

Quantum spacetime fluctuations: Lamb shift and hyperfine structure of the hydrogen atomJ. I. Rivas,^{*} A. Camacho,[†] and E. Göklü[‡]*Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa, Apartado Postal 55-534, CP 09340, México DF, México*
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We consider the consequences of the presence of metric fluctuations upon the properties of a hydrogen atom. Particularly, we introduce these metric fluctuations in the corresponding effective Schrödinger equation and deduce the modifications that they entail upon the hyperfine structure related to a hydrogen atom. We will find the change that these effects imply for the ground state energy of the system and obtain a bound for its size comparing our theoretical predictions against the experimental uncertainty reported in the literature. In addition, we analyze the corresponding Lamb shift effect emerging from these fluctuations of spacetime. Once again, we will set a bound to these oscillations resorting to the current experimental outcomes.

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I. INTRODUCTION

Nowadays gravitational physics faces several profound conundrums. Among them we may consider the quest for a quantum theory of gravity. The present difficulties can be categorized, roughly, as conceptual and mathematical [1,2]. The lack of a consistent theory has several implications, one of them is the absence of testable experimental predictions.

This current condition has spurred the search for information which could provide some clue about the correct direction. This topic is usually denoted as quantum gravity phenomenology, i.e., the observational and experimental search for deviations from Einstein's general relativity or from quantum field theory. It has to be stressed that nowadays it is a very active realm. In this context string theory and loop gravity entail conjectures which imply small modifications from general relativity; for instance, deviations from the $1/r$ potential and violations of the equivalence principle [3,4] or deformed versions of the dispersion relation [5,6].

Both loop gravity [7] and string theory [8,9] imply induced modifications to the field equations governing the motion of spin- $\frac{1}{2}$ particles. Based upon string theory, Kostelecky and co-workers have initiated an intensive study of modifications of the standard model of elementary particle physics [10–12]. In the search of experimental tests the main difficulty lies in the smallness of the predicted effects. The proposed experiments range from modifications to the standard model of elementary particle physics [13,14], interferometric tests [15,16], modification of Maxwell's equations [17], or the use of Bose-Einstein condensates [18] in this context [19–22]. In other words, the proposals run from high energy tests to low energy experiments. A fruitful realm in the direction of precision

tests is atomic physics. Indeed, the Hughes-Drever experiment shows us the power of this resource [23]. One of the advantages of atomic physics is related to the fact that some of the most accurately tested effects lie within this context. Indeed, the relative experimental uncertainty related to the measurement of the hyperfine splitting of the ground state of the hydrogen atom can be considered among the most accurate experiments, i.e., it does not exceed 10^{-12} [24].

The idea in the present work is to take advantage of this high experimental precision for the fine and hyperfine effects and determine bounds for some quantum gravity effects. In particular, we will address the issue of the consequences of the presence of metric fluctuations [25,26] upon the properties of a hydrogen atom. The main ingredient in this aspect corresponds to a Minkowskian background and in addition small spacetime fluctuations are also present. One of the assumptions in this approach is related to the fact that these spacetime fluctuations emerge as classical fluctuations of the background metric.

In addition, we will introduce these metric fluctuations in the corresponding effective Schrödinger equation and deduce the modifications that they entail upon the hyperfine structure related to a hydrogen atom. We will find the change that these effects imply for the ground state energy of the system and set a bound to these oscillations resorting to the current experimental outcomes [24]. It will be shown that, in the simplest case, these fluctuations can be interpreted as redefinitions of the inertial mass.

We also analyze the corresponding Lamb shift effect [27] emerging from these fluctuations of spacetime and obtain a bound for its size comparing our theoretical predictions against the experimental uncertainty reported in the literature. The possibility of the emergence of a Lamb-type-like shift induced by the fluctuations of the metric is the issue to be addressed as a part of the present work. The absence of a quantum electrodynamic theory predicts for the hydrogen atom an accidental degeneracy between the $2S_{1/2}$ and $2P_{1/2}$ levels, i.e., they have the same

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energy. The formulation of a quantum version of electrodynamics breaks down this aforementioned accidental degeneracy. Indeed, the effects of the fluctuations of the electric and magnetic fields with the vacuum entails a perturbation to the solutions stemming from the Coulombian potential. The Lamb shift has been a cornerstone in the development of several areas of physics, among them, atomic physics and quantum electrodynamics. The experimental uncertainty in this realm offers one of the best scenarios for precision tests. For the sake of completeness, let us provide an explanation of how these metric fluctuations can give rise to an effect similar to the Lamb shift. The point here is that in the usual model [27] the electron and proton positions are shifted, due to the fluctuations to the electromagnetic field, $r \rightarrow r + \delta r$. This last and simple comment explains in a very intuitive manner why metric fluctuations shall also impinge upon this aspect. Indeed, the presence of this kind of fluctuations implies that the physical distance between the electron and proton oscillates and therefore the main conditions, required for the Lamb shift, are here also present.

II. ATOMIC STRUCTURE AND SPACETIME FLUCTUATIONS

A. Perturbation procedure

As stated before, this work addresses the relation between metric fluctuations and atomic physics. Let us mention briefly the idea of metric fluctuations. In this direction we have a spacetime which can be regarded as a classical background on which quantum fluctuations exist [25]. Clearly, they emerge as a consequence of a quantum theory of gravity. The effects of these spacetime fluctuations upon our current physics appear, in the first-order effects, in the form of average properties of these oscillations, which modify, for instance, the motion equations. In this general scheme the fluctuations imply a modified Schrödinger equation, in which the Laplacian operator becomes $-\hbar^2/(2m)(\delta^{ij} + \gamma^{ij})\partial_i\partial_j$, where $\gamma^{ij} > 0$ [25,26]. The simplest case involves the so-called conformal fluctuations defined by the following conditions: $\gamma^{ij} = 0$, if $i \neq j$, whereas $\gamma^{xx} = \gamma^{yy} = \gamma^{zz} = \gamma$. In other words, the idea of conformal fluctuations can be easily understood considering them as matrices proportional to the unit matrix. Under these conditions our fluctuations can be comprehended (at least partially) as redefinitions of the inertial mass [26]. For instance, the new inertial mass for the electron (m_e^{eff}) is given by

$$m_e^{\text{eff}} = m_e(1 + \gamma)^{-1}. \quad (1)$$

In this last expression metric fluctuations are encoded in this parameter γ . It has to be mentioned that it has to be considered very small (otherwise its existence would be a proved experimental fact). In addition, we do assume that it has a particular sign, namely, it has to be positive [26]. It

has to be clearly stated that this parameter (γ) depends upon the type of particle.

This interpretation of the kinematical effects of γ as a redefinition of the mass parameter allows us to state that the reduced mass of the system has the form, m_e and m_n are the electronic and nuclear masses, respectively,

$$\mu = \frac{m_e m_n}{m_e + m_n}. \quad (2)$$

To lowest order in the parameter m_e/m_n we have that the new reduced mass of the system (μ^{eff}) shows the effects of the metric fluctuations (here γ is related to the electron). The absence of the corresponding variable for the proton stems from the fact that it appears as a higher-order term, and we keep here the dominant contribution,

$$\mu^{\text{eff}} = \mu(1 + \gamma)^{-1}. \quad (3)$$

This last remark allows us to estimate, roughly, the effects of the metric perturbations, i.e., the functional dependence upon γ . Indeed, a fleeting glimpse at the modifications caused by the fine and hyperfine terms for a hydrogen atom, here we take as an example the case of the $1s$ level, allows us to deduce the fine structure contribution: $\Delta E_f = -\frac{1}{8}\mu c^2 \alpha^2$, whereas the hyperfine modification is given by $\Delta E_h \sim \frac{m_e^2}{m_p} c^2 \alpha^4$. In this sense we may understand $\Delta E \sim \frac{\mu c^2 \alpha^2}{2} \gamma^{-1}$ as a correction to the fine structure contributions, i.e., it goes like $\sim \alpha^2$, and not $\sim \alpha^4$. Here c is the speed of light and α stands for the fine structure constant [28].

The first part of the present work addresses the issue of the effects of these metric fluctuations upon the hyperfine levels of a hydrogen atom. The particular structure of our model reads

$$\hat{W} = \frac{1}{2\mu} \gamma^{ij} \hat{P}_i \hat{P}_j, \quad i, j = x, y, z. \quad (4)$$

In this last expression \hat{P}_i denotes the momentum operator and γ^{ij} are the effects upon the effective Schrödinger equation of the metric fluctuations [25,26], and μ the reduced mass of the hydrogen atom.

This last operator \hat{W} will be considered as a perturbation upon the eigenkets associated to a hydrogen atom. In these eigenkets the fine and hyperfine effects will be included, i.e., our initial eigenkets shall contain the information involving fine and hyperfine structures. At this point we must explain the reasons behind this procedure. Indeed, it is already known that the fine structure Hamiltonian has a larger magnitude than the one related to the hyperfine effects [28], their ratio goes like α^2 , i.e., the square of the fine structure constant. This argument tells us that we must first calculate the modifications upon energies and kets of the hydrogen atom resorting to the fine structure Hamiltonian. Afterwards, the hyperfine terms will be introduced into the energies and kets obtained in the first step. Finally, we assume, from the very beginning, that (4)

is a very tiny contribution to the atomic behavior, i.e., the smallest of all of them, and, in consequence, according to perturbation theory it has to be the last term to be included in this approximation procedure.

The idea is to find a bound for the order of magnitude associated to γ^{ij} resorting to the comparison between our theoretical predictions and the current experimental bounds. As previously mentioned, the relative experimental uncertainty related to the measurement of the hyperfine splitting of the ground state of the hydrogen atom can be considered among the most accurate experiments, i.e., it does not exceed 10^{-12} [24].

Let us for a moment consider only the effects of (4). The most general case, concerning the structure of the space-time fluctuations, does not consider any kind of condition upon the involved parameters, namely, γ^{ij} . Under this general situation it turns out that some properties of the hydrogen atom, stemming from spherical symmetry, will be lost. Let us explain better this last assertion. It is already known that any vector operator, like the momentum operator (P_x, P_y, P_z) , defines, uniquely, a spherical tensor of rank $k = 1$ [29], whose components, for this particular case, read $T_{(q=0)}^{(k=1)} = P_z$ and $T_{(q=\pm 1)}^{(k=1)} = \frac{\mp 1}{\sqrt{2}}\{P_x \pm iP_y\}$. An additional theorem [29] implies that an expression like (4) can be cast as the sum of three different types of spherical tensors, namely, of ranks $k = 0, 1, 2$ (a consequence of the conditions that the Clebsch-Gordan coefficients satisfy). These last arguments imply that, for example, the spherical tensor of rank $k = 2$ associated to (4) will break down the inherent degeneracy of this atom. This can be understood noting that if we take two different kets of the hydrogen atom, with the same energy (same quantum number n) and same angular momentum (same l), then according to Wigner-Eckardt theorem [29]

$$\begin{aligned} \langle n, l, m | T_{(q)}^{(k=2)} | n, l, \hat{m} \rangle \\ = \frac{\langle n, l | | T_{(q)}^{(k=2)} | | n, l \rangle}{\sqrt{2l+1}} \langle l, \hat{m}; k=2, q | l, k=2; l, m \rangle. \end{aligned} \quad (5)$$

Here we follow the usual notation employed in the context of this theorem [28]. For instance, $|l, k=2; l, m\rangle$ denotes an element of the base of the Hilbert space associated to the angular momentum of a system comprising two particles such that this ket is an eigenvector of the total angular momentum of the two particles (J_1 and J_2) but also of the total angular momentum of the system J (here $J = J_1 + J_2$) and of the total projection along the z axis (J_z). The rules satisfied by the Clebsch-Gordan coefficients imply that (5) vanishes if $\hat{m} + q \neq m$ or if $l \notin [k-l, k+l]$ [29]. In other words,

$$\begin{aligned} \langle n=2, l=1, m=+1 | T_{(q)}^{(k=2)} | n=2, l=1, \hat{m}=-1 \rangle \\ \neq \langle n=2, l=1, m=+1 | T_{(q)}^{(k=2)} | n=2, l=1, \hat{m}=+1 \rangle. \end{aligned} \quad (6)$$

According to perturbation theory of degenerate levels the last expression leads us to conclude that (in the subspace of $l=1$) the matrix defined by (5) is not a matrix proportional to the identity matrix, i.e., it has more than one eigenvalue and eigenvector. These last arguments tell us, in a rough way, the modifications due to these metric fluctuations. Notice that for $l=0$, the case in which we are interested, one of the Clebsch-Gordan conditions ($l \notin [k-l, k+l]$) means that only for $k=0$ it could be different from zero, because $0 \notin [2, 2]$ and $0 \notin [1, 1]$. In other words, the fourfold degeneracy of the ground state (taking into account electronic and protonic spins) will not be broken by anisotropic fluctuations. It is readily seen that this last comment entails the fact that spherical symmetry cannot be broken. In general (for nonvanishing values of the orbital angular momentum), the role of metric fluctuations becomes richer if the restriction of conformal condition is released. In this case, spherical symmetry will be broken and the degeneracy, inherent and accidental, can be lost.

In the present work the simplest case will be considered, namely, $\gamma^{ij} = 0$, if $i \neq j$, whereas $\gamma^{xx} = \gamma^{yy} = \gamma^{zz} = \gamma$. This is due to the fact that we are interested in the case $l=0$. Clearly, as already shown, the situation cannot lead to the breakdown of spherical symmetry, though it does not mean that the case is uninteresting. Indeed, it leads to a modification of the ground energy of the hydrogen atom, and the modification of this energy due to the fluctuations has the structure (this statement will be proved latter) $\Delta E \sim \frac{\mu c^2 \alpha^2}{2} (1 + \gamma)^{-1}$, in the leading contribution.

B. Hierarchy of perturbation terms

The fine structure Hamiltonian reads [28]

$$\hat{W}_f = -\frac{P^4}{8\mu^3 c^2} + \frac{1}{2\mu^2 c^2} \frac{1}{r} \frac{dV}{dr} \vec{L} \cdot \vec{S} + \frac{\hbar^2}{8\mu^2 c^2} \nabla^2 V(r). \quad (7)$$

Here $V(r)$ denotes the Coulombian potential. Let us, briefly, explain each one of the three contributions appearing in the right-hand side of this last expression. The first term can be understood as the first relativistic correction to the dispersion relation. The second one takes into account the fact that the electron moves with respect to the nucleus and, therefore, according to special relativity, it must *feel* the magnetic field of the nucleus. Finally, the last term, called Darwin's operator, is a consequence of the *Zitterbewegung* of the electron [28].

There is an additional contribution that has to be included, namely, the hyperfine [28]

$$\begin{aligned} \hat{W}_h = -\frac{\mu_0}{4\pi} \left\{ \frac{q}{\mu r^3} \vec{L} \cdot \vec{M}_I + \frac{1}{r^3} [3(\vec{n} \cdot \vec{M}_I)(\vec{n} \cdot \vec{M}_S) - \vec{M}_S \cdot \vec{M}_I] \right. \\ \left. + \frac{8\pi}{3} \vec{M}_S \cdot \vec{M}_I \delta(r) \right\}. \end{aligned} \quad (8)$$

In this last expression the first term on the right-hand side describes the interaction of the nuclear magnetic moment with magnetic field created by the orbital angular momentum of the electron; the middle operator is related to the dipole-dipole interaction between the magnetic moments of the electron and the nucleus; whereas the last element, called Fermi's contact term, is connected to the fact that the nucleus is not a point, i.e., it has a nonvanishing spatial extension.

The procedure to be followed here is: (i) the initial eigenkets will be those associated to the hydrogen atom [30]. The fine structure Hamiltonian will be used as a perturbation and the corresponding perturbed energies and kets will be obtained. (ii) Then these last results will be employed as original energies and kets and the hyperfine structure Hamiltonian will be introduced as a perturbation. (iii) Once again, the corresponding energies and kets will be deduced and they will be the starting data and (4) will at this point play the role of a time-independent perturbation. Clearly, this entails that the effects of the fluctuations will be calculated in such a way that fine and hyperfine effects are included as fundamental elements of atomic physics.

As a first case we consider conformal fluctuations [25,26], namely, $\gamma^{ij} = 0$, if $i \neq j$, whereas $\gamma^{xx} = \gamma^{yy} = \gamma^{zz} = \gamma$. These conditions reduce (4) to

$$\hat{W} = \frac{1}{2\mu} \gamma \hat{P}^2. \quad (9)$$

$$|1\rangle = \sum_{n=2}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{\langle n; l; m; m_s; m_l | \hat{W}_f | n = 1; l = 0; m = 0; m_s; m_l \rangle}{-\frac{1}{2} \mu c^2 \alpha^2 + \frac{1}{2n^2} \mu c^2 \alpha^2} |n; l; m; m_s; m_l\rangle. \quad (10)$$

There is an additional property which simplifies this last expression. Indeed, the Darwin term vanishes for all states such that $l \neq 0$ [28].

2. Perturbed kets and energies

The modified kets can be written as usual as

$$|\tilde{0}\rangle = |0\rangle + |1\rangle, \quad (11)$$

where $|1\rangle$ is the contribution due to the perturbation. Calculation of this part yields for the new ground state (see Appendix A 1)

$$|\tilde{0}\rangle = |n = 1; l = 0; m = 0; m_s; m_l\rangle + \alpha^2 \sum_{n=2}^{\infty} \frac{n^2}{n^2 - 1} \left(\frac{1}{n^{3/2}} - \frac{1}{n^3} \right) |n; l = 0; m = 0; m_s; m_l\rangle. \quad (12)$$

Notice that this last expression tells us that the dependence of the perturbed ket upon $|n; l = 0; m = 0; m_s; m_l\rangle$, with $n \geq 2$, is much smaller than that related to the case

At this point it seems to be a plain and simple redefinition of the concept of inertial mass, i.e., $\mu \rightarrow \frac{\mu}{1+\gamma}$, and we may wonder if this kind of effect can be detected. The answer to this question is a very simple one and can be understood recalling the general form of the fine structure effect. Indeed, the energy modification due to this contribution is given by $\Delta E_f \sim \frac{1}{8} \mu c^2 \alpha^4$. If we introduce the aforementioned redefinition, we obtain that the new modification reads $\Delta E_f \sim \frac{1}{8} \mu c^2 \alpha^4 (1 + \gamma)^{-1}$. Therefore, in principle, it can be detected.

C. Fine structure

1. General procedure

We will focus on the modifications to the ground state energy, the ionization energy. Since the fine structure effects are larger than the hyperfine one, $|\hat{W}_h/\hat{W}_f| \sim \alpha^2$ [28], then we start our analysis considering first fine structure terms (7). The ground state of the hydrogen atom has a fourfold degeneracy (due to the spin degrees of freedom of the electron and proton). Since $l = 0$, for the ground state, then the spin-orbit coupling does not contribute. In other words, the fine structure cannot entail the breakdown of the spherical symmetry for the ground state. This comment also implies that for $l = 0$ \hat{W}_f has a diagonal matrix. Hence, the four corresponding states move in the same way, namely, the first-order correction to these eigenstates reads

$n = 1$. Indeed, it is readily seen that those kets associated to $n \geq 2$ are multiplied by $\alpha^2 \sim 10^{-4}$. This assertion is a consequence of the fact that the fine structure terms behave as α^4 , and when the corresponding matrix element is divided by the difference between the two involved states ($\Delta E \sim \frac{\mu c^2 \alpha^2}{2}$) we obtain this aforementioned behavior.

D. Hyperfine structure

This new ground state ($|\tilde{0}\rangle$) will be now employed for the deduction of the first-order energy correction due to the hyperfine structure terms (8),

$$E_1 = \langle \tilde{0} | \hat{W}_h | \tilde{0} \rangle. \quad (13)$$

At this point let us rewrite this last energy. In order to do that, let us remember that the definition of the nuclear Bohr magneton, $\mu_n = (g_p \hbar / (2m_p))$, involves this parameter g_p which is approximately equal to 5.585 [28], and then the energy can be cast in the following form:

$$E_1 = -g_p \frac{\mu_e}{m_p} (\mu_e c^2 \alpha^4) \left\{ 1 + \sum_{n=2}^{\infty} \frac{n^2 \alpha^2}{n^2 - 1} \left(\frac{1}{n^3} - \frac{1}{n^{9/2}} \right) + \left[\sum_{n=2}^{\infty} \frac{n^2 \alpha^2}{n^2 - 1} \left(\frac{1}{n^3} - \frac{1}{n^{9/2}} \right) \right]^2 \right\}. \quad (14)$$

Riemann's function [$\xi(\nu) = \sum_{l=1}^{\infty} 1/l^\nu$] allows us to find a simple expression to the first-order energy correction (see Appendix

$$\sum_{n=2}^{\infty} \frac{n^2}{n^s(n^2 - 1)} \approx \frac{4}{3} (\xi(s) - 1). \quad (15)$$

This approximation allows us to write the first-order energy correction as

$$\langle n; l=0; m=0; m_s; m_l | \frac{8\pi}{3} \vec{M}_S \cdot \vec{M}_I \delta(r) | \tilde{n}; l=0; m=0; \tilde{m}_s; \tilde{m}_l \rangle = \frac{8\pi}{3} R_{(n,l=0)}(r=0) R_{(\tilde{n},l=0)}(r=0) \langle m_s; m_l | \vec{M}_S \cdot \vec{M}_I | \tilde{m}_s; \tilde{m}_l \rangle. \quad (17)$$

In this last expression $R_{(n,l=0)}(r)$ denotes the radial part of the corresponding wave function. We now define (as usual, since \vec{M}_S and \vec{M}_I are proportional to \vec{S} and \vec{I} , respectively)

$$\vec{F} = \vec{S} + \vec{I}. \quad (18)$$

Therefore we have that

$$\vec{F}^2 = \vec{S}^2 + \vec{I}^2 + 2\vec{I} \cdot \vec{S}. \quad (19)$$

According to the rules of addition of angular momentum we have $F = 0, 1$. In the eigenkets of \vec{F}^2 (here denoted $|F, m_F\rangle$) we have

$$\begin{aligned} \langle n; F=0, m_F=0 | \hat{W}_h | \hat{n}=1; F=0, m_F=0 \rangle \\ = - \frac{q^2 \hbar^2 g_p \mu_0}{4\pi a_0^3 n^{3/2} \mu_e m_p}, \end{aligned} \quad (20)$$

$$\begin{aligned} |\hat{0}\rangle = |n=1, ; l=0, m_l=0; F=0, m_F=0\rangle + \alpha^2 \sum_{n=2}^{\infty} \frac{n^2}{n^2 - 1} \left(\frac{1}{n^{3/2}} - \frac{1}{n^3} \right) |n; l=0, m_l=0; F=0, m_F=0\rangle \\ + 2 \frac{g_p \mu_e}{m_p} \alpha^2 \sum_{n=2}^{\infty} \frac{n^2}{n^2 - 1} \frac{1}{n^{3/2}} |n; l=0, m_l=0; F=0, m_F=0\rangle + \dots \end{aligned} \quad (22)$$

Now the consequences of the metric fluctuations upon this ground state are deduced

$$\langle \hat{0} | \frac{1}{2\mu} \gamma \hat{P}^2 | \hat{0} \rangle = -\frac{1}{2} \mu c^2 \alpha^2 \gamma \left[1 - \frac{16}{3} \alpha^2 \left[\xi(5/2) - \xi(4) + 2 \frac{g_p \mu_e}{m_p} (\xi(5/2) - 1) \right] + O(\alpha^4) \right]. \quad (23)$$

Finally, the energy of the ground state, which is the ionization energy is

$$E_0 = -\frac{1}{2} \mu_e c^2 \alpha^2 \left[1 + \frac{1}{4} \alpha^2 + 2g_p \frac{\mu_e}{m_p} \alpha^2 (1 - 1.82\gamma) + \gamma (1 - 1.376\alpha^2) \right]. \quad (24)$$

If $\gamma \rightarrow 0$, then we recover the usual result [28]. It is also readily seen that the effects of metric fluctuations appear here as a modification to the ionization energy of the hydrogen atom

$$E_1 = -g_p \frac{\mu_e}{m_p} (\mu_e c^2 \alpha^4) \left[1 + \frac{4\alpha^2}{3} (\xi(3) - \xi(9/2)) \right]. \quad (16)$$

The calculation of the perturbed kets has to be done resorting to (12). Once again, this ground state is fourfold degenerate, nevertheless, let us mention that the term involving $\vec{L} \cdot \vec{M}_I$ vanishes since our ground state implies $l=0$. Similarly, the contribution involving the dipole-dipole interaction turns out to be zero (due to spherical symmetry) [28]. The only term that participates is the last one, the so-called contact term. Here we must calculate terms with the following structure:

and

$$\langle n; F=1, m_F | \hat{W}_h | \hat{n}=1; F=1, m_F \rangle = \frac{q^2 \hbar^2 g_p \mu_0}{12\pi a_0^3 n^{3/2} \mu_e m_p}. \quad (21)$$

We may now write down the perturbed kets, which contain the effects of fine and hyperfine structures. Notice that the correction related to $F=0$ implies a lower energy than those three cases associated to $F=1$. In other words, the ground state now is given by

$$\Delta E_0 = -\frac{1}{2}\mu_e c^2 \alpha^2 \gamma \left(1 - 1.376\alpha^2 - 3.64g_p \frac{\mu_e}{m_p} \alpha^2\right). \quad (25)$$

III. SPACETIME FLUCTUATIONS AND LAMB SHIFT

We now address the issue of a possible connection between metric fluctuations and a Lamb-type-like shift [31]. In addition to the modification imposed by the zero-point fluctuations of the electromagnetic field, since the potential $V(r)$ is a function of r then the presence of these spacetime fluctuations entails a change of the position of the electron (of course, also of the proton), $r \rightarrow r + \delta r$,

$$\begin{aligned} \Delta V &= V(r + \delta r) - V(r) \\ &= \delta \vec{r} \cdot \nabla V(r) + \frac{1}{2}(\delta \vec{r} \cdot \nabla)^2 V(r) + \dots \end{aligned} \quad (26)$$

The method provides the correct order of magnitude of this effect since it reproduces the Bethe formula [31,32]. The assumption of conformal fluctuations implies [25,26] that the average of this change (here denoted by $\langle \Delta V \rangle$)

$$\langle \Delta V \rangle = \langle \frac{1}{2}(\delta \vec{r} \cdot \nabla)^2 V(r) \rangle. \quad (27)$$

The meaning of $\langle \Delta V \rangle$ entails two different averages: (i) an average over metric fluctuations and (ii) a second average over atomic states. Indeed, isotropy leads us to conclude that the average over metric fluctuations

$$\langle \delta \vec{r} \rangle_{(mf)} = 0. \quad (28)$$

Let us now explain how the average over metric fluctuations is to be carried out. Here the background metric is the Minkowskian one,

$$ds^2 = e^{\psi(x)} \eta_{00} dt^2 + e^{\psi(x)} \eta_{ij} dx^i dx^j. \quad (29)$$

We assume (with the condition $|\psi(x)| \ll 1$)

$$\langle \psi(x) \rangle_{(mf)} = 0, \quad (30)$$

$$\langle \partial_\mu \psi(x) \rangle_{(mf)} = 0. \quad (31)$$

Therefore we have

$$\langle \delta x \rangle = \langle e^{\psi(x)} x \eta_{xx} \rangle_{(mf)} = (1 + \frac{1}{2} \langle (\psi)^2 \rangle_{(mf)} + \dots) x \eta_{xx}, \quad (32)$$

$$\langle e^{\psi(x)} \eta_{00} \rangle_{(mf)} = (1 + \frac{1}{2} \langle (\psi)^2 \rangle_{(mf)} + \dots) \eta_{00}, \quad (33)$$

and similarly for the remaining coordinates. The imposed condition (30) implies (28). It is easily seen that these conditions contain isotropy and homogeneity of spacetime. Indeed, it does not define a privileged direction nor a privileged point.

We now notice that, explicitly,

$$\begin{aligned} \frac{1}{2}(\delta \vec{r} \cdot \nabla)^2 V(r) &= \frac{\delta \vec{r}}{2} \cdot [(\delta \vec{r} \cdot \nabla) \nabla V + (\nabla V \cdot \nabla) \delta \vec{r} \\ &\quad + \delta \vec{r} \times \nabla \times (\nabla V) + \nabla V \times \nabla \times \delta \vec{r}]. \end{aligned} \quad (34)$$

The conformal condition imposed upon these fluctuations allow us to simplify the calculations. Indeed, isotropy and independence of the fluctuations along the different directions can be rephrased as follows:

$$\langle \delta x \delta y \rangle_{(mf)} = \langle \delta x \rangle_{(mf)} \langle \delta y \rangle_{(mf)}, \quad (35)$$

$$\langle (\delta x)^2 \rangle_{(mf)} = \frac{1}{3} \langle (\delta \vec{r})^2 \rangle_{(mf)}. \quad (36)$$

Hence, the average over the metric fluctuations can be reduced to

$$\frac{1}{2} \langle (\delta \vec{r} \cdot \nabla)^2 \rangle_{(mf)} = \frac{1}{6} \langle (\delta \vec{r})^2 \rangle_{(mf)} \nabla^2. \quad (37)$$

Until now we have only introduced, explicitly, metric fluctuations ($\langle \dots \rangle_{(mf)}$). At this point we require an assumption for one of our parameters, namely, the behavior of some of the statistical properties of the fluctuations have to be given. We introduce [33]

$$\langle (\delta \vec{r})^2 \rangle_{(mf)} = \sigma^2. \quad (38)$$

In this last expression σ is a constant. We may now conclude

$$\langle \Delta V \rangle = \frac{\sigma^2}{6} \left\langle \nabla^2 \left(\frac{-q^2}{r} \right) \right\rangle_{(at)}. \quad (39)$$

This average ($\langle \dots \rangle_{(at)}$) denotes a calculation over atomic states, i.e.,

$$\frac{\sigma^2}{6} \left\langle \nabla^2 \left(\frac{-q^2}{r} \right) \right\rangle_{(at)} = -\frac{q^2 \sigma^2}{6} \int |\psi_{(n,l,m)}(\vec{r})|^2 \nabla^2 \left(\frac{1}{r} \right) d^3 r. \quad (40)$$

Finally, $\nabla^2 \left(\frac{1}{r} \right) = -4\pi \delta(r)$, and we obtain

$$\langle \Delta V \rangle = 4\pi \frac{q^2 \sigma^2}{6} \int \delta(r) |\psi_{(n,l,m)}(\vec{r})|^2 d^3 r. \quad (41)$$

This last result, as in the usual Lamb shift effect [27], implies that metric fluctuations, in this context, can modify only those states with vanishing angular momentum ($l = 0$), due to the fact that $\psi_{(n,l,m)}(\vec{0}) = 0$ if $l \neq 0$ [28]. Then, for the particular case of $n = 2$ we have (here a_0 denotes Bohr radius)

$$\frac{q^2 \sigma^2}{6} |\psi_{(2,0,0)}(\vec{0})|^2 = -\frac{1}{96} \left(\frac{\sigma}{a_0} \right)^2 \frac{q^2}{a_0}. \quad (42)$$

IV. DISCUSSION AND RESULTS

Let us now discuss the results and their perspectives, always in the context of precision tests.

A. Hyperfine splitting

Our result concerning the ionization energy of the hydrogen atom is provided by (25). The first term $[-(0.5)\mu_e c^2 \alpha^2 \gamma]$ can be comprehended as a consequence of the redefinition of the concept of inertial mass, see (1). Indeed, it is quadratic in the fine structure constant, a fact that discards any relation with the fine or hyperfine structure.

The second contribution $[(0.688)\mu_e c^2 \alpha^4 \gamma]$ has to be related to the fine structure. Of course, the dominant effect (since $\alpha \sim 1/137$) corresponds to $-(0.5)\mu_e c^2 \alpha^2 \gamma$. The emergence of γ in this last term is also a consequence of this redefinition of the inertial mass. Indeed, take, for instance, the Darwin term, $[\hbar^2/(8\mu_e^2 c^2)]\nabla^2 V(r)$. Its average for an unperturbed eigenstate (with quantum numbers n , $l=0$, $m=0$) of the hydrogen atom behaves like $\hbar^2/(8n^2\mu_e^2 c^2 a_0^3)$. The fine structure constant is defined as $\alpha = \hbar/(\mu_e c a_0)$, and therefore, this average has the order of magnitude $\mu_e c^2 \alpha^4/n^2$. If we redefine $\mu^{\text{eff}} = \mu_e(1 + \gamma)^{-1}$, then we deduce that the Darwin term is also modified, namely, $\mu_e c^2 \alpha^4/n^2 \rightarrow \mu_e c^2 \alpha^4(1 + \gamma)^{-1}/n^2$. In other words, this redefinition of the inertial mass is the first modification that emerges in the present context, either in connection with the unperturbed energy levels, or in association with the fine structure terms.

The third and last contribution $(1.82\mu_e c^2 \alpha^4 \gamma g_p \frac{\mu_e}{m_p})$ corresponds to the modifications upon the hyperfine energy due to these fluctuations and, once again, it can be understood as a consequence of this redefinition of the inertial mass. The hyperfine splitting of the ground state of the hydrogen atom can be considered among the most accurately detected physical quantities [24]. The related uncertainty is associated to several possibilities, for instance, correction terms of higher-order QED effects, or the proton electromagnetic structure induced by strong interactions. A very rough bound for the magnitude of γ can be deduced from [24], Eq. (1). Indeed, according to this experimental result the uncertainty related to the hyperfine splitting of the hydrogen atom reads

$$\Delta E_0^{(\text{exp})} = \pm 0.0009 \text{ Hz.} \quad (43)$$

We now relate our third term $(1.82\mu_e c^2 \alpha^4 \gamma g_p \frac{\mu_e}{m_p})$ to the experimental uncertainty

$$1.82\mu_e c^2 \alpha^4 \gamma g_p \frac{\mu_e}{m_p} \leq \hbar \Delta E_0^{(\text{exp})}. \quad (44)$$

In this way we obtain a rough bound for γ :

$$\gamma \leq 10^{-18}. \quad (45)$$

B. Lamb shift

The Lamb shift has been used as a tool for the detection of the radius of the proton, etc. [34]. In our case it allows us to pose, in an independent way from the previous situation, a bound to some statistical properties of the metric fluctuations. Indeed, we may use the uncertainty (ΔE) mentioned in [35] ($\Delta E/\hbar = 4.8$ MHz),

$$\frac{1}{96} \left(\frac{\sigma}{a_0} \right)^2 \frac{q^2}{a_0} \leq \Delta E, \quad (46)$$

and obtain as a bound

$$\sigma \leq 10^{-18} \text{ m.} \quad (47)$$

C. Models of spacetime fluctuations and precision tests

It has to be emphasized that these two bounds [(45) and (47)] cannot be compared directly. Indeed, γ is not equal to σ (γ^{ij} in the general situation) [25,26]. They correspond to different statistical features of the involved fluctuations of spacetime. Of course, they are related and at this point we mention their connection. The effective Schrödinger equation used in the context of hyperfine structure contains an average process of metric fluctuations involving a spacetime interval [see expression (3) in [25]]. The averaging method involved in the calculations of the Lamb shift [33] has a resemblance of the first procedure, though it is not the same kind of fluctuation, as expression (4) in [25] explicitly manifests. Indeed, in this last approach the average of these fluctuations defines a background field, whereas in [33] the average of these fluctuations does not define this parameter. This lack of coincidence in the context of our employed fluctuations shall be no surprise [36], i.e., the possibilities in the type of fluctuations is not restricted to those mentioned in [25] or in [33]. This fact can be considered a drawback of quantum gravity phenomenology since a very large number of options are to be included, as possible cases.

Concerning (45) our parameter γ is closely related (in a weak field approach) to perturbations of the Minkowskian metric, in a similar way as in the case of linear gravitational waves. It can be seen that the present bound is 3 orders of magnitude larger than the strength of a gravitational wave whose source is a stellar binary [37].

In relation with (47) we may also find a bound for $|\langle \delta r \rangle|$. Indeed, we know that the standard deviation is defined as $\Delta r = \sqrt{\sigma^2 - (\langle \delta r \rangle)^2}$. Therefore we find (since $\Delta r \geq 0$) that $|\langle \delta r \rangle| \leq 10^{-18}$ m. Notice that according to (28) we have that $\langle \delta \vec{r} \rangle_{(mf)} = 0$, but this result does not imply that $\delta r = 0$. A physical consequence of $|\langle \delta r \rangle| \leq 10^{-18}$ m is that any distance measurement below this value would be meaningless.

Let us add a final comment concerning the relation between fluctuations and physical effects involved in our paper. Clearly, different fluctuations can be considered as

possible candidates and several effects can be used as tools in this quest for precision tests. Our particular choices in this manuscript have been done looking for the easiest nontrivial cases.

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APPENDIX

1. Calculation of the matrix elements

Let us now provide an explanation that allows us to conclude that the contribution referring to the perturbation of the ground state ket reads

$$|1\rangle = \alpha^2 \sum_{n=2}^{\infty} \frac{n^2}{n^2-1} \left(\frac{1}{n^{3/2}} - \frac{1}{n^3} \right) |n; l=0; m=0; m_s; m_l\rangle. \quad (\text{A1})$$

In this direction notice that $H_0 = \frac{p^2}{2\mu} - \frac{q^2}{r}$, hence $\frac{p^4}{8\mu^3 c^2} = \frac{1}{2\mu c^2} (H_0 + \frac{q^2}{r})^2$, and in consequence we deduce

$$\begin{aligned} \langle n; l, m | \frac{p^4}{8\mu^3 c^2} | \hat{n}; \hat{l}, \hat{m} \rangle \\ = \frac{1}{2\mu c^2} \langle n; l, m | \left(H_0 + \frac{q^2}{r} \right)^2 | \hat{n}; \hat{l}, \hat{m} \rangle. \end{aligned} \quad (\text{A2})$$

From this last condition it turns out

$$\begin{aligned} \frac{1}{2\mu c^2} \langle n; l, m | \left(H_0 + \frac{q^2}{r} \right)^2 | \hat{n}; \hat{l}, \hat{m} \rangle \\ = \frac{1}{2\mu c^2} \left[(E_n)^2 \delta_{n,\hat{n}} \delta_{l,\hat{l}} \delta_{m,\hat{m}} - 2E_n \langle n; l, m | \frac{q^2}{r} | \hat{n}; \hat{l}, \hat{m} \rangle \right. \\ \left. + \langle n; l, m | \frac{q^4}{r^2} | \hat{n}; \hat{l}, \hat{m} \rangle \right]. \end{aligned} \quad (\text{A3})$$

We now mention the fact that these two operators ($\frac{q^2}{r}$ and $\frac{q^4}{r^2}$) are both spherical operators of rank $k=0$, i.e., they cannot modify the orbital angular momentum or the projection of it along the z axis. This last remark entails

$$\langle n; l, m | \frac{1}{r} | \hat{n}; \hat{l}, \hat{m} \rangle = \delta_{l,\hat{l}} \delta_{m,\hat{m}} \int_0^{\infty} R_{(n,l)}(r) R_{(\hat{n},\hat{l})}(r) r dr, \quad (\text{A4})$$

$$\langle n; l, m | \frac{1}{r^2} | \hat{n}; \hat{l}, \hat{m} \rangle = \delta_{l,\hat{l}} \delta_{m,\hat{m}} \int_0^{\infty} R_{(n,l)}(r) R_{(\hat{n},\hat{l})}(r) dr. \quad (\text{A5})$$

Here the wave functions are $\psi_{(n,l,m)} = R_{(n,l)}(r) Y_{(m)}^{(l)}$ [30] and

$$\begin{aligned} R_{(n,l)}(r) = \left[\left(\frac{2}{na_0} \right)^3 \frac{(n-l-1)!}{2n(n+l)!} \right]^{1/2} \exp \left[-\frac{r}{na_0} \right] \\ \times \left(\frac{2r}{na_0} \right)^l \mathcal{L}_{n-l-1}^{2l+1} \left(\frac{2r}{na_0} \right). \end{aligned} \quad (\text{A6})$$

Here $\mathcal{L}_{n-l-1}^{2l+1} \left(\frac{2r}{na_0} \right)$ denotes the Laguerre associated polynomials, and a_0 the Bohr radius [30].

Additionally, it is already known [$\text{Re}(\epsilon) > 0$ and $s > 0$] [38]

$$\int_0^{\infty} e^{-\epsilon x} x^s dx = \frac{s!}{\epsilon^{s+1}}. \quad (\text{A7})$$

Resorting to this integral and the explicit expression for Laguerre polynomials [38], we may write down

$$\begin{aligned} \int_0^{\infty} R_{(n,l)}(r) R_{(\hat{n},\hat{l})}(r) r dr \\ = \frac{1}{n\hat{n}a_0} \left[\left(\frac{(n-l-1)!}{(n+l)!} \right) \left(\frac{(\hat{n}-l-1)!}{(\hat{n}+l)!} \right) \right]^{1/2} \\ \times \sum_{s=0}^{\hat{n}-l-1} \sum_{t=0}^{n-l-1} \left[\frac{(-1)^{s+t} (n+l)! (\hat{n}+l)! (\hat{n}n)^{2l+3+s+t}}{t! s! (n-l-1-t)! (\hat{n}-l-1-s)!} \right. \\ \times \frac{(2l+s+t+1)!}{(s+2l+1)! (t+2l+1)!} \\ \left. \times \frac{2^{2l+2+s+t}}{(n)^{l+t} (\hat{n})^{l+s} (n+\hat{n})^{2l+s+t+2}} \right]. \end{aligned} \quad (\text{A8})$$

In order to calculate our required expressions let us point out that since $H_0 = \frac{p^2}{2\mu} - \frac{q^2}{r}$ we have that

$$\begin{aligned} \langle n; l, m | \frac{p^2}{2\mu} | \hat{n}; \hat{l}, \hat{m} \rangle \\ = -\mu c^2 \alpha^2 \left(\frac{1}{2n^2} \delta_{n,\hat{n}} - \langle n; l, m | \frac{q^2}{r} | \hat{n}; \hat{l}, \hat{m} \rangle \right). \end{aligned} \quad (\text{A9})$$

We mention this expression because it will help us out in the evaluation of (A8). Indeed, the value of this last expression when $n = \hat{n}$ is already known [39],

$$\langle n; l, m | \frac{p^2}{2\mu} | n; l, m \rangle = \frac{\mu c^2 \alpha^2}{2n^2}. \quad (\text{A10})$$

Therefore we conclude that if in (A8) we impose the condition $n = \hat{n}$ (here we drop out the term $1/a_0$ since it plays no role in the evaluation of this summation)

$$\begin{aligned} \frac{1}{n^2} = \frac{1}{n^2} \left[\left(\frac{(n-l-1)!}{(n+l)!} \right) \left(\frac{(n-l-1)!}{(n+l)!} \right) \right]^{1/2} \\ \times \sum_{s=0}^{n-l-1} \sum_{t=0}^{n-l-1} \left[\frac{(-1)^{s+t} (n+l)! (n+l)! (n)^{4l+6+2s+2t}}{t! s! (n-l-1-t)! (n-l-1-s)!} \right. \\ \times \frac{(2l+s+t+1)!}{(s+2l+1)! (t+2l+1)!} \\ \left. \times \frac{2^{2l+2+s+t}}{(n)^{l+t} (n)^{l+s} (2n)^{2l+s+t+2}} \right]. \end{aligned} \quad (\text{A11})$$

Immediately we see that

$$\begin{aligned}
 1 &= \left[\left(\frac{(n-l-1)!}{(n+l)!} \right) \left(\frac{(n-l-1)!}{(n+l)!} \right) \right]^{1/2} \\
 &\times \sum_{s=0}^{n-l-1} \sum_{t=0}^{n-l-1} \left[\frac{(-1)^{s+t} (n+l)! (n+l)! (n)^{4l+6+2s+2t}}{t! s! (n-l-1-t)! (n-l-1-s)!} \right. \\
 &\times \left. \frac{(2l+s+t+1)!}{(s+2l+1)! (t+2l+1)!} \frac{2^{2l+2+s+t}}{(n)^{l+t} (n)^{l+s} (2n)^{2l+s+t+2}} \right]. \quad (\text{A12})
 \end{aligned}$$

Let us, at this point, sum up our conclusions concerning this summation. On one hand, we know the result if $n = \hat{n}$. On the other hand, we point out the fact that in (A8) the summations in s and t are, functionally, the same; they differ only in the upper limit, i.e., it is either $n-l-1$, or $\hat{n}-l-1$. Let us now delve a little bit deeper in this direction. In order to do this let us define

$$\begin{aligned}
 g(s, t; n, \hat{n}) &= \left[\left(\frac{(n-l-1)!}{(n+l)!} \right) \left(\frac{(\hat{n}-l-1)!}{(\hat{n}+l)!} \right) \right]^{1/2} \\
 &\times \left[\frac{(-1)^{s+t} (n+l)! (\hat{n}+l)! (\hat{n}n)^{2l+3+s+t}}{t! s! (n-l-1-t)! (\hat{n}-l-1-s)!} \right. \\
 &\times \frac{(2l+s+t+1)!}{(s+2l+1)! (t+2l+1)!} \\
 &\times \left. \frac{2^{2l+2+s+t}}{(n)^{l+t} (\hat{n})^{l+s} (n+\hat{n})^{2l+s+t+2}} \right]. \quad (\text{A13})
 \end{aligned}$$

This remark concerning the functional dependence upon s and t means that if

$$\sum_{t=0}^{n-l-1} g(s, t; n, \hat{n}) = f(s, n-l; n, \hat{n}), \quad (\text{A14})$$

then

$$\sum_{s=0}^{\hat{n}-l-1} g(s, t; n, \hat{n}) = f(\hat{n}-l, t; n, \hat{n}). \quad (\text{A15})$$

where f is the same function in both equations. Of course, we have, on the right-hand side of (A14) and (A15), the same function as a consequence of this aforementioned equality in the functional dependence in terms of s and t . Clearly, this fact implies that

$$\sum_{s=0}^{\hat{n}-l-1} \sum_{t=0}^{n-l-1} g(s, t; n, \hat{n}) = h(n-l, \hat{n}-l) \quad (\text{A16})$$

is a function of $n-l$ and $\hat{n}-l$ in which the functional dependence upon these two variables is the same. In addition, $h(n-l, n-l) = 1$, and this $\forall n \in \mathbb{N}$, here l is a constant parameter.

We now proceed to prove that $h(n, \hat{n}) = j(n)j(\hat{n})$, i.e., we have $l = 0$. Indeed, notice that our task is the evaluation of the integral shown in (A8). In the mathematical literature there are several variants denoted the second mean

value theorem for integrals. The usual ones cannot be used in the present context since they require as a premise that (at least) one of the two functions under the sign of integral has to be an integrable positive function [40]. In the present case since $R_{(n,l)}(r)$ involves the Laguerre associated polynomials then they may change its sign, and this fact violates the premise of this theorem. The correct theorem is a generalization of the second mean value theorem for integrals done by Okamura [41]; if $f: [a, b] \rightarrow \mathbb{R}$ is a monotonically decreasing function and $g: [a, b] \rightarrow \mathbb{R}$ an integrable function, then there is $c \in (a, b]$ such that

$$\int_a^b f(x)g(x)dx = f(c) \int_a^b g(x)dx. \quad (\text{A17})$$

It is already known that for the case of $l \neq 0$ the wave function for the hydrogen atom vanishes at the origin, this fact is a consequence of the continuity of the solutions to this potential [28,30]. This remark entails that for $l \neq 0$ the radial part of the solution is an increasing function from $r = 0$ to a certain value, say r_0 . This is not the case for those radial parts of the solution associated to $l = 0$, since in this case they do not vanish at $r = 0$ [28,30]. They have a decreasing behavior from $r = 0$ to a certain value given by the corresponding associated Laguerre polynomial. Indeed, if $l = 0$ we have that

$$\begin{aligned}
 R_{(n,l=0)}(r) &= \left[\left(\frac{2}{na_0} \right)^3 \left(\frac{1}{2n^2} \right) \right]^{1/2} \exp \left[-\frac{r}{na_0} \right] \\
 &\times \left[1 - (n-1) \left(\frac{r}{na_0} \right) + (n-1) \left(\frac{r}{na_0} \right)^2 + \dots \right. \\
 &\left. + (-1)^{n-1} (n-1) \left(\frac{r}{na_0} \right)^{n-1} \right]. \quad (\text{A18})
 \end{aligned}$$

This last expression shows us that for $r \in [0, n(n-1)a_0]$, $\forall n \geq 2$, this is a decreasing function. In addition, we know that for large values of r the function is clearly monotonically decreasing, i.e., they represent bound states. These arguments allow us to accept (as a good approximation) that there is $c \in (0, \infty)$:

$$\begin{aligned}
 &\int_0^\infty R_{(n,l=0)}(r) R_{(\hat{n},l=0)}(r) r dr \\
 &= R_{(n,l=0)}(c) \int_0^\infty R_{(\hat{n},l=0)}(r) r dr. \quad (\text{A19})
 \end{aligned}$$

This last expression is the product of a function depending only upon n [$R_{(n,l=0)}(c)$] and another whose independent variable is \hat{n} [$\int_0^\infty R_{(\hat{n},l=0)}(r) r dr$].

This argument proves that $h(n, \hat{n}) = j(n)j(\hat{n})$, i.e., our function $h(n, \hat{n})$ can be written as the product of two functions, one depending on n and the other upon \hat{n} .

Joining these two features we have $h(n, n) = [j(n)]^2 = 1 \Rightarrow j(n) = \pm 1$. This leads us to conclude that

$$\begin{aligned} \pm 1 &= \left[\left(\frac{(n-1)!}{(n)!} \right) \left(\frac{(\hat{n}-1)!}{(\hat{n})!} \right) \right]^{1/2} \\ &\times \sum_{s=0}^{\hat{n}-1} \sum_{t=0}^{n-1} \left[\frac{(-1)^{s+t} (n)! (\hat{n})! (\hat{n}n)^{3+s+t}}{t! s! (n-1-t)! (\hat{n}-1-s)!} \right. \\ &\left. \times \frac{(s+t+1)!}{(s+1)!(t+1)!} \frac{2^{2+s+t}}{(n)^t (\hat{n})^s (n+\hat{n})^{s+t+2}} \right]. \end{aligned} \quad (\text{A20})$$

The ambiguity concerning the sign appearing in this last expression fades away noting that the integral (A8) has to be non-negative, i.e., we must take the plus sign.

We may now write down

$$\int_0^\infty R_{(n,l=0)}(r) R_{(\hat{n},l=0)}(r) r dr = \frac{1}{n\hat{n}a_0}. \quad (\text{A21})$$

The same kind of arguments can be used if the operator $1/r$ is replaced by $1/r^2$. These results are to be introduced in the corresponding matrix elements of (10) and, in this way, we are led to (A1) which corresponds to the particular case in which $\hat{n} = 1$.

We may now, with these results, proceed to the calculation of the perturbed kets and energies.

2. Approximation of the series by Riemann's Zeta function

Let us explain the approximation

$$\sum_{n=2}^\infty \frac{n^2}{n^s(n^2-1)} \approx \frac{4}{3}(\xi(s)-1). \quad (\text{A22})$$

Notice that

$$\begin{aligned} \sum_{n=2}^\infty \frac{n^2}{n^s(n^2-1)} &= \sum_{n=2}^\infty \frac{n^2-1+1}{n^s(n^2-1)} \\ &= \sum_{n=2}^\infty \frac{1}{n^s} + \sum_{n=2}^\infty \frac{1}{n^s(n^2-1)}, \end{aligned} \quad (\text{A23})$$

therefore

$$\sum_{n=2}^\infty \frac{n^2}{n^s(n^2-1)} = \xi(s) - 1 + \sum_{n=2}^\infty \frac{1}{n^s(n^2-1)}. \quad (\text{A24})$$

We now take the second term on the right-hand side of this last expression:

$$\begin{aligned} \sum_{n=2}^\infty \frac{1}{n^s(n^2-1)} &= \frac{1}{3 \times 2^s} + \frac{1}{8 \times 3^s} \dots \\ &\leq \frac{1}{3} \sum_{n=2}^\infty \frac{1}{n^s} = \frac{1}{3}(\xi(s)-1). \end{aligned} \quad (\text{A25})$$

Hence,

$$\sum_{n=2}^\infty \frac{n^2}{n^s(n^2-1)} \leq \frac{4}{3}(\xi(s)-1). \quad (\text{A26})$$

In order to have a deeper understanding of this approximation we have calculated some *exact* results as well as our expression. The relative error between these two cases has also been carried out. This has been done for three different values of s , as the table below shows. The choice for these values of s has been done in terms of their relevance for the final energy expression. It is readily seen that the relative error decreases as s grows, it goes from, approximately, 10% to 2%.

Parameter s	$\sum_{n=2}^\infty \frac{n^2}{n^s(n^2-1)}$	$\frac{4}{3}(\xi(s)-1)$	Relative error
$s = 5/2$	0.411 992 20	0.455 316 4	0.105 157 82
$s = 4$	0.105 065 93	0.109 764 3	0.044 718 588
$s = 5$	0.047 943 09	0.049 237 1	0.026 990 330

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