Kratzer’s molecular potential in quantum mechanics with a generalized uncertainty principle

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Abstract

The Kratzer’s potential $V(r) = g_1/r^2 - g_2/r$ is studied in quantum mechanics with a generalized uncertainty principle, which includes a minimal length $(\Delta X)_\text{min} = \hbar \sqrt{5/\beta}$. In momentum representation, the Schrödinger equation is a generalized Heun’s differential equation, which reduces to a hypergeometric and to a Heun’s equations in special cases. We explicitly show that the presence of this finite length regularizes the potential in the range of the coupling constant $g_1$ where the corresponding Hamiltonian is not self-adjoint. In coordinate space, we perturbatively derive an analytical expression for the bound states spectrum in the first order of the deformation parameter $\beta$. We qualitatively discuss the effect of the minimal length on the vibration-rotation energy levels of diatomic molecules, through the Kratzer interaction. By comparison with an experimental result of the hydrogen molecule, an upper bound for the minimal length is found to be of about 0.01 Å. We argue that the minimal length would have some physical importance in studying the spectra of such systems.

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I. INTRODUCTION

The hypothesis of the existence of a minimal length scale [1, 2] is currently a common finding of several studies in quantum gravity [3–5] and string theory [6–8]. This elementary length is supposed to be of the order of the Planck length ($l_p = 10^{-35}$m), which is a lower bound to all physical length scales, below which distances can not be resolved [9, 10]. For a review of the history and the main motivations for the assumption of a fundamental length scale, see Ref. [11].

The minimal length is introduced in quantum theory by modifying the standard Heisenberg uncertainty principle to the so-called generalized uncertainty principle (GUP) [8, 12]. This GUP implies then a non-zero minimal uncertainty in position, and it involves significant consequences on the mathematical basis of quantum mechanics. The formalism, based on a specific form of the GUP, together with the new concepts it implies, has been extensively discussed by Kempf and co-workers in Refs. [13–16]. Most notably, it has been shown that the GUP can be obtained from a deformed Heisenberg algebra, depending on two small positive parameters $\beta$ and $\beta'$, which are related to the minimal length (see, Sec. II). For the sake of completeness, let us mention that diverse forms of the GUP have been proposed in the literature: there is a GUP which incorporates a minimal length and a minimal momentum [15], a GUP with a Lorentz-covariant algebra [17], and a GUP including a minimal length and a maximal momentum [18, 19].

In recent years, various topics were studied in connection with the GUP. Among others, the Schrödinger equation for: the harmonic oscillator [13, 20, 21], the hydrogen atom, in one [22, 23] and three [20, 24–26] dimensions, the singular inverse square potential [27, 28], and the gravitational quantum well [29, 30]. The minimal length was furthermore introduced in the Dirac equation, with a constant magnetic field [31], with vector and scalar linear potentials [32], with the hydrogen atom potential [33], and the Dirac oscillator [34]. The effect of the GUP was also studied in the context of the Klein-Gordon equation in Refs. [35, 36]. Furthermore, the Casimir effect has been investigated in Ref. [37], the correction to the black body radiation due to a minimal length has been considered in Ref. [38], thermostatic with minimal length has been studied in Ref. [39], Unruh effect with a GUP has been discussed in Ref. [40], and finally, the reconciliation of the Self-Completeness of gravity and the GUP has been addressed in Ref. [41]. For a large number of references in
connection with this subject, see, Ref. [11].

It is important to note that although the minimal length is initially introduced in quantum theory to account for quantum gravitational effects, which arise at Planck’s scales [42], it has been argued that, in quantum mechanics, this elementary length may be associated to the size of the system under study [14, 27]; consequently, the formalism that follows may be useful in the study of complex systems such as quasiparticles, nuclei, and molecules [14]. Another important feature of this finite length is that it provides a natural cutoff for ultraviolet regularization in quantum mechanics [27] and in quantum field theory [16].

In this work, we investigate another problem within the formalism of quantum mechanics with a minimal length, namely the Kratzer’s molecular potential (KP), which has the form $V(r) = g_1/r^2 - g_2/r$. This potential is one of the most important model interaction in quantum physics; it has been first introduced to describe the vibration-rotation spectra of diatomic molecules [43, 44]. Nowadays, KP appears in various fields of physics and chemistry such as molecular physics [45], nuclear physics [46], Liquid-solid interfaces and thermodynamics [47], chemical physics [48], and quantum chemistry [49–53]. From a more formal viewpoint, KP provides a good example for illustrating diverse methods used to solve the Schrödinger equation, such as the Fourier integral representation [54], the algebraic approach [55], the supersymmetry [53], the Nikiforov-Uvarov [49], the asymptotic iteration method [56], and the method of self-adjoint extensions [57], which is used when the coupling constant $g_1$ is such as $2\mu g_1/h^2 \leq -1/4$ ($\mu$ is the particle mass), where the corresponding Hamiltonian operator is not self-adjoint [57].

The aim of this study is twofold, first to examine to what extend the introduction of a minimal length in the Schrödinger equation regularizes the KP in the aforementioned range of the coupling constant $g_1$ where the potential is known to be singular, and second, to compute the bound states energy spectrum, and investigate the effect of this fundamental length on the rovibrational energy levels of diatomic molecules.

The rest of this paper is organized as follows. In Sec. II, we present the main equations of quantum mechanics with a minimal length, that we need in our study. Sec. III is devoted to investigate the KP in this formalism, we study in detail the corresponding Schrödinger equation in momentum representation, then we perturbatively compute the energy spectrum in coordinate space and apply our result to the vibration-rotation of diatomic molecules. In the last section, we summarize our results and conclusions.
II. HEISENBERG ALGEBRA AND REPRESENTATIONS OF THE GUP

As mentioned in Sec. I, diverse topics were studied in quantum mechanics based on the following 3-dimensional modified Heisenberg algebra [13, 14, 21, 27, 28]:

\[
\hat{X}_i, \hat{P}_j = i\hbar[(1 + \beta \hat{P}_i^2)\delta_{ij} + \beta' \hat{P}_i \hat{P}_j], \quad (\beta, \beta') > 0.
\]

\[
[\hat{P}_i, \hat{P}_j] = 0, \quad (1)
\]

\[
[\hat{X}_i, \hat{X}_j] = i\hbar\frac{2\beta - \beta' + \beta(2\beta + \beta')\hat{P}_2}{1 + \beta\hat{P}_2}(\hat{P}_i \hat{X}_j - \hat{P}_j \hat{X}_i).
\]

These commutation relations lead to the following generalized uncertainty principle (GUP) [27]:

\[
(\Delta X_i)(\Delta P_i) \geq \frac{\hbar}{2}\left(1 + \beta\sum_{j=1}^{N}[(\Delta P_j)^2 + \langle \hat{P}_j \rangle^2] + \beta'[\langle (\Delta P_i)^2 + \langle \hat{P}_i \rangle^2 \rangle]\right), \quad (2)
\]

which implies the existence of a minimal length, given by [14]

\[
(\Delta X_i)_{\text{min}} = \hbar\sqrt{3\beta + \beta'}, \quad \forall i. \quad (3)
\]

One of the more important implications of the GUP is the loss of localization in coordinate space as effect of the nonzero minimal uncertainty in position measurements. Consequently, momentum space would be more convenient for solving quantum mechanical problems.

In the literature, one of the most used representations of the position and momentum operators satisfying the commutation relations (1) is [14, 21, 27]

\[
\hat{X}_i = i\hbar[(1 + \beta p^2) \frac{\partial}{\partial p_i} + \beta' p_i p_j \frac{\partial}{\partial p_j} + \gamma p_i], \quad \hat{P}_i = p_i, \quad (4)
\]

where \(\gamma\) is a small positive parameter related to \(\beta\) and \(\beta'\).

The disadvantage of representation (4) is that it considerably complicates the Schrödinger equation, and its solution is not often possible, especially when the potential depends on the position operators in a not too simple way.

To overcome this difficulty, one can alternatively use a perturbative approach to include the minimal length in the Schrödinger equation. So, coordinate space would be more appropriate in this case. This approach was first proposed by Brau to deal with the hydrogen
atom problem [20]. The simplest representation of the operators $\hat{X}_i$ and $\hat{P}_i$ in coordinate space is [20]

$$\hat{X}_i = \hat{x}_i, \quad \hat{P}_i = \hat{p}_i \left(1 + \beta \hat{p}_i^2\right), \quad (5)$$

where $\hat{x}_i$ and $\hat{p}_i$ satisfy the standard commutation relations of ordinary quantum mechanics.

Representation (5), which is valid in the case $\beta' = 2\beta$ up to the first order of $\beta$, is mostly more adequate when applying the perturbation theory to study the deformed Schrödinger equation for a given interaction. As mentioned by Kempf [14], this special case is of particular importance as the commutation relations between the position operators are not modified at the first order in $\beta$, so that the space remains commutative. The deformed algebra (1) takes then the form

$$[\hat{X}_i, \hat{P}_j] = i\hbar[(1 + \beta \hat{P}_j^2)\delta_{ij} + 2\beta \hat{P}_i \hat{P}_j],$$

$$[\hat{P}_i, \hat{P}_j] = 0, \quad [\hat{X}_i, \hat{X}_j] = 0, \quad (6)$$

and the minimal length reads in 3-dimensions as

$$(\Delta X_i)_{\text{min}} = \hbar\sqrt{5\beta}, \quad \forall i.$$ 

The commutators (6) constitute the minimal extension of the Heisenberg algebra [14].

### III. KRATZER POTENTIAL WITH A MINIMAL LENGTH

While several potentials were studied in quantum mechanics with the modified algebra [11], the KP is considered here. We discuss in detail its corresponding deformed Schrödinger equation in momentum representation, we shall be, in particular, interested to the singularity structure of this equation. Then, we perturbatively compute in coordinate space the bound states energy spectrum, and apply our result to the vibration-rotation motion of diatomic molecules.

#### A. Schrödinger equation in momentum representation

The Kratzer potential that we consider in this work has the form [43, 44]

$$V(r) = D_e r_e (r_e/r^2 - 2/r), \quad (7)$$

5
where $D_e$ is the dissociation energy and $r_e$ is the equilibrium internuclear distance of a given diatomic molecule.

First, for convenience and for a later comparison with the hydrogen atom and the inverse square interactions, we write the KP in the general form

$$V(r) = g_1/r^2 - g_2/r.$$  \hspace{1cm} (8)

We proceed our study by writing the Schrödinger equation for the energy function (8) in momentum representation as follows:

$$\left(\hat{R}^2\left(\frac{1}{2\mu}p^2 - E\right) - g_2\hat{R} + g_1\right)\psi(p) = 0,$$  \hspace{1cm} (9)

where $\hat{R}^2 \equiv \hat{R} \times \hat{R} = \sum_{i=1}^{3} \hat{X}_i \hat{X}_i$, and $\mu$ is the particle mass (the reduced mass of the two atoms, in the study of diatomic molecules).

In general, the deformed Schrödinger equation (9) can not be established with the momentum representation (4) of the operators $\hat{X}_i$. The difficulty lies in the definition of the operator $\hat{R}$ because the factorization of $\hat{R}^2$ is not obvious. However, it has been shown in Ref. [26] that, in the case $\beta' = 2\beta$, this operator can be factorized in the first order of $\beta$ for the $s$-waves, and hence the Schrödinger equation can be written in this special case.

In effect, by restricting ourselves to the $\ell = 0$ wave function and by using the momentum representation (4), with $\gamma = 0$, we obtain the following expression for the distance squared operator [26]:

$$\hat{R}^2 = (i\hbar)^2 \left\{1 + \left[1 + (\beta + \beta')p^2\right] \frac{d^2}{dp^2} + \frac{2}{p} \left[1 + (\beta + \beta')p^2\right] \left[1 + (2\beta + \beta')p^2\right] \frac{d}{dp}\right\}.$$  \hspace{1cm} (10)

Since $\beta$ and $\beta'$ are supposed to be small parameters, the distance squared operator can be expressed, in the case $\beta' = 2\beta$, as

$$\hat{R}^2 = (i\hbar)^2 \left\{(1 + 6\beta p^2) \frac{d^2}{dp^2} + \frac{2}{p} (1 + 7\beta^2) \frac{d}{dp}\right\} + O(\beta^2).$$  \hspace{1cm} (11)

Now, with Eq. (11), the square root operator $\hat{R}$ can be defined. Thus, it is easy to check that $\hat{R}^2$ can be written as $\hat{R} \times \hat{R}$, where

$$\hat{R} = i\hbar \left[1 + 3\beta p^2\right] \frac{d}{dp} + \frac{1}{p} \left(1 + \beta p^2\right) + O(\beta^2).$$  \hspace{1cm} (12)

By using formulas (11) and (12) in Eq. (9), we obtain the following differential equation:
\[(p^2 + k^2) (1 + 6 \beta p^2) \frac{d^2 \psi}{dp^2} \quad \{ 2(3 + 19 \beta p^2) + 2 k^2 (1 + 7 \beta p^2) + 2i \sigma_2 (1 + 3 \beta p^2) \} \frac{d\psi}{dp} \]
\[
+ \left\{ 2(3 + 20 \beta p^2) + \frac{2i \sigma_2}{p} (1 + \beta p^2) - \sigma_1 \right\} \psi = 0, \tag{13}
\]
where we have used the notations
\[k^2 = -2 \mu E, \quad \sigma_1 = \frac{2 \mu g_1}{\hbar^2}, \quad \sigma_2 = \frac{\mu g_2}{\hbar}.\]

The singularity of Eq. \((13)\) in \(p = 0\) can be removed by performing the following change of function:
\[\psi(p) = \frac{1}{p} \varphi(p).\]

This leads to the differential equation
\[
(p^2 + k^2) (1 + 6 \beta p^2) \frac{d^2 \varphi}{dp^2} \quad \{ 2 \beta p (p^2 + k^2) + 4 p (1 + 6 \beta p^2) + 2i \sigma_2 (1 + 3 \beta p^2) \} \frac{d\varphi}{dp} \]
\[
+ \left\{ 4(1 + 7 \beta p^2) - 2 \beta (p^2 + k^2) - 2(1 + 6 \beta p^2) - 4i \beta \sigma_2 p - \sigma_1 \right\} \varphi = 0. \tag{14}
\]

Equation \((14)\) is the Schrödinger equation for the KP in momentum space with a minimal length \((\Delta X_i)_{\text{min}} = \hbar \sqrt{5 \beta}\). Before studying this equation, it is important to consider the undeformed case, i.e., the limit \(\beta = 0\).

1. **Undeformed case**

In the special case \(\beta = 0\), Eq. \((14)\) reduces to the following equation:
\[
(p^2 + k^2) \frac{d^2 \varphi}{dp^2} + (4 p + 2i \sigma_2) \frac{d\varphi}{dp} + (2 - \sigma_1) \varphi = 0. \tag{15}
\]

By using the new variable
\[x = 1/2 + ip/2k,\]
equation \((15)\) can be transformed to a hypergeometric differential equation of the form \([58]\)
\[x(1 - x)\varphi'' + [c - (a + b + 1)x] \varphi' - ab \varphi = 0, \tag{16}\]
with the parameters
\[a = 3/2 + \nu, \quad \nu = \sqrt{1/4 + \sigma_1}\]
\[b = 3/2 - \nu, \quad c = 2 + \sigma_2/k.\]
In the vicinity of infinity, the two linearly independent solutions of Eq. (16) are

\[ \varphi_1 (y) = x^{-a} F(a, a - c + 1, a - b + 1; 1/x), \]
\[ \varphi_2 (y) = x^{-b} F(b, b - c + 1, b - a + 1; 1/x), \]

where \( F \) stands for the hypergeometric function.

The two solutions of the Schrödinger equation behave then, in the limit \( (p \gg 1) \), as

\[ \psi_1 (p) \to p^{-5/2 - \nu}, \]  \( \quad (17) \)
\[ \psi_2 (p) \to p^{-5/2 + \nu}. \]  \( \quad (18) \)

In the case where \( \nu \) is real \( (\sigma_1 > -1/4) \), the function \( \psi_2 \) falls off more slowly than \( \psi_1 \), and hence the behavior of the physical solution is that of \( \psi_1 \). This may be understood by the fact that the expectation value of \( \hat{R}^2 \) diverges with the function \( \psi_2 \), as in the case of the relativistic Coulomb problem \[59\].

Then, the solution to the ordinary Schrödinger equation for the KP in momentum space reads

\[ \psi_1 (p) = \frac{N}{p} (1 + ip/k)^{-\frac{3}{2} - \nu} F \left( \frac{3}{2} + \nu, \frac{1}{2} - \frac{\sigma_2}{k} + \nu, 1 + 2\nu; \frac{2}{1 + ip/k} \right), \]  \( \quad (19) \)

where \( N \) is a normalization constant.

The discrete energy spectrum of the KP can be obtained by requiring

\[ 1/2 - \sigma_2/k + \nu = -n, \quad n = 0, 1, 2..., \]  \( \quad (20) \)

so that the wave function \[19\] is square integrable for the whole interval of \( p \). In this case, the hypergeometric series reduces to a polynomial \[58\].

Equation \[20\] is the quantization condition of the energy, it gives the well-known discrete energy spectrum of the KP (see Eq. \[26\], below).

However, when \( \sigma_1 \leq -1/4 \), the parameter \( \nu \) becomes imaginary and thus the spectral condition \[20\] breaks down. Moreover, the asymptotic behaviors of the two solutions, given by Eqs. \[17\] and \[18\], become identical, and both of them are physical. Consequently, the general solution is a linear combination of \( \psi_1 \) and \( \psi_2 \), and thus the wave function and other related observables will now depend on an arbitrary parameter (phase), which is a common feature of singular potentials \[60\].

We mention that the singularity of the KP is due to the inverse square interaction term \( g_1/r^2 \), which is known to be singular in the strong coupling regime \( (\sigma_1 = 2\mu g_1/\hbar^2 \leq -1/4) \).
In this range of the coupling, the Hamiltonian operator corresponding to KP is not self-adjoint, one must then define the self-adjoint extensions of the Hamiltonian, for a recent review, see Ref. [57].

2. Deformed case

We return now to Eq. (14). We first discuss the effect of the minimal length on the singularity structure of this equation. To this end, let us write Eq. (14) in the limit $p \gg 1$ as follows:

$$3p^2 \frac{d^2 \varphi}{dp^2} + 13p \frac{d\varphi}{dp} + 7\varphi = 0,$$

for which the solutions are $\varphi_1 \sim p^{-7/3}$ and $\varphi_2 \sim p^{-1}$.

The solutions of the deformed Schrödinger equation (13) behave then at infinity as

$$\psi_1 \sim p^{-10/3}, \quad \psi_2 \sim p^{-2}.$$

These behaviors are completely different from that of the undeformed case, given by Eqs. (17) and (18). Now, the second solution $\psi_2$ falls off more slowly than $\psi_1$ regardless the value of the "coupling constant" $\sigma_1$. It follows that the physical solution has manifestly the asymptotic behavior of $\psi_1$; one can always reject $\psi_2$ even for $\sigma_1 \leq -1/4$, so that the wave function will not depend on an arbitrary phase, unlike those of singular potentials [60]. Consequently, in the presence of a minimal length, there is no difference between the two ranges of the coupling $g_1$ of the potential: $2\mu g_1/\hbar^2 \leq -1/4$ and $2\mu g_1/\hbar^2 > -1/4$. This might be viewed as an indication of the regularization of the KP by the presence of this elementary length. It is important to note that the rejection of the asymptotic behavior of $\psi_2$ can be, convincingly, reached by requiring that the physical eigenfunctions of the Hamiltonian must behave at large momenta as $p^2 \psi(p)_{p \to \infty} = 0$. This boundary condition emerges naturally from the integral equation corresponding to the differential equation (13); the demonstration is analogous to that given in detail in Ref. [27] for the inverse square potential.

We now discuss the class to which Eq. (14) belongs and its associated properties. After carefully examining this equation, we have shown that it is a Fuchsian differential equation with five regular singular points. In fact, by making the change of variable

$$z = \frac{1}{2}(1 - i\sqrt{6\beta}p),$$
Eq. (14) can be transformed to the following generalized Heun's equation \[61, 62\]:

\[
\frac{d^2 \varphi}{dz^2} + \left(\frac{c}{z} + \frac{d}{(z-1)} + \frac{e}{(z-z_1)} + \frac{f}{(z-z_2)}\right) \frac{d\varphi}{dz} + \left(\frac{abz^2 + \rho_1 z + \rho_2}{z(z-1)(z-z_1)(z-z_2)}\right) \varphi = 0. \tag{22}
\]

The parameters of Eq. (22) are given by

\[
a = 1, \quad b = \frac{7}{3}, \quad \rho_1 = -\frac{7}{3} - \frac{\sigma_1}{3} \sqrt{6\beta}, \quad \rho_2 = \frac{\beta}{2} k^2 + \frac{\sigma_1}{6} \sqrt{6\beta} + \frac{1}{12} + \frac{\sigma_2}{4},
\]

\[
c = \frac{1}{6} + \frac{\sigma_1}{2} \frac{\sqrt{6\beta}}{1 - 6\beta k^2}, \quad d = \frac{1}{6} - \frac{\sigma_1}{2} \frac{\sqrt{6\beta}}{1 - 6\beta k^2}, \quad e = 2 + \frac{\sigma_1}{k} \frac{1 - 3\beta k^2}{1 - 6\beta k^2},
\]

\[
f = 2 - \frac{\sigma_1}{k} \frac{1 - 3\beta k^2}{1 - 6\beta k^2}, \quad z_1 = \frac{1}{2} + \frac{k}{2} \sqrt{6\beta}, \quad z_2 = \frac{1}{2} - \frac{k}{2} \sqrt{6\beta},
\]

which are linked by the Fuchsian condition

\[a + b + 1 = c + d + e + f.\]

Equation (22) belongs to the class of Fuchsian equations: it is a linear homogeneous second-order differential equation with five singular points located at \(z = 0, 1, z_1, z_2, \infty\), all regular. So, it admits power series solutions in the vicinity of each singular point \[62\]. However, to the best of our knowledge, the analytic solutions to the generalized Heun's equation (22) are not known in the literature, i.e., the recurrence relation that determines the coefficients of the series was not established for equations of type (22). It follows that the formulation of a physical problem with this kind of equations is interesting in its own right. This might motivate profound studies on such type of equations.

To end this section, it is important to mention that in the special case \(\sigma_2 = 0\), where the KP reduces to the inverse square potential, Eq. (13) can be transformed to a Heun's differential equation of the form \[63\]:

\[
\frac{d^2 \phi}{d\xi^2} + \left(\frac{c}{\xi} + \frac{d}{\xi-1} + \frac{e}{\xi-\xi_0}\right) \frac{d\phi}{d\xi} + \left(\frac{ab\xi + q}{\xi(\xi-1)(\xi-\xi_0)}\right) \phi = 0, \tag{23}
\]

by using the change of variable \(\xi = \frac{6\beta p^2}{1 + 6\beta p^2}\), and the transformation \(\psi(\xi) = (1-\xi)\phi(\xi)\), with the parameters

\[
a = \frac{11}{6}, \quad b = 1, \quad c = \frac{3}{2}, \quad d = \frac{1}{3}, \quad e = 2, \quad q = -\frac{3}{2} + \frac{\sigma_1/4}{1 + 12\mu \beta E}, \quad \xi_0 = \frac{12\mu \beta E}{1 + 12\mu \beta E}, \tag{24}
\]

where now the Fuchsian condition is \(a + b + 1 = c + d + e\).

The inverse square potential has been already studied in details in Ref. \[27\] with the exact expression of the operator \(\hat{R}^2\), which depends on two deformation parameters \(\beta\) and \(\beta'\).
Whereas, Eq. (23) and their parameters (24) have been obtained by using the approximate expressions of $\hat{R}^2$ and $\hat{R}$ of Ref. [26]. However, one can from Eq. (23) reach all the results and conclusions of Ref. [27], which proves the validity of our approximation.

It turns out that Eq. (14) possesses interesting features, which would be important from a mathematical viewpoint. In particular, the reduction of Eq. (14) to a hypergeometric equation in the case $\beta = 0$ and to a Heun’s equation when $\sigma_2 = 0$ may be useful especially when studying the process of coalescence of the singular points in such generalized Heun’s equations.

To complete our study, it is important to investigate the effect of the minimal length on the energy spectrum of the KP. To this purpose, we will consider the Schrödinger equation in coordinate representation.

**B. Schrödinger equation in coordinate space: Energy spectrum**

Let us now write the Schrödinger equation for the KP (7) in coordinate space by using the representation (5) as follow

$$\left( \frac{\hat{p}^2}{2\mu} + V(r) + \frac{\beta}{\mu} \hat{P}^4 \right) \psi(\vec{r}) = E \psi(\vec{r}),$$

(25)

where terms of order $\beta^2$ have been neglected.

In the ordinary case ($\beta = 0$), Eq. (25) with the KP allows its exact solution for arbitrary quantum number $\ell$. This is an advantage compared to other molecular interactions such the well-known Morse potential [44, 64], for which the Schrödinger equation has exact solution only in the case $\ell = 0$. In coordinate space, the solution of the ordinary Schrödinger equation with the KP can be found in the standard textbooks of quantum mechanics, see, for instance, [44, 65]. The bound states energy eigenvalues and the corresponding normalized eigenfunctions are given by [44, 65]:

$$E_{n\ell}^0 = -\frac{\gamma^2 D_e}{(\lambda + n)^2}, \quad n = 0, 1, 2, ..., \quad \ell = 0, 1, 2, ...,$$

(26)

$$\psi_{n\ell m}^0(r, \theta, \varphi) = NY_{\ell m}^m(\theta, \varphi) \left( r/r_e \right)^{\lambda-1} e^{-\alpha r/r_e} \mathbf{1}_{1} F_{1}(\lambda \varphi; -n, 2\lambda; 2\alpha r/r_e),$$

(27)

where $n$ and $\ell$ are, respectively, the radial (vibrational) and orbital (rotational) quantum numbers, $Y_{\ell m}^m(\theta, \varphi)$ are the orthonormalized spherical harmonics, $\mathbf{1}_{1} F_{1}(\delta, \eta; z)$ is a confluent
hypergeometric function; we have used the following notations:

\[
\gamma = \frac{r_e}{\hbar} \sqrt{2\mu D_e} = \frac{2D_e}{\hbar\omega}, \quad \alpha = \frac{\gamma^2}{(\lambda + n)},
\]

\[
\lambda = 1/2 + \sqrt{(\ell + 1/2)^2 + \gamma^2}, \quad N = \frac{r_e^{-3}(2\alpha)^{\lambda + 1/2}}{\Gamma(2\lambda)} \sqrt{\Gamma(2\lambda + n)} / 2n!(\lambda + n).
\]

with \(\omega\) is the classical frequency for small harmonic vibrations.

In the undeformed case \((\beta \neq 0)\), the solution to Eq. (25) is not obvious. However, we can consider, in Eq. (25), the term \((\beta \mathcal{D}^4)\) as a perturbation to the ordinary Schrödinger equation. Therefore, the use of the perturbation theory allows for the computation of the corrections to the energy levels in the first order of the deformation parameter \(\beta\).

The energy eigenvalues can then be written as

\[
E_{n\ell} = E_{n\ell}^0 + \Delta E_{n\ell},
\]

where \(E_{n\ell}^0\) are the unperturbed levels given by Eq. (26).

In the first order of \(\beta\), the correction \(\Delta E_{n\ell}\) is then

\[
\Delta E_{n\ell} = \frac{\beta}{\mu} \langle \psi_{n\ell}^0 | p^4 | \psi_{n\ell}^0 \rangle \equiv \frac{\beta}{\mu} \langle n\ell m | p^4 | n\ell' m' \rangle.
\]

It has been shown in Ref. [20] that, for central interactions, \(\Delta E_{n\ell}\) can be expressed as follows:

\[
\Delta E_{n\ell} = 4\beta \mu \left[ (E_{n\ell}^0)^2 - 2E_{n\ell}^0 \langle n\ell m | V(r) | n\ell m \rangle + \langle n\ell m | V^2(r) | n\ell m \rangle \right]. \tag{28}
\]

From formula (28) with the KP (8) we get

\[
\Delta E_{n\ell} = 4\beta \mu \left( (E_{n\ell}^0)^2 + 2g_2 E_{n\ell}^0 \langle n\ell m | \frac{1}{r} | n\ell m \rangle + (g_2^2 - 2g_1 E_{n\ell}^0) \langle n\ell m | \frac{1}{r^2} | n\ell m \rangle \right.
\]

\[
-2g_1 g_2 \langle n\ell m | \frac{1}{r^3} | n\ell m \rangle + g_1^2 \langle n\ell m | \frac{1}{r^4} | n\ell m \rangle \right). \tag{29}
\]

Thus, to compute the minimal length correction, one has to evaluate the matrix elements

\[
\langle \frac{1}{r^p} \rangle = N^2 \frac{(2g_2)}{g_1}^{3-p} \int_0^\infty y^{2\lambda-p} e^{-2\alpha y} \left( _1F_1(-n, 2\lambda; 2\alpha y) \right)^2 dy, \quad p = 1, 2, 3, 4,
\]

where we have introduced the dimensionless variable \(y = \frac{2\alpha}{2g_2} r\).

The computation of the above integrals leads to the following results:

\[
\langle \frac{1}{r} \rangle = \frac{\mu g_2}{\hbar^2} \frac{1}{(\lambda + n)^2}, \quad \langle \frac{1}{r^3} \rangle = \frac{\mu g_2}{\hbar^2} \frac{3}{(\lambda + n)^3}
\]

\[
\langle \frac{1}{r^2} \rangle = \frac{(\mu g_2)^2}{\hbar^2} \frac{1}{(\lambda + n)^3}, \quad \langle \frac{1}{r^4} \rangle = \frac{\mu g_2}{\hbar^2} \frac{1}{(\lambda - 1)(\lambda + n)^5}.
\]
By inserting the values of these matrix elements and the expression of $E^0_{n,\ell}$, given by Eq. (26), into Eq. (29), we get

$$
\Delta E_{n\ell} = 4\beta \mu^3 \left( \frac{g_2}{\hbar (\lambda + n)} \right)^4 \left\{ \frac{3}{4} + \frac{\lambda + n}{\lambda - \frac{1}{2}} \left( 1 + \frac{\mu g_1}{\hbar^2} \left( \frac{1}{(\lambda + n)^2} - \frac{2}{\lambda(\lambda - 1)} \right) \right) \right. \\
+ \left. \left( \frac{\mu g_1}{\hbar^2} \right)^2 \frac{1}{(\lambda - \frac{1}{2})(\lambda - 1)(\lambda - \frac{3}{2})(\lambda + n)} \left( 1 + \frac{3n(2\lambda + n)}{\lambda(2\lambda + 1)} \right) \right\}. \quad (30)
$$

In the limit $g_1 = 0$, where KP reduces to the Coulomb potential, and hence

$$
\gamma = \frac{1}{\hbar} \sqrt{2\mu g_1} = 0, \quad \alpha = 0, \quad \lambda = 1/2 + \sqrt{(\ell + 1/2)^2 + \gamma^2} = \ell + 1 \\
E^0_{n\ell}(g_1 = 0) = -\frac{\mu g_2^2}{2\hbar^2 (\ell + 1 + n)^2} = -\frac{\mu g_2^2}{2\hbar^2 n_p^2}, \quad n_p = 1, 2, ...
$$

where, $n_p$ is the principal quantum number. The correction (30) simplifies then to

$$
\Delta E_{n\ell} = \frac{4\beta \mu^3 g_2^4}{\hbar^4 n_p^2} \left( -\frac{3}{4} + \frac{n_p}{\ell + 1/2} \right),
$$

which is exactly the result obtained in Ref. 20 for the hydrogen atom problem.

Finally, the complete energy spectrum of the KP in the presence of a minimal length can be written in terms of Kratzer’s parameters $r_e$ and $D_e$ ($g_2 = 2D_e r_e$, $g_1 = D_e r_e^2$) as follows:

$$
E_{n\ell} = -\frac{\gamma^2 D_e}{(\lambda + n)^2} + \beta \mu D_e^2 \left( \frac{2\gamma}{\lambda + n} \right)^4 \left\{ \frac{3}{4} + \frac{\lambda + n}{\lambda - \frac{1}{2}} \left( 1 + \frac{\gamma^2}{2} \left( \frac{1}{(\lambda + n)^2} - \frac{2}{\lambda(\lambda - 1)} \right) \right) \right. \\
+ \left. \left( \frac{\gamma^4}{4} \frac{1}{(\lambda - \frac{1}{2})(\lambda - 1)(\lambda - \frac{3}{2})(\lambda + n)} \left( 1 + \frac{3n(2\lambda + n)}{\lambda(2\lambda + 1)} \right) \right\}. \quad (31)
$$

Formula (31) shows the effect of this deformed algebra on the energy levels of KP. It can be furthermore used to study several features of diatomic molecules. In particular, it allows us to investigate the effect of the minimal length on the rovibrational energy levels of diatomic molecules.

An application: Vibration-rotation of diatomic molecules

As outlined in Sec. I, the KP is one of the most important molecular interactions; it has long been used to describe the vibration-rotation energy spectrum of diatomic molecules [43, 44]. The importance of this potential lies in that its ordinary Schrödinger equation admits an exact solution for arbitrary rotational quantum number $\ell$. This is an advantage compared to other molecular interactions such as the well-known Morse potential [44]. In addition,
the energy spectrum of the KP is, as we will see, similar to the well-known spectroscopic formula \[66\].

Then Eq. \[31\] can be used to qualitatively investigate the effect of the minimal length on different parts of the rovibrational energy levels of a given diatomic molecule with the KP interaction.

For this purpose, following Ref. \[68\], we use the fact that the dimensionless parameter \(\gamma\), in Eq. \[31\], is so large for most molecules (\(\gamma \gg 1\) \[44\]), we may then expand \(E_{n\ell}\), given by Eq. \[31\], into powers of \(1/\gamma\). This leads to the following expression:

\[
E_{n\ell} = D_e \left( -1 + 2(n + \frac{1}{2}) \frac{1}{\gamma} + (\ell + \frac{1}{2})^2 \frac{1}{\gamma^2} - \frac{3(n + \frac{1}{2})^2 \frac{1}{\gamma^2} + 4(n + \frac{1}{2})^3 \frac{1}{\gamma^3} - 3(n + \frac{1}{2})(\ell + \frac{1}{2})^2 \frac{1}{\gamma^3} \right) + \beta \mu D_e^2 \left( 6 \left( n + \frac{1}{2} \right)^2 + \frac{1}{4} \right) \frac{1}{\gamma^2} + 2(n + \frac{1}{2}) \left\{ -\frac{1}{4} + 4(\ell + \frac{1}{2})^2 - 15(n + \frac{1}{2})^2 \right\} \frac{1}{\gamma^3} + \ldots \tag{32} \]

This formula shows the different parts of the rovibrational energy spectrum, and the corrections that the minimal length introduces in each part. The undeformed spectrum (\(\beta = 0\)) contains three kind of energy: the energy of harmonic vibrations, that is the second term in Eq. \[32\], the third term is the rotational energy levels, the fourth and the fifth terms describe the anharmonicity of vibrations, and the sixth term represents the energy due to the coupling vibration-rotation. The last remaining terms are corrections due to the presence of a minimal length.

As we see, the leading correction induced by the minimal length is proportional to \(1/\gamma^2\), and depends only on the vibrational quantum number \(n\). So, it affects the anharmonicity of vibrations. The next leading contribution brought by this elementary length depends on \(1/\gamma^3\), and carries three corrections: the first affects the energy of harmonic vibrations, which is proportional to \(1/\gamma\), so its effect would not be significant. The second term modifies the energy corresponding to the vibration-rotation coupling, which similarly depends on \(1/\gamma^3\) in the ordinary case. The last term proportional to \(1/\gamma^3\), describes clearly a second correction to the anharmonicity of vibration; it is then less important compared to the previous correction proportional to \(1/\gamma^2\).

Moreover, formula \[32\] might be viewed as an energy spectrum of a three-parameter potential, i.e., \(D_e, r_e\), and \(\beta\). In this sense, the procedure of fitting experimental data used in the case of three-parameter potentials, such as Morse function, can be followed for adjusting the parameters of the "deformed KP" with the spectroscopic data of diatomic
molecules. This viewpoint would be important because it can give not only values of \( \beta \) for any molecule, but also the Kratzer model can be improved with this third parameter. In addition, the introduction of this deformation parameter in the currently most successful models might help in the search for an universal potential function of diatomic molecules, which is of fundamental importance in several areas of physics and chemistry [67].

To end this study, it is important to roughly estimate an upper bound for the minimal length by using formula (31). To this end, we consider the vibrational ground-state energy \( E_{00} \) of the hydrogen molecule (H\(_2\)), which is one of the more remarkably successful predictions of Kratzer potential. So, the comparison of Eq. (31) to accurate experimental results allows to give a value of \( \beta \), by assuming that the effect of the minimal length is included in the gap between the theoretical and the experimental values of \( E_{00} \).

Indeed, the experimental vibrational zero point energy (ZPE \( \equiv G = E_{00} + D_e \)) for the molecule H\(_2\) in the state \( ^1\Sigma_g^+ \) has the value [69]

\[
G^{\exp} = 2179.3(1) \text{ cm}^{-1}.
\]

On the other hand, the theoretical value predicted by Kratzer’s potential can be obtained from Eq. (26), by using the molecular constants [70]: \( D_e = 78844.9005 \text{ cm}^{-1} \), \( r_e = 0.73652 \text{ Å} \), and \( \mu = 0.5039 \text{ uma} \). We then get the result

\[
G^{\beta=0} = E_{00}^0 + D_e = 2174.9 \text{ cm}^{-1}.
\]

The theoretical value is not contained in the error bars. therefore, the discrepancy between \( G^{\exp} \) and \( G^{\beta=0} \) will be entirely attributed to the minimal length correction (\( \Delta E_{00} \)), given by Eq. (30). We then have the natural constraint

\[
\Delta E_{00} < G^{\exp} - G^{\beta=0} = 4.4 \text{ cm}^{-1} \approx 5.4554 \times 10^{-4} \text{ eV},
\]

which leads to the following upper bound of this fundamental length:

\[
(\Delta X)_{\text{min}} = \hbar \sqrt{5\beta} < 1.0186 \times 10^{-2} \text{ Å} \simeq 0.01 \text{ Å}.
\] (34)

This upper bound is, of course, not a stringent limit, because the Kratzer’s potential is far to be the real internuclear potential energy function in the molecule H\(_2\). In addition, many effects, such as relativistic and QED corrections, are also important and must be included in the split (33). There is also the error due to the Born-Oppenheimer approximation. It
follows that a more precise upper limit could be reached if the correction of the minimal length may be included in the currently more developed quantum molecular methods.

Nevertheless, the result (34) can at least be compared to those obtained in the study of fundamental problems of quantum mechanics. The upper bound (34) is weaker than the ones obtained in Refs. [20, 24, 25] for the hydrogen atom. There, the minimal length has been supposed to be related to the finite size of the electron; and an upper bound of about $10^{-7}$-$10^{-6}$ Å has been resulted by using the high-precision experimental data for the transition 1S-2S and for the Lamb shift. It follows that in the study of the vibrations of the molecule H$_2$ (motion of the nuclei), this elementary length would rather be a scale related to the size of the proton not to that of the electron. It is therefore not surprising to find such value to $(\Delta X)_{\text{min}}$. In Ref. [21], the deformed spectrum of the harmonic oscillator has been applied to the motion of electrons in a Penning trap, which led to an upper bound of the same order of magnitude as in the hydrogen atom problem. However, in Ref. [29], the investigation of the effect of the minimal length on the energy levels of ultracold neutrons in the Earth’s gravitational field, led to an upper bound of about 24 Å, which is larger than the value (34).

It turns out that in the study of quantum mechanical problems, this fundamental length would not be close to the Planck scale, but it is rather a scale related to the system being studied and would then depend on its characteristics.

IV. SUMMARY AND CONCLUSION

We have studied the Kratzer’s molecular potential $V(r) = g_1/r^2 - g_2/r$ in quantum mechanics with a deformed Heisenberg algebra characterized by the existence of a minimal length, $(\Delta X)_{\text{min}} = h\sqrt{3\beta + \beta'}$. In the momentum representation, the Schrödinger equation was established in the particular case $\beta' = 2\beta$ in the first order of the deformation parameter $\beta$. It is then transformed to a canonical form of Fuchsian differential equations, namely, a generalized Heun’s equation, which reduces to a hypergeometric equation for $\beta = 0$ and to a Heun’s equation for $g_2 = 0$. The behaviors of the solutions show that the potential becomes regular even for values of the coupling constant $g_1$ such as $2\mu g_1/h^2 \leq -1/4$. In coordinate space, an analytical expression of the energy spectrum has been perturbatively derived in the first order of $\beta$. Through this spectrum, we have explicitly shown the effect of the minimal
length on the rovibrational energy levels of diatomic molecules with KP interaction. The leading correction introduced by the minimal length affects the energy of the anharmonicity of vibrations, and the next-leading contribution concerns the vibration-rotation coupling. However, the energy of harmonic vibrations, which is the principal part of the vibration-rotation spectrum, is not significantly affected, and the rotational levels is absolutely not corrected by this deformed algebra. Furthermore, it has been outlined that the expression of the deformed energy spectrum of KP can be viewed as a formula of a three-parameter potential, and thus the parameter $\beta$ can be determined together with those of Kratzer by fitting the spectroscopic data of diatomic molecules. We have estimated an upper bound of the minimal length of about 0.01 Å by comparing the theoretical and experimental values of the vibrational ground-state energy of the molecule H$_2$. This result shows that the minimal length might be in fact viewed as an intrinsic scale characterizing the system under study, and not a parameter that accounts for quantum gravitational effects, which are extremely small in molecular physics.

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