Investigations on the Minimal-Length Uncertainty Relation

Sándor Zoltán Benczik

Dissertation submitted to the
Faculty of the Virginia Polytechnic Institute and State University
in partial fulfillment of the requirements for the degree of

Doctor of Philosophy
in
Physics

Lay Nam Chang, Chair
Peter Haskell
Mark Pitt
Tatsu Takeuchi
Uwe Täuber

January 22, 2007
Blacksburg, Virginia

Keywords: Minimal length, uncertainty relation, UV/IR mixing.

Investigations on the Minimal-Length Uncertainty Relation

Sándor Zoltán Benczik

Abstract

We consider a modified non-relativistic quantum mechanics, where the position and momentum operators satisfy a non-standard commutation relation of the form $[X_i, P_j] = i\hbar\{(1 + \beta P^2) + \beta' P_i P_j\}$. Such a theory incorporates an absolute minimal length, UV/IR mixing, and non-commutative position space. The possible representations in terms of differential operators are analyzed, and their equivalence to first order is established.

Simple quantum systems, namely the harmonic oscillator, the Coulomb potential and the gravitational well are studied in one of these representations, the pseudo-position one, and results are compared to previously published results. The Coulomb potential is also analyzed by an alternative analytical/numerical method. A constraint of ~ 3 GeV on the scale of the parameters β, β' is obtained from precision experimental data on the atomic hydrogen energy levels.

This work was partially supported by the US Department of Energy grant DE-FG05-92ER40709.

To Gilia

Acknowledgements

First and foremost, my thanks are due to my advisor, Lay Nam Chang, who with his expertise and attention to both detail and the big picture, provided invaluable guidance for my research, all the while being so friendly and straightforward that during our discussions I felt like talking to a fellow graduate student. The material presented here could not have been developed without his assistance.

A considerable part of this work was researched in collaboration with Tatsu Takeuchi and Djordje Minic, and discussions with them and other members of the IPPAP greatly benefitted the entire dissertation. Joseph Slawny provided me with the material leading to the Coulomb numerical simulations.

I would like to thank my committee members for reading the manuscript and interesting observations; they and other faculty members are responsible for the most of the physics I know today.

On a personal note, I would like to acknowledge Chris Thomas going above and beyond her duties in her help in managing bureaucracy and life in the US; also my Blacksburg friends, many of them members of the Hungarian Student Association for making free time pleasant at Virginia Tech.

It is impossible not to mention the moral support I received in many various ways from my family in my quest. I am indebted to my parents for supporting me for years during my studies. My sister helped in varied things ranging from countless discussions, through invaluable help with the graphics, to providing temporary housing for the "two weeks" that turned into a semester. Above all, my thanks go to my wife Gilia for her unwavering love and enduring the separation during my endeavour. This dissertation is dedicated to her.

Contents

List of Figures

Chapter 1

General considerations on quantum theories with minimal length

1.1 Motivation

In usual quantum mechanics, physical observables are described by operators acting on the Hilbert space of states. The most fundamental ones, the position operator $\hat{x}$ and momentum operator $\hat{p}$ satisfy the canonical commutation relation

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar, \tag{1.1}$$

where $\hbar$ is Planck's constant. As a consequence, for the position and momentum uncertainties Δx and Δp of a given state, the Heisenberg uncertainty relation holds:

$$\Delta x \geq \frac{\hbar}{2}\frac{1}{\Delta p}. \tag{1.2}$$

An important consequence is that in order to probe arbitrarily small length-scales, one has to use probes of sufficiently high energy, and thus momentum. This is the principle on which all our accelerators are based. While gravity (and technological and monetary constraints) are neglected, there is in principle no limit to researching smaller and smaller distances using beams of ever increasing energies.

There are reasons to believe, that at high energies, when gravity becomes important, this is no longer true. Namely, increasing a collision's energy above the Planck scale, the extreme energy concentration in a small space will create a black hole with an event horizon behind which we cannot see. It is not unreasonable to suppose that this is not a lack of our experimental sophistication, but nature possesses an absolute *minimal length*.

The formed black hole will evaporate through Hawking radiation. Moreover, the higher the energy of our collision, the heavier the created black hole, and the less energetic the Hawking radiation will be. This is a form of the anticipated *UV/IR correspondence*: high (ultraviolet) energies correspond to low (infrared) ones.

To express this more quantitatively (see e.g. the review [30]), we can imagine trying to probe the transplanckian distance d using energy of order $E \sim 1/d$. A black hole will form, with event horizon radius of $R_S \sim EG \sim G/d$ and temperature of $T \sim 1/R_S \sim d/G$. As a result, the emitted thermal radiation will have a dominant wavelength increasing with the energy of the probing particle, and for transplanckian energies the scale probed is no longer the usual $d \sim 1/E$, but rather $d \sim EG$. It is natural that between the two regimes there will be a minimal observable length.

So far, attempts to incorporate gravity into relativistic quantum field theory run into problems, because taking into account smaller and smaller length-scales yields infinite results. A hypothetical minimal length could serve as a cutoff for a quantum gravity and remove the infinities. Also, research suggests that the position operators corresponding to different coordinates – unlike in ordinary quantum mechanics – will no longer commute in a consistent quantum theory of gravity.

It should be noted that all arguments predict a minimal length which is on a scale comparable to the Planck length, and such the energies involved in probing them are way beyond what we can produce on Earth today. However, there is the possibility that nature possesses large extra dimensions [4, 22, 23]. In such scenarios, the Planck scale and minimal length might be within experimental reach in future accelerators, such as the Large Hadron Collider, under construction at CERN in Geneva, Switzerland, or at the planned International Linear Collider.

Even if large extra dimensions will not be confirmed in the near future and even without a complete theoretical description of quantum gravity, one can gain considerable insight studying a low energy theory incorporating a minimal length. In the first part we will study the possibly simplest modification of quantum mechanics to have the features mentioned, and in the second, apply it to simple quantum mechanical systems and use today's precision data in order to place bound on the minimal length scale.

1.2 The minimal-length uncertainty relation in one dimension

We will mainly investigate the consequences of the following minimal-length relation: [16]

$$[X, P] = i\hbar(1 + \beta P^2), \tag{1.3}$$

where β is a small parameter of dimension of inverse momentum squared. While we will assume that this form is exact, it can also be interpreted as a first order expansion of a relation of the form

$$[X, P] = i\hbar f(P), \tag{1.4}$$

where $f(P)$ is some function, about which it can be naturally assumed that $f(P) \to 1$ as $P \to 0$, (to recover the usual commutation relation in the low-energy limit), and it is positive.

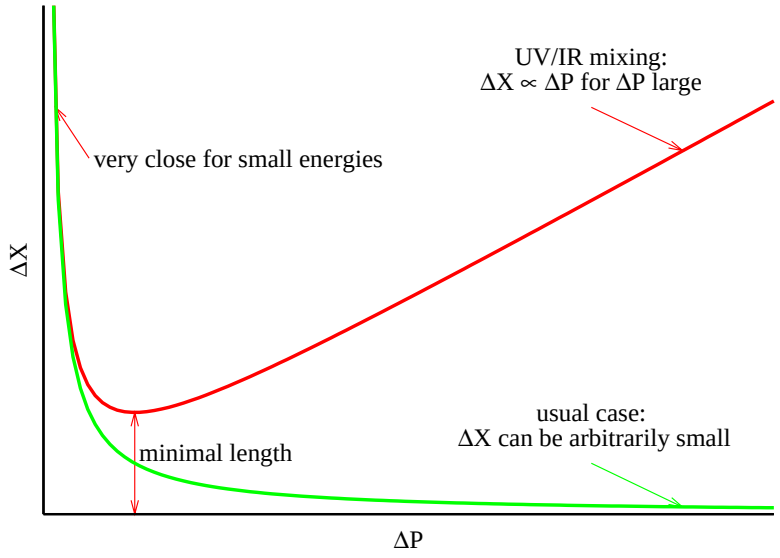

Figure 1.1: *The region allowed by the uncertainty relation is the one above the green line for the standard case and above the red line for the minimal-length case* (1.3)

Under these assumptions, f will have its Taylor expansion around $P = 0$ of the form

$$f(P) = 1 + \beta P^2 + O(P^4), \tag{1.5}$$

so (1.3) will describe to first order the most natural class of possible modifications of the standard commutation relations.

The form of the minimal length relation chosen is motivated *a posteriori* by the uncertainty relation deduced from it. Using the Cauchy-Bunyakovski-Schwartz inequality for a quantum state, the uncertainty relation will read [16]

$$\begin{aligned} \Delta X \Delta P &\geq \frac{\hbar}{2}\left[1 + \beta(\Delta P)^2 + \beta \langle P \rangle^2\right] \\ &\geq \frac{\hbar}{2}\left[1 + \beta(\Delta P)^2\right]. \end{aligned} \tag{1.6}$$

The allowed values for ΔX, ΔP pairs are those situated above the red curve plotted in figure 1.1. We can see that for small momenta $\Delta P \sim \langle P \rangle \sim 0$, the terms involving β can be neglected, and the position uncertainty has the usual behavior

$$\Delta X \gtrsim \frac{\hbar}{2}\frac{1}{\Delta P}. \tag{1.7}$$

In turn, for large values of ΔP, the position uncertainty will satisfy

$$\Delta X \gtrsim \frac{\hbar\beta}{2}\Delta P, \tag{1.8}$$

in concordance with the UV/IR mixing mentioned above.

Moreover, it transpires that we have a minimal position uncertainty of a state of

$$\Delta X \geq \hbar\sqrt{\beta}\big(1+\beta\,\langle P\rangle^2\,\big), \tag{1.9}$$

and an absolute minimum uncertainty of

$$\Delta X \geq \Delta X_{\min} = \hbar\sqrt{\beta}. \tag{1.10}$$

1.3 The uncertainty relation in multiple dimensions

When dealing with more than one dimensions $D > 1$, (1.3) can be generalized tensorially to the form [16]

$$[X_i, P_j] = i\hbar\{\delta_{ij}(1+\beta P^2) + \beta' P_i P_j\}. \tag{1.11}$$

The additional parameter β', with units of inverse momentum squared is again assumed to be small.

With such commutation relations we can no longer assume that both position operators on one hand, and momentum operators, on the other, commute among themselves. The reason for this is that the positions and momenta need to satisfy the Jacobi identity

$$\big[[A,B],C\big] + \big[[C,A],B\big] + \big[[B,C],A\big] = 0, \qquad \forall A,B,C \in \{X_i, P_j\}_{i,j} \tag{1.12}$$

which is necessary for the existence of a representation of the observables as linear differential operators acting on some function space.

As the right-hand side of (1.11) depends explicitly on the momentum operators P_i, it is convenient to assume that they commute,[1]

$$[P_i, P_j] = 0. \tag{1.13}$$

Then the following Jacobi identities involving at least 2 momenta,

$$\big[[P_i, P_j], P_k\big] + \text{circ. perm.} = 0 \tag{1.14}$$

$$\big[[P_i, P_j], X_k\big] + \text{circ. perm.} = 0 \tag{1.15}$$

are automatically satisfied.

From the condition

$$\big[[X_i, X_j], P_k\big] + \text{circ. perm.} = 0 \tag{1.16}$$

one can obtain the commutator of positions up to a term depending on momenta only. It is given by:

$$[X_i, X_j] = \frac{(2\beta-\beta') + (2\beta+\beta')\beta P^2}{1+\beta P^2}\,(P_i X_j - P_j X_i) + f(P_1,\ldots,P_D) \tag{1.17}$$

[1] While this is a just a simplifying choice here, we will see later in Section 1.6 that it is a quite natural assumption.

If one assumes that the P-dependent function f is null, the final Jacobi identity, involving position operators only, is automatically satisfied. While the vanishing of f is sufficient for having a well-defined Heisenberg algebra, it is not obvious if, for arbitrary dimensions, this condition is also necessary. For example, in 3 dimensions, on tensorial considerations alone, a term proportional to

$$\epsilon_{ijk} P_k \, g(P^2) \tag{1.18}$$

is allowed on the right hand side for the commutator $[X_i, X_j]$. This term is odd under the parity transformation $X_i \to -X_i$, and $P_i \to -P_i$. So including this term would have meant that we believe the interactions giving rise to minimal lengths intrinsically violate parity conservation. That is an intriguing possibility, but we will not consider it here; we will assume that the P-dependent function f always vanishes.

The important point is that the position operators for different coordinates can no longer commute and we deal with a non-commutative Heisenberg algebra.[2] It should be noted that this is an extra feature of the theory (not a bug, as a well-known software company would say), as most theories of quantum gravity seem to incorporate non-commutativity in some way.

In summary, the complete set of commutation relations read

$$[X_i, P_j] = i\hbar\{\delta_{ij}(1 + \beta P^2) + \beta' P_i P_j\}, \tag{1.19}$$

$$[P_i, P_j] = 0, \tag{1.20}$$

$$[X_i, X_j] = \frac{(2\beta - \beta') + (2\beta + \beta')\beta P^2}{1 + \beta P^2} \, (P_i X_j - P_j X_i). \tag{1.21}$$

The modification considered here does not destroy rotational invariance. More exactly, the operators

$$L_{ij} = \frac{1}{1 + \beta P^2} \, (X_i P_j - X_j P_i) \tag{1.22}$$

are generators of rotation. That is, they satisfy (see Appendix A.1)

$$[X_i, L_{jk}] = i\hbar(\delta_{ik} X_j - \delta_{ij} X_k), \tag{1.23}$$

$$[P_i, L_{jk}] = i\hbar(\delta_{ik} P_j - \delta_{ij} P_k), \tag{1.24}$$

and

$$[L_{ij}, L_{kl}] = i\hbar(\delta_{ik} L_{jl} + \delta_{jl} L_{ik}. - \delta_{il} L_{jk} - \delta_{jk} L_{il}). \tag{1.25}$$

This is very useful when dealing with systems with rotational symmetry.

[2]This type of non-commutativity should not be confounded with the more usual $[X_i, X_j] = \theta_{ij}$, investigated in detail by both the mathematics and physics community (see e.g. [25] and/or the impressive book by Connes [10]). There the commutator is equal to a c-number θ_{ij}, while in our case to an operator.

1.4 Other forms of minimal-length uncertainty relations

It should be noted that the uncertainty relations considered are not unique; several forms, more or less different, have been considered in the existing literature.

Early papers Apparently the first articles to present a theory with quantized space-time are due to Snyder [26, 27] and Yang [31]. The relative age of these papers, from the late 1940's, is not surprising as their intention was to find a way to remove the infinite results plaguing the early stages in the development of quantum field theory. The renormalization program for Yang-Mills theories provided an alternative way to resolve these problems for the electro-weak and strong interactions, but did not help in quantum gravity, which cannot be renormalized.

In [27], Snyder considers a de Sitter space, with real coordinates $\{\eta_0, \eta_1, \eta_2, \eta_3, \eta_4\}$ satisfying

$$-\eta^2 = \eta_0^2 - \eta_1^2 - \eta_2^2 - \eta_3^2 - \eta_4^2, \tag{1.26}$$

and defines the position and time operators by

$$X_i = ia\left(\eta_4 \frac{\partial}{\partial \eta_i} - \eta_i \frac{\partial}{\partial \eta_4}\right), \qquad i = 1, 2, 3, \tag{1.27}$$

$$T = \frac{ia}{c}\left(\eta_4 \frac{\partial}{\partial \eta_0} + \eta_0 \frac{\partial}{\partial \eta_4}\right), \tag{1.28}$$

acting on a functions of variables $\eta_0, \ldots, \eta_4$, and where a is a natural unit of length, and c is the speed of light. The spectrum of each position operator is discrete, but the theory is Lorentz invariant in the following sense: every linear transformation $(X_i, T) \mapsto (X_i', T')$ that leaves the quadratic form $c^2T^2 - X_1^2 - X_2^2 - X_3^2$ invariant, leaves the operators' spectrum invariant, too.

In addition, the energy and momentum operators are defined as

$$P_i = \frac{\hbar}{a}\left(\frac{\eta_i}{\eta_4}\right), \tag{1.29}$$

$$P_T = \frac{\hbar}{a}\left(\frac{\eta_0}{\eta_4}\right), \tag{1.30}$$

thus the commutators between positions and momenta are given by

$$[X_i, P_i] = i\hbar\left(1 + \frac{a^2}{\hbar^2}P_i^2\right), \tag{1.31}$$

$$[X_i, P_j] = i\hbar\left(\frac{a^2}{\hbar^2}P_i P_j\right). \tag{1.32}$$

This algebra described by Snyder corresponds to our minimal length commutation relation with $\beta = 0$ and $\beta' = (a/\hbar)^2$.

Modified de Broglie relation To incorporate a minimal length scale L_f in their theory, in [12] and subsequent papers, Hossenfelder et al. start out by postulating a non-standard relation between the momentum and wavelength (and thus wave number) of a particle of the form

$$k = k(p), \tag{1.33}$$

where $k(p)$ is an odd function that is close to linear for small values of p, and asymptotically approaches some upper limit $M_f \sim 1/L_f$ for large ones. Such a function will have the small p expansion

$$k(p) = p - \gamma \frac{p^3}{M_f^2}, \tag{1.34}$$

where γ is a unitless coefficient of order one that depends on the exact form of the function $k(p)$, which is not determined from first principles. Postulating canonical commutation relations between x and k, this leads to a generalized uncertainty principle of the form

$$\Delta x \Delta p \geq \frac{\hbar}{2} \left| \left\langle \frac{\partial p}{\partial k} \right\rangle \right| = \frac{\hbar}{2} \left(1 + \gamma \frac{\langle \hat{p}^2 \rangle}{M_f^2} \right), \tag{1.35}$$

and a generalized commutation relation

$$[\hat{x}, \hat{p}] = i \frac{\partial p}{\partial k} = i\hbar \left(1 + \gamma \frac{\hat{p}^2}{M_f^2} \right). \tag{1.36}$$

This is just (1.3) with $\beta = \gamma / M_f^2$.

A minimal momentum also? One problem of the minimal length commutation relation (1.11), even if an aesthetic one, is that it destroys the symmetry between the position and momentum in the Hamiltonian formalism. Indeed, it is possible that nature possesses not only a minimal length, but also a minimal momentum. This can be possible if there held an uncertainty relation of the form

$$\Delta X \Delta P \geq \frac{\hbar}{2} \big(1 + \alpha (\Delta X)^2 + \beta (\Delta P)^2 \big). \tag{1.37}$$

To obtain such an expression, the commutator $[X_i, P_j]$ would need to depend not only on momentum P but also position X. For example, Kempf in [14] considered

$$[X_i, P_j] = i\hbar \delta_{ij} (1 + \alpha X^2 + \beta P^2), \tag{1.38}$$

where the small parameter α has the dimension of inverse length squared, and β that of inverse momentum squared. Obviously this is not the most general tensorial form for arbitrary dimensions. One can include $X_i X_j$ and $P_i P_j$ terms and even crossed ones.

The analysis of such theories is further complicated by the fact that in general neither position nor momentum operators can commute among themselves, and thus there is no representation in which either set is diagonal. Consequently, there are few results pertaining to them. [14, 21]

Alternative approaches with minimal length It should be mentioned that postulating non-standard commutation relations between the position and momentum operators is not the only way to define a theory with minimal length. Two approaches seem to be especially promising.

First, the doubly relativistic Lorentz group studied by Amelino-Camelia [3] and collaborators centers on the group of transformations that have two invariants. In addition to the constant speed of light, it also assumes a constant minimal length.

Second, Padmanabhan and his collaborators [20, 28] study a modified quantum theory by postulating that the path integral is invariant under a duality transformation of the form $x \to L_f^2/x$. This, again, yields a minimal length L_f.

1.5 Differential operator representations

In the following we will look at the representations in terms of differential operators of the minimal-length commutation relations (1.19)–(1.21), [16]

$$[X_i, P_j] = i\hbar\{\delta_{ij}(1+\beta P^2) + \beta' P_i P_j\}, \tag{1.39}$$

$$[P_i, P_j] = 0, \tag{1.40}$$

$$[X_i, X_j] = \frac{(2\beta - \beta') + (2\beta + \beta')\beta P^2}{1+\beta P^2}\,(P_i X_j - P_j X_i). \tag{1.41}$$

While quantum mechanical problems in this context can sometimes be solved by an elegant algebraic approach, for example by introducing ladder operators in the case of harmonic oscillator [15], or by SUSYQM factorization [21], this is not always possible.

The fail proof method, not unlike in regular quantum mechanics, seems to be finding a representation of the operators X_i, P_j in terms of self-adjoint differential operators acting on some Hilbert space of functions. Various papers, treating quantum mechanical systems either analytically or perturbatively, have used quite a number of different representations. The common characteristic, though usually not explicitly stated, is that the representation can be found by a two-step process. First, the operators X_i, P_j are expressed in terms of some operators x_i, p_j that satisfy the commutation relations of the canonical Heisenberg algebra,

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}, \qquad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0. \tag{1.42}$$

Second, for the commutative x_i, p_j, one can use either the momentum representation

$$\hat{x}_i = i\hbar\frac{\partial}{\partial p_i}, \qquad \hat{p}_i = p_i, \tag{1.43}$$

acting on functions of variable p, or the position one

$$\hat{x}_i = x_i, \qquad \hat{p}_j = \frac{\hbar}{i}\frac{\partial}{\partial x_j}, \tag{1.44}$$

acting on functions of variable x.

To differentiate between the two sets of operators, X_i, P_j on one hand, and $\hat{x}_i, \hat{p}_j$ on the other, in this thesis we will always denote noncommutative variables with capital letters, and the *underlying* canonical/commutative ones by lowercase ones. We will also omit the "hat"s from these operators from now on. We will call a particular way of expressing the noncommuting operators in terms of commuting ones a *reduction*.

It should also be mentioned that the physical observables are the non-commuting, "uppercase" ones. The commuting operators are just helper variables; we will see that they depend on the reduction chosen, and one should resist the temptation of assigning them general physical meaning. This should be kept in mind, even when for simplicity we use the terms "underlying position" or "underlying momentum" for them.

Let us review the reductions used so far in the literature, their domain of usability and relative strengths.

The Kempf reduction and momentum representation The original reduction, defined in paper [16] that introduced the form of the commutation relations considered here, is the *Kempf reduction*[3]

$$X_i = x_i + \beta \, \frac{p^2 x_i + x_i p^2}{2} + \beta' \, \frac{p_i p_j x_j + x_j p_i p_j}{2}, \tag{1.45}$$

$$P_i = p_i. \tag{1.46}$$

It can be said that this reduction is somehow the most natural; its expression follows closely the one for the commutation relation $[X_i, P_j]$. The only difference is that on the right hand side the order of operator products is symmetrized. This is done to ensure that, at least formally, the non-commutative operators are self-adjoint.

We will call *momentum representation* this reduction together with a momentum-diagonal representation of the underlying momentum p,

$$x_i = i\hbar \frac{\partial}{\partial p_i}, \qquad p_i = p_i, \tag{1.47}$$

as used first in [16]. Explicitly, it is

$$X_i = i\hbar \left[(1 + \beta p^2) \frac{\partial}{\partial p_i} + \beta' p_i p_j \frac{\partial}{\partial p_j} + \left(\beta + \frac{D+1}{2} \, \beta' \right) p_i \right] , \tag{1.48}$$

$$P_i = p_i \, . \tag{1.49}$$

[3]Two unwritten, but all too often experimentally verified laws of giving name to stuff in exact sciences are that (1) a formula is hardly ever is named after its original inventor, and (2) the same term will mean completely different things when used by a mathematician and a physicist. The only reason I assign names here, in spite of these laws and contrary to my best judgment, is that referring to five different representations by their equation number alone would make the thesis impossible to follow. I do apologize if I failed to give credit where it was due, and for using the expression "reduction" here without any relation to the reduction of, say, Poisson manifolds as used in mathematics.

Refs. [6, 9] also use a closely related representation. There, the operators' expressions are

$$X_i = i\hbar \left[(1+\beta p^2)\frac{\partial}{\partial p_i} + \beta' p_i p_j \frac{\partial}{\partial p_j} + \bar{\gamma}\, p_i \right] , \tag{1.50}$$

$$P_i = p_i \ , \tag{1.51}$$

where $\bar{\gamma}$ is an arbitrary parameter, and the operators are acting on the Hilbert space of functions normalizable with respect to the inner product

$$\langle f|g\rangle_\delta = \int \frac{d^D\mathbf{p}}{[1+(\beta+\beta')p^2]^\delta}\, f^*(\mathbf{p})\, g(\mathbf{p}) \ , \tag{1.52}$$

with

$$\delta = \frac{\beta + \beta'\left(\frac{D+1}{2}\right) - \bar{\gamma}}{\beta+\beta'} \ . \tag{1.53}$$

This reduces to the momentum representation for

$$\bar{\gamma} = \bar{\gamma}_0 := \beta + \beta'\left(\frac{D+1}{2}\right), \tag{1.54}$$

in which case the weight function of the inner product has vanishing exponent $\delta = (\bar{\gamma}_0 - \bar{\gamma})/(\beta+\beta')$, and thus it simplifies to unity.

This apparent generality given by the extra $\bar{\gamma}$ term turns out to be unimportant. Indeed, we can observe at first that $\bar{\gamma}$ can be supposed to be real. Any complex part can be transformed away using a canonical transformation of the form $P_i \mapsto P_i, X_i \mapsto X_i + \gamma P_i$. (See Appendix A.2.)

For real $\bar{\gamma}$, and corresponding δ given by (1.53), one can define $\mathcal{A}$ to be the multiplication operator by $[1+(\beta+\beta')p^2]^{\delta/2}$,

$$\tilde{\psi}(p) \mapsto \mathcal{A}\tilde{\psi}(p) = [1+(\beta+\beta')p^2]^{\frac{\delta}{2}}\tilde{\psi}(p) = \psi(p) \tag{1.55}$$

It is easy to see that a function $\bar{\psi}(p)$ is normalizable under the canonical inner product $\langle\cdot,\cdot\rangle_0$, if and only if $\psi(p) = \mathcal{A}\tilde{\psi}(p)$ is normalizable under $\langle\cdot,\cdot\rangle_\delta$. Thus, the operator A is an isomorphism between the function spaces of physical states defined by the two inner products.

Moreover, $\mathcal{A}$ obviously commutes with the momenta P_i, and for the position operators X_i, it can be verified using (1.50) that

$$X_i\mathcal{A}\tilde{\psi}(p) = X_i\psi(p) = \mathcal{A}\left(\tilde{X}_i\tilde{\psi}(p)\right), \tag{1.56}$$

where

$$\begin{aligned}\tilde{X}_i &= X_i + i\hbar\delta(\beta+\beta')p_i \\ &= i\hbar\left[(1+\beta p^2)\frac{\partial}{\partial p_i} + \beta' p_i p_j\frac{\partial}{\partial p_j} + \left(\bar{\gamma} + \delta(\beta+\beta')\right)p_i\right] \\ &= i\hbar\left[(1+\beta p^2)\frac{\partial}{\partial p_i} + \beta' p_i p_j\frac{\partial}{\partial p_j} + \bar{\gamma}_0\, p_i\right],\end{aligned} \tag{1.57}$$

is just the position operator corresponding to $\bar{\gamma}_0$! This shows that the representation (1.50)–(1.51) with arbitrary $\bar{\gamma}$ is equivalent to the momentum representation through the simple change of variable

$$\psi(p) = [1 + (\beta + \beta')p^2]^{\frac{\delta}{2}} \tilde{\psi}(p). \tag{1.58}$$

In calculational terms this means that, when explicitly trying to solve the differential Scrödinger equation, such a change of variable removes any $\bar{\gamma}$ dependence. An example of this happening appears in [9].

Given the complete equivalence of the members of the family (1.50)–(1.51), the only reason to use any one of them would be if some particular choice of $\bar{\gamma}$ simplified considerably one's calculations, e.g. when $\bar{\gamma} = 0$. Unless this is the case, we will work in the momentum representation, with $\bar{\gamma} = \bar{\gamma}_0 = \beta + \beta'(D+1)/2$, where the position operator is explicitly symmetric and thus formally self-adjoint, and the inner product is the canonical one.

The pseudo-position representation So far we considered the momentum representation of the Kempf reduction (1.45)–(1.46); its main advantage is that the modified momentum and thus the kinetic energy is the same as in the regular quantum mechanics case. The obtained eigenfunctions $\psi(p)$ are in the momentum representation and the variable p can be identified with the momentum of the system. Moreover it is exact, unlike some we will see later.

Its main drawback is that all the complexity arising from the minimal length is contained in the expression for the position operators and thus the potential term of the Schrödinger equation. This can lead to difficulties when the potential depends in a not too straightforward manner on the position operators. For example, in the case of the Coulomb potential, the inverse square root of the operator $X_1^2 + \cdots + X_D^2$ and, in the case of the gravitational well, the condition $X_i > 0$ cannot be expressed easily in terms of the linear differential operators given by (1.50).

In such cases the *pseudo-position* representation can help. This is just the Kempf reduction (1.45)–(1.46), where the underlying variables are expressed in the basis where the underlying position operator is diagonal,

$$x_i = x_i, \qquad p_j = \frac{\hbar}{i}\frac{\partial}{\partial x_j}. \tag{1.59}$$

The pseudo-position representation shifts some of the complexities from the position operator (potential energy) to the momenta (kinetic energy). In exchange it is neither momentum-diagonal, nor position-diagonal as long as the physical variables X_i, P_i are concerned. It only becomes position diagonal in the limiting case when the minimal length parameter $\beta + \beta'$ vanishes. This makes it convenient to use in problems that lend themselves to the position representation in regular quantum mechanics. In such cases, perturbation in the small parameter $\beta + \beta'$ can be used around the regular case.

Similarly to the momentum representation, there is the possibility of an apparently more general representation containing an extra $\bar{\gamma}$-dependent term, of the form

$$\begin{aligned} X_i &= \hat{x}_i(1+\beta\hat{p}^2) + \beta'\hat{x}_j\hat{p}_j\hat{p}_i + \bar{\gamma}p_i, \\ P_i &= \hat{p}_i, \end{aligned}$$

where x_i are diagonal. Such a representation was used in [5], with $\bar{\gamma} = 0$. Again, while this representation is not incorrect, we will refrain from using it in the favor of the explicitly symmetric pseudo-position representation, on a Hilbert function space with canonical inner product.

The Brau reduction The commutators taken between different components of the position X_i have an interesting property: when the minimal-length parameters are such that $\beta' = 2\beta$, then they vanish to first order in β and β'. This choice of parameters has theoretical advantages in that it simplifies the way a translation operator can be defined. [15]

For this particular case, there is a very simple reduction of the form

$$X_i = x_i, \tag{1.60}$$
$$P_i = p_i(1+\beta p^2), \tag{1.61}$$

usually used in the case when the underlying positions are diagonal. For this reduction, defined first in [7], we will use the name *Brau reduction*.

It should be noted that this representation is only correct to the first order in $\beta = 2\beta'$. However, to this order it is position-diagonal. It is particularly convenient for doing perturbation theory around regular position-space eigenfunctions of some systems. Suppose we deal with a Hamiltonian of the general form

$$H = \frac{P^2}{2m} + V(X), \tag{1.62}$$

and we know the exact solution for the $\beta = 0$ case corresponding to $H_0 = p^2/2m + V(x)$. Then, the perturbing potential is simply

$$\begin{aligned} H' &= H - H_0 \\ &= \frac{P^2}{2m} - \frac{p^2}{2m} \\ &= \frac{\beta}{m}p^4 + O(\beta^2). \end{aligned} \tag{1.63}$$

For potentials that are homogeneous of order h, this can be simplified further using the virial theorem, according to which the expectation value of the potential energy with respect to an eigenstate with energy E_n is given by

$$\langle\psi_n|V(x)|\psi_n\rangle = \frac{h}{h+2}E_n. \tag{1.64}$$

Using the Schrödinger equation, the correction to the energy levels then can be expressed as

$$\begin{aligned}\Delta E_n &= \langle H' \rangle \\ &= 4\beta m \left\langle (E_n - V(x))^2 \right\rangle \\ &= 4\beta m \left[\left(\frac{2-h}{2+h} \right) E_n^2 + \left\langle V^2(x) \right\rangle \right].\end{aligned} \tag{1.65}$$

This way, obtaining the energy corrections reduces to the simple problem of calculating the expectation value of the square of the potential energy. This was applied in [7, 8] for the harmonic oscillator, Coulomb potential and the gravitational well.

It should be noted though, that the representation's being correct to first order only can have serious consequences on the obtained results. We will see later, that for the Coulomb potential, the higher order terms can have an effect that should be taken into account.

The general first order reduction family One might be tempted to prescribe the odd behavior of the Brau representation, which corrects the kinetic term instead of the potential ones, to some quirk of the case $\beta' = 2\beta$. It turns out this is not the case.

In [29], Stetsko and Tkatchuk introduced a representation which satisfies the minimal-length commutation relations (1.19)–(1.21) up to first order in β, β' and generalizes the Brau representation for $\beta' \neq 2\beta$. It is given by

$$X_i = x_i + \frac{2\beta - \beta'}{4}(p^2 x_i + x_i p^2), \tag{1.66}$$

$$P_i = p_i \left(1 + \frac{\beta'}{2} p^2 \right). \tag{1.67}$$

Even more generally, we can consider a family of representations with parameter γ,

$$X_i = x_i + (\beta - \gamma) \frac{p^2 x_i + x_i p^2}{2} + (\beta' - 2\gamma) \frac{p_i p_j x_j + x_j p_i p_j}{2}, \tag{1.68}$$

$$P_i = p_i \left(1 + \gamma p^2 \right). \tag{1.69}$$

This *general first order reduction family* generalizes all reductions met so far. It becomes

- the Kempf reduction, (1.45)–(1.46), for $\gamma = 0$;
- the Stetsko-Tkatchuk reduction, (1.66)–(1.67), for $\gamma = \beta'/2$; and
- the Brau reduction, (1.60)–(1.61), for $\gamma = \beta = \beta'/2$.

This proliferation of representations raises several questions. Are these the only representations correct to first order? Are the energy eigenvalues representation-dependent, in particular dependent on the parameter γ?

In this context a general investigation on the expressing of non-commutative operators satisfying minimal-length commutation relations, through underlying commuting variables is certainly warranted. As we will see in the following sections, the answers to the above questions, fortunately, turn out to be negative.

1.6 Reduction of noncommutative variables to commutative ones

Let us consider some Heisenberg algebra of the type (1.19)–(1.21), which introduces a single fundamental parameter ξ^2, with dimension of inverse momentum squared. In the case studied here, this parameter is $\xi^2 = \beta + \beta'$, but the following considerations apply generally, and can be particularized to other Heisenberg algebras easily.

On dimensional basis, the operator X_i will be a sum of terms, that are equal to an underlying position operator x_j, with some index j, multiplied by a dimensionless function. This function can depend on $\xi^2 p_k p_\ell$ only. Note that the index of the x_j operator is not necessarily equal to i, but if it is not, it has to be paired with some p operator's index. To make the indices right, X_i will have the form:

$$X_i = S[x_i G_X(\xi^2 p^2) + x_k(\xi^2 p_k p_i) H_X(\xi^2 p^2)], \tag{1.70}$$

with some reasonably well-behaved functions G_X, H_X. Here $S[\,.\,]$ indicates symmetrization, which should be carried out to make X_i self-adjoint. Similarly, P_j will be given by

$$P_j = p_j F_P(\xi^2 p^2), \tag{1.71}$$

with some function F_P. Note that from this point of view, the vanishing of the commutators of different momenta arises naturally from the fact that P_j does not depend on the underlying position operator; it is no longer a simplifying assumption.

In order to recover in the limit $\xi^2 \to 0$ the usual, commutative algebra, we must impose that

$$G_X(0) = F_P(0) = 1. \tag{1.72}$$

For particular Heisenberg algebras one might also need to impose some conditions on the functions G_X, H_X and F_P, such as positivity or being defined on the whole positive semi-axis to avoid strange effects. Expressing these as general conditions can be complicated, so we will impose only (1.72) and eliminate the unphysical solutions as they arise.

Using that

$$[x_i, f(p)] = i\hbar \frac{\partial f}{\partial p_i}, \qquad [p_j, g(x)] = -i\hbar \frac{\partial g}{\partial x_j}, \tag{1.73}$$

the commutator of X_i and P_j can be calculated

$$\begin{aligned}\frac{[X_i,P_j]}{i\hbar} &= \frac{1}{i\hbar}\big[x_i G_X(\xi^2p^2)+\xi^2 x_k p_k p_i H_X(\xi^2p^2),\, p_j F_P(\xi^2p^2)\big]\\ &= \frac{\partial[p_jF_P(\xi^2p^2)]}{\partial p_i}\,G_X(\xi^2p^2)+\xi^2p_kp_i\frac{\partial[p_jF_P(\xi^2p^2)]}{\partial p_k}\,H_X(\xi^2p^2)\\ &= \delta_{ij}\,F_P(\xi^2p^2)G_X(\xi^2p^2)\\ &\quad+\xi^2p_ip_j\,[2F_P'(\xi^2p^2)G_X(\xi^2p^2)+F_P(\xi^2p^2)H_X(\xi^2p^2)+2\xi^2p^2F_P'(\xi^2p^2)H_X(\xi^2p^2)]\end{aligned} \tag{1.74}$$

Particularizing to our position/momentum commutation relation, (1.19), this should equal

$$\begin{aligned}\frac{[X_i,P_j]}{i\hbar} &= \delta_{ij}(1+\beta P^2)+\beta' P_iP_j\\ &= \delta_{ij}\,[1+\eta\,\xi^2p^2F_P^2(\xi^2p^2)]+\xi^2p_ip_j\,(1-\eta)\,F_P^2(\xi^2p^2),\end{aligned} \tag{1.75}$$

with

$$\eta=\frac{\beta}{\beta+\beta'}. \tag{1.76}$$

Equivalently, $G_X(u), F_P(u)$ and $H_X(u)$, with $u=\xi^2p^2$ should satisfy

$$F_PG_X=1+\eta uF_P^2 \tag{1.77}$$

and

$$2F_P'G_X+F_PH_X+2uF_P'H_X=(1-\eta)F_P^2. \tag{1.78}$$

Any solution of these equations subject to conditions (1.72) will determine a way, — via (1.70) and (1.71), — to reduce the noncommutative variables to commutative ones. We can see that the system is under-determined. In general, any one of the three functions G_X, F_P, H_X can be given and the other two determined from it. Let us look at each in turn.

I. If $F_P(u)$ is given, the other two can be determined in a straightforward way

$$G_X=\frac{1}{F_P}+\eta uF_P, \tag{1.79}$$

$$H_X=\frac{(1-\eta)F_P^3-2F_P'(1+\eta uF_P^2)}{F_P(F_P+2uF_P')}. \tag{1.80}$$

If we choose a constant $F_P(u)$ — which should be equal to unity as $F_P(0)=1$ —, then necessarily

$$G_X(u)=1+\eta u,\qquad H_X(u)=1-\eta, \tag{1.81}$$

which represents the Kempf reduction (1.45)–(1.46).

More generally, one can look for a linear

$$F_P(u) = 1 + \alpha u, \tag{1.82}$$

with some parameter α, which results in

$$G_X(u) = \frac{\eta u(1+\alpha u)^2 + 1}{1+\alpha u}, \tag{1.83}$$

$$H_X(u) = \frac{(1-\eta-2\alpha) + (3-5\eta)\alpha u + (3-7\eta)\alpha^2 u^2 + (1-3\eta)\alpha^3 u^3}{(1+\alpha u)(1+3\alpha u)}. \tag{1.84}$$

The corresponding representation,

$$\begin{aligned} X_i &= x_i[1 + (\beta-\gamma)p^2 + \beta(\beta+\gamma)p^4 + \dots] \\ &\quad + x_k p_k p_i[(\beta' - 2\gamma) + \gamma(8\gamma - 2\beta - \beta')p^2 + \dots], \end{aligned} \tag{1.85}$$

$$P_i = p_i(1+\gamma p^2), \tag{1.86}$$

is just the general first order reduction (1.68)–(1.69) with $\gamma = \alpha\xi^2$. We can see that this is indeed the most general reduction correct to first order, as its name foretold.

Finally, just to sample the variety that can be obtained, if one considers $F_P(u) = e^{\alpha u}$, then

$$G_X(u) = e^{-\alpha u} + \eta u e^{\alpha u}, \tag{1.87}$$

$$H_X(u) = \frac{(1-\eta-2\eta\alpha u)e^{\alpha u} - 2\alpha e^{-\alpha u}}{1+2\alpha u}. \tag{1.88}$$

II. When $G_X(u)$ is given, it can be proven by a rather involved calculation (see Appendix A.3) that the other two defining functions are given by

$$F_P = \frac{G_X - \sqrt{G_X^2 - 4\eta u}}{2\eta u}, \tag{1.89}$$

$$H_X = \frac{4\eta u(1-\eta+G_X' G_X) - (1+\eta)G_X(G_X - \sqrt{G_X^2 - 4\eta u})}{2\eta u(G_X - 2uG_X')}. \tag{1.90}$$

In particular, for $G_X \equiv 1$, one gets

$$F_P(u) = \frac{1-\sqrt{1-4\eta u}}{2\eta u} = 1 + \eta u + 2\eta^2 u^2 + \dots, \tag{1.91}$$

$$H_X(u) = 2(1-\eta) - (\eta+1)\frac{1-\sqrt{1-4\eta u}}{2\eta u} = (1-3\eta) + \eta(1+\eta)u + \dots, \tag{1.92}$$

or

$$X_i = x_i + x_k p_k p_i \left[2\beta' - (2\beta+\beta')\frac{1-\sqrt{1-4\beta p^2}}{2\beta p^2}\right], \tag{1.93}$$

$$P_i = p_i \frac{1-\sqrt{1-4\beta p^2}}{2\beta p^2}. \tag{1.94}$$

This reiterates the important point that the position operators for different directions do not commute. Indeed, if X_i were commuting, we could look for a representation in which $X_i = x_i$ are diagonal. This would correspond to $G_X \equiv 1$ and $H_X \equiv 0$. But setting G_X constant will force a non-zero H_X, and thus noncommuting X_i. We already knew this, but in the approach of this section, the expression $[X_i, X_j]$ was never used!

This leads to one more important observation. The Brau and Stetsko-Tkatchuk representations are correct to first order only. One can safely use them in perturbation theory as long as the higher order terms in the expansion of X_i contribute only higher order corrections to the energy eigenvalues. However, when this is not the case, one should never forget that these higher order terms are always present and they should be taken into account.

III. In general, the most difficult case is when H_X is given. The function G_X can be easily eliminated as

$$G_X = \frac{1}{F_P} + \eta u F_P, \tag{1.95}$$

but F_P will satisfy a differential equation which, in general, cannot be solved analytically.

While it should be clear by now that it is impossible, let us try to force the positions into commuting in yet another way, by imposing $H_X \equiv 0$, akin to the Stetsko-Tkatchuk representation. Then $F_P(u)$ should satisfy the differential equation (1.78),

$$2F_P' \left(\frac{1}{F_P} + \eta u F_P \right) = (1-\eta) F_P^2. \tag{1.96}$$

For $\eta = 1$, (i.e $\beta = 0$), the only solution for $u > 0$ is $F_P'(u) = 0$, or $F_P(u) = \text{const.} = 1$, corresponding to the Kempf reduction, as also treated above. Indeed, in this case the Kempf reduction coincides with the Stetsko-Tkatchuk one.

For $\eta < 1$, eqn. (1.96) is equivalent to the algebraic one

$$u F_P^2 + 1 = (F_P)^{\frac{2}{1-\eta}}. \tag{1.97}$$

The question is whether a solution for this equation exists, and if it does, on *what domain* it can be defined. Then, the solution determines an *exact* reduction,

$$X_i = x_i \, S\left[1 + \frac{2\beta - \beta'}{2} p^2 + \frac{\beta'(6\beta - \beta')}{8} p^4 + \dots \right], \tag{1.98}$$

$$P_i = p_i \left[1 + \frac{\beta'}{2} p^2 + \frac{\beta'(3\beta' - 2\beta)}{8} p^4 + \dots \right], \tag{1.99}$$

which agrees to first order to the Stetsko-Tkatchuk one.

For $\eta = 0$, (i.e. $\beta = 0$), eqn. (1.97) has the solution

$$F_P(u) = \frac{1}{\sqrt{1-u}}, \qquad G_X(u) = \sqrt{1-u}, \tag{1.100}$$

both defined for $u \in [0,1]$ only. That means that (1.99) is convergent only for $p^2 < \frac{1}{\xi^2}$, rather strikingly opposed to our representation, where p can take arbitrary values!

Nevertheless, for $0 < \eta < 1$, $F_P(u)$ is defined for every $u > 0$ and it is increasing as a function of u, and thus defines another exact reduction that agrees with Stetsko-Tkatchuk.

In particular $\eta = \frac{1}{3}$, (i.e. $\beta' = 2\beta$), considered by Brau, eqn. (1.97) is of third order, can be solved exactly and has the real solution

$$\begin{aligned} F_P(u) &= \frac{u^2}{9}\left[\frac{1}{2}\left(1+\frac{2u^3}{27}-\sqrt{1+\frac{4u^3}{27}}\right)\right]^{-1/3} + \frac{u}{3} + \left[\frac{1}{2}\left(1+\frac{2u^3}{27}-\sqrt{1+\frac{4u^3}{27}}\right)\right]^{1/3} \\ &= 1 + \frac{u}{3} + \frac{u^2}{9} + \frac{2u^3}{81} - \dots\,, \end{aligned} \tag{1.101}$$

which seems to be well-defined for every $u > 0$. The corresponding reduction,

$$X_i = x_i(1 + \beta^2 p^4 + \frac{4}{3}\beta^3 p^6 + \dots), \tag{1.102}$$

$$P_i = p_i(1 + \beta p^2 + \beta^2 p^4 + 2\beta^3 p^6 - \dots), \tag{1.103}$$

agrees with Brau's to first order.

As a last example, imposing $H_X \equiv \alpha G_X$, results for $\eta = 1$ in the representation

$$X_i = x_k(\delta_{ij} + \alpha\beta p_k p_i)\frac{1 + (\alpha+1)\beta p^2}{\sqrt{1+\alpha\beta p^2}}, \tag{1.104}$$

$$P_j = \frac{p_j}{\sqrt{1+\alpha\beta p^2}}. \tag{1.105}$$

1.7 First order reductions and perturbation theory

Having shown that the most general reduction, correct to first order is given by the family

$$X_i = x_i + (\beta - \gamma)\,\frac{p^2 x_i + x_i p^2}{2} + (\beta' - 2\gamma)\frac{p_i p_j x_j + x_j p_i p_j}{2}, \tag{1.106}$$

$$P_i = p_i\left(1 + \gamma p^2\right), \tag{1.107}$$

depending on the parameter γ, the next important question is whether this parameter shows up in physically measurable quantities. In particular, we will be verifying if the first order corrections to the energy levels of an arbitrary system do depend in any way on γ.

First, let us observe, that the energy corrections, as calculated with the general first order representation are, in some way, a "combination" of those obtained in the Brau and Kempf

reductions. More exactly, let us consider some quantum mechanical system governed by the Hamiltonian

$$H_0 = \frac{p^2}{2m} + V(x), \tag{1.108}$$

with some arbitrary potential $V(x)$.

In the Kempf reduction, the energy corrections are given by

$$\begin{aligned} \Delta E^K &= \left\langle H^K - H_0 \right\rangle \\ &= \left\langle V(X^K) - V(x) \right\rangle, \end{aligned} \tag{1.109}$$

where, according to (1.46),

$$X_i^K = x_i + \beta \frac{p^2 x_i + x_i p^2}{2} + \beta' \frac{p_i p_j x_j + x_j p_i p_j}{2}. \tag{1.110}$$

The potential $V(X^K)$ can be expanded as

$$V(X^K) = V(x) + \beta V_\beta(x) + \beta' V_{\beta'}(x) + O(\beta, \beta')^2, \tag{1.111}$$

and thus the Kempf correction has the form

$$\Delta E^K = A\beta + B\beta', \tag{1.112}$$

with $A := \langle V_\beta \rangle$ and $B := \langle V_{\beta'} \rangle$.

We have already seen that, in the Brau reduction, where the momentum is defined as $P_i^B = p_i(1 + \beta p^2)$, the energy correction is given by

$$\begin{aligned} \Delta E^B &= \left\langle H^B - H_0 \right\rangle \\ &= \frac{\left\langle (P^B)^2 - p^2 \right\rangle}{2m} \\ &= C\beta, \end{aligned} \tag{1.113}$$

with $C := \langle p^4 \rangle / m$.

In turn, the energy correction in the general first order reduction is given by

$$\begin{aligned} \Delta E^g &= \langle H^g - H_0 \rangle \\ &= \frac{\langle (P^g)^2 - p^2 \rangle}{2m} + \langle V(X^g) - V(x) \rangle. \end{aligned} \tag{1.114}$$

Now, the first of these two terms is the same correction as calculated in the Brau reduction, with the substitution $\beta \mapsto \gamma$. Analogously, the second, potential term is just what was obtained in the Kempf reduction with the replacements $\beta \mapsto \beta - \gamma$, $\beta' \mapsto \beta' - 2\gamma$. Therefore, the energy correction is given by

$$\begin{aligned} \Delta E^g &= C\gamma + A(\beta - \gamma) + B(\beta' - 2\gamma) \\ &= A\beta + B\beta' - (A + 2B - C)\gamma. \end{aligned} \tag{1.115}$$

There is one more interesting observation: the corrections calculated using the Kempf and Brau reductions agree for $\beta' = 2\beta$, if and only if

$$C\beta = (A\beta + B\beta')\big|_{\beta'=2\beta} = (A + 2B)\beta, \tag{1.116}$$

or, equivalently, $A + 2B = C$, that is exactly when the energy correction in the general first order reduction does not depend on γ!

This certainly gives a relatively easy way to check energy corrections' independence from reduction; it is sufficient to compare the results in the Kempf and Brau reductions. Nevertheless, we can prove an even stronger result. Namely, when perturbing around stationary states that vanish at infinity, (which is true for bound states with discrete energy levels), the two reductions indeed agree, i.e. we have

$$A + 2B = C, \tag{1.117}$$

where

$$A = \langle V_\beta \rangle , \qquad B = \langle V_{\beta'} \rangle , \qquad C = \frac{1}{m} \left\langle p^4 \right\rangle , \tag{1.118}$$

and V_β, $V_{\beta'}$ are given by (1.111).

Let us consider the coordinate operator as a function of β, β',

$$X_i(\beta, \beta') = S[x_i(1 + \beta p^2) + \beta' p_i p_j x_j], \tag{1.119}$$

where S is the symmetrization operator, that is defined for a product of (non-commuting) operators by

$$S[a_1 \dots a_n] := \frac{1}{n!} \sum_{\sigma \in S_n} a_{\sigma(1)} \dots a_{\sigma(n)}, \tag{1.120}$$

and extended to arbitrary functions of operators by linearity and continuity. Here S_n is the group of permutations of n elements.

Because

$$\frac{\partial X_i}{\partial \beta}(\beta, \beta') = S[x_i\, p^2], \tag{1.121}$$

$$\frac{\partial X_i}{\partial \beta'}(\beta, \beta') = S[p_i (x \cdot p)], \tag{1.122}$$

the first two coefficients can be calculated from

$$V_\beta = S\left[\frac{\partial V(X_i(\beta, \beta'))}{\partial \beta}\right] = S\left[\frac{\partial V}{\partial x_i}\frac{\partial X_i}{\partial \beta}(\beta, \beta')\right] = S\left[(\operatorname{grad} V \cdot r) p^2\right], \tag{1.123}$$

$$V_{\beta'} = S\left[\frac{\partial V(X_i(\beta, \beta'))}{\partial \beta'}\right] = S\left[\frac{\partial V}{\partial x_i}\frac{\partial X_i}{\partial \beta'}(\beta, \beta')\right] = S\left[(\operatorname{grad} V \cdot p)(x \cdot p)\right]. \tag{1.124}$$

Let us now consider the operator

$$\begin{aligned} a &= S[(x\cdot p)p^2] \\ &= \frac{x_i p_i p_j p_j + p_j p_j p_i x_i}{2}. \end{aligned} \tag{1.125}$$

On one hand, it is well known that with respect to a state that vanishes at infinity, the time evolution of the expectation value of the operator a is determined by its commutator with the Hamiltonian:

$$i\hbar\frac{\partial\langle a\rangle}{\partial t} = \langle [H,a]\rangle\,. \tag{1.126}$$

On the other hand, the commutator can be calculated explicitly using the expression of a to yield

$$\begin{aligned} [H,a] &= i\hbar\left\{-\frac{p^4}{m} + S[(\operatorname{grad}V\cdot x)p^2 + 2(\operatorname{grad}V\cdot p)(x\cdot p)]\right\} \\ &= i\hbar\left(-\frac{p^4}{m} + V_\beta + 2V_{\beta'}\right). \end{aligned} \tag{1.127}$$

where in the last line we have used (1.123) and (1.124). Taking the expectation value of this relation with respect to a stationary state, this can be rewritten

$$A + 2B - C = \frac{\partial\langle a\rangle}{\partial t} \tag{1.128}$$

which vanishes for a stationary state, and so establishes our claim. The proof used here is reminiscent of the proof of the virial theorem with the operator a used instead of the virial operator.

It can be noted that the same proof can be formulated in terms of canonical transformations, without reference to a Hamiltonian. For this, let $\bar{a}$ denote the unitless form of a, namely

$$\bar{a} = i\frac{\xi^2}{\hbar}a, \tag{1.129}$$

Under the unitary transformation $\exp(\tau\bar{a})$ generated by $\bar{a}$, with τ a unitless parameter, the coordinates and momenta transform as

$$X_i \longmapsto e^{\tau\bar{a}}\,X_i\,e^{-\tau\bar{a}} = X_i + \tau[\bar{a},X_i] + O(\epsilon)^2, \tag{1.130}$$

$$P_i \longmapsto e^{\tau\bar{a}}\,P_i\,e^{-\tau\bar{a}} = P_i + \tau[\bar{a},\,P_i] + O(\epsilon)^2, \tag{1.131}$$

where we have used the Baker-Campbell-Hausdorff formula to first order in τ. The $[\bar{a},X_i]$ and $[\bar{a},P_i]$ commutators can be explicitly evaluated, and result in the following transformations for the functions F_X, G_P, H_X in the reduction expression:

$$F_P \longmapsto F_P - \tau(uF_P + 2u^2F_P') \tag{1.132}$$

$$G_X \longmapsto G_X + \tau(uG_X - 2u^2G_X') \tag{1.133}$$

$$H_X \longmapsto H_X + \tau(2G_X + uH_X - 2u^2H_X') \tag{1.134}$$

It can be verified that the differential relations (1.77)–(1.78) between these functions are, to first order in τ, invariant under these transformations. Using this unitary transformation, one can obtain the general first order reduction from the Kempf reduction. It should be noted that this is true to first order only. When including terms to all orders, not all reductions can be obtained in this way. Indeed, we have only one parameter τ, while every F_P, depending on an infinite number of parameters (its expansion coefficients), defines a separate reduction.

The question whether there is some general canonical transformation that relates all reductions to all orders remains open.

1.8 A possible generalization

We conclude this chapter with a heuristic outlook on how these results might be extended in the future to finding a differential operator representation for Heisenberg algebras involving more than one dimensionful parameter. For example one can consider a commutation relation of the type [14]

$$[X_i, P_j] = i\hbar\delta_{ij}(1 + \alpha X^2 + \beta P^2), \tag{1.135}$$

that involves two dimensionful parameters, one with dimensions of inverse length $\chi = \sqrt{\alpha}$ and one of inverse momentum $\xi = \sqrt{\beta}$. As mentioned before, such a problem contains both a minimal length and a minimal momentum.

The most general form of the reduction is

$$X_i = S[x_i G_X + \frac{\xi}{\chi} p_i F_X], \tag{1.136}$$

$$P_j = S[p_j F_P + \frac{\chi}{\xi} x_j G_P], \tag{1.137}$$

where F_X, G_X, F_P, G_P are dimensionless functions, and as such, can depend on the dimensionless parameters

$$u = \chi^2 x^2, \qquad v = \xi^2 p^2, \qquad w = \chi\xi(x \cdot p). \tag{1.138}$$

Note that F_X, which corresponds to wH_X from Section 1.6, no longer requires a factor of w, due to the second dimensional parameter. To recover the regular commutation relations in the limit $\chi, \xi \to 0$ we should impose

$$G_X(u, v, w)\big|_{u=v=w=0} = F_P(u, v, w)\big|_{u=v=w=0} = 1, \tag{1.139}$$

and that the second term in both expressions vanishes in the same limit.

Again, symmetrization (on the orders of factors of operators in the expressions of X_i, P_j) should be carried out to make the non-commutative operators self-adjoint. There is an additional difficulty here. While not mentioned before, the symmetrization operator defined by (1.120) is not unique. One other possibility is to define

$$S'[a_1 a_2 \dots a_n] := \frac{a_1 a_2 \dots a_n + a_n \dots a_2 a_1}{2}. \tag{1.140}$$

These symmetrizations were equivalent in the one parameter case, where the products involved at most one x operator. Here, this is no longer the case. However for a well-chosen symmetrization functional, we can have the following property: for arbitrary operators A, B, the commutator can be calculated as

$$\frac{1}{i\hbar}\big[\, S[A],\, S[B]\,\big] = S\left[\frac{\partial A}{\partial x_k}\frac{\partial B}{\partial p_k} - \frac{\partial B}{\partial x_k}\frac{\partial A}{\partial p_k}\right] =: \{A, B\}_S. \tag{1.141}$$

Introducing the dimensionless

$$\bar{x}_i := \chi x_i, \qquad \bar{X}_i := \chi X_i = \bar{x}_i G_X + \bar{p}_i F_X, \tag{1.142}$$

$$\bar{p}_j := \xi p_j, \qquad \bar{P}_j := \xi P_j = \bar{p}_j F_P + \bar{x}_j G_P, \tag{1.143}$$

the commutator of the position and momentum reads

$$\begin{aligned}\frac{1}{i\hbar}[X_i, P_j] &= S\left[\frac{\partial \bar{X}_i}{\partial \bar{x}_k}\frac{\partial \bar{P}_j}{\partial \bar{p}_k} - \frac{\partial \bar{X}_i}{\partial \bar{p}_k}\frac{\partial \bar{P}_j}{\partial \bar{x}_k}\right] \\ &=: S[\mathcal{C}],\end{aligned} \tag{1.144}$$

where $\mathcal{C}$ has 42 terms, 2 corresponding to δ_{ij}, and 10 each to $x_i x_j, x_i p_j, p_i x_j$, and $p_i p_j$. Explicitly, they are:

$$\begin{aligned}\mathcal{C} = {}& \delta_{ij}(G_X F_P - F_X G_P) \\ &+ x_i x_j \left(2F_P\frac{\partial G_X}{\partial u} - 2F_X\frac{\partial G_P}{\partial u} + 2G_X\frac{\partial G_P}{\partial w} - 2G_P\frac{\partial G_X}{\partial w} + \{G_X, G_P\}_S\right) \\ &+ x_i p_j \left(-2F_X\frac{\partial F_P}{\partial u} - 2G_P\frac{\partial G_X}{\partial v} + 2G_X\frac{\partial F_P}{\partial w} + 2F_P\frac{\partial G_X}{\partial w} + \{G_X, F_P\}_S\right) \\ &+ p_i x_j \left(2F_P\frac{\partial F_X}{\partial u} + 2G_X\frac{\partial G_P}{\partial v} - 2F_X\frac{\partial G_P}{\partial w} - 2G_P\frac{\partial F_X}{\partial w} + \{F_X, G_P\}_S\right) \\ &+ p_i p_j \left(2G_X\frac{\partial F_P}{\partial v} - 2G_P\frac{\partial F_X}{\partial v} - 2F_X\frac{\partial F_P}{\partial w} + 2F_P\frac{\partial F_X}{\partial w} + \{F_X, F_P\}_S\right),\end{aligned} \tag{1.145}$$

where, in terms of u, v, w,

$$\{A, B\}_S = \begin{pmatrix}\partial_u A & \partial_v A & \partial_w A\end{pmatrix}\begin{pmatrix}0 & w & u \\ -w & 0 & -v \\ -u & v & 0\end{pmatrix}\begin{pmatrix}\partial_u B \\ \partial_v B \\ \partial_w B\end{pmatrix}. \tag{1.146}$$

This is the expression of the commutator independent of the exact form of the Heisenberg algebra chosen. Now let us particularize to case of (1.135). The right-hand side, expressed in terms of the dimensionless variables, is

$$1 + \alpha X^2 + \beta P^2 = 1 + (G_P^2 + G_X^2)u + (F_P^2 + F_X^2)v + 2(F_P G_P + F_X G_X)w. \tag{1.147}$$

Imposing that this expression equals to $\mathcal{C}$, (apart form a symmetrization), one obtains five (differential) equations. Solving them is not straightforward, so we might try to find a first order solution only. Let us expand each undetermined function in the form

$$F_X(u,v,w) = f_x + f_{xu}u + f_{xv}v + f_{xw}w + O(u,v,w)^2, \quad \text{etc.} \tag{1.148}$$

We will have a total of 14 parameters: four parameters each for four functions, less two, as $f_p = g_x = 1$ is determined from (1.139). In turn we have to satisfy five relations between the functions, which translate to $4 \times 5 = 20$ equations to solve. So the general case is overdetermined, and not every Heisenberg algebra admits representations in terms of differential operators. In particular, (1.135) seems to have no solution.

Nevertheless, as mentioned before in the RHS one can include other allowable terms, like X_iX_j, etc. A characterization of the forms of the RHS which admit solutions (if any) remains a future task.

Chapter 2

Simple systems with minimal length

2.1 The harmonic oscillator

Probably in every physics framework (classical mechanics, wave mechanics, path integrals etc.) the simplest, though not trivial system is the harmonic oscillator; this happens in the minimal-length quantum mechanics also. It was studied in several papers: the first order corrections to the spectrum were obtained by Kempf [14, 15] in the momentum representation and by Brau [7] in his own representation. Later, Chang, Minic, Okamura, and Takeuchi [9] obtained the exact spectrum and eigenfunctions in the momentum representation.

All results obtained so far are consistent; and according to the first chapter, the pseudo-position representation should be consistent with them too. Nevertheless, we will explicitly calculate the first order correction to the energy spectrum as a "sanity check" for the validity of this new representation.

To recapitulate, the operators X_i, P_j satisfying the minimal-length uncertainty relation

$$[X_i, P_j] = i\hbar[\delta_{ij}(1 + \beta P^2) + \beta' P_i P_j], \tag{2.1}$$

are represented in the pseudo-position representation by

$$\begin{aligned} X_i &= \hat{x}_i + \beta \frac{\hat{p}^2\hat{x}_i + \hat{x}_i\hat{p}^2}{2} + \beta' \frac{\hat{p}_i\hat{p}_j\hat{x}_j + \hat{x}_j\hat{p}_j\hat{p}_i}{2}, \\ P_i &= \hat{p}_i, \end{aligned} \tag{2.2}$$

where the underlying operators $\hat{x}_i, \hat{p}_j$ are given by

$$\hat{x}_i = x_i, \qquad \hat{p}_i = \frac{\hbar}{i}\frac{\partial}{\partial x_i}.$$

satisfying the usual commutation relations

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}. \tag{2.3}$$

The Hamiltonian of the harmonic oscillator is

$$H = \frac{P^2}{2m} + \frac{m\omega^2}{2} R^2, \tag{2.4}$$

and we will interpret it as a small perturbation around the regular Hamiltonian $H_0 = p^2/2m + m\omega^2 r^2/2$. The perturbing potential is thus

$$\begin{aligned} H' &= H - H_0 \\ &= \frac{m\omega^2}{2}\,(R^2 - r^2). \end{aligned} \tag{2.5}$$

The distance-squared operator R^2 in D dimensions can be expanded as

$$\begin{aligned} R^2 &= X_i X_i \\ &= \hat{r}^2 + \beta (R^2)_\beta + \beta' (R^2)_{\beta'} + \beta^2 (R^2)_{\beta^2} + \beta'^2 (R^2)_{\beta'^2} + \beta\beta' (R^2)_{\beta\beta'} \end{aligned} \tag{2.6}$$

where the expansion coefficients are operators given by

$$\begin{aligned} (R^2)_\beta &= 2\hat{r}^2\hat{p}^2 - 4i\hbar(\hat{r}\cdot\hat{p}) - D\hbar^2, \\ (R^2)_{\beta'} &= 2(\hat{r}\cdot\hat{p})^2 - 2Di\hbar(\hat{r}\cdot\hat{p}) - \frac{D(D+1)}{2}\,\hbar^2, \\ (R^2)_{\beta^2} &= \left[\hat{r}^2\hat{p}^2 - 4i\hbar((\hat{r}\cdot\hat{p}) - (D+1)\hbar^2\right]\hat{p}^2, \\ (R^2)_{\beta'^2} &= \left[(\hat{r}\cdot\hat{p})^2 - (D+2)i\hbar(\hat{r}\cdot\hat{p}) - \frac{(D+1)(D+3)}{4}\,\hbar^2\right]\hat{p}^2, \\ (R^2)_{\beta\beta'} &= \left[2(\hat{r}\cdot\hat{p})^2 - 2(D+2)i\hbar(\hat{r}\cdot\hat{p}) - \frac{D^2+3D+4}{2}\,\hbar^2\right]\hat{p}^2, \end{aligned} \tag{2.7}$$

as obtained using the usual commutation relations (2.3).

For the first order energy corrections, we will need $(R^2)_\beta$ and $(R^2)_{\beta'}$ only. These can be brought to a more similar form using the formula

$$r^2p^2 = (\hat{r}\cdot\hat{p})^2 - i\hbar(D-2)(\hat{r}\cdot\hat{p}) + L^2, \tag{2.8}$$

as

$$(R^2)_\beta = 2\hat{r}^2\hat{p}^2 - 4i\hbar(\hat{r}\cdot\hat{p}) - D\hbar^2, \tag{2.9}$$

$$(R^2)_{\beta'} = 2\hat{r}^2\hat{p}^2 - 4i\hbar(\hat{r}\cdot\hat{p}) - \frac{D(D+1)}{2}\,\hbar^2 - 2L^2. \tag{2.10}$$

With the notation $\xi^2 = \beta + \beta'$ and $\eta = \dfrac{\beta}{\beta+\beta'}$, the first order correction to the distance squared operator becomes

$$(R^2)_{\xi^2} = 2\hat{r}^2\hat{p}^2 - 4i\hbar(\hat{r}\cdot\hat{p}) + \frac{\eta D(D-1) - D(D+1)}{2}\,\hbar^2 - 2(1-\eta)L^2. \tag{2.11}$$

Apart from a prefactor of $m\omega^2\xi^2/2$, this is our perturbing potential. The corrections to the energy eigenvalues are given by the expectation values of this operator calculated with respect to the corresponding eigenstates,

$$\Delta E_{n\ell} = \frac{m\omega^2\xi^2}{2}\left\langle (R^2)_{\xi^2}\right\rangle \tag{2.12}$$

The spectrum and eigenfunctions of the unperturbed system, the regular harmonic oscillator, are (relatively) well known in radial coordinates. As with any spherically symmetric observable, the energy eigenfunctions can be factored into a radial and an angular part

$$\Psi_{n\ell m_i}(r,\theta_i) = \psi_{n\ell}(r)Y_{\ell m_i}(\theta_i). \tag{2.13}$$

where $Y_{\ell m}$ are the spherical harmonics and θ_i represent the collection of angular variables.

The operators $\hat{r}^2$, $\hat{p}^2$, $\hat{r}\cdot\hat{p}$ act on the radial part $\psi_{n\ell}(r)$ through

$$\begin{aligned} \hat{r}^2 &= r^2, \\ \hat{p}^2 &= -\hbar^2\frac{\partial^2}{\partial r^2} - \hbar^2\frac{D-1}{r}\frac{\partial}{\partial r} + \frac{L^2}{r^2}, \\ \hat{r}\cdot\hat{p} &= \frac{\hbar}{i}r\frac{\partial}{\partial r}, \end{aligned} \tag{2.14}$$

where $L^2 = \hbar^2\ell(\ell+D-2)$.

For the harmonic oscillator in D dimensions, the energy eigenvalues are given by

$$E_{\nu\ell} = \hbar\omega\left(\frac{D}{2} + 2\nu + \ell\right), \tag{2.15}$$

with corresponding radial eigenfunctions

$$\psi_{\nu\ell}(\rho) = \sqrt{\frac{2n!}{\Gamma(n+\alpha+1)}}\left(\frac{m\omega}{\hbar}\right)^{\frac{D}{4}} e^{-\rho/2}\rho^\ell\, L_\nu^\alpha(\rho^2) \tag{2.16}$$

where ν is a positive integer, and

$$\alpha = \frac{D}{2} + \ell - 1, \qquad \rho = r\sqrt{\frac{m\omega}{\hbar}}. \tag{2.17}$$

The first term in the expectation value of the correction can be rewritten using the Schrödinger equation as

$$\left\langle r^2p^2\right\rangle = 2mE\left\langle r^2\right\rangle - m^2\omega^2\left\langle r^4\right\rangle. \tag{2.18}$$

These in turn can be calculated using the explicit expression of the eigenfunctions and the formulas

$$\int_0^\infty e^{-z} z^{q+2} \left[L_p^{(q)}(z)\right]^2 dz = [2p(p+q) + (2p+q+1)(2p+q+2)] \left[\frac{(p+q)!}{p!}\right] , \tag{2.19}$$

$$\int_0^\infty e^{-z} z^{q+1} \left[L_p^{(q)}(z)\right]^2 dz = (2p+q+1) \left[\frac{(p+q)!}{p!}\right] , \tag{2.20}$$

$$\int_0^\infty e^{-z} z^{q} \left[L_p^{(q)}(z)\right]^2 dz = \left[\frac{(p+q)!}{p!}\right] , \tag{2.21}$$

which are not difficult, if a bit tedious to show using the Rodrigues representation for Laguerre polynomials.

Explicitly, they are

$$\left\langle r^2 \right\rangle = \left(2\nu + \frac{D}{2} + \ell\right) \left(\frac{\hbar}{m\omega}\right) , \tag{2.22}$$

$$\left\langle r^4 \right\rangle = \left[6\nu^2 + (6\nu+1)\left(\frac{D}{2}+\ell\right) + \left(\frac{D}{2}+\ell\right)^2\right] \left(\frac{\hbar}{m\omega}\right)^2 . \tag{2.23}$$

The second term in the expectation value of (2.11) is easier to calculate:

$$\begin{aligned} i\hbar \left\langle r \cdot p \right\rangle &= \hbar^2 \left\langle r \frac{\partial}{\partial r} \right\rangle = \frac{\hbar^2}{2} \int_0^\infty r^D \frac{\partial \psi^2}{\partial r}(r)\, dr = -\frac{D\hbar^2}{2} \int_0^\infty r^{D-1} \psi^2(r)\, dr \\ &= -\frac{D\hbar^2}{2} . \end{aligned} \tag{2.24}$$

The remaining terms are constant. Finally, collecting everything together, and using the expression for L^2, the energy corrections are

$$\Delta E_{\nu\ell} = \frac{m\omega^2\xi^2\hbar^2}{2} \left[\left(2\nu + \ell + \frac{D}{2}\right)^2 + (2\eta - 1)\left(L^2 + \frac{D^2}{4}\right) + (1-\eta)\frac{D}{2}\right] . \tag{2.25}$$

These should be compared to the exact result of [9],

$$E_{n\ell} = \hbar\omega \left[\left(n + \frac{D}{2}\right) \sqrt{1 + \left\{\beta^2 L^2 + \frac{(D\beta + \beta')^2}{4}\right\} \mu^2\hbar^2\omega^2} \right. \tag{2.26}$$

$$\left. + \left\{(\beta+\beta')\left(n+\frac{D}{2}\right)^2 + (\beta-\beta')\left(L^2 + \frac{D^2}{4}\right) + \beta'\frac{D}{2}\right\} \frac{m\hbar\omega}{2}\right] . \tag{2.27}$$

Knowing that their parameters are related by $n = 2\nu + \ell$, $\beta = \eta\xi^2$, and $\beta' = (1-\eta)\xi^2$, these two obviously agree to first order. The result [9] was shown to agree to first

order with [7, 14, 15], also. In particular, the corrections calculated in the pseudo-position representation here are the same of those in the the Brau representation used in [7]. By section 1.7, this means that even in the most general first order representation (1.68)–(1.69) the corrections will be consistent (i.e. independent of γ), and given by (2.25).

In ref. [9], the authors discussed the constraint that can be placed on the parameter β by measuring the energy levels of an electron trapped in a strong magnetic field, i.e. in a so-called *Penning trap*. Even under unrealistic assumptions (e.g. the energy corresponding to level $n = 10^8$ can be measured with accuracy of $\hbar\omega_c$), the hypothetical bound cannot exceed 1GeV.

2.2 The Coulomb potential — perturbation theory

In the last section we had reviewed the harmonic oscillator system under the minimal length hypothesis, but no real constraint can be obtained on the minimal length, presumably because of the softness of the potential at the origin. We could expect a much better bound from precision measurements on hydrogenic atoms. This system has a potential that is singular at the origin, and is therefore particularly sensitive to whether there is a fundamental minimal length. In addition, the energy levels of the hydrogen atom are one of the most precisely measured quantities today.

The Hamiltonian for the Coulomb potential with minimal length is

$$H = \frac{P^2}{2m} - \frac{k}{R}. \tag{2.28}$$

In order to solve this equation, we need the expression for the $1/R$ operator, which is the inverse of the square root of the R^2. Unfortunately, because there is no representation in which R is diagonal, and thus R^2 is in general a differential operator, this is not too easy to determine. One possibility is to work again in the pseudo-position representation, where, at least in the $\beta, \beta' \to 0$ limit, R^2 is diagonal, and attempt to obtain a perturbative result.

2.2.1 First order expression for R^{-1}

From the previous section, the action of the R^2-corrections can be written as (we will set $\hbar = 1$ from now on)

$$\begin{aligned}(R^2)_\beta &= 2(\hat{r}\cdot\hat{p})^2 - 2Di(\hat{r}\cdot\hat{p}) - D + 2L^2 \\ (R^2)_{\beta'} &= 2(\hat{r}\cdot\hat{p})^2 - 2Di(\hat{r}\cdot\hat{p}) - \frac{D(D+1)}{2},\end{aligned}$$

$$
\begin{aligned}
(R^2)_{\beta^2} &= (\hat{r}\cdot\hat{p})^2\hat{p}^2 - (D+2)i(\hat{r}\cdot\hat{p})\hat{p}^2 - (D+1)\hat{p}^2 + L^2\hat{p}^2 \\
(R^2)_{\beta'^2} &= (\hat{r}\cdot\hat{p})^2\hat{p}^2 - (D+2)i(\hat{r}\cdot\hat{p})\hat{p}^2 - \frac{(D+1)(D+3)}{4}\hat{p}^2, \\
(R^2)_{\beta\beta'} &= 2(\hat{r}\cdot\hat{p})^2\hat{p}^2 - 2(D+2)i(\hat{r}\cdot\hat{p})\hat{p}^2 - \frac{D^2+3D+4}{2}\hat{p}^2,
\end{aligned} \tag{2.29}
$$

or in terms of the differential operators (2.14),

$$
\begin{aligned}
(R^2)_{\beta} &= -2r^2\frac{\partial^2}{\partial r^2} - 2(D+1)r\frac{\partial}{\partial r} + 2L^2 - D, \\
(R^2)_{\beta'} &= -2r^2\frac{\partial^2}{\partial r^2} - 2(D+1)r\frac{\partial}{\partial r} - \frac{D(D+1)}{2}, \\
(R^2)_{\beta^2} &= r^2\frac{\partial^4}{\partial r^4} + 2(D+1)r\frac{\partial^3}{\partial r^3} + (D^2+D-2L^2)\frac{\partial^2}{\partial r^2} \\
&\qquad - \frac{2(D-1)L^2}{r}\frac{\partial}{\partial r} + \frac{(D-1+L^2)L^2}{r^2}, \\
(R^2)_{\beta\beta'} &= 2r^2\frac{\partial^4}{\partial r^4} + 4(D+1)r\frac{\partial^3}{\partial r^3} + \frac{(5D^2+3D-4L^2)}{2}\frac{\partial^2}{\partial r^2} \\
&\qquad + \frac{(D-1)(D^2-D-4L^2)}{2r}\frac{\partial}{\partial r} - \frac{(D-1)(D-4)L^2}{2r^2}, \\
(R^2)_{\beta'^2} &= r^2\frac{\partial^4}{\partial r^4} + 2(D+1)\frac{\partial^3}{\partial r^3} + \frac{(5D^2+4D-1-4L^2)}{4}\frac{\partial^2}{\partial r^2} \\
&\qquad + \frac{(D-1)(D^2-1-4L^2)}{4r}\frac{\partial}{\partial r} - \frac{(D-3)(D-1)L^2}{4r^2}.
\end{aligned} \tag{2.30}
$$

We are intent on doing perturbation theory around the solutions of the regular Coulomb Hamiltonian and so we need to determine the expansion of the inverse distance

$$
R^{-1} = r^{-1} + \beta(R^{-1})_{\beta} + \beta'(R^{-1})_{\beta'} + O(\beta,\beta')^2. \tag{2.31}
$$

It should be noted that in order for perturbation theory to work, the perturbing potential should be uniformly bounded with respect to the unperturbed one. This can be problematic in this case as the unperturbed potential $1/r$ is singular as $r \to 0$. This alone will not cause problems, but one can see that the expression for R^2, more exactly its $(R^2)_{\beta\beta'}$ and $(R^2)_{\beta'^2}$ parts, contains terms that are also singular as $r \to 0$. These are the ones involving $\frac{1}{r^2}$ and $\frac{1}{r}\frac{\partial}{\partial r}$. As a result $1/R$ will be regular, and the correction term $k/r - k/R$ will be singular in the small r limit.

Nevertheless, we will go ahead, bearing in mind that our considerations might be true only on some interval $[\epsilon,\infty)$ only instead $(0,\infty)$. Later, we will come back to this point to verify if the extension to the complete positive real semi-axis is warranted or not.

The operator R^{-1} must satisfy the relation $R^{-1}R^2R^{-1} = 1$, which translates into

$$
\begin{aligned}
(R^{-1})_{\beta}\, r + r(R^{-1})_{\beta} &= -r^{-1}(R^2)_{\beta}\, r^{-1}, \\
(R^{-1})_{\beta'} r + r(R^{-1})_{\beta'} &= -r^{-1}(R^2)_{\beta'} r^{-1}.
\end{aligned} \tag{2.32}
$$

Substituting (2.30) we arrive to the equations:

$$\begin{aligned}(R^{-1})_\beta\, r + r(R^{-1})_\beta &= 2\frac{\partial^2}{\partial r^2} + \frac{2(D-1)}{r}\frac{\partial}{\partial r} - \frac{D-2+2L^2}{r^2},\\ (R^{-1})_{\beta'} r + r(R^{-1})_{\beta'} &= 2\frac{\partial^2}{\partial r^2} + \frac{2(D-1)}{r}\frac{\partial}{\partial r} + \frac{D^2-3D+4}{2r^2}.\end{aligned} \tag{2.33}$$

On dimensional grounds we make the ansatz that both $(R^{-1})_\beta$ and $(R^{-1})_{\beta'}$ to be of the form

$$\frac{A}{r}\frac{\partial^2}{\partial r^2} + \frac{B}{r^2}\frac{\partial}{\partial r} + \frac{C}{r^3},$$

where A, B, C are constants to be determined. Substituting this expression into (2.33) and identifying coefficients we obtain:

$$\begin{aligned}(R^{-1})_\beta &= \frac{1}{r}\frac{\partial^2}{\partial r^2} + \frac{D-2}{r^2}\frac{\partial}{\partial r} - \frac{L^2+D-2}{r^3},\\ (R^{-1})_{\beta'} &= \frac{1}{r}\frac{\partial^2}{\partial r^2} + \frac{D-2}{r^2}\frac{\partial}{\partial r} + \frac{D^2-5D+8}{4r^3}.\end{aligned} \tag{2.34}$$

which can be rewritten in terms of the dimensionless $\eta = \beta/(\beta+\beta')$ and $\xi = \sqrt{\beta+\beta'}/a$, with $a = 1/km$ being the Bohr radius as

$$\frac{(R^{-1})_{\xi^2}}{a^{-1}} = a^3\left[\frac{1}{r}\frac{\partial^2}{\partial r^2} + \frac{D-2}{r^2}\frac{\partial}{\partial r} + \frac{(1-\eta)(D^2-5D+8) - 4\eta(L^2+D-2)}{4r^3}\right]. \tag{2.35}$$

As an alternative check, in the expansion of the distance operator

$$R = r + \beta R_\beta + \beta' R_{\beta'} + O(\beta,\beta')^2, \tag{2.36}$$

the correction terms are determined to be:

$$R_\beta = -r\frac{\partial^2}{\partial r^2} - (D-1)\frac{\partial}{\partial r} + \frac{L^2}{r}, \tag{2.37}$$

$$R_{\beta'} = -r\frac{\partial^2}{\partial r^2} - (D-1)\frac{\partial}{\partial r} + \frac{D(1-D)}{4r}. \tag{2.38}$$

Indeed $RR^{-1} = R^{-1}R = 1$ is satisfied, as can be easily checked.

2.2.2 Corrections to the Hydrogen spectrum

The Schrödinger equation for D-dimensional unperturbed Coulomb problem is

$$\left[\frac{\partial^2}{\partial r^2} + \frac{D-1}{r}\frac{\partial}{\partial r} + \frac{2mk}{r} - \frac{L^2}{r^2}\right]\psi(r) = -2m|E|\psi(r), \tag{2.39}$$

which becomes

$$\left[\frac{\partial^2}{\partial\rho^2}+\frac{D-1}{\rho}\frac{\partial}{\partial\rho}+\sqrt{\frac{2m}{|E|}}\frac{k}{\rho}-\frac{L^2}{\rho^2}-1\right]\psi(\rho)=0, \tag{2.40}$$

after changing the variable to the dimensionless $\rho = 2\sqrt{2m|E|}\, r$.

One can see that a normalizable root of eq. (2.40) will have the behavior $\psi(\rho) \sim \rho^\ell$ for $\rho \ll 1$ and $\psi(\rho) \sim e^{-\rho/2}$ for $\rho \gg 1$. Factoring out these contributions

$$\psi(\rho) = \rho^\ell e^{-\rho/2} u(\rho), \tag{2.41}$$

the remaining $u(\rho)$ will satisfy the Laguerre differential equation

$$\rho u''(\rho) + [(2\ell + D - 1) - \rho]u'(\rho) + \frac{1}{2}\left(\sqrt{\frac{2m}{|E|}}k - 2\ell - D + 1\right)u(\rho) = 0. \tag{2.42}$$

In order to obtain a normalizable wave-function, the coefficient of $u(\rho)$ in the previous equation should be an integer. This leads to the eigenvalues

$$E_n = -\frac{k}{2a\bar{n}^2}, \quad n = 1, 2, \ldots, \tag{2.43}$$

where for a given angular momentum number ℓ, only $n > \ell$ is allowed. The normalized eigenfunctions are

$$\psi_{n\ell}(r) = \sqrt{\frac{2^{D-1}}{a^D \bar{n}^{D+1}}\frac{(\bar{n}-\bar{\ell}-1)!}{(\bar{n}+\bar{\ell})!}}e^{\rho/2}\rho^\ell L^{2\bar{\ell}+1}_{\bar{n}-\bar{\ell}-1}(\rho), \tag{2.44}$$

where

$$\begin{aligned}\bar{n} &= n + \frac{D-3}{2},\\ \bar{\ell} &= \ell + \frac{D-3}{2},\\ \rho &= \frac{2r}{a\bar{n}},\end{aligned} \tag{2.45}$$

and $a = 1/mk$ is the Bohr radius. (Note that the exponent of ρ in the wavefunction is ℓ and not $\bar{\ell}$.)

With minimal length, the Hamiltonian of the Coulomb problem is

$$\begin{aligned}H &= \frac{P^2}{2m} - \frac{k}{R}\\ &= \frac{p^2}{2m} - \frac{k}{r} - k\beta(R^{-1})_\beta - k\beta'(R^{-1})_{\beta'} + O(\beta,\beta')^2,\end{aligned} \tag{2.46}$$

so the first order corrections to the energy eigenvalues are given by

$$\Delta E_{n\ell} = -k\beta \left\langle (R^{-1})_{\beta} \right\rangle - k\beta' \left\langle (R^{-1})_{\beta'} \right\rangle . \tag{2.47}$$

Using (2.35), the eigenvalue equation

$$\left(p^2 - \frac{2km}{r} - 2Em \right) \psi_{n\ell}(r) = 0, \tag{2.48}$$

and the expressions for the energy eigenvalues and Bohr radius, eq. (2.47) and can be readily rewritten as:

$$\Delta E_{n\ell} = \frac{a\xi^2}{m} \left[-\frac{1}{a^2\bar{n}^2} \left\langle \frac{1}{r} \right\rangle + \frac{2}{a} \left\langle \frac{1}{r^2} \right\rangle - \left\langle \frac{1}{r^2} \frac{\partial}{\partial r} \right\rangle \right.$$
$$\left. + \frac{4L^2 + (1-\eta)(D^2 - 5D + 8) - 4\eta(L^2 + D - 2)}{4r^3} \left\langle \frac{1}{r^3} \right\rangle \right] . \tag{2.49}$$

As in the previous section, with the help of the Rodrigues representation for Laguerre polynomials,

$$L_p^{(q)}(z) \equiv \frac{1}{p!} e^z z^q \frac{d^p}{dz^p} \left[e^{-z} z^{p+q} \right] , \tag{2.50}$$

it is not too difficult to show in addition to (2.19)–(2.21) that

$$\int_0^\infty e^{-z} z^{q-1} \left[L_p^{(q)}(z) \right]^2 dz = \frac{1}{q} \left[\frac{(p+q)!}{p!} \right] , \tag{2.51}$$

$$\int_0^\infty e^{-z} z^{q-2} \left[L_p^{(q)}(z) \right]^2 dz = \frac{(2p+q+1)}{(q+1)q(q-1)} \left[\frac{(p+q)!}{p!} \right] . \tag{2.52}$$

Using these formulæ, the expectation values $\langle r^{-a} \rangle$ can be calculated to be

$$\begin{aligned} \left\langle \frac{1}{r} \right\rangle &= \frac{1}{a_0\, \bar{n}^2} , \\ \left\langle \frac{1}{r^2} \right\rangle &= \frac{1}{a_0^2\, \bar{n}^3 \left(\bar{\ell} + \frac{1}{2} \right)} , \\ \left\langle \frac{1}{r^3} \right\rangle &= \frac{1}{a_0^3\, \bar{n}^3\, \bar{\ell} \left(\bar{\ell} + \frac{1}{2} \right) \left(\bar{\ell} + 1 \right)} . \end{aligned} \tag{2.53}$$

The last expectation value can be expressed as

$$\begin{aligned} \left\langle \frac{1}{r^2} \frac{\partial}{\partial r} \right\rangle &= \int_0^\infty r^{D-3} \frac{\partial}{\partial r} \left[\psi_{n\ell}(r) \right]^2 dr \\ &= \frac{1}{2} r^{D-3} \left[\psi_{n\ell}(r) \right]^2 \Big|_0^\infty - \frac{D-3}{2} \int_0^\infty r^{D-4} \left[\psi_{n\ell}(r) \right]^2 dr \\ &= -\frac{1}{2} r^{D-3} \left[\psi_{n\ell}(r) \right]^2 \Big|_{r=0} - \frac{D-3}{2} \frac{1}{a_0^3\, \bar{n}^3\, \bar{\ell} \left(\bar{\ell} + \frac{1}{2} \right) \left(\bar{\ell} + 1 \right)} . \end{aligned} \tag{2.54}$$

The first term cancels when $\ell + \frac{D-3}{2} = \bar{\ell} > 0$, that is either $l \neq 0$ or $D > 3$. In this case collecting everything together, we finally arrive to

$$\frac{\Delta E_{n\ell}}{|E_0|} = \frac{2\xi^2}{\bar{n}^3}\left[\frac{(D-1)\,(3\eta-1)}{4\bar{\ell}(\bar{\ell}+1)(\bar{\ell}+\frac{1}{2})} + \frac{\eta+1}{\bar{\ell}+\frac{1}{2}} - \frac{1}{\bar{n}}\right], \tag{2.55}$$

or in terms of β and β',

$$\Delta E_{n\ell} = \frac{1}{ma^4\bar{n}^4}\left\{\left[\frac{(D-1)\left(\beta-\frac{\beta'}{2}\right)}{2\bar{\ell}(\bar{\ell}+1)(\bar{\ell}+\frac{1}{2})} + \frac{2\beta+\beta'}{\bar{\ell}+\frac{1}{2}}\right]\bar{n} - (\beta+\beta')\right\}. \tag{2.56}$$

For $D = 3$ and $\ell = 0$, which is the case of most interest to us, the s-states of the 3D Hydrogen atom, the last two expectation values are formally infinite.

This is a good place to return to the convergence problem mentioned in the beginning of the section. While the expansion is apparently in ξ^2, a quick calculation of higher-order terms confirms what is expected on dimensional grounds, namely, that the expansion parameter is $\beta/r^2 \sim \xi^2/\rho^2$. The ξ-quartic part in the expansion (2.6) of R^2 contains terms of the type ξ^4/ρ^2 and $(\xi^4/\rho)\partial_\rho$. Therefore, the approximation (2.35) for R^{-1} is no longer good for $\rho \lesssim \xi$. The actual expression of the operator R^{-1} for r small is a mystery (to the author, at least), but there is no singularity at the origin[1] as (2.35) would led us to believe.

What we have been doing by calculating expectation values over $(0,\infty)$, was *extrapolating* the approximation (2.35), valid only on some interval $[\rho_c\xi,\infty)$, where $\rho_c \equiv r_c/a_0 \sim 1$, to the whole positive semi-axis. This is allowable only if the error introduced, that is the expectation value of (2.35), calculated over $[0,\rho_c\xi]$ is negligible.

Let us estimate the error made by this extrapolation. The largest discrepancy between (2.49) and the actual value comes from the expectation value of $1/\rho^3$ calculated over the interval $[0,\rho_c\xi]$. For an angular momentum state ℓ, this is of the order

$$\begin{aligned}\xi^2\int_0^{r_c\xi}\frac{R^2_{n\ell}(r)}{r^3}r^{D-1}dr &\sim \xi^2\int_0^{r_c\xi} r^{2\ell+D-4}dr \\ &\sim \xi^{2\ell+D-1}, \qquad \text{for } \ell>0 \text{ or } D>3.\end{aligned} \tag{2.57}$$

For $D > 3$ or $\ell \neq 0$, this exponent is $2\ell + D - 1 > 2$, and consequently the error made is higher order when compared to the leading ξ^2. Thus it is safe to use (2.49), and (2.55) is justified. It should be noted that this expression generalizes the result of Ref. [7] for arbitrary η and D. For the particular case $D = 3$ and $\eta = 1/3$ (i.e., $\beta' = 2\beta$), it reduces to the one obtained there, as long as $\ell \neq 0$.

When $D = 3$ and $\ell = 0$, the integral (2.57) is infinite:

$$\xi^2\int_0^{r_c\xi}\frac{dr}{r} = \infty. \tag{2.58}$$

[1]This is quite general. Any P-dependent commutation relation is expected to expand like (1.3) and to exhibit this behavior.

In this case we were introducing an infinite error by extrapolating. No wonder we got a formally infinite result! To re-emphasize, the infinity obtained did not come from some peculiarity of the physical system, but was introduced by us using an approximation which was wrong on some domain.

Nevertheless, we can obtain at least the general form of the correction by approximating R^{-1} with (2.35) on the interval it can be trusted, $[r_c\xi, \infty)$, and supposing that R^{-1} is bounded on $[0, r_c\xi]$, which is plausible. The leading order contribution will come from the $1/r^3$ term of $(R^{-1})_{\xi^2}$, that is

$$\begin{aligned}\int_{r_c\xi}^{\infty} \psi_{1s}(r)(R^{-1})_{\xi^2}\psi_{1s}(r)r^2dr &\sim \int_{\rho_c\xi}^{\infty}\left(\frac{a\xi^2}{m}\right)\left(\frac{1-3\eta}{2\rho^3}\right)\frac{4}{(na)^3}e^{-\rho}\rho^2 d\rho \\ &= \frac{4(1-3\eta)}{n^3}\left(\frac{1}{2ma^2}\right)\xi^2 E_1(\rho_c\xi),\end{aligned} \tag{2.59}$$

where $E_1(\rho_c\xi) = -\ln\xi - (\gamma + \ln\rho_c) + O(\xi)$ is the exponential integral function.

As a result the corrections will have the expansion

$$\frac{\Delta E_{n\ell}}{|E_0|} = \frac{4(3\eta-1)}{n^3}\xi^2\ln(\xi) + C\xi^2 + O(\xi^3). \tag{2.60}$$

The coefficient of the ξ^2 term gets contributions from several parts. First, there are the remaining terms in (2.49). Second, the actual value of R^{-1}, bounded on the interval $[0, \rho_c\xi]$, can contribute another term of order ξ^2. Lastly, the exact choice of the cutoff value ρ_c also contributes a ξ^2 term. Because we do not know the exact form of R^{-1} for r small, we cannot calculate analytically the second of these contributions. We will see later that when needed, C can be determined numerically, by fitting relation (2.60) to the numerical results of the next section at a sufficiently low value of ξ^2.

Finally, let us mention that the expansion of R^{-1} can be calculated to arbitrary order with enough patience or with the help of an algebraic manipulation program such as MATHEMATICA. The next order, $(R^{-1})_{\xi^4}$ will contain terms that are even more singular, such as $1/r^5$, which formally contribute additional infinities in the expectation value. Nevertheless, if these terms could be resummed, than one can get a finite result.

An interesting attempt in this sense is the recent paper [29], but the method there seems incomplete. Namely, the authors find a finite perturbation, whose expansion will reproduce the exact coefficient of the $1/r^3$ term. More exactly they work in the Stetsko-Tkatchuk basis (1.66)–(1.67), and their perturbing potential is

$$H' = \frac{\beta' p^4}{2m} - k\left(\frac{1}{\sqrt{r^2 + (D-1)\left(\beta - \frac{\beta'}{2}\right)}} - \frac{1}{r} - \left(\beta - \frac{\beta'}{2}\right)\frac{r^{-1}p^2 + p^2 r^{-1}}{2}\right). \tag{2.61}$$

The interesting part is the $(r^2+b^2)^{-1/2}$ term, which, when expanded in a series in $1/r$,

$$\begin{aligned}(r^2+b^2)^{-1/2} &= \frac{1}{r}\left(1+\frac{b^2}{r^2}\right)^{-\frac{1}{2}} \\ &= \frac{1}{r}-\frac{b^2}{2}\left(\frac{1}{r^3}\right)+O\left(\frac{1}{r}\right)^5,\end{aligned} \tag{2.62}$$

agrees with the R^{-1} expansion up to order $(1/r)^3$. However it is not clear that the higher order corrections will also agree, or at least their contribution is negligible. To put it in another way, if $(r^2+b^2)^{-1/2}$ is replaced by, say,

$$\frac{1}{r}\exp\left(-\frac{b^2}{2r^2}\right), \tag{2.63}$$

will the result still be the same?

It seems that the same problem occurs in the case of Brau's [7], which uses the representation where R is diagonal to first order. The exact representation will have to include these higher order terms, and it is again unclear if their contribution is negligible.

2.3 The Coulomb potential — analytical/numerical approach

There is the possibility of solving the Coulomb potential exactly. The idea is the following. First, diagonalize the radial distance squared operator and find its eigenvalues ρ_n^2 corresponding to eigenfunctions $|\psi_n\rangle$. These eigenfunctions form a basis of the physical states, and the action of the inverse distance operator appearing in the Coulomb potential is simply multiplication by $1/\rho_n$. A candidate eigenfunction can be expanded in terms of this basis, and the action of the Coulomb Hamiltonian on it expressed exactly. The boundary condition of normalizability will translate, as we will see, into a second order linear recursion with variable coefficients,[2] which can be solved numerically.

This will also allow us to estimate the so far undetermined coefficients for the s-states of the 3 dimensional Hydrogen atom.

[2]The procedure of diagonalizing the radial distance squared operator and obtaining this linear recursion was developed by Tatsu Takeuchi and Joseph Slawny in an unpublished paper. I am indebted to them for making their notes available to me.

2.3.1 Diagonalization of R^2

We will work in the momentum representation, more exactly in the one given by (1.50) with $\bar{\gamma} = 0$, that is

$$X_i = i\hbar \left[(1+\beta p^2) \frac{\partial}{\partial p_i} + \beta' p_i p_j \frac{\partial}{\partial p_j} \right], \tag{2.64}$$

$$P_i = p_i, \tag{2.65}$$

where the operators are acting on the Hilbert space of functions normalizable under the inner product of weight factor

$$\int \frac{d^D \mathbf{p}}{[1+(\beta+\beta')p^2]^\delta} = \int d\Omega_p \int_0^\infty \frac{p^{D-1} dp}{[1+(\beta+\beta')p^2]^\delta}, \tag{2.66}$$

with

$$\begin{aligned} \delta &= \frac{1}{\beta+\beta'} \left(\beta + \frac{D+1}{2} \beta' \right) \\ &= \frac{D+1}{2} - \eta \frac{D-1}{2}, \end{aligned} \tag{2.67}$$

using again the dimensionless $\eta = \beta/(\beta+\beta')$.

Due to rotational symmetry, we can again factor the R^2 operator's eigenfunctions into a radial and angular part. The radial part $R(p)$ satisfies the eigenvalue equation:

$$\begin{aligned} -\hbar^2 \Bigg[\left\{ [1+(\beta+\beta')p^2] \frac{\partial}{\partial p} \right\}^2 + \frac{(D-1)(1+\beta p^2)}{p} \left\{ [1+(\beta+\beta')p^2] \frac{\partial}{\partial p} \right\} \\ - \frac{L^2 (1+\beta p^2)^2}{p^2} \Bigg] R(p) = r^2 R(p), \end{aligned} \tag{2.68}$$

where the operator L^2 acts on the subspace of functions with definite angular momentum ℓ through multiplication by

$$L^2 = \ell(\ell + D - 1). \tag{2.69}$$

The change of variable

$$\theta \equiv \tan^{-1} \sqrt{\beta+\beta'}\, p\,, \tag{2.70}$$

with shorthand notations

$$s \equiv \sin\theta, \qquad c \equiv \cos\theta, \tag{2.71}$$

transforms the integration measure into

$$\int_0^\infty \frac{p^{D-1} dp}{[1+(\beta+\beta')p^2]^\delta} = (\beta+\beta')^{-D/2} \int_0^1 ds\, s^{D-1} c^{-[1+\eta(D-1)]}, \tag{2.72}$$

while the eigenvalue equation becomes

$$\left[\frac{\partial^2}{\partial\theta^2}+(D-1)\left(\frac{c}{s}+\eta\frac{s}{c}\right)\frac{\partial}{\partial\theta}+\left\{\rho^2-L^2\left(\frac{c}{s}+\eta\frac{s}{c}\right)^2\right\}\right]R(\theta)=0, \tag{2.73}$$

where ρ is the dimensionless form of the radial eigenvalue r^2,

$$\rho^2\equiv\frac{r^2}{\hbar^2(\beta+\beta')}\,. \tag{2.74}$$

Using $R(\theta)=c^\lambda f(s)$, with λ to be determined, the equation for $f(s)$ becomes

$$\begin{aligned}(1-s^2)f''+\left[-\{2\lambda+1+(D-1)(1-\eta)\}\,s+\frac{D-1}{s}\right]f'\\ +\left[\left\{\rho^2-(2\eta-1)L^2-\lambda D\right\}-\frac{L^2}{s^2}+\left\{\lambda^2-\lambda[1+(D-1)\eta]-\eta^2L^2\right\}\frac{s^2}{c^2}\right]f=0.\end{aligned} \tag{2.75}$$

We can choose λ to cancel the tangent squared term by imposing

$$\lambda^2-\lambda[1+(D-1)\eta]-\eta^2L^2=0, \tag{2.76}$$

with solution

$$\lambda=\frac{1+(D-1)\eta}{2}\pm\sqrt{\frac{\{1+(D-1)\eta\}^2}{4}+\eta^2L^2}\,. \tag{2.77}$$

Please note that the integration measure (2.72) is singular as $c\to 0$ (i.e. $\theta\to\pi/2$). Moreover, this singularity is an apparent one due to the choice of variables, because the weight factor expressed in terms of p, c.f. (2.66), is regular as $p\to\infty$. Therefore, for a normalizable $R(p)$, we will chose λ large enough such that the singularity is canceled out in the norm of $R(\theta)$. This translates into $2\lambda-[1+\eta(D-1)]\geq 0$, or

$$\lambda>\frac{1+(D-1)\eta}{2}, \tag{2.78}$$

which eliminates the solution with the negative sign in (2.77).

Next, we can eliminate the centrifugal barrier term L^2/s^2 with the substitution $f(s)=s^\ell g(s)$, resulting in the equation

$$\begin{aligned}(1-s^2)g''+\left[-\{2\lambda+2\ell+1+(D-1)(1-\eta)\}s+\frac{2\ell+D-1}{s}\right]g'\\ +\left[\rho^2-2\eta L^2-(2\ell+D)\lambda+\ell\{(D-1)\eta-1\}\right]g=0.\end{aligned} \tag{2.79}$$

Finally, the change of variable

$$z=2s^2-1 \tag{2.80}$$

yields the integration measure

$$\int_0^1 ds\, s^{D-1} c^{-[1+\eta(D-1)]} = 2^{-\frac{(D+1)-(D-1)\eta}{2}} \int_{-1}^1 dz\, (1-z)^{-\frac{1+(D-1)\eta}{2}} (1+z)^{\frac{D}{2}-1}, \tag{2.81}$$

and leads to the equation

$$(1-z^2)\frac{d^2g}{dz^2} + \Big[(b-a) - (a+b+2)z\Big]\frac{dg}{dz} + \frac{1}{4}\left[\rho^2 - 2\eta L^2 - (2\ell+D)\lambda + \ell\{(D-1)\eta - 1\}\right] g = 0, \tag{2.82}$$

where we set

$$a \equiv \lambda - \frac{1+(D-1)\eta}{2} \;=\; \sqrt{\frac{\{1+(D-1)\eta\}^2}{4} + \eta^2 L^2}\,, \tag{2.83}$$

$$b \equiv \frac{D}{2} + \ell - 1\,. \tag{2.84}$$

Assuming that the normalizable solutions of this equation are the polynomial ones, the condition the distance squared eigenvalues have to satisfy is

$$\frac{1}{4}\left[\rho^2 - 2\eta L^2 - (2\ell+D)\lambda + \ell\{(D-1)\eta - 1\}\right] = n(n+a+b+1)\,, \tag{2.85}$$

with $n = 0, 1, 2, \ldots$ in which case the solutions of (2.84) are just the Jacobi polynomials

$$g(z) = P_n^{(a,b)}(z)\,. \tag{2.86}$$

The eigenvalues are given by

$$\rho^2 = \left\{2n + \left(\frac{D}{2} + \ell + \sqrt{\frac{\{(D-1)\eta+1\}^2}{4} + \eta^2 L^2}\right)\right\}^2 - (1-\eta)^2\left\{L^2 + \frac{(D-1)^2}{4}\right\}, \tag{2.87}$$

while the eigenfunctions are

$$R_{n\ell}(p) = N_{n\ell}\, c^\lambda s^\ell\, P_n^{(a,b)}(z), \tag{2.88}$$

where the normalization factor $N_{n\ell}$, (with the sign included for later convenience) is

$$N_{n\ell} = (-1)^n(\beta+\beta')^{D/4}\sqrt{\frac{2(2n+a+b+1)\,n!\,\Gamma(n+a+b+1)}{\Gamma(n+a+1)\Gamma(n+b+1)}}, \tag{2.89}$$

and

$$\begin{aligned} c = \cos\theta \;&=\; \frac{1}{\sqrt{1+(\beta+\beta')p^2}}\,, \\ s = \sin\theta \;&=\; \frac{\sqrt{\beta+\beta'}\,p}{\sqrt{1+(\beta+\beta')p^2}}\,, \\ z = 2s^2 - 1 \;&=\; \frac{(\beta+\beta')p^2 - 1}{(\beta+\beta')p^2 + 1}. \end{aligned} \tag{2.90}$$

2.3.2 The expansion of Coulomb wavefunctions

Having diagonalized R^2, we can now turn to solving the Schrödinger equation for the Coulomb potential. Let us suppose that $\Psi(p)$ (or, expressed in terms of z, $\Psi(z)$) is an eigenfunction corresponding to energy E, that is

$$\left(\frac{P^2}{2m} - \frac{k}{R}\right)\Psi = E\Psi. \tag{2.91}$$

If, for some fixed ℓ, the function Ψ is expanded in the orthonormal basis $R_n = R_{n\ell}$ as

$$\Psi = \sum_{n=0}^{\infty} f_n R_n, \tag{2.92}$$

then the action of Hamiltonian can be calculated exactly. The kinetic term, in terms of the variable z is just multiplication by

$$\frac{P^2}{2m} = \frac{1}{2m(\beta+\beta')}\left(\frac{1+z}{1-z}\right) . \tag{2.93}$$

while $1/R$ acts as

$$\Psi = \sum_{n=0}^{\infty} f_n R_n \;\stackrel{1/R}{\longmapsto}\; \sum_{n=0}^{\infty} f_n \frac{R_n}{r_n} = \frac{1}{\hbar\sqrt{\beta+\beta'}} \sum_{n=0}^{\infty} \frac{f_n}{\rho_n} R_n, \tag{2.94}$$

so the Schrödinger equation becomes

$$\sum_{n=0}^{\infty} f_n \left[\frac{1}{2m(\beta+\beta')}\left(\frac{1+z}{1-z}\right) - \frac{1}{\hbar\sqrt{\beta+\beta'}}\frac{k}{\rho_n} + (-E)\right] R_n = 0 . \tag{2.95}$$

Multiplying through by $2m(\beta+\beta')(1-z)$ and introducing the dimensionless

$$\xi \equiv \sqrt{2m(\beta+\beta')(-E_0)} = \frac{\hbar\sqrt{\beta+\beta'}}{a_0} , \tag{2.96}$$

$$\epsilon \equiv 2M(\beta+\beta')(-E) = \xi^2\left(\frac{E}{E_0}\right) . \tag{2.97}$$

defined in terms of the Bohr radius $a_0 = 1/mk$ and regular energy $E_0 = -k/2a_0$, the equation reads

$$\sum_{n=0}^{\infty} f_n \left[\left(1+\epsilon-\frac{2\xi}{\rho_n}\right) + \left(1-\epsilon+\frac{2\xi}{\rho_n}\right) z\right] R_n(z) = 0. \tag{2.98}$$

We can observe that in addition to the orthonormal $R_n(z)$ functions, now term involving $zR_n(z)$ appear. These can be re-expressed in terms of $R_n(z) = N_n\, c^{\lambda} s^{\ell}\, P_n^{(a,b)}(z)$ by using the

recursion relation for the Jacobi polynomials [1, Eqn. 22.7.1], in the form

$$\begin{aligned} z\,\frac{R_n(z)}{N_n} = &\frac{2(n+1)(n+a+b+1)}{(2n+a+b+1)(2n+a+b+2)}\frac{R_{n+1}(z)}{N_{n+1}} \\ &- \frac{a^2-b^2}{(2n+a+b)(2n+a+b+2)}\frac{R_n(z)}{N_n} \\ &+ \frac{2(n+a)(n+b)}{(2n+a+b+1)(2n+a+b)}\frac{R_{n-1}(z)}{N_{n-1}}\,. \end{aligned} \tag{2.99}$$

Plugging in the expression for the normalization factors N_n given by (2.89), we obtain

$$z\,R_n(z) = a_n R_{n+1}(z) + b_n R_n(z) + c_n R_{n-1}(z), \tag{2.100}$$

where

$$a_n = -\frac{2}{(2n+a+b+2)}\sqrt{\frac{(n+1)(n+a+1)(n+b+1)(n+a+b+1)}{(2n+a+b+1)(2n+a+b+3)}} = c_{n+1}, \tag{2.101}$$

$$b_n = -\frac{a^2-b^2}{(2n+a+b)(2n+a+b+2)}\,, \tag{2.102}$$

$$c_n = -\frac{2}{(2n+a+b)}\sqrt{\frac{n(n+a)(n+b)(n+a+b)}{(2n+a+b-1)(2n+a+b+1)}} = a_{n-1}. \tag{2.103}$$

Finally, substituting these into the Scrödinger equation (2.98), we obtain the recursion relation

$$(s_{n+1}c_{n+1})f_{n+1} + (2 - s_n + s_n b_n)f_n + (s_{n-1}a_{n-1})f_{n-1} = 0, \tag{2.104}$$

where $f_{-1} = 0$, and

$$s_n = 1 - \epsilon + \frac{2\xi}{\rho_n}. \tag{2.105}$$

Note that the the coefficients f_n, as determined by this recursion relation above, depend on the energy eigenvalues through ϵ. Since the functions $R_n(z)$ are orthonormal, the condition for a normalizable solution $\Psi(z) = \sum_{n=0}^{\infty} f_n R_n(z)$ is

$$\|\Psi\|^2 = \sum_{n=0}^{\infty} f_n^2 = \text{finite}. \tag{2.106}$$

This condition determines the eigenvalues of the energy.

Let us look at the behavior of this recursion relation as $n \to \infty$. The coefficients of f_n have the limits

$$a_n = c_{n+1} \to \frac{1}{2}, \qquad b_n \to 0, \qquad s_n \to 1 - \epsilon, \tag{2.107}$$

so (2.104) is asymptotically equivalent to the one with constant coefficients

$$(1-\epsilon)f_{n+1} + 2(1+\epsilon)f_n + (1-\epsilon)f_{n-1} = 0. \tag{2.108}$$

This has the characteristic equation

$$(1-\epsilon)\lambda^2 + 2(1+\epsilon)\lambda + (1-\epsilon) = 0, \tag{2.109}$$

with solutions

$$\lambda_\pm = \frac{1 \pm \sqrt{\epsilon}}{1 \mp \sqrt{\epsilon}}, \tag{2.110}$$

and thus the asymptotic behavior of the sequence f_n is

$$f_n(\epsilon) \sim C_+(\epsilon)\,\lambda_+^n + C_-(\epsilon)\,\lambda_-^n\,. \tag{2.111}$$

The root $\lambda_+ > 1$, while $\lambda_- < 1$. For a normalizable solution we need $f_n \to 0$; this can be achieved only if $C_+(\epsilon) = 0$. While we were not able to find a closed form expression for $C_+(\epsilon)$, its zeros — which determine the energy spectrum — can be calculated numerically.

2.3.3 Numerical results

In order to determine the values of ϵ for which C_+ vanishes, two different algorithms were used.

The direct algorithm. The first, "direct", algorithm (see also Appendix A.4) is based on forward evaluation of the recurrence (2.104). It starts with $f_{-1} = 0$ and an $f_0 = 1$ —, the value of f_0 does not matter as it will only contribute an overall factor to the remaining f_n — and determines the the values of ϵ, in terms of parameters D, ξ, and ℓ for which (2.104) converges to zero. The main difficulty is that, due to the inexact internal representation of the real floating point numbers, the coefficient C_+ will never be exactly null and the term corresponding to it will eventually dominate the sequence.

An example is shown in Fig. 2.1. There the parameters are $D = 3$, $\xi = 0.1$, $\ell = 0$ and $\eta = 0$, and the values of f_n are calculated for two different ϵ, namely those corresponding to $E/E_0 = 0.248$ (blue line) and $E/E_0 = 0.249$ (red line). These bracket the exact energy eigenvalue of $E_{2s}/E_0 = 0.24867\ldots$

In the top graph the actual values of the f_n are plotted. It can be seen that for $n \gtrsim 100$, the $C_+\lambda_+^n$ term begins to dominate. This is confirmed by the bottom graph that shows the logarithm of the absolute value of f_n. It can be seen that the high n behavior of f_n is opposite to each other. Indeed it is due to the fact that C_+ changes sign, and this can be used to determine the energy eigenvalues to arbitrary accuracy by a bisecting method.

There is one more observation to be made: the number of places where f_n changes sign (marked by light blue vertical lines) shows the position of ϵ with respect to the energy

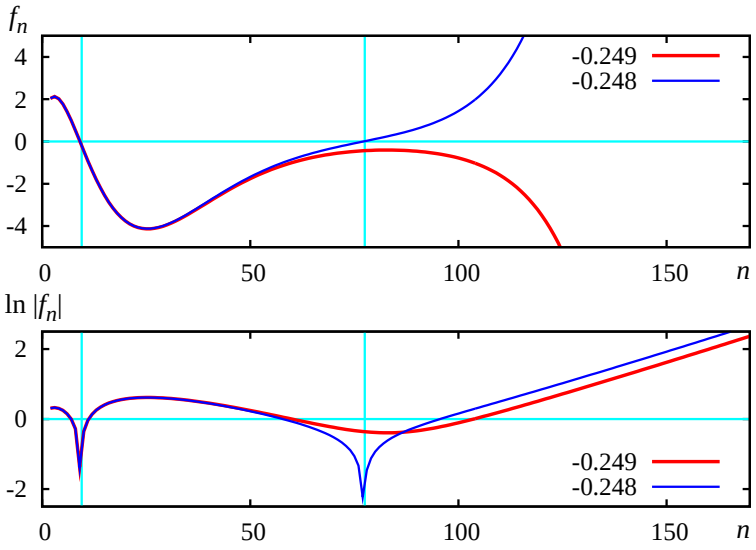

Figure 2.1: *The behavior of the recursion terms in the direct algorithm*

eigenvalues. More precisely, f_n does not change sign when ϵ is above the energy with largest absolute value; this is $|E_{1s}|$ for $\ell = 0$.[3] The recursion has one sign-change when ϵ is between the two largest energies, that is between $E_{1\mathrm{s}}$ and $E_{2\mathrm{s}}$, for example in the red line's case in the figure. The recursion has two sign changes when ϵ is between $E_{2\mathrm{s}}$ and $E_{3\mathrm{s}}$ (see e.g. the blue plot in figure) and so on. In the actual program this property, rather than the switch in the high-n behavior, was used to determine the energy eigenvalues.

The other difficulty in the method is to determine where to stop evaluating the f_n's. While visually it seems obvious when the $C_+\lambda_+^n$ became dominant, in an algorithm it is not so easy to find the proper time to stop. One possibility is to stop after a predetermined, fairly large n. This has the drawback that it can fail when the $C_+\lambda_+^n$ terms becomes dominant late. This happens when C_+ is small (i.e. ϵ is close to the energy eigenvalues) or when $\lambda_+ \simeq 1$ (the minimal length is small), exactly the cases in which that interest us most. In turn, increasing the number of evaluation steps increases considerably the simulation time.

As a result, we determine dynamically the time to stop. We evaluate the ratio f_{n+1}/f_n at every step, and we stop when the relative difference between this ratio and λ_+ is smaller than some value (taken to be 1%) for a sufficiently large number of steps (taken greater of 20 and 10% of total steps). There is one additional heuristic correction, in that the "relative difference" is evaluated using

$$\frac{\dfrac{f_{n+1}}{f_n} - \lambda_+}{\lambda_+ - 1}\,. \tag{2.112}$$

[3]Obviously, the energy level with largest magnitude is $|E_{2\mathrm{p}}|$ for $\ell = 1$, and $|E_{3\mathrm{d}}|$ for $\ell = 2$, etc.

This adds some needed extra security for small values of the minimal length ξ, when $\lambda_+ \simeq 1$. With this correction, the algorithm is robust for ξ as low as 10^{-4}, every value of η, and at least the first five energy levels.

This algorithm is also quite fast. On a contemporary PC with clock speed of ~ 2 GHz, the determination for an energy level corresponding to $\xi \simeq 10^{-3}$ takes less than a minute; for higher values of ξ, where the convergence is much faster, only a few seconds.

The reverse algorithm The alternative algorithm is a "reverse" one, where one starts at some high n with an (almost) null f_n and the recursion is evaluated backwards in an attempt to recover $f_{-1} = 0$ for suitable values of ϵ.

More exactly, the recursion relation (2.104) is rewritten in terms of

$$\lambda_n = \frac{f_{n+1}}{f_n}, \tag{2.113}$$

as

$$(s_{n+1}c_{n+1})\lambda_n\lambda_{n-1} + (2 - s_n + s_n b_n)\lambda_{n-1} + s_{n-1}a_{n-1} = 0, \tag{2.114}$$

which gives the inverse recursion

$$\lambda_{n-1} = -\frac{s_{n-1}a_{n-1}}{(s_{n+1}c_{n+1})\lambda_n + 2 - s_n + s_n b_n}\,. \tag{2.115}$$

For an ϵ corresponding to an energy eigenvalue, the sequence λ_n should have the limit $\lambda_- = \frac{1-\sqrt{\epsilon}}{1+\sqrt{\epsilon}}$ so we start for with a value of $\lambda_n = \lambda_-$ for sufficiently high n. For a consistency check the reverse recursion is evaluated also for a starting value of $\lambda'_n = \lambda_-^{(n)} \simeq \lambda_-$, where $\lambda_-^{(n)}$ is the root of the equation

$$(s_{n+1}c_{n+1})\lambda^2 + (2 - s_n + s_n b_n)\lambda + s_{n-1}a_{n-1} = 0. \tag{2.116}$$

and the solution discarded if the two recurrences give seriously different results.

For the choice of the starting point of the backward recursion, the value of $n = 10\xi/\epsilon \sim 1/\epsilon\Delta_{\min}$ strikes a good balance between reliability and speed. For this value the algorithm works well in the domain described above ($\xi \gtrsim 10^{-4}$, $n \leq 5$, η arbitrary) and its speed is comparable, if a little bit slower than the direct algorithm.

For a given ξ and ϵ the values of of $\lambda_{n-1}, \lambda_{n-2}, \ldots, \lambda_0$ are evaluated successively using (2.115). The boundary condition for the energy eigenvalues is $f_{-1} = 0$, or equivalently

$$(2 - s_1 + s_1 b_1)\lambda_0 + s_0 a_0 = 0. \tag{2.117}$$

Thus, in order to determine the energy spectrum, the values of candidate ϵ are varied over an interval, and when a sign change in the previous expression is detected, the procedure enters a bisecting phase to determine the eigenvalue to pre-set accuracy. Finally, the coefficients f_n can be recovered from the formula

$$f_n = \lambda_{n-1} \ldots \lambda_1 \lambda_0. \tag{2.118}$$

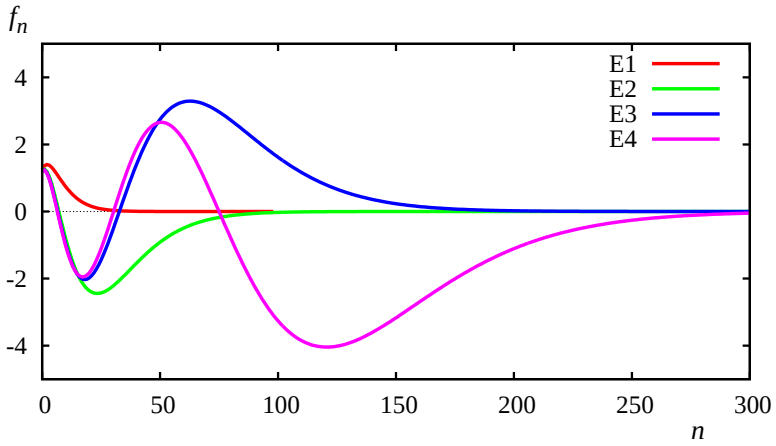

Figure 2.2: *The behavior of the recursion terms in the reverse algorithm*

An example on the behavior of the coefficients f_n is shown in Figure 2.2. There $\xi = 0.1$, $\eta = 0$ and $\ell = 0$ as in Figure 2.1. The values chosen for ϵ, however, are those corresponding to the first four energy eigenvalues. We can see again that the number of "wiggles" on the graph of the f_n's corresponds to the energy level.

Results In general the two algorithms give consistent results. There are, however, small differences in their domain of usability. The reverse algorithm works slightly better for large values of ξ, that is when $\xi \gtrsim 1$. There, the direct algorithm fails in its present form for $\epsilon > 1$, when λ_+ becomes negative. It can also miss some of the sign changes of the f_n sequence, and thus "skipping" some energy levels. This can happen with the second algorithm also: as ξ increases, the energy levels become more densely packed, and while scanning over ϵ, one or more energy levels can be overlooked.

In both cases the problems can be mended, for example by a finer granulation of the scanning in the reverse case. There is not much reason to do so, though. Large values of ξ means a minimal length of an order of magnitude larger than that of the Bohr radius, which is obviously unphysical.

Both algorithms can give inaccurate results when ξ becomes very small, but this is not that easily corrected. The reason is that for small ξ, the convergence of f_n becomes slow and during the recursive evaluation of an increased number of terms the numerical errors will invariably accumulate. To get an estimate on the lowest ξ for which the programs are reliable, they were recompiled using a double-double (quad) precision floating point variables. This results in a huge hit in execution time, but shows that the programs with regular, double precision variables can be trusted down to $\xi = 10^{-4}$. To be on the safe side, our analysis uses values ξ of 10^{-3} or higher.

The results are sampled in Figures 2.3 and 2.4. In Figure 2.3, the energy values are

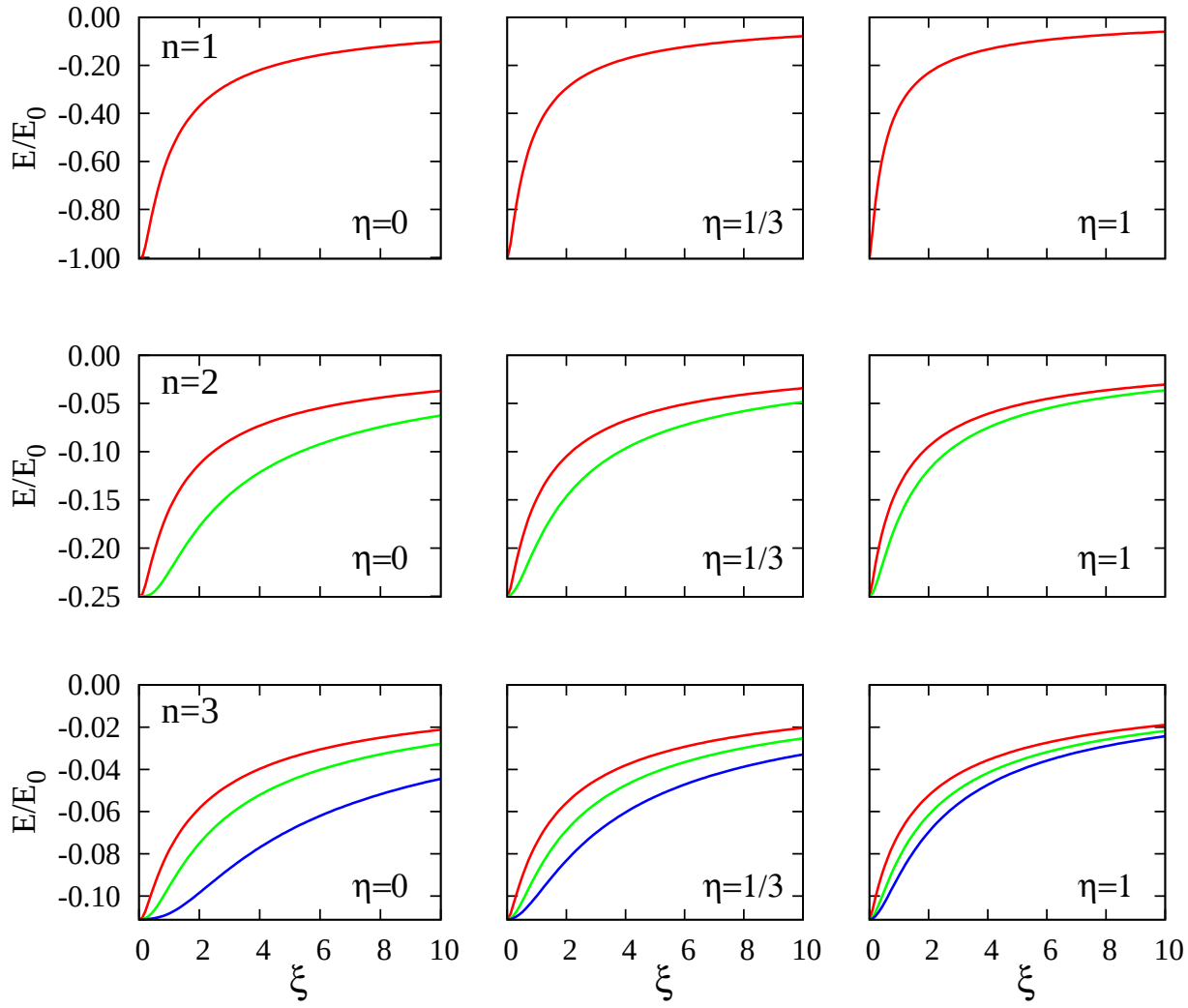

Figure 2.3: *Energy corrections for the Coulomb spectrum, as a function of the minimal length* $0 < \xi \leq 10$. *The red, green, and blue lines represent* s, p, *and* d *states, respectively. The columns correspond to different* $\beta'/(\beta+\beta')$ *ratios, and the lines to different energy levels* n.

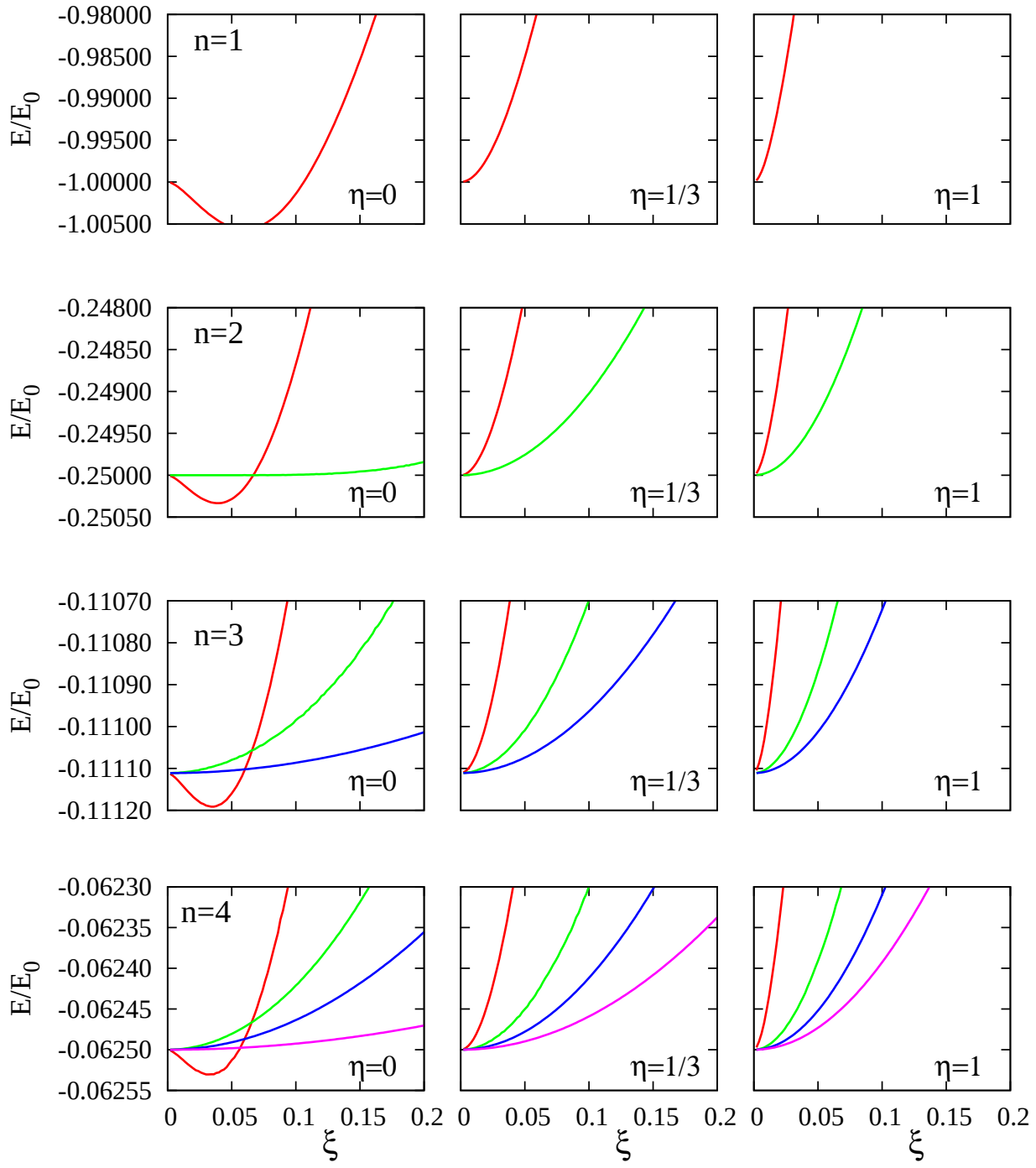

Figure 2.4: *Energy corrections for the Coulomb spectrum, as a function of the minimal length* $0 < \xi \leq 0.2$. *The red, green, blue, and magenta lines represent* s, p, d, *and* f *states, respectively. The columns correspond to different* $\beta'/(\beta+\beta')$ *ratios, and the lines to different energy levels* n.

plotted as a function of the minimal length $\sqrt{\beta+\beta'}$ in units of the Bohr radius a, for $\xi = \sqrt{\beta+\beta'}/a < 10$. The first three energy levels are plotted with angular momentum number varying between $\ell = 0$ and $\ell = 2$. Figure 2.4 shows magnifications of these plots, for the most interesting region of small minimal length ξ, with the addition of a fourth energy level and $\ell = 3$. In both panels, the $\eta = \beta/(\beta+\beta')$ is also varied, the left column corresponding to $\beta = 0$, the center one to $\beta' = 2\beta$ and the right one to $\beta' = 0$.

We can see that the degeneracy among different angular momentum states is lifted: higher-ℓ states get smaller corrections. The only exceptions are the S states for $\beta' > 2\beta$ and $D = 3$. These states start out with the lowest, negative correction for small $\xi < 0.2$, but cross the higher-angular-momentum levels as ξ increases. Another important remark, expected but not readily transparent in the representation used, is that the energy values converge to the usual result in the limit when the minimal length is taken to zero.

Comparison with previous results For non-s states the energy corrections obtained in previous section (2.55) agreed with the results obtained previously by Brau for $\beta' = 2\beta$ in [7]. The agreement with the numerical results is excellent, as it can be seen in Figure 2.5 (a), for the case of $2P$ states. For other non-S states the agreement of the three results is similarly good, also.

For vanishing angular momentum and three dimensions, there are two disagreeing partial results published previously, [7] for $\beta' = 2\beta$, and [2] for arbitrary η and $\ell = 0$. In the last section we determined the general form of the correction, but its coefficients were not fixed. It was

$$\frac{\Delta E_{n\ell}}{E_0} = \frac{4(3\eta-1)}{n^3}\xi^2 E_1(\rho_c\xi) + C\xi^2 + O(\xi^3), \tag{2.119}$$

Let us see if this approximation is reproduced by the numerical results. In Figure 2.6 the quantity

$$\frac{\xi^2 \log(\xi)}{\Delta E_{1s}} \tag{2.120}$$

is plotted against very small values of the minimal length ξ, obtained from the direct method,[4] for $\eta = 1$. If the form (2.119) is correct, this quantity should converge to the value of the leading order coefficient. This coefficient is $-1/8$ for the case considered, and is represented by the red line in the graph. It can be seen that over 4 orders of magnitude in ξ — or, equivalently, 8 orders in $\beta+\beta'$, — the quantity is indeed approximatively constant and close to the expected value.

This confirms the actual form of the s-level corrections, and C can be determined numerically, by fitting relation (2.60) to the numerical results at a sufficiently low value of ξ^2. We have used the value of $\xi = 10^{-3}$, corresponding to $\beta+\beta' = 10^{-6}a$. With these fits, the agreement with the numerical results is good. [See Figure 2.5 (b) and (c).] For $\beta' = 2\beta$, the

[4]It should be noted that for $\xi \lesssim 10^{-4}$, the values are unconfirmed by alternative methods, and as such the errors might be larger for the first two data points.

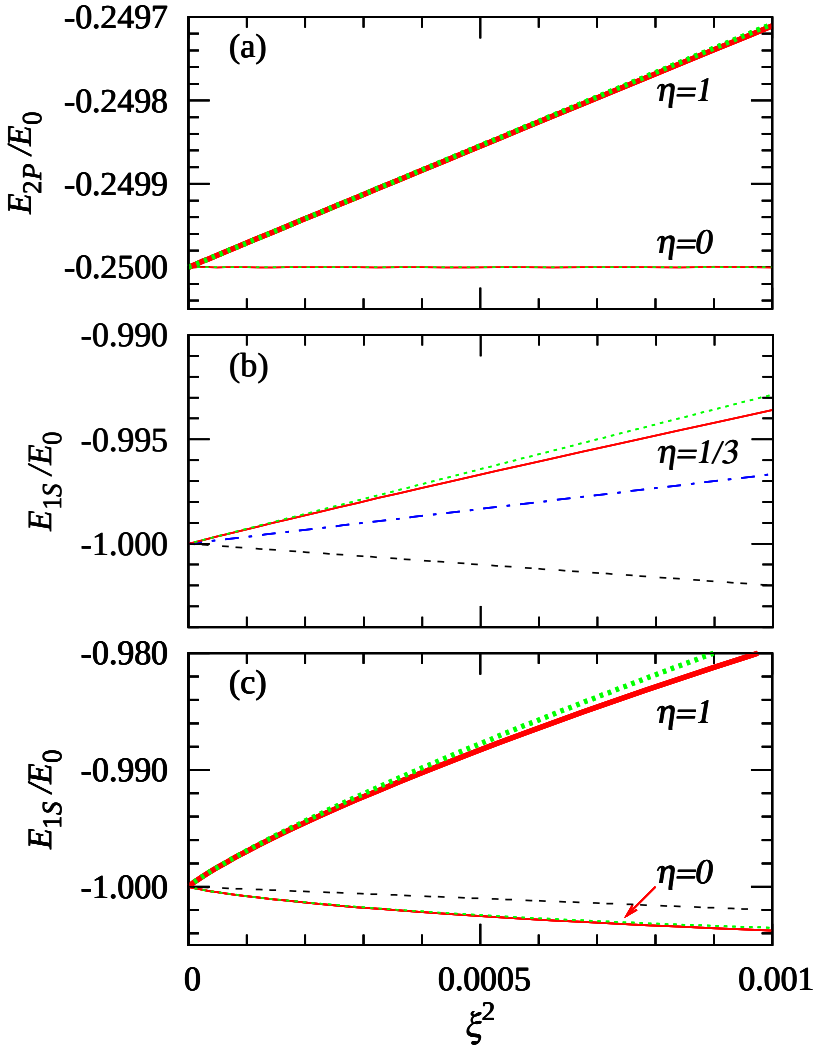

Figure 2.5: *Comparison of different results for for the energy corrections to the* $1S$ *and* $2P$ *Coulomb states: (a)* $2P$ *state with* $\eta = 0, 1$*; (b)* $1S$ *state with* $\eta = 1/3$*; (c)* $1S$ *state with* $\eta = 0, 1$*.*

- *Solid red lines: numeric result;*
- *dotted green lines: perturbative result;*
- *dash-dotted blue lines: Ref. [7];*
- *double-dashed black lines: Ref. [2].*

The perturbative expression is given for (a) by (2.55) *and for (b), (c) by formula* (2.60)*, with the coefficient* C *chosen such that it agrees with the numerics at* $\xi^2 = 10^{-6}$*.*

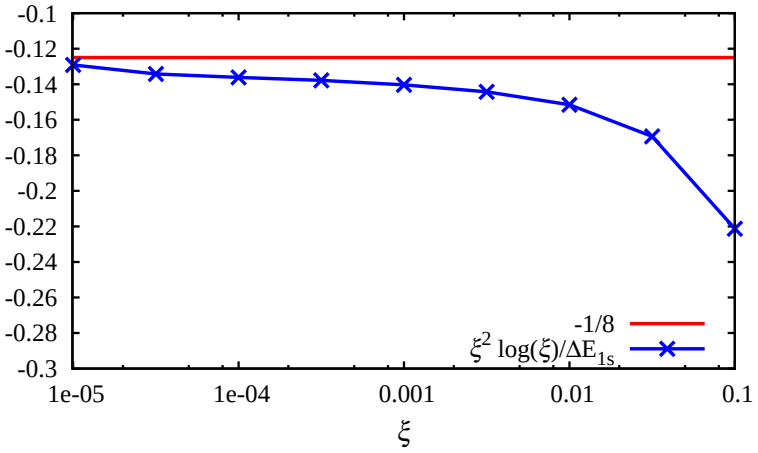

Figure 2.6: *Behavior of the S-state corrections for very small values of* ξ

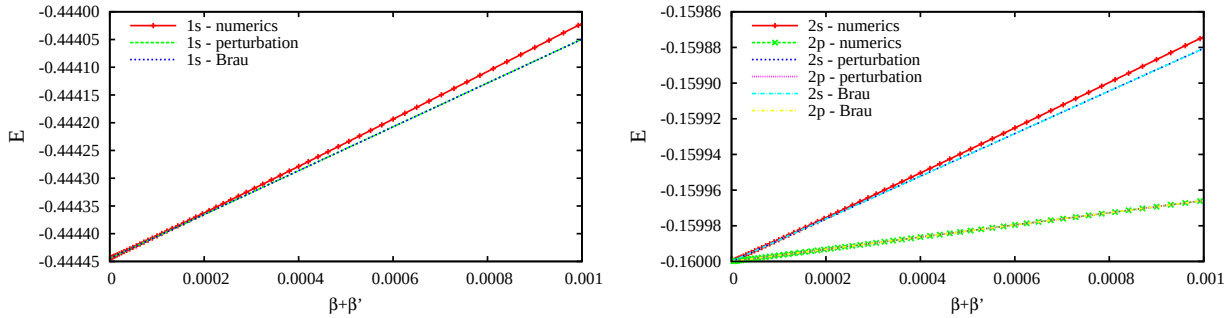

Figure 2.7: *Comparison of Coulomb energy corrections in* $D = 4$ *dimensions. Left:* $n = 1$ *states, right:* $n = 2$ *states.*

coefficient of the leading $\xi^2 \ln(\xi)$ vanishes, and ξ^2 becomes the leading term, as in [7]. The coefficient of it obtained from the fit, however, disagrees with that calculated by Brau. As mentioned before, this might be due to his neglecting higher order terms in the expansion of R^2.

Reference [2] arrives at a different expression, which is independent of η. However, we could neither account for the discrepancy nor reproduce those results.

It should be noted or $D > 3$, in the perturbative method the $\langle 1/\rho^3 \rangle$ integrals are convergent, and the approximate solutions agree with [7] and are reproduced nicely with the corresponding numerical results, even for $\ell = 0$, as it can be seen Figures 2.7 and 2.8, both plotted for $\eta = 1/3$.

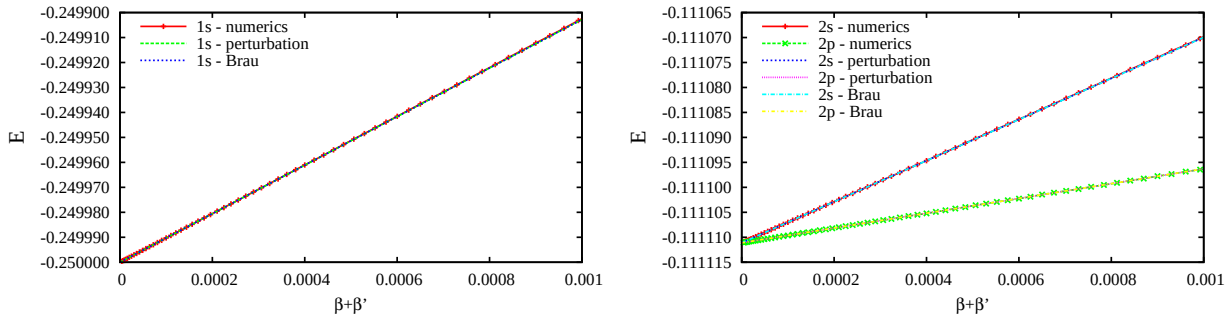

Figure 2.8: *Comparison of Coulomb energy corrections in $D = 5$ dimensions. Left: $n = 1$ states, right: $n = 2$ states.*

2.3.4 A bound on the minimal length

If the corrections due to the minimal length are large enough, their contribution will be seen in precision spectroscopy of hydrogen-like atoms. Conversely, the lack of such experimental fingerprints would impose limits on the value of the perturbation parameter β.

A naive estimate, obtained by requiring that the corrections are smaller than the experimental error on the value of the hydrogen $1S$-$2S$ splitting, gives $\Delta x_{\min} \gtrsim 300$ GeV (cf. [7]). Unfortunately, this estimate would be correct only if the measured value of the physical observable agreed with the theoretical prediction, and the main source of error were the experimental one. This is certainly not the case for the $1S$-$2S$ splitting in hydrogen: known to 1.8 parts in 10^{14}, it is one of the most precisely measured quantities today and is considered a *de facto* standard [19]. The value of the Rydberg constant is determined using this measurement as an input, and thus the theoretical uncertainty is orders of magnitude above the experimental one.

The only reasonable requirement is that the corrections due to the (hypothetical) minimal length are smaller than the difference between the measured and theoretical values. To do so, we include the minimal length contributions in the Lamb shifts. As a reminder, by convention, the energy levels of a hydrogenic state is composed of two parts. The main contribution is given by the solution of the Dirac equation together with the first order nuclear recoil correction. All other corrections, including those due to QED, the proton charge radius or the hypothetical minimal length uncertainty constitute the *Lamb shift* corresponding to this level.

The strongest constraint is expected from the $1S$ Lamb shift, being the one determined most precisely and getting the largest correction. Today's best theoretical prediction for the $1s$ state Lamb shift is [17]

$$L_{1s}^{\text{th}} = 8172.731(40)\text{MHz}$$

The experimental value of the $1S$ Lamb shift in Hydrogen together with the Rydberg constant are extracted from the the measurement of two splittings: the $1S$-$2S$ on one hand

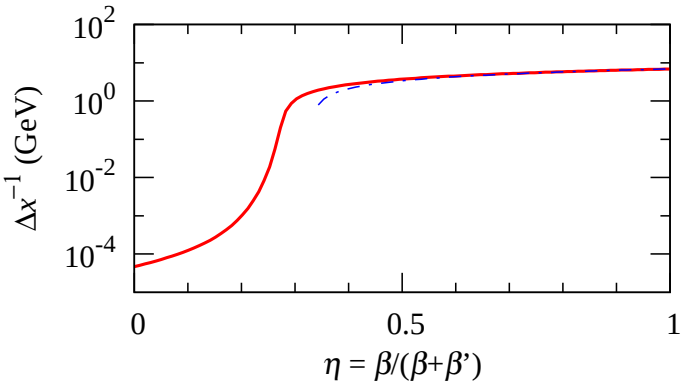

Figure 2.9: *Constraint on the minimal length obtained as a function of η, including the two highest-order terms (continuous line) and just the leading-order term (dash-dotted line).*

and a $2S$ to some high nS/nD on the other. As said before, the $1S$-$2S$ splitting in the atomic hydrogen is one of the most precisely measured quantities today; the experimental values of the Lamb shifts are known less exactly due to the somewhat larger error on the second splitting and uncertainties in the values of physical constants (electron-proton mass ratio, fine structure constant) needed in calculating them. Even so, the measured Lamb shift [24] of

$$L_{1s}^{\rm exp} = 8172.837(22)\text{MHz} \tag{2.121}$$

is larger than the theoretical value by about 5σ experimental uncertainties.

If we attribute the discrepancy entirely to the minimal length correction to the $1S$ state, the bound as a function of η, obtained using the first two terms in (2.60), is shown in Fig. 2.9. It is 1.75 GeV for $\eta = 1/3$ and increases to 6.87 GeV for $\eta = 1$. Below $\eta = 1/3$, the constraint relaxes rapidly. Indeed, in this case the leading-order term in (2.60) is negative, and only the contribution from the next term can account for the observed difference. As a comparison, including only the leading term, we can obtain a bound only for $\eta > 1/3$, with consistent results for $\eta \gtrsim 0.5$.

We should point out that the Lamb shift theoretical predictions are somewhat frail because of the uncertainties in the nuclear structure. Most importantly, the correction due to the proton charge radius has the same order of magnitude that the ones discussed here. There was some controversy in the recent literature on the exact value of the charge radius (see [11] for a review), and a possible shift in this value could influence strongly our results. Thus one should consider our results rather as upper limits for the minimal length.

To avoid the effects of nuclear structure, one could look into muonium spectroscopy. Here only the $1S$-$2S$ splitting is measured with good accuracy, but the current limits are still weak for our purposes. If proposed experiments [13] could bring down the experimental uncertainty by more than two orders of magnitude below the 100KHz level they could provide us with a better limit on β or an independent signal of physics beyond the Standard Model,

possibly manifested by the existence of a minimal length.

2.4 The gravitational well

In [18] and subsequent papers the authors report a first experiment to identify the quantum states of a system in a gravitational well. In their setup, ultra-cold neutrons are flying above a mirror in the Earth's gravitational field and their ground state can be conclusively identified.

In a first approximation, such a setup can be described by the potential of a perfectly reflecting mirror,

$$V(z) = \begin{cases} mgz, & z > 0, \\ \infty, & z \leq 0. \end{cases} \tag{2.122}$$

The solution of the Schrödinger equation of such a system is well known. Along the z axis, the energy spectrum is

$$E^0_{z,n} = -\frac{mg}{\gamma}\alpha_n, \tag{2.123}$$

where α_n represent the zeros of the Airy function $\mathrm{Ai}(z)$ and $\gamma = (2m^2g)^{1/3}$ is the characteristic momentum scale of the system. (We set $\hbar = 1$.) The normalized eigenfunctions are

$$\psi_{z,n}(z) = \frac{\sqrt{\gamma}}{|\,\mathrm{Ai}'(\alpha_n)|}\,\mathrm{Ai}(\gamma z + \alpha_n). \tag{2.124}$$

In the experiment, the most probable heights of the flying neutrons are measured. These are given by

$$h^0_n = \frac{E^0_{z,n}}{mg} = -\frac{\alpha_n}{\gamma} \tag{2.125}$$

Along the y axis the particle is free, with continuous spectrum. Here we will assume that the eigenfunction is just a plane wave,

$$\psi_y(y) = e^{ip_y y}, \tag{2.126}$$

with energy eigenvalue

$$E^0_y = \frac{p_y^2}{2m}, \tag{2.127}$$

but extension to a superposition of plane waves is straightforward.

The complete eigenstate of the system is

$$\psi(y,z) = \psi_y(y)\psi_z(z), \tag{2.128}$$

and has total energy

$$E^0 = E^0_y + E^0_{z,n}. \tag{2.129}$$

One can raise the question if modifications of quantum mechanics, such as those leading to a hypothetical minimal length, can have a measurable effect on the obtained energy level(s). The problem was considered by Brau and Buisseret in [8], where perturbative corrections were obtained for the $\beta' = 2\beta$ case. Here our aim is to obtain a solution for arbitrary β and β'. We will see that for $\beta' = 0$ the Schrödinger equation can be solved exactly, and perturbative corrections can be obtained for arbitrary $\beta, \beta' > 0$.

We will represent these operators X_i, P_j through the pseudo-position representation

$$X_i = \hat{x}_i(1 + \beta\hat{p}^2) + \beta'\hat{x}_j\hat{p}_j\hat{p}_i + \bar{\gamma}p_i, \tag{2.130}$$

$$P_i = \hat{p}_i, \tag{2.131}$$

in terms of the operators

$$\hat{x}_i = x_i, \qquad \hat{p}_j = \frac{1}{i}\frac{\partial}{\partial x_j}, \tag{2.132}$$

satisfying the usual commutation relations

$$[\hat{x}_i, \hat{p}_j] = i\delta_{ij}, \qquad [\hat{p}_i, \hat{p}_j] = [\hat{x}_i, \hat{x}_j] = 0, \tag{2.133}$$

where $\bar{\gamma}$ is an arbitrary constant.

The Hamiltonian for the problem considered is (with $Z = X_3$)

$$H = \frac{P_y^2 + P_z^2}{2m} + V(Z), \tag{2.134}$$

with the potential

$$V(Z) = \begin{cases} mgZ, & Z > 0, \\ \infty, & \text{otherwise.} \end{cases} \tag{2.135}$$

In terms of the representation above, the Hamiltonian is:

$$H = -\left(\frac{1}{2m} + mg\beta z\right)\frac{\partial^2}{\partial y^2} - mg\beta' y\frac{\partial^2}{\partial y \partial z} - \left(\frac{1}{2m} + mg(\beta + \beta')z\right)\frac{\partial^2}{\partial z^2} - \bar{\gamma}mg\frac{\partial}{\partial z} + mgz. \tag{2.136}$$

The Hamiltonian is a second order linear partial differential operator with variable coefficients. As a first step we can determine the domains where it is elliptic, parabolic or hyperbolic. Its discriminant is

$$\begin{aligned} \Delta &= (mg\beta' y)^2 - 4\left(\frac{1}{2m} + mg\beta z\right)\left(\frac{1}{2m} + mg(\beta + \beta')z\right) \\ &= \frac{1}{m^2}\left\{\left[(1-\eta)\frac{y}{z_0}\right]^2 - 4\left(\frac{1}{2} + \eta\frac{z}{z_0}\right)\left(\frac{1}{2} + \frac{z}{z_0}\right)\right\} \\ &= \frac{1}{m^2}\left[(1-\eta)^2\left(\frac{y}{z_0}\right)^2 - 4\eta\left(\frac{z}{z_0}\right)^2 - 2(\eta+1)\left(\frac{z}{z_0}\right) - 1\right], \end{aligned} \tag{2.137}$$

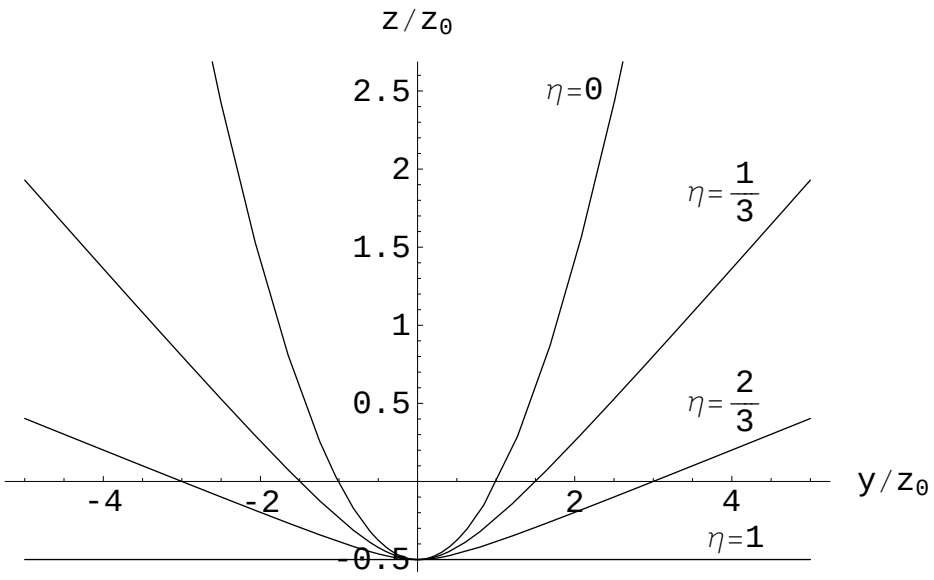

Figure 2.10: *Domains of ellipticity of the Schrödinger equation for the gravitational well. For given η, and $z > 0$, the Schrödinger equation is parabolic on the curve, elliptic in the region above it and hyperbolic below it.*

where in the second line we introduced

$$\eta = \frac{\beta}{\beta + \beta'} \quad \text{and} \quad z_0 = \frac{1}{(\beta + \beta')m^2 g}. \tag{2.138}$$

The condition for ellipticity, $\Delta < 0$, can be readily solved then to yield (for $z > 0$)

$$\frac{z}{z_0} > \begin{cases} \frac{(1-\eta)\sqrt{4\eta(y/z_0)^2+1}-(\eta+1)}{4\eta}, & \eta > 0, \\ \frac{(y/z_0)^2-1}{2}, & \eta = 0. \end{cases} \tag{2.139}$$

In Figure 2.4, the curves corresponding to the interface where the equation switches from elliptic to hyperbolic are drawn for a few values of η. The coordinates are in units of z_0. Please note that the only curve not intersecting the horizontal axis is the one for $\beta' = 0$ (i.e $\eta = 1$).

We can observe that, independent of η, the equation is elliptic for $|y| < z_0$. The value of z_0 in terms of $\Delta x_{\min} = \sqrt{\beta + \beta'}$ can be calculated as

$$z_0 \text{ (in meters)} \simeq \left[\frac{2 \times 10^{-8}}{\Delta x_{\min} \text{ (in meters)}}\right]^2. \tag{2.140}$$

Even for $\Delta x_{\min}$ as high as 6.6×10^{-17} m, corresponding roughly to the bound of $(3 \text{ GeV})^{-1}$ derived in Section 2.3.4 and [5],

$$z_0 \simeq 10^{17} \text{ m} \simeq 10 \text{ light-years}, \tag{2.141}$$

at which distance the effect of our table-top experiment and the Earth's gravitational pull can be neglected. One way to proceed is to restrict ourselves to the domain where the Schrödinger equation is elliptic, and solve it subject to the condition that the wavefunction vanishes at the boundary of this domain.

There is one case where we can avoid resorting to an approximation or the rather complicated procedure of solving a mixed type equation. As one can see from the figure above or from (2.139), when $\eta = 1$ or, equivalently, $\beta' = 0$, the half-plane $z > 0$ is situated entirely above the interface, and as such the equation is elliptic in the complete domain we are interested in.

2.4.1 Exact result for $\beta' = 0$

When $\beta' = 0$, the mixed derivative term in the Hamiltonian vanishes and the Scrödinger equation simplifies considerably and can be solved explicitly. It reduces to

$$\left[-\left(\frac{1}{2m}+mg\beta z\right)\frac{\partial^2}{\partial y^2}-\left(\frac{1}{2m}+mg\beta z\right)\frac{\partial^2}{\partial z^2}-mg\bar{\gamma}\frac{\partial}{\partial z}+mgz\right]\psi(y,z)=E\psi(y,z). \tag{2.142}$$

The functions $y \mapsto e^{ip_y y}$, with real p_y satisfy

$$\frac{\partial^2}{\partial y^2}e^{ip_y y}=-p_y^2 e^{ip_y y}, \tag{2.143}$$

and can be used to expand ψ as

$$\psi(y,z)=\int \frac{dp_y}{2\pi}\, a_{p_y}(z)e^{ip_y y}. \tag{2.144}$$

The coefficients a_{p_y}, as a function of z, will then satisfy

$$\left[-\left(\frac{1}{2m}+mg\beta z\right)\frac{\partial^2}{\partial z^2}-mg\bar{\gamma}\frac{\partial}{\partial z}+mg(1+p_y^2\beta)z+\frac{p_y^2}{2m}-E\right]a_{p_y}(z)=0. \tag{2.145}$$

For $z \to \infty$, this equation is asymptotically equivalent to

$$-\beta a''_{p_y}+(1+p_y^2\beta)a_{p_y}=0, \tag{2.146}$$

with normalizable solution $a_{p_y}(z) \sim \exp\left(-z\sqrt{p_y^2+1/\beta}\right)$. This suggests changing the dependent variable to

$$b_{p_y}(z)=a_{p_y}(z)e^{z\sqrt{p_y^2+\frac{1}{\beta}}}. \tag{2.147}$$

The eigenvalue equation for b_{p_y},

$$\left[-\left(1+2m^2g\beta z\right)\frac{\partial^2}{\partial z^2}+2\left((1+2m^2g\beta z)\sqrt{p_y^2+\frac{1}{\beta}}-m^2g\bar{\gamma}\right)\frac{\partial}{\partial z}\right.$$
$$\left.-2mE-\frac{1}{\beta}+2m^2g\bar{\gamma}\sqrt{p_y^2+\frac{1}{\beta}}\right]b_{p_y}(z)=0, \tag{2.148}$$

is equivalent, via a change of variable of the form

$$\zeta = \alpha(1 + 2m^2 g\beta z), \tag{2.149}$$

with α to be determined, to

$$\left[\frac{\alpha m^2 g\beta}{\sqrt{p_y^2 + \frac{1}{\beta}}}\,\zeta\frac{\partial^2}{\partial\zeta^2} + \left(\frac{\alpha m^2 g\bar{\gamma}}{\sqrt{p_y^2 + \frac{1}{\beta}}} - \zeta\right)\frac{\partial}{\partial\zeta} + \lambda\right] b_{p_y}(z) = 0, \tag{2.150}$$

where

$$\lambda = \frac{-2m^2 g\bar{\gamma}\sqrt{\beta(\beta p_y^2 + 1)} + 2mE\beta + 1}{4m^2 g\beta\sqrt{\beta(\beta p_y^2 + 1)}}. \tag{2.151}$$

However, by taking

$$\alpha = \frac{1}{m^2 g\beta}\sqrt{p_y^2 + \frac{1}{\beta}} \quad \text{i.e.} \quad \zeta = \sqrt{p_y^2 + \frac{1}{\beta}}\left(2z + \frac{1}{m^2 g\beta}\right), \tag{2.152}$$

this equation is just Kummer's differential equation, (see e.g. [1, Chap. 13]),

$$\zeta b''_{p_y}(\zeta) + (\nu - \zeta)b'_{p_y}(\zeta) + \lambda b_{p_y}(\zeta) = 0, \tag{2.153}$$

for the particular case $\nu = \bar{\gamma}/\beta$, and has the solution

$$b_{p_y}(\zeta) = C_1 U\left(-\lambda, \frac{\bar{\gamma}}{\beta}, \zeta\right) + C_2 M\left(-\lambda, \frac{\bar{\gamma}}{\beta}, \zeta\right). \tag{2.154}$$

Here C_1, C_2 are arbitrary constants, U a confluent hypergeometric function of the first kind, and M is Kummer's function.[5]

For non-integer λ, Kummer's function increases asymptotically as [1, Eqn. 13.1.4]

$$M(-\lambda, \tfrac{\bar{\gamma}}{\beta}, \zeta) \sim \zeta^{-\lambda - \frac{\bar{\gamma}}{\beta}} e^{\zeta}, \qquad \zeta \to \infty, \tag{2.155}$$

so the corresponding solution a_{p_y} increases exponentially, and thus is non-normalizable. In addition, for integer λ, the two primary solutions agree,

$$U(-\lambda, \tfrac{\bar{\gamma}}{\beta}, \zeta) = M(-\lambda, \tfrac{\bar{\gamma}}{\beta}, \zeta), \tag{2.156}$$

so we can safely assume $C_2 = 0$.

[5]For integer λ and ν, Kummer's function reduces to the generalized Laguerre polynomial $M(-\lambda, \nu, \zeta) = L_\lambda^{\nu-1}(\zeta)$. As a result, sometimes the term "Laguerre differential equation" is used for (2.153), and $M(-\lambda, 1, \zeta)$ is called a Laguerre function or, confusingly enough, Laguerre polynomial for arbitrary λ, even though it is not even a polynomial in general.

The confluent hypergeometric function's asymptotic behavior is [1, Eqn. 13.1.8]

$$U(-\lambda, \tfrac{\bar{\gamma}}{\beta}, \zeta) \sim \zeta^{-\lambda}, \qquad \zeta \to \infty, \tag{2.157}$$

and thus the resulting a_{p_y} is normalizable for arbitrary λ. The function U has a singularity for $\zeta = 0$, but this is of no concern to us, because from (2.152) we can see that ζ is strictly positive for $z \geq 0$.

In summary, the normalizable eigenfunctions are

$$a_{p_y}(z) = C_1\, U\left(\frac{\bar{\gamma}}{2\beta} - \frac{E + \frac{1}{2m\beta}}{2mg\beta\sqrt{p_y^2 + \frac{1}{\beta}}},\ \frac{\bar{\gamma}}{\beta},\ \left(2z + \frac{1}{m^2 g\beta}\right)\sqrt{p_y^2 + \frac{1}{\beta}}\right) e^{-z\sqrt{p_y^2 + \frac{1}{\beta}}}. \tag{2.158}$$

This expression holds when $Z > 0$. When $Z < 0$, the potential is infinite and the eigenfunction vanishes. The boundary condition $a_{p_y}(z) = 0$ for $Z = 0$ fixes the energy spectrum.

The $Z = 0$ condition can be expressed easily when $\bar{\gamma} = 0$. Then, $X_i = x_i(1 + \beta\hat{p}^2)$, so $Z = 0$ whenever $z = 0$. As a result, for $\bar{\gamma} = 0$, the boundary condition is simply $a_{p_y}(0) = 0$. Using the dimensionless

$$\bar{E} = \frac{\gamma}{mg}E, \tag{2.159}$$

$$\bar{\beta} = \gamma^2\beta, \tag{2.160}$$

$$\bar{p}_y = \frac{p_y}{\gamma}, \tag{2.161}$$

where $\gamma = \sqrt{2m^2 g}$ is the characteristic scale of the system, this condition is equivalent to

$$U\left(-\frac{\bar{E} + \frac{1}{\bar{\beta}}}{2\sqrt{\bar{\beta}(\bar{\beta}\bar{p}_y^2 + 1)}},\ 0,\ \frac{2\sqrt{\bar{\beta}(\bar{\beta}\bar{p}_y^2 + 1)}}{\bar{\beta}^2}\right) = 0. \tag{2.162}$$

This equation is exact; its solutions in E for arbitrary parameters β and p_y can be determined straightforwardly, e.g. with a C program using the implementation of confluent hypergeometric functions and root-solving algorithms of the GNU Scientific Library.[6]

In Figure 2.11, the first six energy eigenvalues (for $\bar{E} \in [0, 10]$) are plotted against $0 < \bar{\beta} \leq 1$. In the experiments the energy levels along z axis are measured; along the y axis the particle is approximately free, and so the spectrum is continuous. In turn, (2.162) gives the total energy of the system. Consequently, for a more useful result, in the plot we subtracted the kinetic energy along y axis,

$$E_y = \frac{p_y^2}{2m} \tag{2.163}$$

[6]The only caveat is that extended range confluent hypergeometric function should be used. The function $U(-\lambda, 1, \zeta)$ oscillates wildly for large values of λ and ζ, and because of this the regular implementation results in overflow for small values of β.

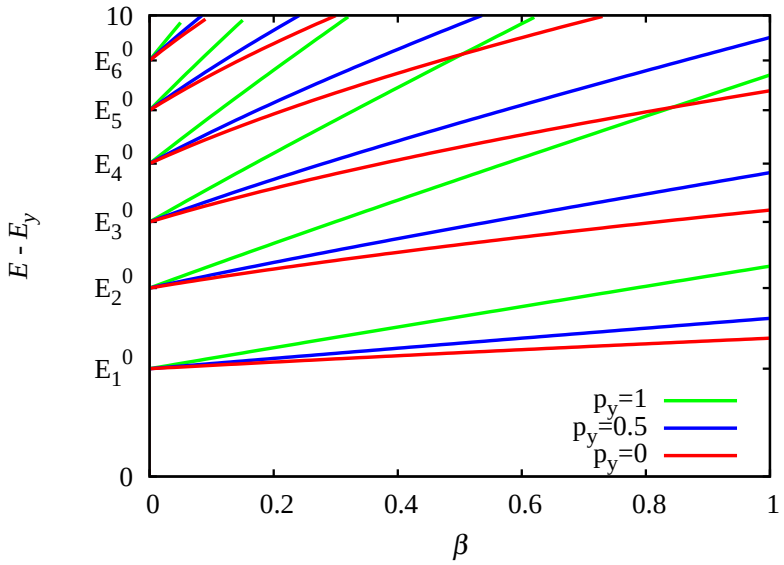

Figure 2.11: *Energy eigenvalues of the gravitational well as a function of the minimal-length parameter β, for $\beta' = 0$ and various horizontal momenta p_y. The kinetic energy in the horizontal direction, $\bar{E}_y = \bar{p}_y^2$ was subtracted from the total energy. The energies are expressed in units of γ/mg, and β in units of $1/\gamma^2$, where $\gamma = \sqrt{2m^2 g}$.*

(or equivalently $\bar{E}_y = \bar{p}_y^2$) from the obtained total energy.

One interesting thing to look for is the behavior of the energy eigenvalues in the limit of the usual quantum mechanics, that is as $\beta \to 0$. Passing to this limit in (2.162) is not straightforward. Both the first and the third argument of the confluent hypergeometric function U has infinite limit. Nevertheless, from the plot it is obvious that as $\beta \to 0$, we indeed recover the values obtained in the usual quantum mechanics,

$$\bar{E}_n^0 = -\alpha_n, \tag{2.164}$$

marked on the vertical axis.

2.4.2 Perturbation theory

While (2.162) is exact, it is not very convenient for obtaining numerical estimates for small values of β and it is restricted to the case $\beta' = 0$. For this reason, let us compute the the first order corrections for the energy eigenvalues in naive perturbation theory. We use $H = H_0 + H'$, where the unperturbed Hamiltonian is

$$H_0 = -\frac{1}{2m}\frac{\partial^2}{\partial y^2} - \frac{1}{2m}\frac{\partial^2}{\partial z^2} + \underbrace{mgz}_{V(z)}, \tag{2.165}$$

and the correction terms are

$$H' = -mg\left[\beta z\frac{\partial^2}{\partial y^2} + (\beta+\beta')z\frac{\partial^2}{\partial z^2} + \beta' y\frac{\partial^2}{\partial y\partial z} + \bar{\gamma}\frac{\partial}{\partial z}\right]. \tag{2.166}$$

To calculate the energy corrections ΔE_n we will need a few expectation values. First,

$$\langle z\rangle = \frac{1}{mg}\langle V(z)\rangle = \frac{2}{3mg}E^0_{z,n}, \tag{2.167}$$

applying the virial theorem, $\langle V(z)\rangle = 2E^0_{z,n}/3$, to the homogeneous potential mgz. This can also be verified explicitly by using the expression of the eigenfunctions (2.124). Next, using the change of variables $\bar{z} = \gamma z + \alpha_n$, the differential relation $\mathrm{Ai}''(z) = z\,\mathrm{Ai}(z)$ satisfied by the Airy function, and the value of the unperturbed energies (2.123),

$$\left\langle\frac{\partial}{\partial z}\right\rangle = \frac{\gamma}{\mathrm{Ai}'(\alpha_n)^2}\int_{\alpha_n}^{\infty} d\bar{z}\,\mathrm{Ai}(\bar{z})\,\mathrm{Ai}'(\bar{z}) = \frac{\gamma}{\mathrm{Ai}'(\alpha_n)^2}\,\frac{\mathrm{Ai}(z)^2}{2}\bigg|_{\alpha_n}^{\infty} = 0, \tag{2.168}$$

and

$$\begin{aligned}\left\langle z\frac{\partial^2}{\partial z^2}\right\rangle &= \frac{\gamma}{\mathrm{Ai}'(\alpha_n)^2}\int_{\alpha_n}^{\infty} d\bar{z}\;(\bar{z}-\alpha_n)\,\mathrm{Ai}(\bar{z})\,\mathrm{Ai}''(\bar{z})\\ &= \frac{\gamma}{\mathrm{Ai}'(\alpha_n)^2}\left[\int_{\alpha_n}^{\infty} d\bar{z}\;\bar{z}^2\,\mathrm{Ai}(\bar{z})^2 - \alpha_n\int_{\alpha_n}^{\infty} d\bar{z}\;\bar{z}\,\mathrm{Ai}(\bar{z})^2\right]\\ &= \left(\frac{1}{5}-\frac{1}{3}\right)\gamma\alpha_n^2 = -\frac{2\gamma^3}{15m^2g^2}(E^0_{z,n})^2.\end{aligned} \tag{2.169}$$

We can see that the parameter $\bar{\gamma}$, with no physical meaning, drops out, as it should.

Along the y axis we can suppose that we take the expectation values with respect to a state with definite momentum $p_y = \sqrt{2mE^0_y}$. Then we have on one hand

$$\left\langle\frac{\partial^2}{\partial y^2}\right\rangle = -2mE^0_y. \tag{2.170}$$

On the other hand, $\left\langle y\frac{\partial}{\partial y}\right\rangle$ is undetermined; it can be calculated using a more rigorous wave-packet approach. Nevertheless, for our purpose it is sufficient that this expectation value is finite, because it will get multiplied by the vanishing $\left\langle\frac{\partial}{\partial z}\right\rangle$.

Collecting everything together,

$$\begin{aligned}\Delta E_n &= \langle H'\rangle\\ &= -mg\left[\beta\left(\frac{2E^0_{z,n}}{3mg}\right)(-2mE^0_y) + (\beta+\beta')\left(-\frac{2\gamma^3}{15m^2g^2}\right)(E^0_{z,n})^2\right]\\ &= \frac{4\beta m}{3}E^0_{z,n}E^0_y + \frac{4(\beta+\beta')m}{15}(E^0_{z,n})^2.\end{aligned} \tag{2.171}$$

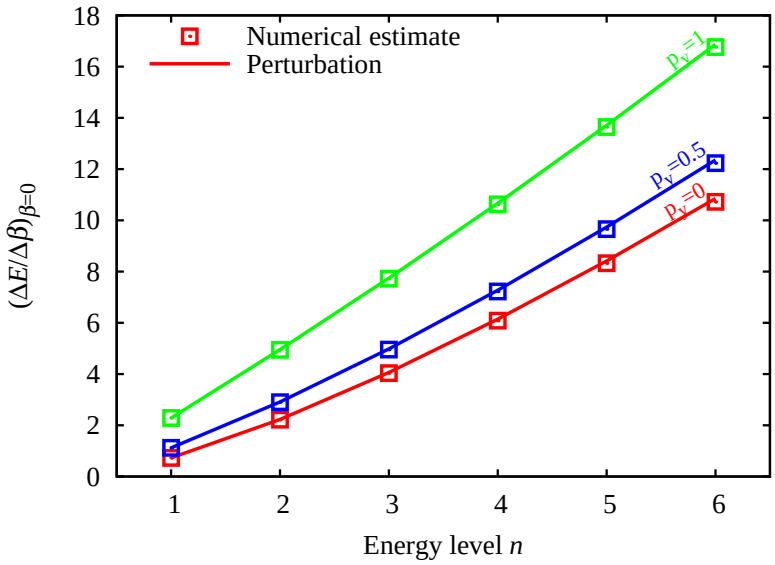

Figure 2.12: *Comparison of the first order correction to the energy eigenvalues of the gravitational well, as obtained from perturbation theory in* (2.172) *and estimated from the numerical values of the exact result for* $\beta' = 0$*, for various energy levels and values of horizontal momentum* p_y*.*

This is the main result of this section. It can be compared with the exact result obtained in the previous section plotted in Figure 2.11. In unitless form and for $\beta' = 0$, (2.171) can be rewritten as

$$\begin{aligned} \left.\frac{\partial \bar{E}_n}{\partial \bar{\beta}}\right|_{\bar{\beta}=0} &= \frac{2}{3}\bar{E}^0_{z,n}\bar{E}^0_y + \frac{2}{15}(\bar{E}^0_{z,n})^2 \\ &= \frac{2}{15}\alpha_n(\alpha_n - 5\bar{p}_y^2). \end{aligned} \tag{2.172}$$

The derivative can also be estimated from the slope of the graphs in Figure 2.11, calculated between the two leftmost points, $\bar{\beta} = 0.001$ and $\bar{\beta} = 0.01$. As it can be seen in Figure 2.12, the agreement is excellent.

Finally, let us comment on the gravitational well in the original, momentum-diagonal, representation introduced in [16]. Here the calculation of energy corrections is not as straightforward, as the momentum operator is diagonal while the boundary conditions are manifestly position-dependent. Nevertheless, because the perturbative method is used in the undeformed Heisenberg algebra of p_i's and q_i's, one can employ Fourier analysis to argue that the expectation values, and, as a consequence, the energy correction will be the same as above. For example, the unperturbed energy eigenfunctions are given by the Fourier transform of

(2.124), which can be written as

$$\begin{aligned}\psi(p_z) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(z)e^{-izp_z}dz \\ &= \frac{A_n}{\gamma}\sqrt{\frac{\pi}{2}}\exp\left[i\left(\frac{\alpha_n p_z}{\gamma}+\frac{p_z^3}{3\gamma^3}\right)\right]+\frac{iA_n}{2\pi}\int_{-\infty}^{\infty}\frac{\exp\left[i\left(\alpha_n t+\frac{t^3}{3}\right)\right]}{\gamma t-p_z}dt,\end{aligned} \tag{2.173}$$

where we have used the integral representation of the Airy function,

$$\mathrm{Ai}(\bar{z}) = \int_{-\infty}^{\infty}\exp\left[i\left(\bar{z}t+\frac{t^3}{3}\right)\right]dt. \tag{2.174}$$

Comparison with a former result In [8], the authors calculated the first order corrections to the energy spectrum of the quantum gravitational well, for the case $\beta' = 2\beta$, using the Brau representation (1.60)–(1.61). The result obtained there,[7]

$$\Delta E_n = \beta m\left[\frac{8}{3}E_{z,n}^0 E_y^0+\frac{4}{5}(E_{z,n}^0)^2\right], \tag{2.175}$$

disagrees with (2.171), which, for $\beta' = 2\beta$, reduces to

$$\Delta E_n = \beta m\left[\frac{4}{3}E_{z,n}^0 E_y^0+\frac{4}{5}(E_{z,n}^0)^2\right], \tag{2.176}$$

The source of discrepancy seems to be a subtle mistake the authors of [8] make interpreting their result.

When including the minimal length, one always have to consider the whole multidimensional system in question and thus the total energy, because the system cannot be reconstructed from its 1-dimensional components by adding energies and taking tensor products of one dimensional wavefunctions, as usual. The minimal length effectively mixes the different dimensions.

On the other hand, the experiment described in [18] is sensitive to the energy along the vertical direction only, not the total energy. Because perturbation theory is applied to a system with continuous spectrum (along the horizontal direction the energy being arbitrary), utmost care should be taken to compare the right states before and after the perturbation.

As we compare the results we have obtained using the pseudo-position representation (2.130)–(2.131), with those obtained by Brau, we need to avoid interpretations that are specific to a given choice of the dynamical variables. So for example, in the one chosen in our analysis, the operator $P_y = p_y$ refers to the actual translation operator inherent in the minimal length algebra. The quantity p_y has actually no meaning apart from the

[7] The paper in question uses the notation E_n^0 for $E_{z,n}^0$ and E_c for E_y^0.

identification with P_y, and in this representation, it is in fact the displacement generating operator.

By contrast, in Brau's representation, $P_i = p_i\,(1 + \beta p^2)$, and while P_i is the displacement generating operator in the presence of a minimal length, p_i is not. Consequently, the eigenvalues associated with p_i have no independent meaning, and cannot be interpreted as components of momentum.

A second point to bear in mind is that within the context of the total Hamiltonian H given by (2.134), eigenvalues of P_y cannot be specified in the basis where the energy is diagonal, since these two operators have a non-vanishing commutator, and are not simultaneously diagonalizable. So we cannot specify the perturbed energy by using the eigenvalues of p_y, which have no meaning in the Brau representation; nor can we use those of P_y. At best, we can do so only in terms of the *expectation* of P_y^2 with respect to the energy eigenvectors of the unperturbed Hamiltonian.

Following [8], the correction of the total energy $\Delta E = E - E^0$ can be calculated as follows. The representation, valid for the case $\beta' = 2\beta$, is

$$X_i = x_i, \tag{2.177}$$
$$P_i = p_i(1 + \beta p^2), \tag{2.178}$$

so the perturbing term, up to first order in β is

$$\begin{aligned} H - H_0 &= \left(\frac{P^2}{2m} + V(Z)\right) - \left(\frac{p^2}{2m} + V(z)\right) \\ &= \frac{\beta}{m} p^4, \end{aligned} \tag{2.179}$$

and the correction is

$$\begin{aligned} \Delta E &= \frac{\beta}{m} \left\langle p^4 \right\rangle \\ &= \frac{\beta}{m} \left[\left\langle p_z^4 \right\rangle + 2 \left\langle p_y^2 \right\rangle \left\langle p_z^2 \right\rangle + \left\langle p_y^4 \right\rangle \right] \\ &= 4\beta m \left[(E_{z,n}^0)^2 - 2E_{z,n}^0 \left\langle V(z) \right\rangle + \left\langle V^2(z) \right\rangle + 2E_y^0 \big(E_{z,n}^0 - \left\langle V(z) \right\rangle \big) + (E_y^0)^2 \right], \end{aligned} \tag{2.180}$$

where in the last line we have used the Schrödinger equation in the form

$$p_y^2 = 2mE_y^0, \tag{2.181}$$
$$p_z^2 = 2m\big(E_{z,n}^0 - V(z)\big). \tag{2.182}$$

Please note that, unlike [8], at this point we do not neglect the $(E_y^0)^2$ term. The expectation value for the potential is

$$\left\langle V(z) \right\rangle = \frac{2}{3} E_{z,n}^0 \tag{2.183}$$

from the virial theorem, while the one for the square of the potential can be calculated to be

$$\left\langle V^2(z)\right\rangle = \frac{8}{15}(E^0_{z,n})^2. \tag{2.184}$$

This results in a correction to the *total* energy of

$$\Delta E = \beta m\left[\frac{4}{5}(E^0_{z,n})^2 + \frac{8}{3}E^0_{z,n}E^0_y + 4(E^0_y)^2\right], \tag{2.185}$$

as obtained in [8], with the exception of the last term.

The subtlety is that the expression of the momentum operator is different in the unperturbed and perturbed system, which leads to a change in the horizontal energy of the system. Namely, in the unperturbed system $P_i = p_i$, so

$$E^0_y = \frac{p_y^2}{2m}, \tag{2.186}$$

while in the perturbed one it is

$$\begin{aligned} E_y &= \left\langle \frac{P_y^2}{2m}\right\rangle \\ &= \frac{p_y^2}{2m}(1 + 2\beta p_y^2 + 2\beta\left\langle p_z^2\right\rangle) \\ &= E^0_y + 4m\beta(E^0_y)^2 + \frac{4m\beta}{3}E^0_y E^0_{z,n}, \end{aligned} \tag{2.187}$$

using (2.181)–(2.182) Finally, the correction to the energy levels along the vertical direction, the ones to which the experiment is sensitive, are given by

$$\begin{aligned} \Delta E_{z,n} &= E_{z,n} - E^0_{z,n} \\ &= (E - E_y) - (E^0 - E^0_y) \\ &= \Delta E - (E_y - E^0_y) \\ &= \beta m\left[\frac{4}{3}E^0_{z,n}E^0_y + \frac{4}{5}(E^0_{z,n})^2\right]. \end{aligned} \tag{2.188}$$

Notice how, after the perturbation corrections are grouped together to form the expectation value of P_y, the results from the two representations now completely agree.

There is a similar situation that arises in the analysis of the motion of an electron in a homogeneous external magnetic field. If the field $\vec{B}$ is pointing the z-direction, then we may choose to work in the gauge where the vector potential is given by $A_x = -By$, with all other components vanishing. In substituting into the Hamiltonian, there will appear a term proportional to p_x^2, and one is tempted to identify this with the momentum along the x-direction. That would be an error. Indeed, the quantity associated with p_x is actually

part of the operator that specifies the y-component of the quantum analog of the circular orbit. The corresponding x-component is related to p_y, and since the two operators do not commute, the system indeed possesses a minimal length, the magnetic length $\sqrt{1/eB}$.

To be specific, the Hamiltonian in the Landau gauge for an electron trapped in a constant field B along the z-direction is obtained by the usual substitution

$$p_i \mapsto P_i = p_i - eA_i, \tag{2.189}$$

and thus is given by

$$\begin{aligned} H &= \frac{(p_x - eA_x)^2}{2m} + \frac{p_y^2}{2m} \\ &= \frac{p_x^2}{2m} + eB\frac{p_x y}{m} + \frac{p_y^2}{2m} + \frac{m}{2}\left(\frac{eB}{m}\right)^2 y^2. \end{aligned} \tag{2.190}$$

This is the Hamiltonian for a simple harmonic oscillator in 1-D, with frequency $\omega = eB/m$. The remaining terms can be re-grouped into

$$y_0 = -\frac{p_x}{eB}, \tag{2.191}$$

so that the Hamiltonian takes the form

$$H = \frac{p_y^2}{2m} + \frac{m}{2}\left(\frac{eB}{m}\right)^2 (y - y_0)^2, \tag{2.192}$$

with energy eigenvalues $(n + 1/2)\omega$. The quantity y_0 signifies the equilibrium point of the 1-D oscillation. On the other hand, had we considered p_x to be a measurable parameter, and attempted to do perturbation in this quantity, we would have gotten a null result for the first order, and a mysterious cancellation in the second order. The meaning of p_x, as fixing the center of oscillation, and therefore a degeneracy parameter, would be obscured. It does not signify the momentum in the x-direction, which by itself, would not be gauge invariant.

In the final part of this study of the gravitational well with minimal length, let us look at the possible bounds on the minimal length that could be extracted from the experimental results. These were considered rather extensively in [8], and its conclusions, that the experiment's sensitivity is several orders of magnitude below that needed to extract any meaningful bound, are not changed radically by a correcting factor of $\approx$2. This, after all, is hardly surprising. It was quite an achievement showing experimentally that the energy levels of the quantum gravitational well are indeed discrete, and we should not expect precision phenomenology from a measurement with an error >10%.

Conclusions

In the present thesis we reviewed the basic development of a non-relativistic quantum theory that includes an absolute minimal length, by postulating a simply modified commutation relation of the form

$$[X_i, P_i] = i\hbar\big\{\delta_{ij}(1+\beta P^2) + \beta' P_i P_j\big\},$$

between the position and momentum operators.

Apart from a minimal length, such a theory contains other attractive features, such as UV/IR mixing, and a non-commutative position operator algebra. It could also be accessible experimentally if the universe possessed large extra dimensions. It is closely related to other theories that include a minimal length, and can also be interpreted as a first order expansion of any meaningful modification of the canonical Heisenberg algebra.

One of the main advantages of the approach considered is that the entire theory follows from this simple algebraic relation, with few, very natural assumptions. The commutation relations among position operators are determined by the Jacobi identity. Differential operator representations can be characterized by simple differential equations, based only on simple tensorial and dimensional considerations.

The differential operator representations can be obtained in a two-step process: first one expresses the non-commutative variables in terms of commutative ones, and then uses one of the usual representation for these underlying variables. It is good to know that these reductions to canonical Heisenberg algebras are equivalent to first order, at least, so the algebraic structure considered again seems to determine the theory completely.

In the second chapter, using mostly the pseudo-position representation several quantum problems were treated, namely the harmonic oscillator, the Coulomb potential and the gravitational well. It can be seen that this representation has a clear advantage for problems where the potential depends in some intricate way on the position operators. In addition, it is exact, it works for arbitrary β, β', and the physical momenta are expressed in the same way as in the regular position representation.

In the case of the harmonic oscillator, the pseudo-position treatment does not add much to the solutions already obtained in different representations; it was mainly presented just as a simple introductory example. For the Coulomb potential, and the gravitational well, however, it exposes several subtleties that can be overlooked in other representations. In the case of the S states of a hydrogen-like atom it underlines the importance of the higher

order terms in the expansion of R^2. While in the Brau representation the corrections coming from the infrared domain of the underlying r can be easily calculated, it overlooks the extra correction due to the ultraviolet domain $r \sim 0$ that is the most important one for the zero angular momentum states. Numerical calculations confirmed the importance of these ultraviolet corrections.

For the gravitational well, the pseudo-position representation emphasized that allocating energy between different directions is no longer straightforward, because the momentum component operators generally no longer commute with the Hamiltonian, and thus the energy can only be defined in terms of expectation values.

We also considered the bounds that can be obtained from precision measurements on simple systems. As expected, the strongest constraint comes from the energy level measurements of the hydrogen atoms, which are the most exactly determined, and for which the singularity of the potential at the origin magnifies the effects of the minimal length. The fact that only a bound of ~ 3 GeV can be obtained is due to the fact that the today's generally accepted theoretical and experimental values for the $1S$ Lamb shift differ considerably.

Notwithstanding its results, probably the most important conclusion that can be drawn from this exposition is that it is possible to write down a consistent non-relativistic quantum theory that incorporates UV/IR mixing and minimal length. As long as the minimal length is relatively small, the resulting modifications are mild, not radically altering experimentally established facts. Moreover, the main algebraic structure is conserved, e.g. there still exists a rotation generating L_{ij} satisfying the usual commutation relations with X_i, P_j. Analogously, the P_i operator can still be interpreted as generating translations.

The next logical step is extension to the relativistic domain and to many-body systems, that invariably appear at energies at which pair-production is possible. The exact form of such a theory is unclear. In usual relativistic quantum theory, the main ingredients are fields defined on a position space. The non-commutativity of position operators makes this harder to implement. Most probably, a similar algebraic approach has the greatest promise. Indeed, as a first promising step, it seems possible to define a gauge-invariant vector potential related to the electro-magnetic field by a similar algebraic relation.

Finally, it should be repeated that the general idea of an absolute minimal-length is somewhat speculative because, even though it is theoretically pleasing, no experimental confirmation for it exists so far. Possibly the problems it seems to cure, like the renormalizability of quantum gravity, will be solved by other advances in physics. If confirmed by experiment, though, we expect that its low energy limit will be very similar to the one presented here.

Appendices

A.1 Proof of (1.23)

While the the relation (1.24),

$$[P_i, L_{jk}] = i\hbar(\delta_{ik}P_j - \delta_{ij}P_k), \tag{1.24}$$

can be obtained easily, because the momenta commute, (1.23) is far from obvious. It can be proven starting from the definition (1.22) of L_{ij} written as

$$(1 + \beta P^2)L_{ij} = (X_i P_j - X_j P_i), \tag{A.1}$$

and taking the commutator with X_k, which leads to

$$\begin{aligned} &- [X_k, X_i]P_j - X_i[X_k, P_j] + [X_k, X_j]P_i + X_j[X_k, P_i] \\ &\qquad + \beta[X_k, P^2]L_{ij} + (1 + \beta P^2)[X_k, L_{ij}] = 0. \end{aligned} \tag{A.2}$$

Using Jacobi's identity the second term can be re-expressed as

$$\begin{aligned} -X_i[X_k, P_j] &= -\big[X_i, [X_k, P_j]\big] - [X_k, P_j]X_i \\ &= \big[X_k, [P_j, X_i]\big] + \big[P_j, [X_i, X_k]\big] - [X_k, P_j]X_i \\ &= \big[X_k, [P_j, X_i]\big] + P_j[X_i, X_k] - [X_i, X_k]P_j - [X_k, P_j]X_i, \end{aligned} \tag{A.3}$$

and similarly the fourth one as

$$X_j[X_k, P_i] = -\big[X_k, [P_i, X_j]\big] - P_i[X_j, X_k] + [X_j, X_k]P_i + [X_k, P_i]X_j. \tag{A.4}$$

Substituting the last two relations into (A.2), canceling the common terms, and finally expressing expressing $[X., X_k]$ through (1.20), L_{ij} through (1.22), leads straightforwardly to the desired result,

$$[X_k, L_{ij}] = i\hbar(\delta_{jk}X_i - \delta_{ik}X_j). \tag{1.23}$$

Relation (1.25) can be the obtained easily from (1.23) and (1.24).

A.2 Quantum canonical transformations

To exemplify how a canonical transformation leaves invariant the energy spectrum of a Hamiltonian, we will choose two representation related by such a transformation, and work out the solution of the Schrödinger equation for a simple problem, namely the harmonic oscillator, in regular quantum quantum mechanics *without* minimal length. This will also show that such freedom in the choice of the variables is not a new feature due to the minimal length commutation relations.

The Hamiltonian for the harmonic oscillator is

$$H = \frac{\tilde{p}^2}{2m} + \frac{m\omega^2}{2}\tilde{x}^2,$$

where $\tilde{x}$ and $\tilde{p}$ satisfy the usual commutation relations.

In particular, the funny representation

$$\tilde{x} = x + \gamma p, \quad \tilde{p} = p,$$

where

$$x = x, \quad p = \frac{\hbar}{i}\frac{\partial}{\partial x},$$

satisfies $[\tilde{x}, \tilde{p}] = i\hbar$ and $[\tilde{x}, \tilde{x}] = [\tilde{p}, \tilde{p}] = 0$ so it should result in the same energy eigenvalues as the equation in x, p.

In this representation the Hamiltonian reads

$$H = \frac{1 + m^2\omega^2\gamma^2}{2m}p^2 + \frac{m\omega^2}{2}(2\gamma xp - \gamma i\hbar + x^2).$$

With the change of variables

$$\xi = \sqrt{\frac{m\omega}{\hbar}}\,\frac{x}{\sqrt{1 + m^2\omega^2\gamma^2}},$$

and denoting $\epsilon = E/\hbar\omega$, the Schrödinger equation takes the dimensionless form

$$\left[\frac{\partial^2}{\partial\xi^2} + im\omega\gamma\left(2\xi\frac{\partial}{\partial\xi} + 1\right) + 2\epsilon - (1 + m^2\omega^2\gamma^2)\xi^2\right]\psi(x) = 0. \tag{A.5}$$

The definition of ξ has an extra factor of $1/\sqrt{1 + m^2\omega^2\gamma^2}$ compared to the usual case, that is included for later convenience. Please note, that using the alternative ladder operators

$$\tilde{a}, \tilde{a}^\dagger = \frac{1}{\sqrt{2}}(\tilde{x} \pm i\tilde{p}),$$

one can easily prove that $\epsilon_n = n + \frac{1}{2}$, but we will not use this.

The eigenfunction ψ obviously has non-vanishing imaginary part, and it can be factored as $\psi(\xi) = e^{i\phi(\xi)}R(\xi)$, where ϕ will be determined later and R is not necessarily real. Substituting into (A.5) and canceling out the common $e^{i\phi(\xi)}$ phase factor one gets the equation

$$R'' + \left[-(\phi')^2 - 2m\omega\gamma\xi\phi' + 2\epsilon - (1 + m^2\omega^2\gamma^2)\xi^2\right] R + \\ i[\phi'' R + 2\phi' R' + 2m\omega\gamma\xi R' + m\omega\gamma R] = 0,$$

or equivalently

$$R'' + \left[-(\phi' + m\omega\gamma\xi)^2 + 2\epsilon - \xi^2\right] R + \frac{i}{R}\frac{\partial}{\partial\xi}\left[(\phi' + m\omega\gamma\xi)R^2\right] = 0.$$

(Prime denotes derivative with respect to ξ.)

Thus, if we take ϕ such that

$$\phi'(\xi) = -m\omega\gamma\xi,$$

and substitute back, we immediately arrive to

$$R'' + \left(2\epsilon - \xi^2\right) R = 0,$$

which is nothing else than the version of Hermite's equation that appears in the solution using the regular position representation, and which, apart from an overall phase factor, has the normalizable solutions

$$R(\xi) = e^{-\xi^2/2} H_{\epsilon - 1/2}(\xi),$$

where $n = \epsilon - 1/2$ is a non-negative integer and H_n are the Hermite polynomials. In other words, apart from a physically unimportant phase factor, the wavefunction is the usual one with its variable scaled down by $\frac{1}{\sqrt{1+m^2\omega^2\gamma^2}}$.

It is interesting to see what happens in the momentum representation

$$p = p, \qquad x = i\hbar\frac{\partial}{\partial p}.$$

As $\tilde{p} = p$, we expect that $\tilde{p}$ can still be interpreted as the momentum of the system, and the eigenfunction $\psi(p)$ represents an amplitude for the momentum distribution for the energy eigenstates. In other words, the eigenfunction's variable should not be scaled as in the position representation.

Indeed, the Hamiltonian can be written in the form

$$H = \frac{1 + m^2\omega^2\gamma^2}{2m}p^2 + \frac{m\omega^2}{2}(2\gamma px + \gamma i\hbar + x^2).$$

With the change of variables

$$\eta = \frac{p}{\sqrt{m\omega\hbar}},$$

the Scrödinger equation reads

$$\left[\frac{\partial^2}{\partial\eta^2} - im\omega\gamma\left(2\xi\frac{\partial}{\partial\eta}+1\right) + 2\epsilon - (1+m^2\omega^2\gamma^2)\eta^2\right]\psi(x) = 0,$$

which is the same as (A.5), with γ replaced by $-\gamma$. It's solution therefore is of the form

$$\psi(\eta) = e^{i\phi(\eta)}R(\eta),$$

where

$$\begin{aligned}\phi'(\eta) &= m\omega\gamma\eta,\\ R(\eta) &= e^{-\eta^2/2}H_{\epsilon-1/2}(\eta),\end{aligned}$$

as we expected.

Please note that the phase factor is the generating function for the canonical transformation $(x,p) \mapsto (\tilde{x},\tilde{p})$. This is generally true in quantum mechanics where canonical transformations correspond to unitary transformations of the x and p operators.

A.3 Proof of (1.89)–(1.90)

A relatively simple way to obtain $F_P(u)$ and $H_X(u)$, when $G_X(u)$ is given, is as follows. The second order equation (1.77), or

$$\eta u F_P^2 - G_X F_P + 1 = 0, \tag{A.6}$$

has the the two solutions

$$F_P = \frac{G_X \pm \sqrt{G_X^2 - 4\eta u}}{2\eta u}. \tag{A.7}$$

As $G_X(0) = 1$, the solution with the plus sign diverges as $u \to 0$, so we will keep only the other one,

$$F_P = \frac{G_X - \sqrt{G_X^2 - 4\eta u}}{2\eta u}, \tag{A.8}$$

which corresponds to (1.89).

From (1.78), H_X can be expressed as

$$H_X = \frac{(1-\eta)F_P^2 - 2F_P' G_X}{F_P + 2uF_P'}. \tag{A.9}$$

Using (A.8), the denominator can be rewritten as

$$F_P + 2uF_P' = F_P\frac{G_X - 2uG_X'}{\sqrt{G_X^2 - 4\eta u}}, \tag{A.10}$$

and thus

$$F'_P = \frac{F_P}{2u}\left[-1 + \frac{G_X - 2uG'_X}{\sqrt{G_X^2 - 4\eta u}}\right]. \tag{A.11}$$

Plugging this into (A.9), reducing a factor of F_P, and finally expressing F_P through (A.8) leads to

$$H_X = \frac{4\eta u(1 - \eta + G'_X G_X) - (1+\eta)G_X\left(G_X - \sqrt{G_X^2 - 4\eta u}\right)}{2\eta u(G_X - 2uG'_X)}, \tag{A.12}$$

i.e. (1.90).

A.4 Example code listing

In this section we will present some example code used to determine numerically the eigenvalues of the Coulomb potential with the hypothesis of the minimal-length. Because these files were developed for "in-house" usage, almost no error checking is done.

The first file, `defs.cpp`, contains the general definitions that are used in every algorithm. They closely follow the definitions of Section 2.3, though some differences in the notation exists. These are clarified in the comments.

```
/**** File: defs.cpp ****/

typedef long double myDouble;

/* For quad precision, uncomment the following lines;
 * needs the LBNL high precision library QD;
 * see http://crd.lbl.gov/~dhbailey/mpdist/
 */

//#include "qd/include/qd.h"
//typedef dd_real myDouble;

using namespace std;


//*** GLOBALS ***
const myDouble D = 3.0;
myDouble       l;
myDouble     Lsq;
myDouble     eta;       // eta = beta / (beta + beta')
myDouble       a;
myDouble       b;
```

```
myDouble alpha;  // beta is here; alpha = min. length/ Bohr radius
                 // alpha is denoted xi in notes
myDouble eps;    // and here is the energy in units of e^2/2a_0 / alpha^2
//*** End GLOBALS ***


//*** FORMULAS ***
inline myDouble square(myDouble arg)
{ return arg*arg; }

// nu are the R eigenvalues, denoted by \rho in the notes
inline myDouble nu(const int n)
{ return
    sqrt( square(2.0*n + D/2.0 + l + sqrt( square(eta*(D-1.0)+1.0)/4.0
   + eta*eta*Lsq ))
  - square(1.0-eta)*( Lsq + (D-1.0)*(D-1.0)/4.0 ) );
}

inline myDouble theta(const int n)
{ return 2.0* alpha / nu(n); }

// these are c_n from the notes
inline myDouble cm(const int n_int)
{ myDouble n = (myDouble)n_int;
 return -2.0 / (2.0*n + a + b)
   * sqrt( (a+n)*(b+n)*(b+a+n)*n/(2.0*n+a+b-1.0)/(2.0*n+a+b+1.0) );  }

// these are b_n from the notes
inline myDouble bm(const int n)
{ return (b*b-a*a) / (2.0*n+a+b) / (2.0*n+a+b+2.0); }

// these correspond to s_n a_n from the notes;
// s(n-1) is the coefficient of f(n-1)
inline myDouble  s(const int n)
{ return (1.0 - eps + theta(n)) * cm(n+1); }

// these correspond to 2 - s_n + s_n b_n from the notes;
// t(n) is the coefficient of f(n)
inline myDouble  t(const int n)
{ return (1.0 + eps - theta(n)) + (1.0 - eps + theta(n)) * bm(n); }
```

```
// these correspond s_n c_n from the notes;
// u(n+1) is the coefficient of f(n+1)
inline myDouble  u(const int n)
{ return (1.0 - eps + theta(n)) * cm(n); }
//*** End FORMULAS ***

//*** General procedures ***
// initialization after change in l, eta (or D)
void init() {
  Lsq = l*(l+D-2.0);
  a = sqrt( (1.0 + (D-1.0)*eta)*(1.0 + (D-1.0)*eta)/4.0 + eta*eta*Lsq  );
  b = D/2.0 + l - 1.0;
}

/**** End of file: defs.cpp ****/
```

The second file, `forlib.cpp` contains the procedures used in the "direct" or "forward" method. One function is `zero()`, which progressively evaluates the f_n terms, stopping when it deems that the exponential tail was reached, and returning the number of zeros (sign changes of f_n) encountered.

The other function is `deteps()`, which looks for ϵ corresponding to the `level`'th energy level in the interval $(0, \texttt{seed})$. It assumes the energy level in question is indeed in this interval.

```
/**** File: forlib.cpp ****/

#include <iostream>

const double prec_tail = 0.01;   // precision for identifying the tail
const  int   SIGUR  = 20;        // minimal length of tail
const myDouble precizie = 1e-5;  // precision of eigenvalues


int zero() {
  // const long double eps passed as global

  myDouble prev, current, next;
  current = 1;
  next = - current * t(0) / u(1);

  int n = 1;
  int sigur = SIGUR; // counts the tail
  int zeros = 0;     // counts the number of zeros
```

```
  myDouble lambdap = (1.0+sqrt(eps))/(1.0-sqrt(eps));

  do {
    prev = current;
    current = next;

    // f[n+1] = - ( f[n]*t(n) + f[n-1]*s(n-1) ) / u(n+1);
    next = - ( current * t(n) + prev * s(n-1) ) / u(n+1);

    if (next * current < 0.0) {
      zeros++;
      // cout << "\n  -> zero detected between n="
      //      << n << " & n=" << n+1;
    }

    if ( abs( (next/current - lambdap)/(lambdap-1.0) ) < prec_tail)
      sigur--;
    else
      sigur = ((n < 200) ? SIGUR : (n / 10));
    n++;
  }
  while ((sigur > 0) && (n < 1e8));
  // clog << "n=" << n << "\n";
  return zeros;
}

myDouble deteps(const myDouble seed, const int level) {
  /* epsilon is scanned over (0, seed);
   * level is the level of energy
   * const myDouble alpha passed as global
   */

  eps = seed / 2.0;
  for (myDouble corr = eps/2.0;
       corr > precizie*alpha*alpha*alpha; corr /= 2.0) {
    if (zero() < level)
      eps -= corr;
    else
      eps += corr;
  }
  return eps;
}
```

```
/**** End of file: forlib.cpp ****/
```

The last listing is an example of a main file, that is a simple interface for the functions in the two files presented above. It determines and lists the eigenvalues corresponding to a single set of parameters that are read from the command line. These should be, in order, (1) $\eta = \beta/(\beta + \beta')$, (2) the angular momentum number ℓ, (3) the minimal length ξ and finally the ordinal number of the (4) lowest and (5) largest energy level to be determined.

```
/**** File: oneener.cpp ****/
// Usage: ‘oneener eta ell xi min_level max_level’

#include <iostream>
#include <iomanip>
#include "defs.cpp"
#include "forlib.cpp"


int main(int argc, char ** argv) {
  eta = atof(argv[1]);
  l = atof(argv[2]);
  init();

  alpha = atof(argv[3]);

  eps = 1;
  for (int i = atoi(argv[4]); i <= atoi(argv[5]); i++) {
    eps = deteps(eps, i-int(l));
    cout << i << "\t" << setiosflags(ios::left)
         << setprecision(10) << -eps/alpha/alpha
         << "\n";
  }
}

/**** End of file: oneener.cpp ****/
```

Bibliography

[1] Abramowitz, M., and Stegun, I. A. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, ninth dover printing, tenth gpo printing ed. Dover, New York, 1964.

[2] Akhoury, R., and Yao, Y. P. Minimal length uncertainty relation and the hydrogen spectrum. *Phys. Lett. B572* (2003), 37–42.

[3] Amelino-Camelia, G. Doubly-special relativity: First results and key open problems. *Int. J. Mod. Phys. D11* (2002), 1643.

[4] Arkani-Hamed, N., Dimopoulos, S., and Dvali, G. R. The hierarchy problem and new dimensions at a millimeter. *Phys. Lett. B429* (1998), 263–272.

[5] Benczik, S., Chang, L. N., Minic, D., and Takeuchi, T. The hydrogen atom with minimal length. *Phys. Rev. A72* (2005), 012104.

[6] Benczik, S., et al. Short distance vs. long distance physics: The classical limit of the minimal length uncertainty relation. *Phys. Rev. D66* (2002), 026003.

[7] Brau, F. Minimal length uncertainty relation and hydrogen atom. *J. Phys. A32* (1999), 7691–7696.

[8] Brau, F., and Buisseret, F. Minimal length uncertainty relation and gravitational quantum well. *Phys. Rev. D74* (2006), 036002.

[9] Chang, L. N., Minic, D., Okamura, N., and Takeuchi, T. Exact solution of the harmonic oscillator in arbitrary dimensions with minimal length uncertainty relations. *Phys. Rev. D65* (2002), 125027.

[10] Connes, A. *Noncommutative geometry*. Academic Press, 1994.

[11] Eides, M. I., Grotch, H., and Shelyuto, V. A. Theory of light hydrogenlike atoms. *Phys. Rept. 342* (2001), 63–261.

[12] Hossenfelder, S., et al. Collider signatures in the planck regime. *Phys. Lett. B575* (2003), 85–99.

[13] Jungmann, K. P. Past, present and future of muonium. In *Proceedings of the Memorial Symposium in Honor of Vernon Willard Hughes* (2004), pp. 134–153.

[14] Kempf, A. Uncertainty relation in quantum mechanics with quantum group symmetry. *J. Math. Phys. 35* (1994), 4483–4496.

[15] Kempf, A. Nonpointlike particles in harmonic oscillators. *J. Phys. A30* (1997), 2093–2102.

[16] Kempf, A., Mangano, G., and Mann, R. B. Hilbert space representation of the minimal length uncertainty relation. *Phys. Rev. D52* (1995), 1108–1118.

[17] Mallampalli, S., and Sapirstein, J. Perturbed orbital contribution to the two-loop lamb shift in hydrogen. *Phys. Rev. Lett. 80*, 24 (Jun 1998), 5297–5300.

[18] Nesvizhevsky, V. V., et al. Quantum states of neutrons in the earth's gravitational field. *Nature 415* (2002), 297–299.

[19] Niering, M., Holzwarth, R., Reichert, J., Pokasov, P., Udem, T., Weitz, M., Hänsch, T. W., Lemonde, P., Santarelli, G., Abgrall, M., Laurent, P., Salomon, C., and Clairon, A. Measurement of the hydrogen $1s$- $2s$ transition frequency by phase coherent comparison with a microwave cesium fountain clock. *Phys. Rev. Lett. 84*, 24 (Jun 2000), 5496–5499.

[20] Padmanabhan, T. Hypothesis of path integral duality. 1. quantum gravitational corrections to the propagator. *Phys. Rev. D57* (1998), 6206–6215.

[21] Quesne, C., and Tkachuk, V. M. Harmonic oscillator with nonzero minimal uncertainties in both position and momentum in a susyqm framework. *J. Phys. A36* (2003), 10373–10391.

[22] Randall, L., and Sundrum, R. An alternative to compactification. *Phys. Rev. Lett. 83* (1999), 4690–4693.

[23] Randall, L., and Sundrum, R. A large mass hierarchy from a small extra dimension. *Phys. Rev. Lett. 83* (1999), 3370–3373.

[24] Schwob, C., Jozefowski, L., de Beauvoir, B., Hilico, L., Nez, F., Julien, L., Biraben, F., Acef, O., Zondy, J.-J., and Clairon, A. Optical frequency measurement of the $2s - 12d$ transitions in hydrogen and deuterium: Rydberg constant and lamb shift determinations. *Phys. Rev. Lett. 82*, 25 (Jun 1999), 4960–4963.

[25] Seiberg, N., and Witten, E. String theory and noncommutative geometry. *JHEP 09* (1999), 032.

[26] Snyder, H. S. The electromagnetic field in quantized space-time. *Phys. Rev. 72* (1947), 68–71.

[27] Snyder, H. S. Quantized space-time. *Phys. Rev. 71* (1947), 38–41.

[28] Srinivasan, K., Sriramkumar, L., and Padmanabhan, T. The hypothesis of path integral duality. ii: Corrections to quantum field theoretic results. *Phys. Rev. D58* (1998), 044009.

[29] Stetsko, M. M., and Tkachuk, V. M. Perturbation hydrogen-atom spectrum in deformed space with minimal length. e-print hep-ph/9609357.

[30] Susskind, L. The paradox of quantum black holes. *Nature Phys. 2* (2006), 665–677.

[31] Yang, C. N. On quantized space-time. *Phys. Rev. 72* (1947), 874.

Vita

Sándor Zoltán Benczik is Hungarian from Arad, in the Western part of Romania known as Transylvania. He received a bachelor's and master's degree in mathematics from the West University of Timişoara. He is doctoral student under the guidance of professor Lay Nam Chang, his research area being elementary particle theory, in particular the possibility of the existence of a minimal length and the properties of neutrinos. He is a founding member and former president of the Hungarian Student Association at Virginia Tech. He is happily married to Gilia, but does not have any children yet.