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ORIGINAL PAPER

Spectrum of the Kratzer-type molecule in non-commutative spaces

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Abstract: An analytical formulation to determine the non-relativistic energy spectrum associated with the Kratzer potential has been exploited using the Bopp shift method within the framework of non-commutative geometry. A necessary analysis of the Kratzer potential is performed, identifying corrections to the second-order degenerate states, which are influenced by the non-commutative coefficient θ. To accomplish this ambitious task, we focused mainly on solving the Schrödinger equation with separated variables, always within the framework of non-commutative geometry.

Keywords: Non-commutative geometry space; The star-product; Bopp's shift method; Kratzer potential

1. Introduction

Over the past century, two revolutionary theories of physics have transformed our understanding of the universe: general relativity and quantum mechanics. General relativity, formulated by Albert Einstein in 1916, provides a comprehensive framework for understanding the behavior of objects on a cosmic scale. In contrast, quantum mechanics (QM), developed by pioneers such as Niels Bohr, Werner Heisenberg, Erwin Schrödinger, and Paul Dirac, addresses the phenomena occurring at the microscopic level.

Dirac's work in 1927 unified these two approaches into a single mathematical framework known as state vectors, which included the Heisenberg and Schrödinger formulations introduced successively in 1925 and 1926 [1].

In 1928, Dirac merged his state vector mechanics with special relativity, leading to the prediction of antimatter in 1930. Historically, the transition from non-relativistic to relativistic quantum mechanics involved the generalization of the Schrödinger equation where solving this equation is essential to study microscopic systems by determining over time the wave function and energy spectrum of possible states.

This work will explore the Schrödinger equation using the method of separation of variables, focusing on its application within non-commutative space. The fundamental constant of quantum mechanics $\hbar = h/2\pi$ named in honor of Max Planck is the foundation of physical theory and is integral to the Heisenberg uncertainty principle expressed as $\Delta x.\Delta p \simeq h/2$. This principle highlights the commutation relations of position and momentum operators within a Hilbert space:

$$\left[\,\hat{x}_i, \hat{x}_j\right] = 0, \qquad \left[\hat{p}_i, \hat{p}_j\right] = 0, \qquad \left[\hat{x}_i, \hat{p}_j\right] = i\hbar\delta_{ij}. \tag{1}$$

Quantum mechanics in non-commutative space involves the examination of the Hamiltonian that depends on the position and momentum operators [2], which adhere to a noncanonical commutation algebra. The study of exactly solvable models in quantum mechanics can help us better understand some phenomena occurring in non-commutative quantum field theory.

Non-commutative geometry, which emerged in 1947 through the work of Snyder [3], introduces a novel perspective where the coordinates of spacetime do not follow traditional commutation rules. Unlike conventional geometry, which relies on commutative algebraic structures (where $ab = ba$). Non-commutative geometry [4–7] involves algebraic structures where $ab \neq ba$. This framework reshapes our understanding of spatial and temporal interactions, as reflected in the noncommuting behavior of position and momentum operators:

$$\left[\,\hat{x}_i, \hat{x}_j\right] \neq 0, \qquad \left[\hat{p}_i, \hat{p}_j\right] \neq 0. \tag{2}$$

Our aim in this work is to present a study of the energy corrections to the spectrum of a Kratzer-type molecule in a

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*Corresponding author, E-mail: mourad.debabi@univ-msila.dz non-commutative space, obtained by solving the Schrödinger equation with separated variables.

2. Non-commutative geometry

2.1. Non-commutative space time algebra

The three non-commutativity relations below can encapsulate the entirety of non-commutative algebra and its fundamental principles [8–10]:

$$\begin{cases} \left[\widehat{x}_i, \widehat{x}_j\right] = i\theta_{ij} \\ \left[\widehat{p}_i, \widehat{p}_j\right] = i\sigma_{ij}\ . \\ \left[\widehat{x}_i, \widehat{p}_j\right] = i\hbar\delta_{ij} \end{cases} \tag{3}$$

The quantities θ_{ij} and σ_{ij} are real anti-symmetric parameters that may depend on the operators $\widehat{p}$ and $\widehat{x}$, subject to the following conditions: $\theta_{ij} = \varepsilon_{ij}\theta$ and $\sigma_{ij} = \varepsilon_{ij}\sigma$ with $\varepsilon_{ij} = -\varepsilon_{ji} = 1$. When we set $(\theta, \sigma) \to (0, 0)$, we obtain the relationships of ordinary quantum mechanics.

Non-commutativity is only achieved on positional operators by means of parameters (positional non-commutativity) [8]. Therefore, the algebra above is rewritten as:

$$\begin{cases} \left[\hat{x}_i\ , \hat{x}_j\right] = i\theta_{ij} \\ \left[\hat{p}_i, \hat{p}_j\right] = 0 \quad . \\ \left[\hat{x}_i, \hat{p}_j\right] = i\hbar\delta_{ij} \end{cases} \tag{4}$$

Where θ_{ij} is an anti-symmetric tensor with real elements:

$$\theta_{ij} = \begin{pmatrix} 0 & -\theta & 0 & 0 \\ \theta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{5}$$

2.2. Weyl quantization

Weyl quantization is a technique used to describe quantum mechanics based on the phase space of classical mechanics. It enables the association of quantum operators with classical functions that depend on phase space variables, particularly canonical variables. This method offers a systematic approach to describe non-commutative spaces and to investigate field theories formulated within them.

2.2.1. The star-product

The star-product formalism, initially developed by Weyl and Wigner, provides a way to describe quantum mechanics using the phase space. Unlike the operator-based approach, it revolves around deforming the product of phase space variables. This formalism can be applied effectively with the aid of the Fourier transform [10–14]:

$$\begin{aligned} f(x) =& (2\pi)^{-D/2} \int d^D k e^{-ik_i x^i} \widetilde{f}(k) \Longleftrightarrow \widetilde{f}(k) \\ =& (2\pi)^{-D/2} \int d^D k e^{ik_i x^i} f(x). \end{aligned} \tag{6}$$

The Weyl symbol is defined as:

$$W(f) = (2\pi)^{-D/2} \int d^D k e^{ik_i x^i} \widetilde{f}(k). \tag{7}$$

If $f(x)$ are real functions, then the Weyl operator is Hermitian.

According to [8, 9, 15, 16], we can write the star-product of two functions at the first order of θ as follows:

$$\begin{aligned} f * g =& f(x) \exp\left(\frac{i}{2} \overleftarrow{\partial_i}\, \theta^{ij} \overrightarrow{\partial_j}\right) g(y)\ |_{x=y} \\ =& f(x)g(x) + \frac{i}{2}\theta^{ij}\partial_i f(x)\partial_j g(y) + O(\theta^2)\ |_{x=y}\ . \end{aligned} \tag{8}$$

If $\theta = 0$, the star-product of two functions is equal to the ordinary product of these functions, which corresponds to the commutative case.

$$f(x) * g(x) = f(x)g(x). \tag{9}$$

2.3. Schrödinger equation in non-commutative space

In D-dimensional non-commutative space-time, we replace wave function products with the star-product. The Schrödinger equation on non-commutative spacetime takes the following form [15, 17]:

$$\hat{H}(\widehat{p}, \overrightarrow{\widehat{x}}) * \Psi(\overrightarrow{\widehat{x}}, t) = E\Psi(\overrightarrow{\widehat{x}}, t), \tag{10}$$

$$i\hbar\frac{\partial\Psi}{\partial t}(\overrightarrow{\widehat{x}}, t) = \left[\frac{\overrightarrow{p}^2}{2m} + V(\overrightarrow{\widehat{x}})\right] * \Psi(\overrightarrow{\widehat{x}}, t). \tag{11}$$

The star-product between the potential operator and the wave function is defined as:

$$V(\overrightarrow{x}).\Psi(\overrightarrow{x}, t) \to V(\overrightarrow{\widehat{x}}) * \Psi(\overrightarrow{\widehat{x}}, t). \tag{12}$$

In his research, Mezincescu [18] demonstrated that the following relationship holds true:

$$V(\overrightarrow{x}) * \Psi(\overrightarrow{x}) = V(\overrightarrow{\widehat{x}} - \frac{\widetilde{p}}{2})\Psi(\overrightarrow{\widehat{x}}). \tag{13}$$

2.4. The “Bopp shift” formula

In the context of non-commutative spacetime, we can establish a relationship between the operators $\widehat{x}_i$ and $\widehat{p}_i$, which represent position and momentum, and their conventional counterparts x_i and p_i [19] through the transformation [15, 18]:

$$\widehat{x}_i = x_i - \frac{\theta_{ij}}{2\hbar} p_j, \tag{14}$$

$$\widehat{p}_j = p_j. \tag{15}$$

The last transformation is referred to as the 'Bopp shift'.

3. Schrodinger equation with solutions for a Kratzer-type molecule

Generally, in QM the determination of exact analytical solutions to the Schrödinger equations is difficult and ongoing task, which is not always the case and the search for approximate solutions is necessary. In atomic and molecular physics, as well as in chemistry, the Kratzer potential [20, 21] is one of the most effective potential energy models used in quantum mechanics to describe molecular interactions, due to its central role in determining the energy of bound states.

The Kratzer potential [22], formed by combining the Coulomb potential with the inverse square potential, plays an important role in quantum chemistry, taking into account the influence of the nucleus (Coulomb term) and internal electrons (represented by an additional term) [23].

In quantum mechanics, where analytically solvable problems are limited [24], the Kratzer potential is one of the few for which an exact solution exists [25–28].

Bayrak [29] presented a comprehensive analytical demonstration, emphasizing the significance and practical value of obtaining the eigenvalues explicitly in theoretical chemistry problems.

On the other hand, we noticed in the literature that many researchers had addressed the study of this potential within the framework of relativistic and non-relativistic quantum mechanics [30–32] and non-commutative quantum mechanics [33–39]. Furthermore, an intriguing study on two-dimensional and three-dimensional space has been conducted [40, 41] within the non-commutative quantum mechanics framework.

These features have made it a subject of interest, and researchers have extensively examined Kratzer potential in Refs. [20, 22, 29, 42]:

$$V(r) = -2D\left(\frac{a}{r} - \frac{1}{2}\frac{a^2}{r^2}\right), \tag{16}$$

With a minimum of $V(r) = -D$ and D is the bond interaction dissociation energy between two atoms in the diatomic molecules separated by an equilibrium inter nuclear distance a Fig. 1. Where one of the two atoms can be much heavier than the other [22].

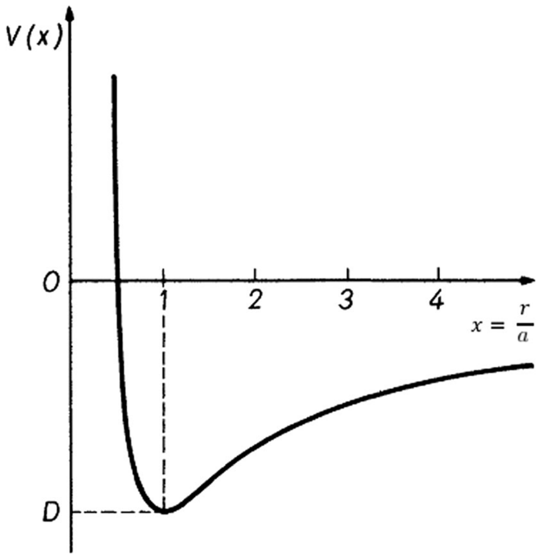

Fig. 1 Kratzer potential

3.1. Non-commutative case

Solving Schrödinger's equation with the kratzer potential in non-commutative space first requires the introduction of the Bopp shift relation (14) into Eq. (16).

We have:

$$\widehat{x}_i = x_i - \frac{\theta_{ij}}{2\hbar}\widehat{p}_j, \tag{17}$$

where [43–46]:

$$r = \sqrt{\widehat{x}_i\widehat{x}_i}. \tag{18}$$

Now it is recommended that the relationship be maintained [47]:

$$V^{NC}(r) = -2D_e\left(\frac{r_e}{\sqrt{\widehat{x}_i\widehat{x}_i}} - \frac{r_e^2}{2(\widehat{x}_i\widehat{x}_i)}\right) \tag{19}$$

$$\begin{aligned}
&= -2D_e\left(\frac{r_e}{\sqrt{(x_i - \frac{\theta_{ij}}{2\hbar}\widehat{p}_j)(x_i - \frac{\theta_{ij}}{2\hbar}\widehat{p}_j)}} - \frac{r_e^2}{2(x_i - \frac{\theta_{ij}}{2\hbar}\widehat{p}_j)(x_i - \frac{\theta_{ij}}{2\hbar}\widehat{p}_j)}\right)\\
&= -2D_e\left(\frac{r_e}{(r^2 - \frac{\theta_{ij}}{\hbar}\widehat{p}_j x_i + \vartheta(\theta^2))^{\frac{1}{2}}} - \frac{r_e^2}{2(r^2 - \frac{\theta_{ij}}{\hbar}\widehat{p}_j x_i + \vartheta(\theta^2))}\right)\\
&= -2D_e\left(\frac{r_e}{(1 - \frac{\theta_{ij}}{\hbar r^2}\widehat{p}_j x_i + \vartheta(\theta^2))^{\frac{1}{2}}} - \frac{r_e^2}{2r^2(1 - \frac{\theta_{ij}}{\hbar r^2}\widehat{p}_j x_i + \vartheta(\theta^2))}\right)\\
&= \frac{-2D_e r_e}{r}(1 + \frac{\theta_{ij}}{2\hbar r^2}\widehat{p}_j x_i + \vartheta(\theta^2)) + \frac{2D_e r_e^2}{2r^2}\left(1 + \frac{\theta_{ij}}{\hbar r^2}\widehat{p}_j x_i + \vartheta(\theta^2)\right)\\
&= \frac{-2D_e r_e}{r} + \frac{2D_e r_e^2}{2r^2} - 2D_e r_e\frac{\sum \varepsilon_{ijk}\theta_k\widehat{p}_j x_i}{4\hbar r^3} + 2D_e r_e^2\frac{\sum \varepsilon_{ijk}\theta_k\widehat{p}_j x_i}{4\hbar r^4},
\end{aligned} \tag{20}$$

where $\vartheta(\theta^2)$ expresses the second-order term that will be neglected. Since:

$$\theta_{ij} = \frac{\varepsilon_{ijk}\theta_k}{2}. \tag{21}$$

We have:

$$\begin{aligned}\sum \varepsilon_{ijk}\,\theta_k\,\hat{p}j\,x_i &= (x_2\,p_3 - x_3\,p_2)\theta_1 \\ &+ (x_3\,p_1 - x_1\,p_3)\theta 2 + (x_1\,p_2 - x_2\,p_1)\theta_3 \\ &= L_1\theta_1 + L_2\theta_2 + L_3\theta_3 \\ &= \vec{L}\cdot\vec{\theta}.\end{aligned} \tag{22}$$

Then:

$$V^{NC}(r) = -2D_e\left(\frac{r_e}{r} - \frac{r_e^2}{2r^2}\right) - \frac{D_e r_e \overrightarrow{L}\,\overrightarrow{\theta}}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right), \tag{23}$$

we find:

$$V^{NC}(r) = V^C(r) - \frac{D_e r_e \overrightarrow{L}\,\overrightarrow{\theta}}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right). \tag{24}$$

We can write the Hamiltonian operator in non-commutative space as follows:

$$\widehat{H} = \frac{\widehat{p}^2}{2m} + V^{NC}(r). \tag{25}$$

The Schrödinger equation in non-commutative space:

$$\widehat{H}\Psi(\overrightarrow{r},\theta,\varphi) = E\Psi(\overrightarrow{r},\theta,\varphi), \tag{26}$$

by substituting Eq. (23) into Eq. (26):

$$\begin{aligned}&\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{\widehat{L}^2}{\hbar^2 r^2}\right) - 2D_e\left(\frac{r_e}{r} - \frac{r_e^2}{2r^2}\right)\right. \\ &\left.-\frac{D_e r_e \overrightarrow{L}\,\overrightarrow{\theta}}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right)\right]\Psi(\overrightarrow{r},\theta,\varphi) = E\Psi(\overrightarrow{r},\theta,\varphi),\end{aligned} \tag{27}$$

we have:

$$\Psi(\overrightarrow{r},\theta,\varphi) = R_{nl}(r)Y_{lm}(\theta,\varphi). \tag{28}$$

Right now, and by substituting (28) into (27):

$$\begin{aligned}&\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{\widehat{L}^2}{\hbar^2 r^2}\right) - 2D_e\left(\frac{r_e}{r} - \frac{r_e^2}{2r^2}\right)\right. \\ &\left.-\frac{D_e r_e \overrightarrow{L}\,\overrightarrow{\theta}}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right)\right]R_{nl}(r)Y_{lm}(\theta,\varphi) = ER_{nl}(r)Y_{lm}(\theta,\varphi),\end{aligned} \tag{29}$$

where:

$$\widehat{L}^2 Y_{lm}(\theta,\varphi) = \hbar^2 l(l+1)Y_{lm}(\theta,\varphi). \tag{30}$$

Finally, we have:

$$\begin{aligned}&\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{\widehat{L}^2}{\hbar^2 r^2}\right) - 2D_e\left(\frac{r_e}{r} - \frac{r_e^2}{2r^2}\right)\right. \\ &\left.-\frac{D_e r_e \overrightarrow{L}\,\overrightarrow{\theta}}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right)\right]R_{nl}(r)Y_{lm}(\theta,\varphi) = ER_{nl}(r)Y_{lm}(\theta,\varphi).\end{aligned} \tag{31}$$

In this context, we can see that the angular part is the same as in the commutative case, where $Y_{lm}(\theta,\varphi)$ represents:

$$Y_{lm}(\theta,\varphi) = \sqrt{\left(\frac{2}{4\pi}\right)^3\frac{(l-m)!}{(l+m)!}}(-1)^m p_l^m(\cos\theta)e^{im\varphi}. \tag{32}$$

On the other hand, the radial part is completely different from the commutative radial part. So:

$$\begin{aligned}&\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right) - 2D_e\left(\frac{r_e}{r} - \frac{r_e^2}{2r^2}\right)\right. \\ &\left.-\frac{D_e r_e \overrightarrow{L}\,\overrightarrow{\theta}}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right)\right]R_{nl}(r) = ER_{nl}(r),\end{aligned} \tag{33}$$

where n and l denote the radial and orbital angular momentum quantum numbers, r is the inter nuclear separation of the diatomic molecules.

Using the following change of variable:

$$R_{nl}(r) = \frac{U(r)}{r}, \tag{34}$$

we find:

$$\begin{aligned}&\frac{\partial^2}{\partial r^2}U(r) - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2} \\ &\left(-2D_e\left(\frac{r_e}{r} - \frac{r_e^2}{2r^2}\right) - \frac{D_e r_e \overrightarrow{L}\,\overrightarrow{\theta}}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right) - E\right)U(r) = 0.\end{aligned} \tag{35}$$

The Hamiltonian $\widehat{H}_\theta$ becomes:

$$\widehat{H}_\theta = \frac{\widehat{p}^2}{2m} - 2D_e\left(\frac{r_e}{r} - \frac{r_e^2}{2r^2}\right) - \frac{D_e r_e \overrightarrow{L}\,\overrightarrow{\theta}}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right). \tag{36}$$

From the last relationship, we can be observe that non-commutativity appears in the form of a perturbation.

$$\widehat{W}_\theta = -\frac{D_e r_e \overrightarrow{L}\,\overrightarrow{\theta}}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right), \tag{37}$$

becomes

$$\widehat{W}_\theta = -\frac{D_e r_e L_z \theta}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right). \tag{38}$$

We observe that the expression above closely resembles that which describes spin-orbit coupling.

$$\widehat{W}_{s.o} = -\frac{e^2}{2m^2c^2}\left(\frac{\overrightarrow{L}\cdot\overrightarrow{S}}{r^3}\right). \tag{39}$$

By identifying the non-commutativity constant θ with the spin angular momentum S, it becomes evident that the non-commutativity constant assumes the role of spin. In simpler terms, one can state that spin derives from the non-commutativity of space.

In the following discussion, we will treat non-commutativity as a perturbation in order to identify and estimate the corrections to the energy levels of the Kratzer potential.

3.2. Energy corrections

Applying usual perturbation theory, the main corrections for energy levels resulting from non-commutativity, i.e. first order perturbation and the tree-level contributions in field theory, can be expressed as:

$$\triangle E_n^{(1)} = \left\langle \psi n, l, m_l \mid \widehat{W}_\theta \mid \psi_{n,l,m_l}\right\rangle, \tag{40}$$

$$\triangle E_n^{(1)} = -\frac{D_e r_e \theta}{2\hbar}\int_0^\infty drr^2 \int_0^{4\pi} \left[\left\langle \psi^+_{n,l,m_l} \mid \frac{L_z}{r^3} \mid \psi_{n,l,m_l}\right\rangle - \left\langle \psi^+_{n,l,m_l} \mid \frac{r_e L_z}{r^4} \mid \psi_{n,l,m_l}\right\rangle\right] d\Omega. \tag{41}$$

Let's use the following notation:

$$\mid \psi_{n,l,m_l}\rangle = \mid n, l, m_l\rangle, \tag{42}$$

Equation (40) becomes

$$\triangle E_n^{(1)} = \left\langle n, l, m_l \mid -\frac{D_e r_e L_z \theta}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right) \mid n, l, m_l\right\rangle. \tag{43}$$

We find:

$$\triangle E_n^{(1)} = -\frac{D_e r_e \theta m_l}{2}\left(\left\langle n, l, m_l \mid \frac{1}{r^3} \mid n, l, m_l\right\rangle - \left\langle n, l, m_l \mid \frac{r_e}{r^4} \mid n, l, m_l\right\rangle\right), \tag{44}$$

because:

$$\langle n, l, m_l \mid L_z \mid n, l, m_l\rangle = m_l \hbar. \tag{45}$$

It is observed that:

$$\left\langle n, l, m_l \mid \frac{1}{r^3} \mid n, l, m_l\right\rangle = \int_0^\infty drr^2 R^*_{nl}(r)\frac{1}{r^3}R_{nl}(r) = \langle\frac{1}{r^3}\rangle. \tag{46}$$

Since:

$$\int_0^\infty drr^2 R^*_{nl}(r) R_{nl}(r) = 1. \tag{47}$$

According to [48]

Concerning mean values $\langle r^k\rangle_{nl}$, distinctions among different radial eigenfunctions become particularly evident when we compute the mean value of r, the distance between the electron and the nucleus, raised to various powers. The mean value $\langle r^k\rangle_{nl}$ is defined as:

$$\frac{k+1}{n^2}\langle r^k\rangle_{nl} - (2k+1)\frac{a_0}{z}\langle r^{k-1}\rangle_{nl} + k\left[l(l+1) + \frac{1-k^2}{4}\right]\langle r^{k-2}\rangle_{nl} = 0. \tag{48}$$

Now, let's calculate the first energy correction $\triangle E_n^{(1)}$ by substituting Eqs. (100) and (101) into (44):

$$\triangle E_n^{(1)} = -\frac{D_e r_e \theta m_l}{2}\left(\left\langle\frac{1}{r^3}\right\rangle - \left\langle\frac{r_e}{r^4}\right\rangle\right) \tag{49}$$

$$= -\frac{D_e r_e \theta m_l}{2}\left(\frac{Z^3}{a_0^3 n^3 (l+1)(l+\frac{1}{2})l} - \frac{r_e Z^4 \frac{1}{2}[3n^2 - l(l+1)]}{a_0^4 n^5 (l+\frac{3}{2})(l+1)(l+\frac{1}{2})l(l-\frac{1}{2})}\right), \tag{50}$$

$$\begin{aligned} &= -\frac{D_e r_e \theta m_l}{2}\left(\frac{Z^3}{a_0^3 n^3 (l+1)(l+\frac{1}{2})l} - \frac{r_e Z^4 \frac{1}{2}[3n^2 - l(l+1)]}{a_0^3 n^3 (l+1)(l+\frac{1}{2}) l a_0 n^2 (l+\frac{3}{2})l(l-\frac{1}{2})}\right) \\ &= -\frac{D_e r_e \theta m_l}{2}\left(\frac{Z^3 a_0 n^2 (l+\frac{3}{2})l(l-\frac{1}{2})}{a_0^3 n^3 (l+1)(l+\frac{1}{2}) l a_0 n^2 (l+\frac{3}{2})l(l-\frac{1}{2})} - \frac{\frac{1}{2} r_e Z^4 [3n^2 - l(l+1)]}{a_0^3 n^3 (l+1)(l+\frac{1}{2}) l a_0 n^2 (l+\frac{3}{2})l(l-\frac{1}{2})}\right) \\ &= -\frac{D_e r_e \theta m_l}{2}\left(\frac{Z^3 a_0 n^2 (l+\frac{3}{2})l(l-\frac{1}{2}) - r_e Z^4 \frac{1}{2}[3n^2 - l(l+1)]}{a_0^4 n^5 (l+\frac{3}{2})(l+1)(l+\frac{1}{2})l(l-\frac{1}{2})}\right). \end{aligned} \tag{51}$$

We put:

$$\begin{cases} g_1 = \frac{D_e Z^4 r_e^2}{a_0^4} \\ g_2 = \frac{2D_e Z^3 r_e}{a_0^3} \end{cases}, \tag{52}$$

therefore:

$$\triangle E_n^{(1)} = -\frac{g_2 \theta m_l}{4n^3 (l+1)(l+\frac{1}{2})} + \frac{g_1 \theta m_l [3n^2 - l(l+1)]}{4n^5 (l+\frac{3}{2})(l+1)(l+\frac{1}{2})(l-\frac{1}{2})l}. \tag{53}$$

When $g_1 = 0$, the Kratzer potential reduces to the Coulomb potential, and thus Eq. (53) becomes:

$$\triangle E_n^{(1)} = -\frac{g_2\theta m_l}{4n^3(l+1)(l+\frac{1}{2})l}, \tag{54}$$

this last equation yields the same result for the first-order energy spectrum of the hydrogen atom [43, 49, 50].

$$g_2 = 1$$

$$\triangle E_n^H = -\frac{\theta m_l}{4n^3 l(l+1)(l+\frac{1}{2})}. \tag{55}$$

According to perturbation theory. The Eq. (53) shows how non-commutativity affects energy levels of Kratzer-type molecules up to the first order. We denote the states of diatomic molecules through n, l, and m_l quantum numbers, this enables us to qualitatively evaluate the non-commutativity constant of space through by studying of its effects on energy levels in diatomic molecules as a whole.

For $n = 1$ the energy levels (53) are as follows when $l = 1 \;\; \rightarrow -l \leq m \leq l \;\; \rightarrow \;\; m = -1, 0, 1,$ we examine three cases:

$\cdot\ l = 1,\ m = -1$

$$\triangle E_n^{(1)} = +\frac{g_2\theta}{12} - \frac{g_1\theta}{15}, \tag{56}$$

$\cdot\ l = 1, m = 0$

$$\triangle E_n^{(1)} = 0, \tag{57}$$

$\cdot\ l = 1, m = +1$

$$\triangle E_n^{(1)} = -\frac{g_2\theta}{12} + \frac{g_1\theta}{15}. \tag{58}$$

Indeed [43, 44, 49, 50], it is crucial to recognize that the total angular momentum is conserved in such situations. Therefore, for a comprehensive treatment of this subject necessitates consideration of both orbital and spin quantum numbers, which can be achieved by replacing the states $\mid n, l, m_l\rangle$ with $\mid n, j, j_z\rangle$. It should be noted that $j = l + s$ represents the total angular momentum quantum number.

Now, we will amend the relationship (43) to align with the concept presented in the previous paragraph.

$$\triangle E_n^{(1)} = \left\langle n, j, j_z \mid -\frac{D_e r_e \theta_z \widehat{L}_z}{2\hbar}\left(\frac{1}{r^3} - \frac{r_e}{r^4}\right) \mid n, j, j_z \right\rangle. \tag{59}$$

Taking into account the Clebsch-Gordan coefficients and Refs. [43, 49, 51] we have

$$\left\langle n, j, j_z \mid \widehat{L}_z \mid n, j, j_z \right\rangle = \begin{cases} \left(1 - \frac{1}{2l+1}\right) j_z\hbar \text{for } j = l + \frac{1}{2} \\ \left(1 + \frac{1}{2l+1}\right) j_z\hbar \text{ for } j = l - \frac{1}{2} \end{cases}. \tag{60}$$

With this in mind, we can writing the first-order energy levels as follows:

$$\triangle E_n^{(1)} = -\frac{D_e r_e \theta_z j_z}{2}\left(1 \mp \frac{1}{2l+1}\right) \left(\left\langle n, l', j, j'_z \mid \frac{1}{r^3} \mid n, l, j, j_z \right\rangle - \left\langle n, l', j, j'_z \mid \frac{r_e}{r^4} \mid n, l, j, j_z \right\rangle\right). \tag{61}$$

The energy shift level using relation (52), is given by

$$\triangle E_n^{(1)} = \frac{\theta_z j_z}{4}\left[\frac{g_1[3n^2 - l(l+1)]}{n^5(l+\frac{3}{2})(l+1)(l+\frac{1}{2})l(l-\frac{1}{2})} - \frac{g_2}{n^3(l+1)(l+\frac{1}{2})l}\right] \left(1 \mp \frac{1}{2l+1}\right), \tag{62}$$

for

$$j = l \pm \frac{1}{2}. \tag{63}$$

Despite the conservation of total angular momentum, our earlier approximation (20) was seemingly violated and this in order to achieve a satisfactory outcome, as evidenced by the analysis of Eq. (61).

4. Spin orbit coupling and fine structure

The total angular momentum of an atom is defined as the sum of its orbital and spin angular momenta:

$$\mathbf{J} = \mathbf{L} + \mathbf{S}, \tag{64}$$

which is a conserved quantity in a central field, in contrast to **L** or **S** separately. By squaring this sum to yield the following result:

$$\mathbf{J}^2 = \mathbf{L}^2 + \mathbf{S}^2 + 2\mathbf{L} \cdot \mathbf{S}. \tag{65}$$

L and **S** are commuting operators. Then

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right). \tag{66}$$

As the eigenvectors of the Hamilton operator are eigenvectors of all the three operators $\mathbf{J}^2$, $\mathbf{L}^2$ and $\mathbf{S}^2$ with the respective eigenvalues $\hbar^2 j(j+1)$, $\hbar^2 l(l+1)$, $\hbar^2 s(s+1)$, where the j indicates coupled angular momentum and the energy is different for each j.

The fine structure is a relativistic correction to the kinetic energy. On the other hand the magnetic field interacts with the electron's internal magnetic moment, causing an additional energy shift $\Delta E = -m\mathbf{B} = \frac{Ze_0^2}{2m_0c^2}\frac{\mathbf{L}\cdot\mathbf{S}}{r^3}$. In contrast, in view of the aforementioned Eq. (38), we can express the energy correction due to the spin orbit interaction can be formulated as follows:,

$$\Delta E=\frac{Dr_eL_z\theta}{2\hbar}\left(\frac{1}{r^3}-\frac{r_e}{r^4}\right). \tag{67}$$

4.1. The Lamb shift and noncommutative correction

According to relativistic quantum theory the actual energy levels of the $n=2$; the $2S_{1/2}$ level should be exactly degenerate with $2P_{1/2}$, but in reality there is an energy interval between them, $E(2S_{1/2})-E2(P_{1/2})\simeq 1GH_z$. The shift of the $2S_{1/2}$ level to a higher energy than the E_{Dira} is about one tenth of the interval between the two fine-structure levels $E(2P_{3/2})-E(2P_{1/2})\simeq 11GH_z$. Although small, this discrepancy in hydrogen was of great historical importance in physics, As a result energies of $|n=2,l=1,s=1/2\rangle$ which are split according to [50, 52]

$$j=\begin{cases}3/2 & \rightarrow {}^2P_{3/2}\\ 1/2 & \rightarrow {}^2P_{1/2}\end{cases}, \tag{68}$$

and $|n=2,l=0,s=1/2\rangle$ having,

$$j=1/2 \qquad \rightarrow \ {}^2S_{1/2} \tag{69}$$

the explanation of this Lamb shift goes beyond relativistic quantum mechanics and requires quantum electrodynamics (QED).

Back to the Eq. (62) this last is in fact dependent on l, n and j_z where $j_z=-j,\ -j+1.....+j$, It is evident that the presence of j_z indicates that energy will be further divided according to its value, but it is not the same as the spectrum of a hydrogen atom [50].

This is due to the second term of Eq. (62) resulting from the Kratzer potential in non-commutative space. Notably, the first terms of Eq. (62) for ${}^2S_{1/2}$ and ${}^2P_{1/2}$ undergo a correction as follows:

$${}^2P_{1/2}=\begin{cases}{}^2P_{+1/2}\\ {}^2P_{-1/2}\end{cases},\quad {}^2S_{1/2}=\begin{cases}{}^2S_{+1/2}\\ {}^2S_{-1/2}\end{cases}, \tag{70}$$

and the second term of Eq. (62), represented by the ${}^2P_{2/3}$ level where undergoes a correction as follows:

$${}^2P_{3/2}=\begin{cases}{}^2P_{+3/2}\\ {}^2P_{1/2}\\ {}^2P_{-1/2}\\ {}^2P_{-3/2}\end{cases}. \tag{71}$$

This last is a Spectrum of the Kratzer molecule in non-commutative spaces.

As a "toy" example, we can propose a spectral series to illustrate the effect of space non-commutativity in the case of the Kratzer molecule. In Fig. 2, since the limit approaches the hydrogen atom (see Eq. (55)), the "energy" levels correspond to those of the hydrogen atom, with the non-commutative effect becoming apparent only at the end. We also note that in Fig. 2, there is a great similarity with the Zeeman effect, Paschen effect, and other phenomena where interaction with a magnetic field and the atomic magnetic moment removes degeneracy and multiplies the initial atomic spectrum. Overall, we can predict a causal relationship between space non-commutativity and the degeneracy of atomic or molecular energy levels.

It is evident that the selection rules dictate that there are only transitions from ${}^2S_{1/2}$ to ${}^2P_{1/2}$ and from ${}^2P_{2/3}$ to ${}^2S_{1/2}$, respectively. Furthermore, we can see that this Spectrum corresponds to the hydrogen atom spectrum in non-commutative space when $g_1=0$ in the Eq. (62); where the upper part of the spectrum disappears. This confirms our findings in Eq. (55), this, in turn, corresponds to the [49, 50].

In the end, our efforts have culminated in the derivation of the energy spectrum for a diatomic molecule, characterized by Kratzer potential interaction in a non-commutative space, now taking into account the influence of spin to provide a more accurate result.

5. Conclusion

With this approach, our main objective was to solve the Schrödinger equation for the Kratzer potential within the limits of non-commutative space geometry. This non-commutativity was treated as a time-independent perturbation. It results in a simple shift of the position vector x_i to an equivalent vector $\widehat{x_i}$ defined by the relation $\widehat{x_i}=x_i-\frac{\theta_{ij}}{2\hbar}p_j$, which depends on the non-commutative parameter θ. Our study has revealed energy corrections up to the second order, directly contingent he depends the non-commutativity coefficient θ. Our results highlight the inherent complexity of understanding these corrections and thus underline the ongoing nature of research in this area.

Appendix 1

In this Appendix, we will calculate the commutators between the coordinates in phase and spatial space.

When dealing with a spatial dimension of $D=2$, the aforementioned relationships can be represented as follows: $(\theta_{ij}=\varepsilon_{ij}\theta$ and $\varepsilon_{ij}=-\varepsilon_{ji}=1)$

$$\widehat{x}=x-\frac{\theta_{ij}}{2\hbar}p_y=x-\frac{\theta}{2\hbar}p_y, \tag{72}$$

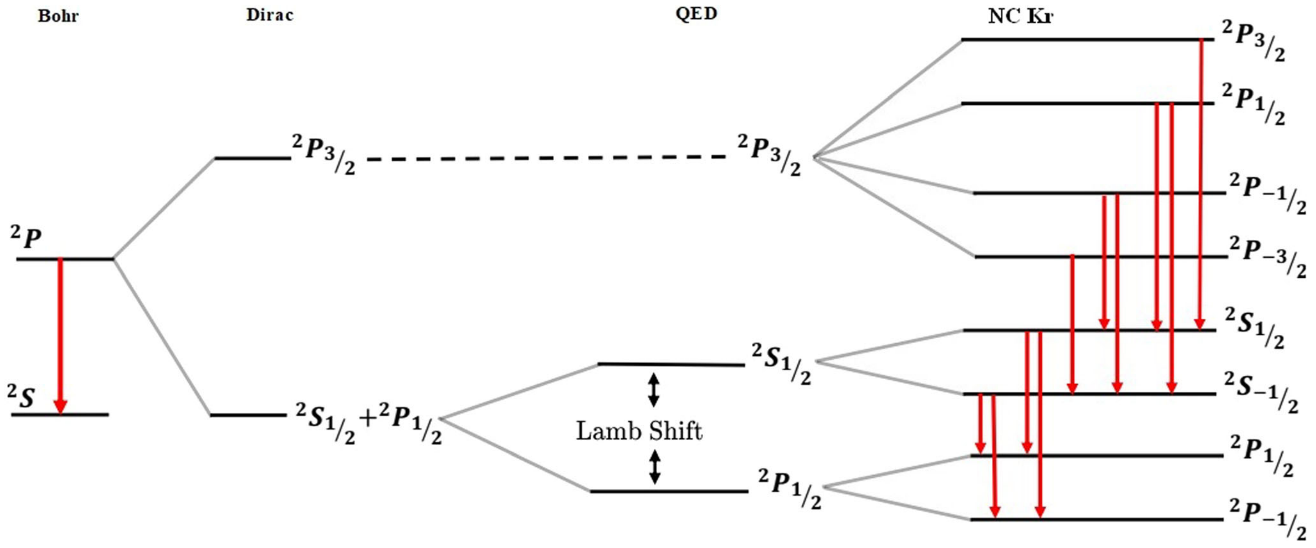

Fig. 2 Spectrum of the Kratzer molecule in non-commutative spaces

$$\widehat{y} = y - \frac{\theta_{ji}}{2\hbar}p_x = y + \frac{\theta_{ij}}{2\hbar}p_x = y_t + \frac{\theta}{2\hbar}p_x, \tag{73}$$

$$\widehat{p}_x = p_x, \tag{74}$$

$$\widehat{p}_y = p_y. \tag{75}$$

Let's use Eqs. (14) and (15) to calculate the commutators:

$$[x_i, x_j], [x_i, p_j], [p_i, p_j]. \tag{76}$$

We find the commutation laws between coordinates in the classical case

$$\begin{aligned}
[x_i, x_j] &= \left[\widehat{x}_i + \frac{\theta_{ij}}{2\hbar}\widehat{p}_j, \widehat{x}_j + \frac{\theta_{ij}}{2\hbar}\widehat{p}_i\right] \\
&= [\widehat{x}_i, \widehat{x}_j] + \frac{\theta_{ji}}{2\hbar}[\widehat{x}_i, \widehat{p}_i] + \frac{\theta_{ij}}{2\hbar}[\widehat{p}_i, \widehat{x}_i] + \frac{\theta_{ij}}{2\hbar}\frac{\theta_{ji}}{2\hbar}[\widehat{p}_j, \widehat{p}_i] \\
&= i\theta_{ij} + \frac{\theta_{ji}}{2\hbar}(i) + \frac{\theta_{ij}}{2\hbar}(-i) + \frac{\theta_{ij}}{2\hbar}\frac{\theta_{ji}}{2\hbar}(0) \\
&= i\theta_{ij} + \frac{-\theta_{ij}}{2\hbar}(i) + \frac{\theta_{ij}}{2\hbar}(-i) + 0 \\
&= 0,
\end{aligned} \tag{77}$$

$$\Longrightarrow [x_i, x_j] = 0. \tag{78}$$

$$\begin{aligned}
[x_i, p_j] &= \left[\widehat{x}_i + \frac{\theta_{ij}}{2\hbar}\widehat{p}_j, \widehat{p}_j\right] \\
&= [\widehat{x}_i, \widehat{p}_j] + \frac{\theta_{ij}}{2\hbar}[\widehat{p}_j, \widehat{p}_j] \\
&= i\hbar\delta_{ij} + \frac{\theta_{ij}}{2\hbar}(0) \\
&= i\hbar\delta_{ij},
\end{aligned} \tag{79}$$

$$\Longrightarrow [x_i, p_j] = i\hbar\delta_{ij}. \tag{80}$$

$$[p_i, p_j] = [\widehat{p}_i, \widehat{p}_j] = 0. \tag{81}$$

Appendix 2

This part of the Appendix we will proof of the recurrence relation (48):

In the context of a hydrogen-like atom with quantum numbers n and l, the expectation values of $\langle r^k \rangle_{nl}$ for different powers of the radial variable r are calculated using Eq. (48).

$$\langle r^k \rangle_{nl} = \int_0^\infty r^k [R_{nl}(r)]^2 r^2 dr. \tag{82}$$

$R_{n.l}(r)$ represents the solutions to the radial differential equation $HR(r) = ER(r)$we demonstrate that these values are linked by the recurrence relation (48). To simplify the concept, let's define the real function $u(r)$ us $u = rR_{n.l}$ and denote its first and second derivatives as $u'$and u''. The Eq. (82) then takes the form:

$$\langle r^k \rangle_{nl} = \int_0^\infty r^k u^2 dr. \tag{83}$$

Since we have:

$$\frac{\partial R_{nl}(r)}{\partial r} = \frac{u'}{r} - \frac{u}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R_{nl}(r)}{\partial r}\right) = ru''. \tag{84}$$

Starting from the relationship:

$$HR(r) = ER(r), \tag{85}$$

it becomes:

$$u^{''} = \left[\frac{l(l+1)}{r^2} - \frac{2z}{a_0 r} + \frac{z^2}{n^2 a_0^2}\right] u. \tag{86}$$

With the introduction of the energy equation $E_n = -\frac{ze^2}{2a_0 n^2}$, we begin by first deriving the useful relationship before directly deriving Eq. (48). Let's consider the integral:

$$\int_0^\infty r^\nu u u' dr. \tag{87}$$

We perform integration by parts:

$$\int_0^\infty r^\nu u u' \partial r = r^\nu u^2 \mid_0^\infty - \int_0^\infty u \frac{\partial}{\partial r}(r^\nu u) dr. \tag{88}$$

The first part of the integral disappears because when $R(r) \longrightarrow 0$ exponentially as $r \longrightarrow \infty$, and $u(r) \longrightarrow 0$ as $r \longrightarrow 0$.

Expanding the derivative in the integral on the right-hand side, we get

$$\int_0^\infty r^\nu u u' dr = -\nu \int_0^\infty r^{\nu-1} u^2 dr - \int_0^\infty r^\nu u u' dr. \tag{89}$$

By combining the integral on the left-hand side with the last one on the right-hand side, we get the result

$$\int_0^\infty r^\nu u u' dr = -\frac{\nu}{2}\langle r^{\nu-1}\rangle_{nl}. \tag{90}$$

To obtain the recurrence relation (48), we multiply the Eq. (86) by $r^{k+1}u'$ and integral over r.

$$\begin{aligned}
\int_0^\infty r^{k+1} u' u'' dr =& l(l+1) \int_0^\infty r^{k-1} u u' dr \\
& - \frac{2z}{a_0} \int_0^\infty r^k u u' dr + \frac{z^2}{n^2 a_0^2} \int_0^\infty r^{k+1} u u' dr \\
=& \frac{l(l+1)(k-1)}{2}\langle r^{k-2}\rangle_{nl} \\
& + \frac{kz}{a_0}\langle r^{k-1}\rangle_{nl} - \frac{(k+1)z^2}{2n^2 a_0^2}\langle r^k\rangle_{nl}.
\end{aligned} \tag{91}$$

The left-hand integral of Eq. (91) can be integrated as:

$$\begin{aligned}
\int_0^\infty r^{k+1} u' u'' \partial r =& -\int_0^\infty u' \frac{\partial}{\partial r}(r^{k+1} u') dr \\
=& -(k+1)\int_0^\infty r^k u' u' dr - \int_0^\infty r^{k+1} u' u'' dr \\
=& (k+1)\int_0^\infty u \frac{\partial}{\partial r}(r^k u') dr - \int_0^\infty r^{k+1} u' u'' dr \\
=& k(k+1)\int_0^\infty r^{k-1} u u' dr + (k+1)\int_0^\infty r^k u u'' dr \\
& - \int_0^\infty r^{k+1} u' u'' dr.
\end{aligned} \tag{92}$$

The integral on the left-hand side and the last integral on the right-hand side can be combined to yield:

$$\int_0^\infty r^{k+1} u' u'' dr = -\frac{k(k-1)(k+1)}{4}\langle r^{k-2}\rangle_{nl} + \frac{(k+1)}{2}\int_0^\infty r^k u u'' dr. \tag{93}$$

Here we use the Eq. (90) in the first integral on the right-hand side.

Let's Substitution of Eq. (86) for u'' in the last integral on the right-hand side of (93):

$$\begin{aligned}
\int_0^\infty r^{k+1} u' u'' dr =& -\frac{(k-1)k(k+1)}{4}\langle r^{k-2}\rangle_{nl} \\
& + \frac{(k+1)l(l+1)}{2}\langle r^{k-2}\rangle_{nl} \\
& - \frac{(k+1)Z}{a_0}\langle r^{k-1}\rangle_{nl} + \frac{(k+1)Z^2}{2n^2 a_0^2}\langle r^k\rangle_{nl}.
\end{aligned} \tag{94}$$

Finally, by combining Eqs. (91) and (94), we arrive at the recurrence relation (48).

Now, by using the relation (48) for $k = (0, 1, -1)$, we obtain [48] For $k = 0$

$$\langle r^{-1}\rangle = \frac{Z}{a_0 n^2}. \tag{95}$$

For $k = 1$

$$\frac{2}{n^2}\langle r\rangle - \frac{3a_0}{Z} + l(l+1)\frac{a_0^2}{Z^2}\langle r^{-1}\rangle = 0, \tag{96}$$

$$\langle r\rangle = \frac{a_0}{2Z}[3n^2 - l(l+1)]. \tag{97}$$

For $k = -1$

$$\langle\frac{1}{r^3}\rangle = \frac{Z}{l(l+1)a_0}\langle\frac{1}{r^2}\rangle. \tag{98}$$

and from [48, 53] we have

$$\langle\frac{1}{r^2}\rangle = \frac{Z^2}{a_0^2 n^3 (l+\frac{1}{2})}. \tag{99}$$

We replace (99) in (98):

$$\langle\frac{1}{r^3}\rangle = \frac{Z^3}{a_0^3 n^3 (l+1)(l+\frac{1}{2})l}. \tag{100}$$

Finally [54]:

$$\langle\frac{1}{r^4}\rangle = \frac{Z^4[3n^2 - l(l+1)]}{2a_0^4 n^5 (l+\frac{3}{2})(l+1)(l+\frac{1}{2})l(l-\frac{1}{2})}. \tag{101}$$

where $a_0 = \frac{\hbar^2}{2me^2}$ is the 1st Bohr radius.

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