shift only between states of opposite parity so the linear shift depends on the presence of degenerate states. Therefore the ground-state first-order effect vanishes and hence the energy shifts start at the quadratic order, the quadratic Stark effect. In both linear and quadratic Stark effects one uses the ordinary perturbation theory. If the external field is strong, perturbation theory is not justified, and one may use the WKB method (see, e.g., Bekenstein and Krieger (1969)). The combined Coulomb and the external potential felt by an electron implies that there are no absolutely stable bound states, and there is a possibility of quantum tunnelling. If the field is increased enough, then the states become unbound, leading to the ionization (see, e.g., Yamabi *et al* (1977)).

Here we are interested in studying the Stark effect in noncommutative quantum mechanics of the H-atom in the ground state for which one can safely use the ordinary perturbation theory. In this direction, the linear Stark effect has been studied by Chaichian *et al* (2001a) in which they showed that there is no Stark shift linear in the electric field induced by the noncommutativity of the coordinates and in particular the ground state remains unchanged, in the linear Stark effect. In the physical literature there are many papers dealing with noncommutative analogues of different dynamical models (see, e.g., Chaichian *et al* (2001b), Falomir *et al* (2002)). Like the ordinary Stark effect of the hydrogen atom, in order to obtain correction for ground-state energy one has to go to the second order in perturbation theory. In this paper we compute the noncommutative quadratic Stark energy shift using two methods. The first one is to use the second order in perturbation theory that we just mentioned, which contains an infinite summation over the excited states. The other method available is the Dalgarno–Lewis method (Dalgarno and Lewis 1955) which is exact and does not contain any summations over the excited states. In doing so we show that there is a noncommutative quadratic Stark effect which results in a lowering of the ground-state energy like the ordinary quadratic Stark effect. Both of these energies contribute additively to the polarization of the hydrogen atom and as a result of the noncommutativity of the polarization tensor is no longer diagonal. When equating the two expressions for the noncommutative quadratic Stark shift in energy obtained by the two methods, we obtain the sum rule on the mean oscillator strength for the Lyman series.

2. The noncommutative quadratic Stark effect for the ground state of the H-atom

Noncommutative quantum mechanics is defined through the following commutation relations:

$$\begin{aligned}[][\mathbf{x}_i, \mathbf{x}_j] &= \mathrm{i}\theta_{ij} \\ [\mathbf{x}_i, \mathbf{p}_j] &= \mathrm{i}\hbar\delta_{ij} \\ [\mathbf{p}_i, \mathbf{p}_j] &= 0\end{aligned} \tag{1}$$

where θ_{ij} is the noncommutative parameter and is of dimension of (length)^2. It is convenient, however, for computational reasons to change to the new coordinate system,

$$x_i = \mathbf{x}_i + \frac{1}{2\hbar}\theta_{ij}\mathbf{p}_j, \qquad p_i = \mathbf{p}_i, \tag{2}$$

where the new coordinates satisfy the usual canonical commutation relations:

$$[x_i, x_j] = 0, \qquad [x_i, p_j] = \mathrm{i}\hbar\delta_{ij}, \qquad [p_i, p_j] = 0. \tag{3}$$

When the electron in the H-atom is subjected to a uniform electric field E in the positive z-direction, its potential energy is $eE\mathbf{z}$, therefore using equation (2) the total Hamiltonian of this system that takes into account the noncommutative coordinates is

$$H = \frac{p^2}{2m} - \frac{e^2}{r} + eEz + \frac{e}{4\hbar}(\vec{\theta} \times \vec{p}) \cdot \vec{E}. \tag{4}$$

The term eEz is the ordinary Stark potential whereas the term $+\frac{e}{4\hbar}(\vec{\theta} \times \vec{p}) \cdot \vec{E}$ in the above equation corresponds to the noncommutative Stark potential energy. The components of the vector $\vec{\theta}$ are written in terms of the noncommutative parameter θ_{ij} as $\theta_i = \varepsilon_{ijk}\theta_{jk}$. Therefore, $(\vec{\theta} \times \vec{p})_i = -2\theta_{ij}p_j$. As a result the noncommutative Stark potential, apart from the θ_{ij} term, is the interaction between the induced electric dipole moment of the electron and the external electric field. Note that, though the model in question is introduced in a noncommutative guise it is essentially commutative. It is well known that at first order in perturbation theory there is no shift in the ground-state energy of the H-atom due to the perturbing term eEz. Similarly the noncommutative Stark perturbing potential does not change the ground-state energy in the first order of perturbation theory (Chaichian *et al* 2001a). Like the ordinary Stark effect one needs to go to the second order in perturbation theory in order to find the correction to the ground-state energy, this is the quadratic Stark effect. Using the fact that $p_i = \frac{m}{\mathrm{i}\hbar}[x_i, H_0]$, where $H_0 = \frac{p^2}{2m} - \frac{e^2}{r}$ the correction to the ground-state energy then is

$$\begin{aligned} E_1^{2(\mathrm{NC})} &= \sum_{n\neq 1,l,m} \frac{|\langle n,l,m|H^{(\mathrm{NC})}|1,0,0\rangle|^2}{E_n^0 - E_1^0} \\ &= \sum_{n\neq 1,l,m} \frac{|\langle n,l,m|\frac{e}{4\mathrm{i}\hbar^2}(\vec{E}\times\vec{\theta})_1([x_1,H_0] + (\vec{E}\times\vec{\theta})_2[x_2,H_0])|1,0,0\rangle|^2}{E_n^0 - E_1^0}, \end{aligned} \tag{5}$$

where we have used $(\vec{\theta}\times\vec{p})\cdot\vec{E} = (\vec{E}\times\vec{\theta})\cdot\vec{p}$. The states $|n,l,m\rangle$ form a complete set of eigenstates of the free Hamiltonian, $H_0|n,l,m\rangle = E_n^0|n,l,m\rangle$ and $E_n^0 = \frac{E_1^0}{n^2}$, E_1^0 is the ground-state energy. Using the identities $x \pm y = r\sin\theta\exp(\pm\mathrm{i}\phi) = \mp r\sqrt{\frac{8\pi}{3}}\mathbf{Y}_1^{\pm 1}$, where $\mathbf{Y}_l^m$ are the spherical harmonics for $l = 1$ and $m = \pm 1$. Then x, y in terms of the spherical harmonics are

$$\begin{aligned} x &= r\sqrt{\frac{2\pi}{3}}\left[\mathbf{Y}_1^{-1}(\theta,\phi) - \mathbf{Y}_1^1(\theta,\phi)\right] \\ y &= \mathrm{i}r\sqrt{\frac{2\pi}{3}}\left[\mathbf{Y}_1^{-1}(\theta,\phi) + \mathbf{Y}_1^{+1}(\theta,\phi)\right], \end{aligned}$$

and hence by orthonormality of the spherical harmonics, the selection rules are, $\Delta m = \pm 1, \Delta l = 1$. Using the selection rules and doing the angular integration, equation (5) becomes

$$E_1^{2(\mathrm{NC})} = \frac{e^2 m^2 E_1^0}{16\hbar^4}|\vec{E}\times\vec{\theta}|^2 \frac{1}{3}\sum_{n\neq 1}\frac{n^2-1}{n^2}\left|\int_0^\infty \mathbf{R}_{n1} r^3 \mathbf{R}_{10}\,\mathrm{d}r\right|^2, \tag{6}$$

where $\mathbf{R}_{nl}$ are the radial wavefunctions for the hydrogen atom, corresponding to the principal quantum number n and the orbital quantum number l. The radial integration is already computed and is given in Bethe and Salpeter (1957), the results are

$$\left|\int_0^\infty \mathbf{R}_{n1} r^3 \mathbf{R}_{10}\,\mathrm{d}r\right|^2 = \frac{2^8 n^7 (n-1)^{2n-5}}{(n+1)^{2n+5}} a^2,$$

where $a = \frac{\hbar^2}{me^2} = -\frac{e^2}{2E_1^0}$ is the Bohr radius. Finally, the noncommutative quadratic Stark effect for the hydrogen atom at the ground state reads

$$E_1^{2(\mathrm{NC})} = -\frac{e^2 m}{32\hbar^2}|\vec{E}\times\vec{\theta}|^2 \frac{1}{3}\sum_{n\neq 1}\frac{2^8 n^5 (n-1)^{2n-4}}{(n+1)^{2n+4}}. \tag{7}$$

Therefore there is a contribution to the Stark effect from the noncommutativity of coordinates which were not present in the first order in perturbation theory. Note also like the ordinary Stark effect the noncommutative quadratic Stark effect also results in a reduction of the ground-state energy. This means that the contribution to the Stark effect would be the addition of the usual quadratic Stark effect $E_1^{2(C)} = -\frac{9a^3}{4}|\vec{E}|^2$ and that given by equation (7). There is no contribution from the crossed term of the full potential,

$$V_{\mathrm{Stark}} = eEz + \frac{e}{4\hbar}(\vec{\theta}\times\vec{p})\cdot\vec{E}.$$

One can check this using the selection rules. In the following section using the method due to Dalgarno and Lewis (1955), we will show that the exact contribution to the noncommutative quadratic Stark effect is $E_1^{2(\mathrm{NC})} = -\frac{e^2 m}{32\hbar^2}|\vec{E}\times\vec{\theta}|^2$.

3. The exact computation

In this section we will briefly review the method due to Dalgarno and Lewis (1955), then use it to carry out the computation for the noncommutative quadratic Stark effect. In this method the goal is to find the perturbed ground state ψ_1^1 which is assumed to be related to the ground state in the form, $\psi_1^1 = F\psi_1$ where F is a scalar function of the variables that occur in the Hamiltonian, and then use the relation, $E_1^{2(\mathrm{NC})} = \langle\psi_1|H'|\psi_1^1\rangle - E_1^{1(\mathrm{NC})}\langle\psi_1|\psi_1^1\rangle = \langle\psi_1|H'|\psi_1^1\rangle$ (the first-order correction $E_1^{1(\mathrm{NC})} = 0$) to compute the second-order correction, H' being the noncommutative perturbing Hamiltonian and ψ_1 is the ground-state wavefunction for the hydrogen atom. The first-order equation in perturbation theory is given by

$$(H_0 - E_1)\psi_1^1 + \left(H' - E_1^1\right)\psi_1. \tag{8}$$

Setting $\psi_1^1 = F\psi_1$ where F is a scalar function of the variables that occur in the Hamiltonian, and defining a reduced potential by $V' = H' - E_1^1 = H' - \langle\psi_1|H'|\psi_1^1\rangle$ then the first-order perturbation equation it can be written as

$$[H_0, F]\psi_1 + V'\psi_1 = 0, \tag{9}$$

where $H_0 = -\frac{\hbar^2}{2m}\nabla^2 + u(r)$ is the free Hamiltonian for the H-atom and $u(r)$ is the Coulombic potential. Because $u(r)$ and F commute then one can show (e.g., see Hmmeka (1981)) that the function F is the solution to the following differential equation:

$$\frac{\hbar^2}{2m}\nabla^2 F\psi_1 - \frac{2}{a}\Omega F\psi_1 = \left(\frac{V'\psi_1}{\psi_1}\right), \tag{10}$$

where Ω is the differential operator defined by

$$\Omega = \frac{x}{r}\frac{\partial}{\partial x} + \frac{y}{r}\frac{\partial}{\partial y} + \frac{z}{r}\frac{\partial}{\partial z}. \tag{11}$$

The reduced potential in our case is the noncommutative Stark potential as the first-order correction $E_1^{1(\mathrm{NC})} = 0$. By acting by the operator $V_{\mathrm{Stark}}^{(\mathrm{NC})} = \frac{e}{4\hbar}(\vec{\theta} \times \vec{p}) \cdot \vec{E}$ on the ground-state wavefunction, $\psi_1 = (\pi a^3)^{-1/2} \exp -(r/a)$ the differential equation (10) is then

$$-\frac{\hbar^2}{2m}\nabla^2 F - \frac{2}{a}\Omega F = \frac{e}{4\mathrm{i}}\left[(\vec{E} \times \vec{\theta})_x \frac{x}{r} + (\vec{E} \times \vec{\theta})_y \frac{y}{r}\right]. \tag{12}$$

From the following relations

$$\begin{aligned} &\nabla^2(xr) = \tfrac{4x}{r}, && \Omega(xr) = 2x \\ &\nabla^2(x) = 0, && \Omega(x) = \tfrac{x}{r} \\ &\nabla^2(yr) = \tfrac{4y}{r}, && \Omega(yr) = 2y \\ &\nabla^2(y) = 0, && \Omega(y) = \tfrac{y}{r}, \end{aligned}$$

the solution to our differential equation would be of the form

$$F = \alpha x + \beta(xr) + \gamma y + \delta(yr), \tag{13}$$

where α, β, γ and δ are constants to be found. Substituting this expression into equation (12), then we find

$$F = \frac{em}{4\mathrm{i}\hbar^2}[(\vec{E} \times \vec{\theta})_x x + (\vec{E} \times \vec{\theta})_y y]. \tag{14}$$

Having found the expression for F, the second correction to the ground-state energy will be given by an integration rather than summation,

$$\begin{aligned} E_1^{2(\mathrm{NC})} &= \langle\psi_1|H'|F\psi_1\rangle \\ &= \frac{em}{4i\hbar^2}\langle\psi_1|[(\vec{E}\times\vec{\theta})_x p_x + (\vec{E}\times\vec{\theta})_y p_y][(\vec{E}\times\vec{\theta})_x x + (\vec{E}\times\vec{\theta})_y y]|\psi_1\rangle \\ &= -\frac{em}{16\hbar^2}\left[|\vec{E}\times\vec{\theta}|^2 + |(\vec{E}\times\vec{\theta})_x|^2\langle\psi_1|x\frac{\partial}{\partial x}|\psi_1\rangle + |(\vec{E}\times\vec{\theta})_y|^2\langle\psi_1|y\frac{\partial}{\partial y}|\psi_1\rangle\right]. \end{aligned} \tag{15}$$

Note that we have dropped the terms $\left\langle\psi_1 y\frac{\partial}{\partial x}\psi_1\right\rangle$ and $\left\langle\psi_1 yx\frac{\partial}{\partial y}\psi_1\right\rangle$ as they vanish by orthogonality of the spherical harmonics. Writing both x and y in the spherical harmonics then doing the angular and radial integration we obtain the following exact result for the noncommutative quadratic Stark effect:

$$E_1^{2(\mathrm{NC})} = -\frac{e^2 m}{32\hbar^2}|\vec{E}\times\vec{\theta}|^2. \tag{16}$$

Comparing this result with that obtained in the last section using the second-order perturbation theory given by equation (7) we conclude that

$$\frac{1}{3}\sum_{n\neq 1}\frac{2^8 n^5 (n-1)^{2n-4}}{(n+1)^{2n+4}} = 1. \tag{17}$$

Indeed this is the case, this sum is nothing but the sum rule of the mean oscillator strength for the Lyman series (Bethe and Salpeter 1957) which is equal to 1 as one can check by setting $l = 0$ in equation (61.5) for the ground state (Bethe and Salpeter 1957). Therefore, equating the exact computation for the energy contribution in the noncommutative quadratic Stark effect with that computed in the last section we derived the sum rule for the mean oscillator strength. This quantity is a dimensionless quantity and proportional to the frequency times the dipole moment.

Adding the noncommutative quadratic Stark shift energy to the ordinary Stark shift we have

$$E_1^{\mathrm{Stark}} = -\frac{9a^3}{4}|\vec{E}|^2 - \frac{e^2 m}{32\hbar^2}|\vec{E}\times\vec{\theta}|^2 - \frac{3555a^7}{64}|\vec{E}|^4 + O(|\vec{E}|^6). \tag{18}$$

This energy in terms of polarizability is

$$E_1^{\mathrm{Stark}} = -\tfrac{1}{2}\varepsilon_{ij}E_iE_j, \tag{19}$$

where ε_{ij} is the polarizability tensor. In general ε_{ij} is a function of external field, however, up to second order it is electric field independent. One can easily read off ε_{ij} from equation (18):

$$\varepsilon_{ij} = \frac{9}{2}\delta_{ij}a^3 + \frac{e^2 m}{16\hbar^2}(\theta^2\delta_{ij} - \theta_i\theta_j). \tag{20}$$

From this equation we make the following remarks, first noncommutative polarizability is not proportional to δ_{ij} it has a more complicated tensorial structure. In other words the noncommutative Stark effect is direction dependent. It is due to the fact that an electron (in general any charged particle) in noncommutative space also has an electric dipole moment. The second remark is that $\varepsilon_{ij}^{(\mathrm{NC})}$ has a zero eigenvalue ($\varepsilon_{ij}\theta_j = 0$). Physically it means that the noncommutative Stark effect vanishes if the external electric field is parallel to $\vec{\theta}$. This is explicitly seen from equation (16). The third remark we make is of observational significance; although the present experimental data on the Stark effect are not updated and precise enough to improve the current bounds on noncommutativity coming from other experiments

(Chaichian *et al* (2001a)). One may still study observational prospects of the noncommutative Stark effect. It is convenient to present our results as the the ratio of noncommutative to commutative results, i.e.

$$\begin{aligned}\Delta_{\mathrm{NC}} &= \frac{E^{(\mathrm{NC})}}{E^{C}} \\ &= \frac{\frac{e^2 m}{32\hbar^2}|\vec{E}\times\vec{\theta}|^2}{\frac{9a^3}{4}|\vec{E}|^2} = \frac{|\vec{\theta}|^2}{72a^4}\sin^2\phi,\end{aligned} \tag{21}$$

where ϕ is the angle between $\vec{\theta}$ and $\vec{E}$. It is worth noting that the above ratio is independent of α_{QED}. If the precision of the Stark effect is P_{Stark}, the ratio Δ_{NC} should be within the error bars of the experiment or $\Delta_{\mathrm{NC}} \preceq P_{\mathrm{Stark}}$. From this one can infer an upper bound on θ, or equivalently a lower bound on the noncommutativity scale.

4. Conclusion

In this paper we have shown that there is a contribution to the quadratic Stark effect due to the noncommutativity of the coordinates. We have obtained the correction to the ground-state energy using two methods and by combining the two we have derived the sum rule of the mean oscillator strength. If the external electric field $\vec{E}$ is parallel to $\vec{\theta}$ then there will be no shift in the ground-state energy of the H-atom, therefore in this case we have only the ordinary quadratic Stark effect. If the two vectors are not parallel then the polarization of the ground state is no longer diagonal. From which we may infer some lower bound on the noncommutativity scale.

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