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NONASSOCIATIVE QUANTUM MECHANICS

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Martinus van Kuppeveld

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The dissertation of Martinus van Kuppeveld was reviewed and approved by the following:

Martin Bojowald
Professor of Physics
Dissertation Advisor
Chair of Committee

Murat Gunaydin
Professor of Physics

Ping Xu
Professor of Mathematics

Nigel Higson
Evan Pugh Professor of Mathematics

Nitin Samarth
Professor of Physics
Head of the Department of Physics

Abstract

Nonassociative operator observable algebras, like those that occur in the presence of small magnetic monopole charges and non-geometric backgrounds in string theory, can not be represented as linear operators on a Hilbertspace, creating difficulties in extracting physics from these systems. This thesis is a compilation of three papers [1–3] that start with a more robust definition of an eigenstate and uses inequalities between moments following from positivity of the state to find the spectra of several operators. This is done without making any reference to wave functions or density matrices, and can thus be applied tot nonassociative operator algebras as well. From this we find a new bound on the magnetic charge of the muon ($g \leq 4.7 \cdot 10^{-18}\text{Am} = 1.4 \cdot 10^{-9} g_{\text{Dirac}}$).

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Chapter 1
Introduction

This thesis is based on three papers that explore a moment based approach to quantum mechanics, with the aim of extracting physics of systems with non-associative observable algebras. These algebras arise in anomalous gauge theories [4–6], in non-geometric backgrounds of string theory, and in Non-commutative geometry [7]. These algebras are typically dismissed as un-physical as they can not be represented with Hilbert space operators. However, with effective theories based on higher moments in quantum systems[1], it turns out we can still ask physically meaningful questions, and investigate non-associative deformations of our theories which may represent a very large, unexplored theory space.

The simplest system in which these non-associative algebras appear is in the description of an electrically charged particle in the presence of certain magnetic monopoles [5, 11, 12]. This can be seen directly from the fact that the Jacobi identity does not hold for the momentum operators, meaning that $(\hat{p}_i\hat{p}_j)(\hat{p}_k) \neq (\hat{p}_i)(\hat{p}_j\hat{p}_k)$ can not hold for all i, j, k.
As such, we can not represent these operators with linear maps on a Hilbert space, as these are automatically associative[2]. This means that states can no longer be represented as an element of a Hilbert space.

There is however a natural definition of states in terms of normalized, positive functionals on C^* - algebras, and this can be generalized in a straightforward way to non-associative

[1] Constructions like these are also useful in the context of deriving effective equations for higher moments in constrained systems [8], and have been applied in gravitational context [9, 10]

[2] Monopoles that satisfy the Dirac quantization condition, like those we see in most GUTs, can still be described with the standard formalism involving Hilbert spaces. The simplest way to see this is by noting that these field configurations can be realized in the standard theories by using more exotic fibre bundles [13]. However, these constructions are related to integer topological invariants (elements of certain homotopy groups), and are not available for arbitrary magnetic charges.

algebras. In concrete terms, this means we define a state by the expectation values it gives for all observables. The set of states is then characterized by the fact that these expectation values have to satisfy properties like $\langle 1 \rangle = 1$ and $\langle A^\dagger A \rangle \geq 0$. By defining an eigenstate of the Hamiltonian as a state for which $\langle \hat{X}(\hat{H} - E) \rangle = 0$ for a fixed E and all operators$\hat{X}$, it is then possible to extract an energy spectrum even in a non-associative setting.

Applying this in the context of the harmonic oscillator directly led to a relation between natural generalizations of the uncertainty principle and energy eigenstates, one which was maintained under perturbations [3], and this is what the paper in chapter 2 is about. Furthermore, applying this technique to a hydrogen-like atom whose nucleus had some small magnetic charge allowed us to get the first characterization of the spectrum of a non-associative Hamiltonian, which led to an improved upper bound on the magnetic charge of a muon [2], as described in chapter 3. Extending this work in [1] led to a new analytical method that allows for the full reconstruction of the negative energy states, as shown in chapter 4.

Chapter 2
Moments and saturation properties of eigenstates: Oscillator Systems

Martin Bojowald, Jonathan Guglielmon, Martijn van Kuppeveld

Eigenvalues are defined for any element of an algebra of observables and do not require a representation in terms of wave functions or density matrices. A systematic algebraic derivation based on moments is presented here for the harmonic oscillator, together with a perturbative treatment of anharmonic systems. In this process, a collection of inequalities is uncovered which amount to uncertainty relations for higher-order moments saturated by the harmonic-oscillator excited states. Similar saturation properties hold for anharmonic systems order by order in perturbation theory. The new method, based on recurrence relations for moments of a state combined with positivity conditions, is therefore able to show new physical features.

2.1 Introduction

The usual derivation of eigenvalues in model systems of quantum mechanics seems to suggest that spectral properties are a direct consequence of boundary conditions imposed on wave functions. However, boundary conditions are a property of representations of an algebra of observables $\mathcal{A}$ (with a unit $\mathbb{I}$), while the spectrum of an operator does not refer to a representation: For any algebra element $\hat{a} \in \mathcal{A}$, it can be defined as the set of all $\lambda \in \mathbb{C}$ such that $\hat{a} - \lambda\mathbb{I}$ does not have an inverse in $\mathcal{A}$. The main purpose of this article is to show that it is not only possible to define the spectrum directly for an algebra, but

also to compute it without using a specific representation.

While this statement may seem formal, there are several useful implications for physical considerations. In particular, (i) the algebraic derivation works for all possible representations of the algebra, (ii) it applies equally to pure states and mixed states, and (iii) it is available in systems of non-associative quantum mechanics that cannot be represented on a Hilbert space [5,11,14]. The latter arena has recently led to a new upper bound on the magnetic charge of elementary particles [2] and is therefore physically meaningful. Here, we demonstrate the new method used in the latter result for standard associative systems, in which we rederive known spectra but find new identities for moments of eigenstates that can be interpreted as saturation conditions of higher-order uncertainty relations. This result helps to demonstrate a relationship between excited states and generalized coherent states.

Our starting point is the algebraic definition of a state as a (normalized) positive linear functional on the $*$-algebra $\mathcal{A}$ of observables, that is a linear map $\langle\cdot\rangle\colon \mathcal{A}\to\mathbb{C}$ with $\langle\hat{a}^\dagger\hat{a}\rangle\geq 0$ for all $\hat{a}\in\mathcal{A}$ (and $\langle\mathbb{I}\rangle=1$). (We denote the $*$-relation by a $\dagger$, following standard physics notation in quantum mechanics.) Physically, the positivity condition implies not only that fluctuations $\langle\hat{a}^2\rangle-\langle\hat{a}\rangle^2\geq 0$ of self-adjoint algebra elements are positive, but also, and slightly less obviously, that observations are subject to uncertainty relations; see for instance [15]: Any positive state obeys the Cauchy–Schwarz inequality

$$\langle\hat{a}^\dagger\hat{a}\rangle\langle\hat{b}^\dagger\hat{b}\rangle\geq|\langle\hat{a}^\dagger\hat{b}\rangle|^2 \tag{2.1}$$

from which uncertainty relations can be derived by making suitable choices for $\hat{a}$ and $\hat{b}$.

The $*$-relation on $\mathcal{A}$ may be abstractly defined, or given by the usual adjoint if $\mathcal{A}$ is represented on a Hilbert space. For basic generators $\hat{x}_i$ of $\mathcal{A}$, such as positions and momenta, one can parameterize a state by its basic expectation values $\langle\hat{x}_i\rangle$ and central moments

$$\Delta(x_1^{a_1}\cdots x_n^{a_n})=\langle(\hat{x}_1-\langle\hat{x}_1\rangle)^{a_1}\cdots(\hat{x}_n-\langle\hat{x}_n\rangle)^{a_n}\rangle_{\text{Weyl}} \tag{2.2}$$

using completely symmetric (or Weyl) ordering. Coupled equations of motion for basic expectation values and moments follow from an extension of Ehrenfest's theorem. For instance, for canonical $(x_i)=(q,p)$ with $[\hat{q},\hat{p}]=i\hbar\mathbb{I}$, in addition to

$$\frac{\mathrm{d}\langle\hat{q}\rangle}{\mathrm{d}t}=\frac{\langle[\hat{q},\hat{H}]\rangle}{i\hbar}\quad,\quad\frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t}=\frac{\langle[\hat{p},\hat{H}]\rangle}{i\hbar} \tag{2.3}$$

we have

$$\frac{\mathrm{d}\Delta(q^2)}{\mathrm{d}t} = \frac{\mathrm{d}(\langle\hat{q}^2\rangle - \langle\hat{q}\rangle^2)}{\mathrm{d}t} = \frac{\langle[\hat{q}^2,\hat{H}]\rangle}{i\hbar} - 2\langle\hat{q}\rangle\frac{\mathrm{d}\langle\hat{q}\rangle}{\mathrm{d}t} \tag{2.4}$$

for the position variance $\Delta(q^2) = (\Delta q)^2$. As usual, the time dependence in Ehrenfest-type equations may reside in the states used to compute expectation values (Schrödinger picture) or in the operators (Heisenberg picture). To be specific, we take the former viewpoint because it helps to avoid addressing mathematical questions about suitable topologies on the algebra that would be required to define a time derivative of operators. Depending on the Hamiltonian, the right-hand sides of (2.3) and (2.4) can be expanded in moments and usually involve asymptotic series of terms (unless the Hamiltonian is quadratic in basic operators).

This formulation is especially useful for canonical effective theories [16] and semiclassical expansions because the condition $\Delta(x_1^{a_1}\cdots x_n^{a_n}) = O(\hbar^{(a_1+\cdots+a_n)/2})$ provides a general definition of semiclassical (but possibly non-Gaussian) states and allows tractable approximations of the equations of motion order by order in $\hbar$. In the present paper, as another new conceptual insight, we show that interesting properties that can be obtained in this way are not restricted to semiclassical ones: Harmonic and perturbative eigenvalues can be derived as well, together with relationships between their moments.

Uncertainty relations play a crucial role in this context, as can be seen by the simple example of the ground state of the harmonic oscillator with Hamiltonian

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{q}^2\,. \tag{2.5}$$

Using moments, the ground-state energy can be derived from two conditions, namely that (i) the moments be time independent for a stationary state, and (ii) the standard uncertainty relation be saturated. Indeed, in this case the second-order moments obey a closed set of evolution equations

$$\frac{\mathrm{d}\Delta(q^2)}{\mathrm{d}t} = 2\frac{\Delta(qp)}{m} \tag{2.6}$$

$$\frac{\mathrm{d}\Delta(qp)}{\mathrm{d}t} = \frac{1}{m}\Delta(p^2) - m\omega^2\Delta(q^2) \tag{2.7}$$

$$\frac{\mathrm{d}\Delta(p^2)}{\mathrm{d}t} = -2m\omega^2\Delta(qp)\,. \tag{2.8}$$

Condition (i) implies $\Delta(qp) = 0$ and $\Delta(p^2) = m^2\omega^2\Delta(q^2)$. Condition (ii) then determines $\Delta(q^2) = \hbar/(2m\omega)$ and $\Delta(p^2) = \frac{1}{2}m\omega\hbar$. Therefore, the energy expectation value in such a

state (with $\langle\hat{q}\rangle = 0 = \langle\hat{p}\rangle$ by condition (i)),

$$\langle\hat{H}\rangle = \frac{1}{2m}\Delta(p^2) + \frac{1}{2}m\omega^2\Delta(q^2) = \frac{1}{2}\hbar\omega\,, \tag{2.9}$$

agrees with the ground-state energy. It is not necessary to compute the full ground-state wave function in order to find the energy. However, the question of how to compute the energy eigenvalues of excited states using moments is more difficult: Their eigenstates are not Gaussian and therefore do not saturate the standard uncertainty relation.

For the ground state of the harmonic oscillator, the condition that Heisenberg's uncertainty relation be saturated can be replaced by a lesson from the variational principle. The expectation value of the Hamiltonian is minimized in the ground state. Since (2.9) is linear in second-order moments, which take values in a region bounded by the uncertainty relation, the expectation value is minimized at the boundary allowed by this relation. Saturation therefore need not be assumed but can be derived from a fundamental principle. But again, for excited states such a derivation based on moments seems to be more complicated because one would somehow have to restrict the moments to belong to a wave function orthogonal to the ground state and all lower-excited states. However, orthogonality relations are not available for states at the algebraic level. Our procedure will instead lead to certain higher-order uncertainty relations that, regarding energy eigenstates, split the state space into subsets much like the usual orthogonality conditions do for wave functions.

For some time and in a slightly different context, moments have been known to be useful for numerical approximations of eigenvalues of excited states [17–20]. (See also [21,22] for recent work.) Here, we use some of the same relations between moments of eigenstates, but in a different way. As a result, our constructions have a more fundamental flavor because they can serve as new definitions of eigenvalues and eigenstates in the algebraic perspective, even while they do provide new computational schemes as well. We are aware of at least two examples for settings in which our constructions may be useful: In canonical quantum gravity, the problem of time [23–25] often makes explicit constructions of physical Hilbert spaces and wave functions untractable, while moment methods have been shown to present certain computational advantages [26–29]. And in non-associative quantum mechanics, which plays a role in models with magnetic monopoles [30] or of certain flux compactifications in string theory [31–35], operators on wave functions (and therefore the usual definition of eigenvalues) are in general unavailable [33, 36–39], but moments may still be used [2, 56, 70].

The main new result we will be able to uncover here for associative systems is a saturation property for any harmonic-oscillator eigenstate. (For a detailed non-associative example, see [40].) As part of our procedure, we impose a set of inequality constraints involving the moments, so as to ensure that they belong to an actual state (a *positive* linear functional). These constraints include the standard uncertainty principle as well as a series of inequalities involving higher moments. Upon imposing these conditions, we find that some of them are not only satisfied but also saturated by a harmonic-oscillator eigenstate. This feature is reminiscent of the saturation of Heisenberg's uncertainty relation by the ground state. As a related result, we show that excited states of the harmonic oscillator are (limits of) generalized coherent states as defined by Titulaer and Glauber [41]. In an extension to anharmonic oscillators, we confirm that such saturation properties continue to hold order by order in perturbation theory by the anharmonicity.

At present, it is not clear how feasible it would be to extend this method to non-harmonic systems beyond perturbation theory. As an alternative, still algebraic procedure, we therefore show how eigenvalues can be derived from convergence conditions for certain recurrence relations derived from positivity and boundedness conditions of expectation values. The positivity of states used in this construction is also the origin of uncertainty relations, but in the alternative procedure we do not directly impose uncertainty relations and therefore do not obtain new saturation properties. However, the algebraic derivation of eigenvalues and eigenstates is more tractable in this case and applies not only to the harmonic example presented here but also to the standard hydrogen problem [40]. Finally, our appendix presents an instructive finite-dimensional example given by a fermionic system.

2.2 Eigenvalues from Moments

In the standard presentation of the problem, using wave functions, eigenvalues λ and eigenstates ψ_λ of a given operator $\hat{H}$ are determine by a single equation,

$$\hat{H}\psi_\lambda = \lambda\psi_\lambda\,. \tag{2.10}$$

This equation immediately implies that that all expectation values of the form

$$\langle\hat{O}(\hat{H}-\lambda\mathbb{I})\rangle_\lambda = \langle\psi_\lambda|\hat{O}(\hat{H}-\lambda\mathbb{I})\psi_\lambda\rangle = 0 \tag{2.11}$$

vanish for any operator $\hat{O}$ such that ψ_λ is in the domain of $\hat{O}^\dagger$. In our derivation, operators $\hat{O}$ polynomial in basic operators $\hat{q}$ and $\hat{p}$ will be found to be sufficient. Even with this restriction, an algebraic derivation of eigenvalues is not obvious and requires two ingredients: (i) A way of organizing infinitely many equations implied by (2.11) for sufficiently many choices of $\hat{O}$, and (ii) the imposition of a condition that the expectation value in (2.11) indeed refers to an admissible, that is, positive state.

In this section we present two methods for the same system that differ in how both (i) and (ii) are addressed. In our first derivation, we rewrite (2.11) as a system of recurrence relations for moments of an eigenstate and impose positivity through (generalized) uncertainty relations. In an alternative derivation in Section 2.2.3 we use generating functions and impose positivity more indirectly through continuity and boundedness conditions on a suitably defined object.

2.2.1 Notation

Equation (2.11) immediately implies that eigenstates of a self-adjoint $\hat{H}$ are stationary:

$$\begin{aligned} \frac{\mathrm{d}\langle\hat{O}\rangle_\lambda}{\mathrm{d}t} &= \frac{\langle[\hat{O},\hat{H}]\rangle_\lambda}{i\hbar} \\ &= \frac{\langle\hat{O}(\hat{H}-\lambda\mathbb{I})\rangle_\lambda - \langle\hat{O}^\dagger(\hat{H}-\lambda\mathbb{I})\rangle_\lambda^*}{i\hbar} = 0\,. \end{aligned} \tag{2.12}$$

For the harmonic oscillator, this equation applied to $\hat{q}$ and $\hat{p}$ implies that $\langle\hat{q}\rangle = 0$ and $\langle\hat{p}\rangle = 0$. Instead of using central moments as in the introduction, we can therefore work directly with bare moments and zero basic expectation values. We define

$$\hat{T}_{m,n} := (\hat{q}^m\hat{p}^n)_{\mathrm{Weyl}} \tag{2.13}$$

where $\hat{q}$ and $\hat{p}$ are the canonical position and momentum operators, m and n are non-negative integers, and the subscript indicates, as before, that the product is taken in completely symmetric ordering. Note that through the commutation relation $[\hat{q},\hat{p}] = i\hbar$, products of the form $\hat{T}_{m,n}\hat{T}_{m',n'}$ can always be rewritten as sums over individual $\hat{T}_{m'',n''}$ of order $m+n+m'+n'$ or less. See [42] for an explicit statement of the relevant reordering identity.

Given a particular state, we define the bare moments (about the origin) as:

$$T_{m,n} := \langle\hat{T}_{m,n}\rangle. \tag{2.14}$$

The collection of all such moments for a given state provides a complete description of the state in the sense that given the moments, it is possible (in principle) to reconstruct the wave function. However, the moments are not completely free. They must satisfy certain inequalities, such as Heisenberg's uncertainty relation, as well as a number of other constraints involving higher moments. A necessary and sufficient condition for a collection of moments $\{T_{m,n}\}$ to correspond to a genuine quantum state has been given in [43]. More recently, a similar result has been developed from a different perspective in [44], providing a generalized uncertainty principle that imposes inequality constraints on higher moments. These results are key for our further constructions.

Consider the column vector, $\hat{\xi}_J$, consisting of all operators $\hat{T}_{m,n}$ up to order $m+n = 2J$, where J is an integer or half-integer. The generalized uncertainty principle states that the $(J+1)(2J+1) \times (J+1)(2J+1)$ dimensional square matrix $M_J = \langle \hat{\xi}_J \hat{\xi}_J^\dagger \rangle$ is positive semi-definite,

$$M_J = \langle \hat{\xi}_J \hat{\xi}_J^\dagger \rangle \geq 0 \tag{2.15}$$

where the expectation value is taken element by element. Prior to taking the expectation value, the matrix elements are products of the form $\hat{T}_{m,n}\hat{T}_{m',n'}$. As mentioned above, these products can be rewritten as linear combinations of individual $T_{m'',n''}$. The elements of M_J are thus functions of the moments. Since $M_J \geq 0$ implies non-negativity of its principal minors, the generalized uncertainty principle yields a set of inequalities involving the moments.

As discussed in [45], it is useful to bring this matrix to block diagonal form

$$M_J \to \begin{pmatrix} A_0 & & & \\ & A_1 & & \\ & & \ddots & \\ & & & A_{2J} \end{pmatrix} \tag{2.16}$$

where A_n is an $n+1$ by $n+1$ matrix that contains moments up to order $2n$. This can be achieved by repeatedly applying the following identity

$$L \begin{pmatrix} A & C^\dagger \\ C & B \end{pmatrix} L^\dagger = \begin{pmatrix} A & 0 \\ 0 & B - CA^{-1}C^\dagger \end{pmatrix} \tag{2.17}$$

to M_J, where

$$L = \begin{pmatrix} 1 & 0 \\ -CA^{-1} & 1 \end{pmatrix}. \tag{2.18}$$

This identity holds whenever the matrix on the left-hand side of Eq. (2.17) is Hermitian. We then have that $M_J \geq 0$ if and only if $A_n \geq 0$ for all $n \leq 2J$. The generalized uncertainty principle may thus be rephrased as

$$A_n \geq 0 \text{ for all } n \geq 0. \tag{2.19}$$

If the state under consideration is known to be an eigenstate of a Hamiltonian, $\hat{H}$, then we can obtain an additional set of constraints. For all $m, n \geq 0$ we have

$$\langle \hat{T}_{m,n}(\hat{H} - \lambda \mathbb{I}) \rangle_\lambda = 0 \tag{2.20}$$

where λ is the eigenvalue of the state $\langle \cdot \rangle_\lambda$ under consideration. In order to rewrite this set of equations as a collection of constraints on the moments, we express $\hat{H}$ in terms of the $\hat{T}_{m,n}$ and reorder the product $\hat{T}_{m,n}\hat{H}$ into a sum over individual $\hat{T}_{m',n'}$. Equation (2.20) then implies recurrence relations for $T_{m,n}$ which depend on the system under consideration.

2.2.2 Application to the harmonic oscillator

We now show how the considerations outlined above can be used to find the eigenvalues of the harmonic-oscillator Hamiltonian. The idea is to use (2.20) to solve for the moments in terms of the eigenvalue λ and then apply (2.15) to obtain information concerning the allowed values of λ (as yet unspecified). This combination is the basis of our new method.

2.2.2.1 Recurrence relations

For the sake of mathematical clarity, we use the Hamiltonian $\hat{H} = (\hat{p}^2 + \hat{q}^2)/2$. The usual parameters given by the mass m and frequency ω can be reintroduced by a suitable canonical transformation of q, p if we also understand $\hat{H}$ as the energy divided by ω. Our q and p then both have units of $\sqrt{\hbar}$, such that $T_{m,n}$ has units of $\hbar^{(m+n)/2}$. Imposing (2.20) results in the following relations between the moments

$$\begin{aligned} T_{m+2,n} + T_{m,n+2} &= 2\lambda T_{m,n} + \frac{n(n-1)}{4}\hbar^2 T_{m,n-2} \\ &\quad + \frac{m(m-1)}{4}\hbar^2 T_{m-2,n} \qquad (2.21) \\ nT_{m+1,n-1} &= mT_{m-1,n+1} \qquad (2.22) \end{aligned}$$

which hold for all $m, n \geq 0$. Two constraints are obtained because (2.20) — defined without symmetric ordering of the product $\hat{T}_{m,n}\hat{H}$ — has both real and imaginary parts. From (2.22), starting with $m = 0$ or $n = 0$, we find that the moments are zero unless both m and n are even. For even and non-zero $m = 2j$ and $n = 2k$, we then define $S_{j,k}$ such that

$$T_{2j,2k} = \frac{(2j)!(2k)!}{j!k!} S_{j,k} \,. \tag{2.23}$$

For these coefficients, (2.22) implies the simple relation

$$S_{j+1,k} = S_{j,k+1} \,, \tag{2.24}$$

which in turn implies that $S_{j,k}$ depends only on $j + k$. There are, therefore, dimensionless coefficients b_j depending only on a single integer, such that

$$T_{2j,2k} = \frac{(2j)!(2k)!}{j!k!} \hbar^{j+k} b_{j+k} \,. \tag{2.25}$$

For convenience, it is useful to define a second set of coefficients, a_j, such that

$$b_{j+k} = \frac{(j+k)!}{(2j+2k)!} a_{j+k} \,, \tag{2.26}$$

or

$$T_{2j,2k} = \frac{(2j)!(2k)!(j+k)!}{j!k!(2j+2k)!} \hbar^{j+k} a_{j+k} \,. \tag{2.27}$$

For instance,

$$T_{2j,0} = \hbar^j a_j \tag{2.28}$$

and

$$T_{2j,2} = \hbar^{j+1} \frac{a_{j+1}}{2j+1} \tag{2.29}$$

have more compact coefficients than the equivalent expressions in terms of b_j.

As a consequence of (2.21), the remaining coefficients, a_ℓ, are subject to a difference equation in a single independent variable:

$$a_{\ell+1} = \frac{\lambda \hbar^{-1}(2\ell+1)}{\ell+1} a_\ell + \frac{(2\ell+1)(2\ell)(2\ell-1)}{8(\ell+1)} a_{\ell-1} \,. \tag{2.30}$$

Given the two initial values $a_0 = 1$ (as a consequence of normalization of the state, $T_{0,0} = 1$) and $a_1 = \lambda/\hbar$ (as a consequence of $2\hbar a_1 = T_{2,0} + T_{0,2} = 2\langle \hat{H} \rangle_\lambda = 2\lambda$), (2.30) determines all orders of moments in terms of the parameter λ. It is clear from the

recurrence and its initial values that a_ℓ is a polynomial in λ of degree ℓ. It has only even terms for ℓ even, and only odd terms for ℓ odd.

In terms of b_ℓ, the recurrence relation is slightly simpler,

$$(\ell+1)b_{\ell+1} - \frac{\lambda}{2\hbar}b_\ell - \frac{1}{16}\ell b_{\ell-1} = 0\,, \tag{2.31}$$

and can be solved via the generating function $f(x) = \sum_{\ell=0}^{\infty} b_\ell x^\ell$ subject to the differential equation

$$\left(1 - \frac{1}{16}x^2\right) f'(x) = \frac{1}{2}\left(\frac{\lambda}{\hbar} + \frac{1}{8}x\right) f(x) \tag{2.32}$$

and initial conditions $f(0) = b_0 = 1$, $f'(0) = b_1 = \frac{1}{2}\lambda$. The solution,

$$f(x) = \frac{(1+x/4)^{\lambda/\hbar - 1/2}}{(1-x/4)^{\lambda/\hbar + 1/2}}\,, \tag{2.33}$$

has the Taylor expansion

$$\begin{aligned} f(x) \;\; = \;\; & \sum_{\ell=0}^{\infty} \left(\frac{-x}{4}\right)^\ell \frac{(\ell - \lambda/\hbar - 1/2)!}{(-\lambda/\hbar - 1/2)!\ell!} \\ & \times {}_2F_1(\lambda/\hbar + 1/2, -\ell; \lambda/\hbar + 1/2 - \ell; -1) \end{aligned} \tag{2.34}$$

and determines the b_ℓ in terms of hypergeometric functions.

2.2.2.2 Positivity

We now apply the generalized uncertainty principle (2.15) to these moments. Note that $M_J \geq 0$ implies that $M'_J \geq 0$, where M'_J is a matrix formed by deleting from M_J any number of rows and their corresponding columns. Equivalently, M'_J may be defined as the matrix formed by deleting entries from $\hat{\xi}_J$ to form a new vector $\hat{\xi}'_J$ and then taking

$$M'_J = \langle \hat{\xi}'_J \hat{\xi}'^\dagger_J \rangle\,. \tag{2.35}$$

In particular, consider the matrix M'_J formed by taking $\hat{\xi}'_J$ to contain only operators of the form $\hbar^{-m/2}\hat{T}_{m,0}$ and $\hbar^{-m/2}\hat{T}_{m-1,1}$ up to $m = 2J$. While $\hat{\xi}_J$ has

$$N_J = (J+1)(2J+1) \tag{2.36}$$

components, $\hat{\xi}'_J$ has

$$N'_J = 4J + 1 = N_J - J(2J-1) \tag{2.37}$$

components. (The number N'_J is by definition given by one plus twice the maximum number $2J$ of factors of $\hat{q}$ included in $\hat{T}_{m,0}$ for a given $\hat{\xi}_J$. It also equals $N'_J = N_J - N_{J-1}$.) Therefore, $M'_J \neq M_J$ if and only if $J \geq 1$.

For example, for $J = 0$ we have $M'_0 = 1$, not implying any non-trivial uncertainty relation. For $J = 1/2$, we have

$$M'_{1/2} = M_{1/2} = \left\langle \begin{pmatrix} 1 & \hat{q}/\sqrt{\hbar} & \hat{p}/\sqrt{\hbar} \\ \hat{q}/\sqrt{\hbar} & \hat{q}^2/\hbar & \hat{q}\hat{p}/\hbar \\ \hat{p}/\sqrt{\hbar} & \hat{p}\hat{q}/\hbar & \hat{p}^2/\hbar \end{pmatrix} \right\rangle \tag{2.38}$$

where the expectation value is taken element by element. A suitable minor of $M'_{1/2}$ being positive semidefinite,

$$\begin{aligned} \det \begin{pmatrix} \langle \hat{q}^2 \rangle & \langle \hat{q}\hat{p} \rangle \\ \langle \hat{p}\hat{q} \rangle & \langle \hat{p}^2 \rangle \end{pmatrix} &= T_{2,0}T_{0,2} - \left(T_{1,1} + \frac{1}{2}i\hbar\right)\left(T_{1,1} - \frac{1}{2}i\hbar\right) \\ &= T_{2,0}T_{0,2} - T_{1,1}^2 - \frac{\hbar^2}{4} \geq 0\,, \end{aligned} \tag{2.39}$$

is equivalent to Heisenberg's uncertainty relation. Taking $J = 1$ as another example (the simplest case in which $M'_J \neq M_J$), we have

$$\hat{\xi}'_1 = \begin{pmatrix} 1 \\ \hat{T}_{1,0}/\sqrt{\hbar} \\ \hat{T}_{0,1}/\sqrt{\hbar} \\ \hat{T}_{2,0}/\hbar \\ \hat{T}_{1,1}/\hbar \end{pmatrix} \tag{2.40}$$

which gives

$$M'_1 = \left\langle \begin{pmatrix} 1 & \hat{T}_{1,0}/\sqrt{\hbar} & \hat{T}_{0,1}/\sqrt{\hbar} & \hat{T}_{2,0}/\hbar & \hat{T}_{1,1}/\hbar \\ \hat{T}_{1,0}/\sqrt{\hbar} & \hat{T}_{1,0}\hat{T}_{1,0}/\hbar & \hat{T}_{1,0}\hat{T}_{0,1}/\hbar & \hat{T}_{1,0}\hat{T}_{2,0}/\hbar^{3/2} & \hat{T}_{1,0}\hat{T}_{1,1}/\hbar^{3/2} \\ \hat{T}_{0,1}/\sqrt{\hbar} & \hat{T}_{0,1}\hat{T}_{1,0}/\hbar & \hat{T}_{0,1}\hat{T}_{0,1}/\hbar & \hat{T}_{0,1}\hat{T}_{2,0}/\hbar^{3/2} & \hat{T}_{0,1}\hat{T}_{1,1}/\hbar^{3/2} \\ \hat{T}_{2,0}/\hbar & \hat{T}_{2,0}\hat{T}_{1,0}/\hbar^{3/2} & \hat{T}_{2,0}\hat{T}_{0,1}/\hbar^{3/2} & \hat{T}_{2,0}\hat{T}_{2,0}/\hbar^2 & \hat{T}_{2,0}\hat{T}_{1,1}/\hbar^2 \\ \hat{T}_{1,1}/\hbar & \hat{T}_{1,1}\hat{T}_{1,0}/\hbar^{3/2} & \hat{T}_{1,1}\hat{T}_{0,1}/\hbar^{3/2} & \hat{T}_{1,1}\hat{T}_{2,0}/\hbar^2 & \hat{T}_{1,1}\hat{T}_{1,1}/\hbar^2 \end{pmatrix} \right\rangle \tag{2.41}$$

where as before the expectation value is taken element by element.

In order to derive the generic structure of M'_J, we use the relations

$$\hat{T}_{k,0}\hat{T}_{\ell,1} = \hat{T}_{k+\ell,1} - \frac{1}{2}ik\hbar\hat{T}_{k+\ell-1,0} \tag{2.42}$$

$$\hat{T}_{k,1}\hat{T}_{\ell,1} = \hat{T}_{k+\ell,2} + \frac{1}{2}i(\ell-k)\hbar\hat{T}_{k+\ell-1,1} + \frac{1}{4}k\ell\hbar^2\hat{T}_{k+\ell-2,0} \tag{2.43}$$

which follow from the general ordering equations given in [42] (or [45]). For fixed J, we can express the non-constant components of $\hat{\xi}'_J =: \hat{\xi}'$ as

$$\hat{\xi}'_n = \hbar^{-n/4} \cdot \begin{cases} \hat{T}_{n/2,0} & \text{if } n \text{ even} \\ \hbar^{1/4}\hat{T}_{(n-3)/2,1} & \text{if } n \text{ odd} \end{cases} \tag{2.44}$$

where $2 \leq n \leq 4J+1$. Excluding (for now) the first row and column of $\hat{M}'_J$ which contain at most one factor of $\hat{T}_{m,n}$ and therefore do not require any reordering, this operator-valued matrix has the components

$$\begin{aligned} \hat{M}'_{mn} = \hat{\xi}'_m\hat{\xi}'^{\,\dagger}_n &= \hbar^{-(m+n)/4} \cdot \begin{cases} \hat{T}_{(m+n)/2,0} & \text{if } m,n \text{ even} \\ \hbar^{1/4}\hat{T}_{(m-3)/2,1}\hat{T}_{n/2,0} & \text{if } m \text{ odd and } n \text{ even} \\ \hbar^{1/4}\hat{T}_{m/2,0}\hat{T}_{(n-3)/2,1} & \text{if } m \text{ even and } n \text{ odd} \\ \hbar^{1/2}\hat{T}_{(m-3)/2,1}\hat{T}_{(n-3)/2,1} & \text{if } m,n \text{ odd} \end{cases} \\ &= \hbar^{-(m+n)/4} \cdot \begin{cases} \hat{T}_{(m+n)/2,0} & \text{if } m,n \text{ even} \\ \hbar^{1/4}\hat{T}_{(m+n-3)/2,1} + \frac{1}{4}in\hbar^{5/4}\hat{T}_{(m+n-5)/2,0} & \text{if } m \text{ odd and } n \text{ even} \\ \hbar^{1/4}\hat{T}_{(m+n-3)/2,1} - \frac{1}{4}im\hbar^{5/4}\hat{T}_{(m+n-5)/2,0} & \text{if } m \text{ even and } n \text{ odd} \\ \hbar^{1/2}\hat{T}_{(m+n-6)/2,2} + \frac{n-m}{4}i\hbar^{3/2}\hat{T}_{(m+n-8)/2,1} & \\ \quad + \frac{(m-3)(n-3)}{16}\hbar^{5/2}\hat{T}_{(m+n-10)/2,0} & \text{if } m,n \text{ odd} \end{cases} \end{aligned} \tag{2.45}$$

Taking expectation values and setting all $T_{m,n} = 0$ unless m and n are even, we obtain

$$M'_{mn} = \hbar^{-(m+n)/4} \cdot \begin{cases} T_{(m+n)/2,0} & \text{if } m,n \text{ even} \\ \frac{1}{4}in\hbar^{5/4}T_{(m+n-5)/2,0} & \text{if } m \text{ odd and } n \text{ even} \\ -\frac{1}{4}im\hbar^{5/4}T_{(m+n-5)/2,0} & \text{if } m \text{ even and } n \text{ odd} \\ \hbar^{1/2}T_{(m+n-6)/2,2} + \frac{1}{16}(m-3)(n-3)\hbar^{5/2}T_{(m+n-10)/2,0} & \text{if } m,n \text{ odd} \end{cases} \tag{2.46}$$

Some components M'_{mn} are zero for certain values of m and n, which can be seen by refining the parameterization such that $m = 4q + \alpha$ and $n = 4r + \beta$ with integer q and r

and $0 \le \alpha, \beta \le 3$. For fixed q and r, we obtain the 4×4 block

$$\hbar^{q+r} M'_{4q+\alpha,4r+\beta} = \tag{2.47}$$
$$\begin{pmatrix} T_{2(q+r),0} & -iq\hbar T_{2(q+r-1),0} & 0 & 0 \\ ir\hbar T_{2(q+r-1),0} & T_{2(q+r-1),2} & 0 & 0 \\ & +(q-\frac{1}{2})(r-\frac{1}{2})\hbar^2 T_{2(q+r-2),0} & & \\ 0 & 0 & \hbar^{-1}T_{2(q+r+1),0} & -i(q+\frac{1}{2})T_{2(q+r),0} \\ 0 & 0 & i(r+\frac{1}{2})T_{2(q+r),0} & \hbar^{-1}T_{2(q+r),2} \\ & & & +qr\hbar T_{2(q+r-1),0} \end{pmatrix}$$

where rows and columns are arranged according to the values of α and β. (The full 4×4-blocks appear in M'_J only for $q \ge 1$ and $r \ge 1$, while parts of these blocks make up the first three rows and columns of M'_J.) Using (2.28) and (2.29), we obtain the blocks

$$\hbar^{q+r} M'_{4q+\alpha,4r+\beta} = \tag{2.48}$$
$$\begin{pmatrix} a_{q+r} & -iqa_{q+r-1} & 0 & 0 \\ ira_{q+r-1} & \frac{a_{q+r}}{2(q+r)-1} + (q-\frac{1}{2})(r-\frac{1}{2})a_{q+r-2} & 0 & 0 \\ 0 & 0 & a_{q+r+1} & -i(q+\frac{1}{2})a_{q+r} \\ 0 & 0 & i(r+\frac{1}{2})a_{q+r} & \frac{a_{q+r+1}}{2(q+r)+1} + qra_{q+r-1} \end{pmatrix}$$

If $J = 1$, for instance, we have the matrix

$$M'_1 = \begin{pmatrix} 1 & 0 & 0 & a_1 & 0 \\ 0 & a_1 & \frac{1}{2}i & 0 & 0 \\ 0 & -\frac{1}{2}i & a_1 & 0 & 0 \\ a_1 & 0 & 0 & a_2 & ia_1 \\ 0 & 0 & 0 & -ia_1 & \frac{1}{3}a_2 + \frac{1}{4} \end{pmatrix}. \tag{2.49}$$

It is block-diagonalized by identifying $C^\dagger$ in (2.17) with the vector $C_1^\dagger = (0, 0, a_1, 0)$:

$$L_1 M'_1 L_1^\dagger = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & a_1 & \frac{1}{2}i & 0 & 0 \\ 0 & -\frac{1}{2}i & a_1 & 0 & 0 \\ 0 & 0 & 0 & a_2 - a_1^2 & ia_1 \\ 0 & 0 & 0 & -ia_1 & \frac{1}{3}a_2 + \frac{1}{4} \end{pmatrix}. \tag{2.50}$$

Its determinant is equal to

$$\begin{aligned} & \det(L_1 M_1' L_1^\dagger) \\ = \; & \frac{1}{4}(\lambda/\hbar + 1/2)^2(\lambda/\hbar - 1/2)^2(\lambda/\hbar + 3/2)(\lambda/\hbar - 3/2) \end{aligned} \tag{2.51}$$

using the solution $a_2 = \frac{3}{2}(\lambda^2/\hbar^2 + 1/4)$ of the recurrence relation (2.30).

2.2.2.3 Eigenvalues

For any J, we may block diagonalize M_J' as in Equation (2.16), except that each A_n' will be a 2×2 matrix since we are working with the reduced matrix, M_J'. We then have

$$\det(A_n') \geq 0 \tag{2.52}$$

for all n. For a fixed n, this inequality is a constraint involving moments up to order $2n$. All of these moments can in turn be written in terms of λ using (2.27) and (2.30). From explicit computations, we infer the general result

$$d_n = \det(A_n') = \frac{1}{4^{n-1}} \prod_{k=1}^{n} (\lambda/\hbar - \alpha_k)(\lambda/\hbar + \alpha_k) \tag{2.53}$$

where $\alpha_k = (2k-1)/2$ are the odd half-integer multiples. (The polynomial (2.51) is equal to $d_1 d_2$.) Considered as a function of λ, this expression has nodes at the α_k up to some maximum k that depends on the particular value of n. Between nodes, the function is non-zero, and it alternates in sign depending on the value of n. In particular, because $d_{n+1} = \frac{1}{4} d_n(\lambda^2/\hbar^2 - \alpha_k^2)$ implies $\operatorname{sgn} d_{n+1} = -\operatorname{sgn} d_n$ if $|\lambda|/\hbar < \alpha_n$, sending $n \to n+1$ causes the sign to alternate. This behavior combined with the non-negativity of $\det(A_n')$ implies that the only allowable values for λ occur at the nodes. We can exclude negative values of λ by appealing to the non-negativity of the first leading principal minor of A_1' (which in this case is a 1×1 "block" consisting simply of λ), which gives the constraint $\lambda \geq 0$. We thus have that the only possible values for λ are

$$\lambda = \frac{1}{2}\hbar, \frac{3}{2}\hbar, \frac{5}{2}\hbar, \ldots \tag{2.54}$$

in agreement with the well-known eigenvalues of the harmonic-oscillator Hamiltonian (divided by ω).

Since eigenvalues occur at the nodes of positivity conditions, all excited states obey

saturation conditions of higher-order uncertainty relations. We will explore these relations further in Section 2.3, but first give an alternative moment-based derivation of eigenvalues because we have found it to be difficult to construct a general analytic proof of our crucial equation (3.4).

2.2.3 Alternative derivation

We now present an alternative algebraic derivation of eigenvalues and eigenstates of the harmonic oscillator that appears to be more tractable but does not give as direct access to saturation properties as the previous method. We still impose the two main conditions stated at the beginning of this section, equation (2.11) combined with positivity of states, but do so in an alternative way. The recurrence relations for moments will be replaced by recurrence relations for coefficients of a suitable generating function, and positivity will be evaluated by means of boundedness and continuity of a certain expectation value of a 1-parameter family of operators.

Given an energy eigenstate of the harmonic oscillator with eigenvalue λ, consider the function

$$L_\lambda(\gamma) = \left\langle \exp\left((1+\gamma)\hat{q}^2/\hbar\right)\right\rangle_\lambda \,. \tag{2.55}$$

For fixed λ, this function of γ is well defined for $\gamma \leq -1$ because $\exp\left((1+\gamma)\hat{q}^2/\hbar\right)$ is then an algebra element that quantizes a bounded function, with $L_\lambda(-1) = 1$ by normalization and $\lim_{\gamma\to-\infty} L_\lambda(\gamma) = 0$. (Any positive state is continuous [46].) Positivity of the state also implies that $L_\lambda(\gamma)$ increases monotonically. We will show that these properties, implied by boundedness and positivity, can replace the uncertainty relations used in the preceding section in an algebraic derivation of eigenvalues. This method can also be applied to non-harmonic systems, including the standard hydrogen problem [40].

2.2.3.1 Recurrence relations

The moment expansion

$$\begin{aligned} L_\lambda(\gamma) &= \sum_{j=0}^{\infty} \hbar^{-j}\langle\hat{q}^{2j}\rangle_\lambda \frac{(1+\gamma)^j}{j!} \\ &= \sum_{j=0}^{\infty} a_j \frac{(1+\gamma)^j}{j!} \end{aligned} \tag{2.56}$$

is readily obtained from the Taylor series of the exponential function, followed by the identification $\hbar^{-j}\langle\hat{q}^{2j}\rangle = \hbar^{-j}T_{2j,0} = a_j$ according to (2.28). Using the recursion relation

(2.30) for the a_j we obtain the differential equation

$$3L_\lambda+3(9+9\gamma+4\lambda/\hbar)L'_\lambda+8(2+\lambda/\hbar+\gamma(6+3\gamma+\lambda/\hbar))L''_\lambda+4\gamma(1+\gamma)(2+\gamma)L'''_\lambda=0 \quad (2.57)$$

where primes indicate derivatives by γ. Motivated by the behavior of $L_\lambda(\gamma)$ as $\gamma \to -\infty$, we rewrite this function as

$$L_\lambda(\gamma) = \sum_{n=0}^{\infty} \alpha_{n,s}(-\gamma)^{-n-s} \quad (2.58)$$

where the constant s takes into account a possible root-like pole at $\gamma \to -\infty$. The $\alpha_{n,s}$ are then subject to the relation

$$8(n+s)(n+s-\lambda/\hbar)\alpha_{n,s} - (1+2n+2s)\Big((3+6n+6s-4\lambda/\hbar)\alpha_{n+1,s} - (3+2n+2s)\alpha_{n+2,s}\Big) = 0\,.$$

Inserting $n=-1$ and requiring that this sequence of numbers terminates before $n=0$ in backwards recurrence implies $s=\frac{1}{2}$. With this knowledge we can rewrite L as

$$L_\lambda(\gamma) = \sum_{n=0}^{\infty} A_n(-\gamma)^{-n-\frac{1}{2}} \quad (2.59)$$

where $A_n = \alpha_{n,1/2}$. The preceding recurrence relation then turns into

$$(1+2n)(1+2n-2\lambda/\hbar)A_n - 2(1+n)\Big((3+3n-2\lambda/\hbar)A_{n+1} - (2+n)A_{n+2}\Big) = 0 \quad (2.60)$$

In the large-n limit, equation (2.60) simplifies to $4A_n - 6A_{n+1} + 2A_{n+2} = 0$. Therefore, for very large n, $A_n \approx c_1 + 2^n c_2$. If $c_1 \neq 0$ or $c_2 \neq 0$, this asymptotic behavior is problematic as it would cause

$$\begin{aligned} L_\lambda(\gamma) &\approx \sum_{n=0}^{M-1} A_n(-\gamma)^{-n-\frac{1}{2}} + \sum_{n=M}^{\infty}\Big(c_1(-\gamma)^{-n-\frac{1}{2}} + 2^n c_2(-\gamma)^{-n-\frac{1}{2}}\Big) \\ &= \sum_{n=0}^{M-1} A_n(-\gamma)^{-n-\frac{1}{2}} - (-\gamma)^{\frac{1}{2}-M}\left(\frac{c_1}{1+\gamma} + \frac{2^M c_2}{2+\gamma}\right) \end{aligned} \quad (2.61)$$

to diverge on values of γ, $\gamma=-1$ and $\gamma=-2$, where it ought to be between zero and one.

Therefore, both c_1 and c_2 have to be strictly zero: after a certain n all the A_n should vanish. Let N be the lowest integer such that $A_N = 0$. (Such an N always exists because

the normalization condition $L_\lambda(-1) = 1$ cannot be satisfied if all A_n are zero.) We then obtain the consistency equation

$$(2N-1)(2N-1-2\lambda/\hbar)A_{N-1} = 0 \tag{2.62}$$

from inserting $n = N-1$ in (2.60). By definition A_{N-1} is nonzero. Combined with the fact that N is an integer greater than zero, we find the familiar spectrum (2.54).

2.2.3.2 Coefficients

Based on this result, the coefficients introduced in (4.109) seem to be more tractable in the eigenvalue problem compared with our original a_j. These sets are strictly related to each other, but not in a simple way. Using Cauchy's formula to invert (4.109), we first write

$$\begin{aligned} A_n &= \frac{(-1)^{n+1}}{2\pi} \oint_{|z|=1} L_\lambda(z) z^{n-\frac{1}{2}} \mathrm{d}z \\ &= i(-1)^{n+1} \sum_{j=0}^{\infty} \frac{a_j}{2\pi j!} \int_0^{2\pi} (1+e^{i\theta})^j e^{i(n+1/2)\theta} \mathrm{d}\theta \\ &= i \sum_{j=0}^{\infty} \frac{a_j}{\pi j!} B(-1; n+1/2, j+1) \end{aligned} \tag{2.63}$$

using also (2.58), where B is the incomplete beta function.

In order to check convergence, we write $(1+e^{i\theta})^j = 2^j e^{ij\theta/2} \cos(\theta/2)^j$ and show that the second factor can be approximated as $\cos(\theta/2)^j \approx \exp(-j\theta^2/8)$. It is straightforward to confirm that these two expressions match to second order of a Taylor expansion in θ around $\theta = 0$. The local maxima of the difference of $\cos(\theta/2)^j$ and $\exp(-j\theta^2/8)$ are at some $\theta_{\max}$ such that

$$\begin{aligned} 0 &= \partial_\theta \left(\cos(\theta/2)^j - \exp(-j\theta^2/8) \right)_{\theta=\theta_{\max}} \\ &= \frac{j}{4} \left(\theta_{\max} \exp(-j\theta_{\max}^2/8) - 2\tan(\theta_{\max}/2) \cos(\theta_{\max}/2)^j \right) \end{aligned}$$

or

$$\cos(\theta_{\max}/2)^j = \frac{\theta_{\max}/2}{\tan(\theta_{\max}/2)} \exp(-j\theta_{\max}^2/2)\,.$$

Therefore, the difference is bounded by

$$\begin{aligned}\Delta_j &:= \sup_{\theta\in[-\pi,\pi]} |\cos(\theta/2)^j - \exp(-j\theta^2/8)| \\ &= |\cos(\theta_{\max}/2)^j - \exp(-j\theta_{\max}^2/8)| \\ &= \left(1 - \frac{\theta_{max}/2}{\tan(\theta_{max}/2)}\right)\exp(-j\theta_{max}^2/8)\,.\end{aligned}$$

This expression goes to zero for large j because of the exponential factor, unless $\theta_{\max} \to 0$ in which case the first factor in Δ_j approaches zero. We conclude that the difference of the two functions $\cos(\theta/2)^j$ and $\exp(-j\theta^2/8)$ converges to zero in $L^\infty[-\pi,\pi]$ when j goes to infinity.

Now, writing

$$(1+e^{i\theta})^j \le 2^j \exp(-j\theta^2/8 + ij\theta/2) + 2^j e^{ij\theta/2}\Delta_j$$

in the incomplete beta function and using $(-1)^n \int_{-\pi}^{\pi} \exp(i(n+(j+1)/2)\theta)\mathrm{d}\theta \le 2\pi$, we have

$$\begin{aligned}&B(-1; n+\tfrac{1}{2}, j+1) = \frac{(-1)^n}{2}\int_{-\pi}^{\pi}(1+e^{i\theta})^j e^{i(n+1/2)\theta}\mathrm{d}\theta \\ &\le \frac{(-1)^n}{2}\int_{-\infty}^{\infty} 2^j \exp(-j\theta^2/8 + ij\theta/2)e^{i(n+1/2)\theta}\mathrm{d}\theta \\ &\qquad +2^j\pi\Delta_j \\ &= \sqrt{2\pi}(-1)^n \frac{2^j}{\sqrt{j}}\exp\left(-\frac{(1+j+2n)^2}{2j}\right) + 2^j\pi\Delta_j\,. \qquad (2.64)\end{aligned}$$

The first term goes to zero for fixed n and large j. From the recursion relation for the a_j, we then see that the series (2.63) for A_n has to converge as well, as the numerator grows at most exponentially with j, while the denominator contains a $j!$.

Conversely, we have

$$\begin{aligned}a_j &= \left(\frac{\mathrm{d}^j}{\mathrm{d}\gamma^j}L_\lambda(\gamma)\right)\Big|_{\gamma=-1} \\ &= \sum_{n=0}^{\infty} A_n \left(\frac{\mathrm{d}^j}{\mathrm{d}\gamma^j}(-\gamma)^{-n-\frac{1}{2}}\right)\Big|_{\gamma=-1} \\ &= (-1)^j \sum_{n=0}^{\infty} A_n \left(-n-\frac{1}{2}\right)^{(j)} \qquad (2.65)\end{aligned}$$

where $x^{(n)}$ is the nth Pochhammer polynomial. As we have seen, only a finite number of the A_n are nonzero, and therefore this sum is clearly well defined.

2.2.3.3 Probability density

The alternative method based on (2.55) allows a more direct derivation of the probability density of eigenstates compared with reconstruction from the moments of Section 2.2.2.

In order to reconstruct the probability density of the N^{th} energy level, we first solve the recurrence relation for the coefficients A_n. Once N is fixed for a given eigenstate, we know that the N^{th} coefficient, A_N, is the highest non-zero one. Its exact value will be fixed later by normalization. Running through the recursion relation (2.60) with the known eigenvalue $\lambda = \hbar(N + \frac{1}{2})$, we can then work backward, starting with $n = N - 1$, until we reach the 0^{th} coefficient A_0 using (2.60) for $n = 0$. After that, the recurrence terminates automatically: For $n = -1$ in (2.60), we obtain $A_{-1} = 0$ because of an overall factor of $(1 + n)$ in the second part of (2.60), and for $n = -2$ we obtain $A_{-2} = 0$ because A_{-1} is zero, as just shown, and there is a factor of $(n + 2)$ in front of the $A_0 = A_{n+2}$ in this case. All coefficients of orders less than -2 then vanish because the recurrence is of second order. As an example, we consider $N = 4$ and find

$$\begin{aligned} A_3 &= -\frac{12}{7}A_4 \\ A_2 &= \frac{6}{5}A_4 \\ A_1 &= -\frac{12}{35}A_4 \\ A_0 &= \frac{3}{5}A_4\,. \end{aligned}$$

The coefficients A_n then determine the function $L_\lambda(\gamma)$, in which we can impose normalization by requiring $L_\lambda(-1) = \langle \mathbb{I} \rangle_\lambda = 1$. Continuing with our example of $N = 4$, we find

$$L_{\lambda_4} = \frac{35 + 60\gamma + 42\gamma^2 + 12\gamma^3 + 3\gamma^4}{8(-\gamma)^{9/2}}\,. \tag{2.66}$$

The probability density then requires an inversion of the integral that defines the expectation value taken in $L_\lambda(\gamma)$.

In order to do so, we first note that the Hamiltonian commutes with the parity operator, such that the probability density of any eigenstate has to be even. We therefore write

$$L_\lambda(\gamma) = 2\int_0^\infty \exp\left(\frac{1+\gamma}{\hbar}x^2\right) P_\lambda(x)\mathrm{d}x \tag{2.67}$$

in order to introduce the probability density $P_\lambda(x)$. Subsituting $u = x^2$ and $t = -(1+\gamma)/\hbar$, where all expressions are well-defined if $\mathrm{Re}(t) > 0$, we obtain

$$L_\lambda(-1-\hbar t) = \int_0^\infty e^{-tu} \frac{P_\lambda(\sqrt{u})}{\sqrt{u}} \mathrm{d}u \,. \tag{2.68}$$

The probability density is therefore obtained by an inverse Laplace transform, for which we can use Mellin's inverse formula (with a suitable δ):

$$\begin{aligned} P_\lambda(x) &= \frac{x}{2\pi i} \lim_{T\to\infty} \int_{\delta-iT}^{\delta+iT} e^{tx^2} L_\lambda(-1-\hbar t) \mathrm{d}t \\ &= \sum_{n=0}^{N} \frac{x}{2\pi i} \lim_{T\to\infty} \int_{\delta-iT}^{\delta+iT} e^{tx^2} A_n (1+\hbar t)^{-n-\frac{1}{2}} \mathrm{d}t \\ &= \sum_{n=0}^{N} \frac{A_n n! (2x)^{2n} \exp(-x^2/\hbar)}{\sqrt{\pi}(2n)!\hbar^{n+\frac{1}{2}}} \,. \end{aligned} \tag{2.69}$$

Proceeding again for our example of $N = 4$, we have

$$\begin{aligned} P_{\lambda_4}(x) &= \frac{\exp(-x^2/\hbar)}{\sqrt{\pi\hbar}} \left(\frac{3}{8} - \frac{12}{8}\frac{2x^2}{\hbar} + \frac{42}{8}\frac{4x^4}{3\hbar^2} - \frac{60}{8}\frac{8x^6}{15\hbar^3} + \frac{35}{8}\frac{16x^8}{105\hbar^4} \right) \\ &= \frac{\exp(-x^2/\hbar)}{24\sqrt{\pi\hbar}} \left(3 - 12\frac{x^2}{\hbar} + 4\frac{x^4}{\hbar} \right)^2 = \frac{\exp(-x^2/\hbar)}{\sqrt{\pi\hbar} 2^4 4!} H_4\left(\frac{x}{\sqrt{\hbar}}\right)^2 = |\psi_4(x)|^2 \end{aligned} \tag{2.70}$$

The method introduced in the present subsection is more efficient than the moment method, and perhaps more powerful because it provides a more direct route to probability densities of eigenstates. However, the key definition (2.55) of the function $L_\lambda(\gamma)$ was made with the benefit of knowing that the operator $\exp((1+\gamma)\hat{q}^2/\hbar)$ should be useful, based on the known form of wave functions for harmonic-oscillator eigenstates. While this alternative method is fully algebraic, just like the moment method, it is not completely independent of standard derivations of eigenstates.

We note at this point that other algebraic derivations of eigenvalues and eigenstates of the harmonic oscillator exist in the literature, such as [47]. However, they are based on ladder operators in Hilbert space and therefore require representations of the algebra of observables.

2.3 Saturation of inequalities

An interesting result that emerges from the solutions in Section 2.2.2 is a saturation property of the first n eigenstates that obey $d_n = 0$, and therefore saturate the generalized uncertainty relation $\det(A'_n) \geq 0$ given in (3.4). For $n = 1$, this condition is just the well-known statement that the harmonic-oscillator ground state saturates Heisenberg's uncertainty relation. For each $n > 1$, we have an inequality involving higher moments that is saturated by the first n eigenstates. (This saturation property is different from the one found in [48]. Moreover, it sharpens a saturation property found in [45], which is true for all energy eigenstates of the harmonic oscillator.) Motivated by this finding, we return to the full generalized uncertainty principle and analyze its behavior for the harmonic oscillator eigenstates, as well as related properties.

2.3.1 Principal minors and pure states

As is evident from our derivations in the previous section, we need to make use of only a submatrix of M_J, corresponding to moments in $\hat{\xi}'_J$ with at most one insertion of a momentum operator. (A related computational fact is that M_J has an eigenvalue zero with degeneracy $D = J(2J-1)$.) Computational experiments indicate that the remaining conditions do not impose additional restrictions on the allowed values of λ, which is consistent with the fact that (2.54) is the full set of harmonic-oscillator eigenvalues.

Still, for an application of the method without prior knowledge of the spectrum, it would be of interest to understand these features in more detail. In particular, it remains unclear to us how a suitable subset of independent inequalities can be selected from the generalized uncertainty principle that would be sufficient for determining all eigenstates of a given Hamiltonian.

The observation that the matrices M'_J suffice to find all relevant conditions on eigenvalues can be interpreted as follows: For pure states, the moments $T_{m,0} = \langle \hat{q}^m \rangle$ allow one to reconstruct the norm of the wave function according to the Hamburger problem, while the additional moments $T_{n,1} = \langle \hat{q}^n \hat{p} \rangle$ with a single momentum operator can be used to determine the phase; see for instance [16, 49]. The other moments are therefore not independent parameters if the state is known to be pure. (They would be independent for mixed states.) The observation that M'_J suffices to find all conditions on eigenvalues, at least for the harmonic oscillator, can therefore be interpreted as saying that mixed states cannot provide eigenstates in this case.

2.3.2 Saturation from ladder operators

With hindsight, it is possible to obtain a saturation result for energy eigenstates of the harmonic oscillator by means of the usual ladder operators,

$$\hat{a} = \frac{1}{\sqrt{2\hbar}}(\hat{q} + i\hat{p}) \quad , \quad \hat{a}^\dagger = \frac{1}{\sqrt{2\hbar}}(\hat{q} - i\hat{p})\,. \tag{2.71}$$

(We still assume $m = 1$ and $\omega = 1$.) Let $\hat{a}$ be the lowering operator and take

$$\hat{f} = \hat{a}^n + \hat{a}^{\dagger n} \quad , \quad \hat{g} = \hat{a}^n - \hat{a}^{\dagger n}\,. \tag{2.72}$$

If a state $|\psi\rangle$ is a linear combination of the first n eigenstates of the harmonic oscillator, then $\hat{f}|\psi\rangle = -\hat{g}|\psi\rangle$, which implies $\langle\hat{f}^\dagger\hat{f}\rangle\langle\hat{g}^\dagger\hat{g}\rangle = \langle\hat{f}^\dagger\hat{g}\rangle\langle\hat{g}^\dagger\hat{f}\rangle$. Thus, the Cauchy-Schwarz inequality

$$\langle\hat{f}^\dagger\hat{f}\rangle\langle\hat{g}^\dagger\hat{g}\rangle \geq |\langle\hat{f}^\dagger\hat{g}\rangle|^2 \tag{2.73}$$

is saturated. Explicit expressions for given n imply higher-order uncertainty relations, which must then also be saturated by the first n energy eigenstates of the harmonic oscillator.

The first three inequalities obtained in this way are as follows. The n^{th} inequality is saturated by any linear combination of the first n harmonic-oscillator eigenstates. For $n = 1$,

$$\left\langle\hat{q}^2\right\rangle\left\langle\hat{p}^2\right\rangle \geq \hbar^2/4 + \langle\hat{q}\hat{p}\rangle^2_{\text{Weyl}} \tag{2.74}$$

for $n = 2$,

$$\begin{aligned}&\left(\langle\hat{p}^4\rangle + \langle\hat{q}^4\rangle - 2\langle\hat{p}^2\hat{q}^2\rangle_{\text{Weyl}} + \hbar^2\right)\left(\langle\hat{p}^2\hat{q}^2\rangle_{\text{Weyl}} + \frac{\hbar^2}{4}\right)\\ &\geq \hbar^2\left(\langle\hat{p}^2\rangle + \langle\hat{q}^2\rangle\right)^2 + \left(\langle\hat{p}\hat{q}^3\rangle_{\text{Weyl}} - \langle\hat{p}^3\hat{q}\rangle_{\text{Weyl}}\right)^2\end{aligned} \tag{2.75}$$

and for $n = 3$,

$$\begin{aligned}&\left(\frac{1}{9}\left\langle\hat{q}^6\right\rangle - \frac{2}{3}\left\langle\hat{p}^2\hat{q}^4\right\rangle_{\text{Weyl}} + \left\langle\hat{p}^4\hat{q}^2\right\rangle_{\text{Weyl}} + \hbar^2\left\langle\hat{q}^2\right\rangle + \hbar^2\left\langle\hat{p}^2\right\rangle\right)\\ &\times\left(\frac{1}{9}\left\langle\hat{p}^6\right\rangle - \frac{2}{3}\left\langle\hat{p}^4\hat{q}^2\right\rangle_{\text{Weyl}} + \left\langle\hat{p}^2\hat{q}^4\right\rangle_{\text{Weyl}} + \hbar^2\left\langle\hat{p}^2\right\rangle + \hbar^2\left\langle\hat{q}^2\right\rangle\right)\end{aligned} \tag{2.76}$$

$$\geq \hbar^2 \left(\frac{\hbar^2}{3} + \frac{1}{2} \left\langle \hat{p}^4 \right\rangle + \frac{1}{2} \left\langle \hat{q}^4 \right\rangle + \left\langle \hat{p}^2 \hat{q}^2 \right\rangle_{\rm Weyl} \right)^2 + \tag{2.77}$$

$$\left(\frac{1}{3} \left\langle \hat{p}^5 \hat{q} \right\rangle_{\rm Weyl} + \frac{1}{3} \left\langle \hat{p} \hat{q}^5 \right\rangle_{\rm Weyl} - \frac{10}{9} \left\langle \hat{p}^3 \hat{q}^3 \right\rangle_{\rm Weyl} \right)^2 . \tag{2.78}$$

Except for $n = 1$, there is no obvious relationship with minors of the matrices M'_J introduced in (2.35), which were found to be relevant for eigenstates in our previous analysis.

2.3.3 Generalized coherent states

The saturation property of the harmonic-oscillator ground state, which by definition satisfies $\hat{a}\psi = 0$, is maintained by coherent states defined by $\sqrt{2\hbar}\hat{a}\psi = \alpha\psi$ with a complex number $\alpha = \langle \hat{q} \rangle + i\langle \hat{p} \rangle$. Similarly, saturation properties of higher-order uncertainty relations obeyed by the first $n-1$ excited states, all subject to the condition $\hat{a}^n\psi = 0$, can be maintained by generalized coherent states, for which

$$(\sqrt{2\hbar}\,\hat{a})^n \psi = \alpha^n \psi \,. \tag{2.79}$$

We will first show that these generalized coherent states indeed obey higher-order uncertainty relations.

As in the case of $\alpha = 0$ in the preceding subsection, we introduce two new operators, $\hat{f} := (2\hbar)^{n/2}(\hat{a}^n + \hat{a}^{\dagger n}) - \alpha^n$ and $\hat{g} := (2\hbar)^{n/2}(\hat{a}^n - \hat{a}^{\dagger n}) - \alpha^n$. In a state ψ that satisfies (2.79), we again obtain $\hat{f}\psi = -\hat{g}\psi$ and therefore

$$\langle \hat{f}^\dagger \hat{f} \rangle \langle \hat{g}^\dagger \hat{g} \rangle = \langle \hat{f}^\dagger \hat{g} \rangle \langle \hat{g}^\dagger \hat{f} \rangle = |\langle \hat{f}^\dagger \hat{g} \rangle|^2 \tag{2.80}$$

saturating (2.73) as before.

The form of these uncertainty relations saturated by a generalized coherent state depends on the parameter $\alpha = \langle \hat{q} \rangle + i\langle \hat{p} \rangle$. For instance, for $n = 1$, we do not directly obtain the standard uncertainty relation but rather compute

$$\begin{aligned}
\langle \hat{f}^\dagger \hat{f} \rangle &= \langle 4\hat{q}^2 - 2(\alpha + \alpha^*)\hat{q} + |\alpha|^2 \rangle \\
&= 4(\Delta q)^2 + \langle \hat{q} \rangle^2 + \langle \hat{p} \rangle^2 && (2.81) \\
\langle \hat{g}^\dagger \hat{g} \rangle &= 4(\Delta p)^2 + \langle \hat{q} \rangle^2 + \langle \hat{p} \rangle^2 && (2.82) \\
\langle \hat{f}^\dagger \hat{g} \rangle &= 4i\langle \hat{q}\hat{p} \rangle - 2\left(\alpha \langle \hat{q} \rangle + i\alpha^* \langle \hat{p} \rangle\right) + |\alpha|^2
\end{aligned}$$

$$= iC_{qp} - 2\hbar - \langle\hat{q}\rangle^2 - \langle\hat{p}\rangle^2 \tag{2.83}$$

with the covariance $C_{qp} = \Delta(qp)$. The saturated uncertainty relation obtained immediately from (2.80) then takes the form

$$\begin{aligned}&(\Delta q)^2(\Delta p)^2 - C_{qp}^2 \\ &+\frac{1}{4}\left(\langle\hat{q}\rangle^2 + \langle\hat{p}\rangle^2\right)\left((\Delta q)^2 + (\Delta p)^2 - \hbar\right) = \frac{1}{4}\hbar^2\,.\end{aligned} \tag{2.84}$$

This equation is equivalent to saturation of the standard uncertainty relation because $(\Delta q)^2 = \hbar/2 = (\Delta p)^2$ in a coherent state such that (2.79) holds with $n = 1$.

It is possible to evaluate the condition for generalized coherent states explicitly in terms of energy eigenstates, following the usual procedure for $n = 1$. We will denote these states as $|\alpha, k\rangle$, anticipating the presence of a second (integer) parameter k because the condition (2.79) does not uniquely determine a state for $n > 1$ even if α has been fixed. Using the energy eigenstates $|m\rangle$ as a basis, we first compute, for integer $0 \leq \ell < k$, the inner products

$$\begin{aligned}\langle kn+\ell|\alpha,k\rangle &= \frac{1}{\sqrt{(kn+\ell)!}}\left((\hat{a}^\dagger)^{kn+\ell}|0\rangle\right)^\dagger|\alpha,k\rangle \\ &= \frac{1}{(2\hbar)^{kn/2}}\frac{\alpha^{kn}}{\sqrt{(kn+\ell)!}}\langle 0|\hat{a}^\ell|\alpha,k\rangle \\ &= \frac{\alpha^{kn}}{(2\hbar)^{kn/2}}\frac{\sqrt{\ell!}}{\sqrt{(kn+\ell)!}}\langle\ell|\alpha,k\rangle \\ &=: \alpha^{kn}\frac{\sqrt{\ell!}}{\sqrt{(kn+\ell)!}}C_\ell\end{aligned} \tag{2.85}$$

with k independent constants C_ℓ (which are related to one another only by normalization). We then write

$$\begin{aligned}|\alpha,k\rangle &= \sum_{m=0}^{\infty}\langle m|\alpha,k\rangle|m\rangle \\ &= \sum_{\ell=0}^{k-1}C_\ell\sqrt{\ell!}\sum_{n=0}^{\infty}\frac{\alpha^{kn}}{\sqrt{(kn+\ell)!}}|kn+\ell\rangle \\ &= \sum_{\ell=0}^{k-1}C_\ell\frac{\sqrt{\ell!}}{\alpha^\ell}\sum_{n=0}^{\infty}\frac{(\alpha\hat{a}^\dagger)^{kn+\ell}}{(kn+\ell)!}|0\rangle\,.\end{aligned} \tag{2.86}$$

The infinite series $\sum_{n=0}^{\infty}(\alpha\hat{a}^\dagger)^{kn+\ell}/(kn+\ell)!$ in this last expression is related to the exponential function applied to multiples of $\alpha\hat{a}^\dagger$, but it is not a single such function because n in the usual series is replaced here by $kn+\ell$. The series encountered here therefore makes use of only a subset of the expansion terms of a single exponential function. Using the basic k-th root of unity $u_k = e^{2\pi i/k}$, it is possible to write our series as a superposition of exponential functions,

$$\sum_{n=0}^{\infty}\frac{(\alpha\hat{a}^\dagger)^{kn+\ell}}{(kn+\ell)!} = \frac{1}{k}\sum_{j=0}^{k-1} u_k^{-j\ell}\exp(u_k^j\alpha\hat{a}^\dagger) \tag{2.87}$$

in which coefficients have been chosen so as to make unwanted terms cancel out. Indeed,

$$\sum_{j=0}^{k-1} u_k^{-j\ell}\exp(u_k^j\alpha\hat{a}^\dagger) = \sum_{N=0}^{\infty}\frac{1}{N!}\left(\sum_{j=0}^{k-1} u_k^{j(N-\ell)}\right)(\alpha\hat{a}^\dagger)^N \tag{2.88}$$

implies the desired equation (2.87) because

$$\sum_{j=0}^{k-1} u_k^{j(N-\ell)} = \begin{cases} k & \text{if } N-\ell = kn \text{ for some integer } n \\ 0 & \text{otherwise} \end{cases} \tag{2.89}$$

thanks to properties of roots of unity, u_k.

We can therefore continue our derivation of $|\alpha,k\rangle$ and write

$$\begin{aligned} |\alpha,k\rangle &= \sum_{\ell=0}^{k-1} C_\ell\frac{\sqrt{\ell!}}{\alpha^\ell}\frac{1}{k}\sum_{j=0}^{k-1} u_k^{-jl}\exp(u_k^j\alpha\hat{a}^\dagger)|0\rangle \\ &= \frac{1}{k}e^{\frac{1}{2}|\alpha|^2}\sum_{j=0}^{k-1} D_j|u_k^j\alpha\rangle \end{aligned} \tag{2.90}$$

with the standard coherent states $|\beta\rangle = e^{-\frac{1}{2}|\beta|^2}\exp(\beta\hat{a}^\dagger)|0\rangle$ and new constants

$$D_j = \sum_{\ell=0}^{k-1}\frac{\sqrt{\ell!}}{\alpha^\ell}u_k^{-j\ell}C_\ell\,. \tag{2.91}$$

Multiplying the parameter $\alpha = \langle\hat{q}\rangle + i\langle\hat{p}\rangle$ of a standard coherent state with a power of a basic root of unity u_k in the superposed coherent states $|u_k^j\alpha\rangle$ of (2.90) rotates the peak position $(\langle\hat{q}\rangle,\langle\hat{p}\rangle)$ in phase space by a multiple of a fixed angle $2\pi/k$. According to (2.90), a generalized coherent state $|\alpha,k\rangle$ is therefore a superposition of k standard coherent states with peaks $(\langle\hat{q}\rangle,\langle\hat{p}\rangle)$ placed at equal distances on a circle of radius $|\alpha|$.

The k-th eigenstate of the harmonic oscillator is the limit of such a state in which these peaks approach one another at the center, for suitable C_ℓ. Using [50], these generalized coherent states are the same as those introduced by Titulaer and Glauber in [41]; see also [51]. However, to the best of our knowledge, the relation to saturated uncertainty relations and energy eigenstates is new.

2.4 Anharmonic oscillators

We now demonstrate that the methods developed in Section 2.2 can be used to find perturbed eigenvalues for an anharmonic oscillator. Here we take $H = \frac{1}{2}(q^2 + p^2) + \epsilon q^4$.

2.4.1 Moment method

Using the same techniques as for the harmonic oscillator (but now setting $\hbar = 1$), we obtain the following recurrence relations for the moments:

$$\begin{aligned} T_{m+2,n} &+ T_{m,n+2} - \frac{n(n-1)}{4} T_{m,n-2} - \frac{m(m-1)}{4} T_{m-2,n} - 2\lambda T_{m,n} \\ &+ \epsilon \left(2\hat{T}_{m+4,n} - 3n(n-1) T_{m+2,n-2} + \frac{1}{8} n(n-1)(n-2)(n-3) T_{m,n-4} \right) = 0 \end{aligned} \tag{2.92}$$

and

$$m\hat{T}_{m-1,n+1} = n\hat{T}_{m+1,n-1} + \epsilon \left(4n\hat{T}_{m+3,n-1} - n(n-1)(n-2) T_{m+1,n-3} \right) . \tag{2.93}$$

Setting $n = 0$ in (2.92) and $n = 1$ in (2.93) while shifting m to $m + 1$, and combining to eliminate $T_{m,2}$ gives

$$\frac{(m+2)}{(m+1)} T_{m+2,0} - 2\lambda T_{m,0} - \frac{m(m-1)}{4} T_{m-2,0} + 2\epsilon \frac{(m+3)}{(m+1)} T_{m+4,0} = 0 . \tag{2.94}$$

Then using (2.93) with n shifted to$n + 1$ and m to $m - 1$ results in

$$T_{m-2,n+2} = \frac{(n+1)}{(m-1)} T_{m,n} + \epsilon \left(4\frac{(n+1)}{(m-1)} T_{m+2,n} - \frac{(n+1)(n)(n-1)}{(m-1)} T_{m,n-2} \right) . \tag{2.95}$$

We now assume an expansion for the moments in powers of ϵ

$$T_{m,n} = \sum_k T^{(k)}_{m,n} \epsilon^k \tag{2.96}$$

and similarly for the eigenvalues,

$$\lambda = \sum_k \lambda_{(k)} \epsilon^k. \tag{2.97}$$

Using Equations (2.94)–(2.97), we can solve order by order for the moments in terms of the $\lambda_{(k)}$.

For the odd moments, we first note that, at zeroth order, all of them are zero (as we know well from the harmonic oscillator):

$$T^{(0)}_{\text{odd,odd}} = T^{(0)}_{\text{odd,even}} = T^{(0)}_{\text{even,odd}} = 0\,. \tag{2.98}$$

Then setting $m = 0$ and $n = 1$ in (2.93) gives $T^{(1)}_{1,0} = 0$. Using this and (2.94) with m odd gives $T^{(1)}_{\text{odd},0} = 0$. Taking $n = 0$ in (2.93) gives $T_{m,1} = 0$ at all orders in ϵ. Combining these two results with (2.95) implies that the rest of the odd moments vanish:

$$T^{(1)}_{\text{odd,odd}} = T^{(1)}_{\text{odd,even}} = T^{(1)}_{\text{even,odd}} = 0\,. \tag{2.99}$$

We can apply this argument repeatedly to find that the odd moments vanish at all orders in ϵ.

Using the recurrence relations following the procedure detailed in Section 2.2, we find to first order in ϵ

$$\begin{aligned}
\det\left(A'_1\right) &= \left(\lambda_{(0)} - \frac{1}{2}\right)\left(\lambda_{(0)} + \frac{1}{2}\right) - \frac{1}{4}\epsilon\lambda_{(0)}\left(12\lambda^2_{(0)} - 8\lambda_{(1)} + 3\right) + O(\epsilon^2) && (2.100)\\
\det(A'_2) &= \frac{1}{4}\left(\lambda_{(0)} - \frac{3}{2}\right)\left(\lambda_{(0)} - \frac{1}{2}\right)\left(\lambda_{(0)} + \frac{1}{2}\right)\left(\lambda_{(0)} + \frac{3}{2}\right) \\
&\quad -\frac{1}{32}\epsilon\lambda_{(0)}\left(80\lambda^4_{(0)} - 32(\lambda_{(1)} + 4)\lambda^2_{(0)} + 40\lambda_{(1)} + 3\right) + O(\epsilon^2)\,. && (2.101)
\end{aligned}$$

At zeroth order in ϵ, we recover our results for the harmonic oscillator. Setting $\lambda_{(0)} = 1/2$, we find:

$$\begin{aligned}
\det\left(A'_1\right) &= \epsilon\left(\lambda_{(1)} - \frac{3}{4}\right) + O(\epsilon^2) && (2.102)\\
\det\left(A'_2\right) &= \epsilon\left(\frac{3}{8} - \frac{1}{2}\lambda_{(1)}\right) + O(\epsilon^2)\,. && (2.103)
\end{aligned}$$

Positivity of these determinants then yields $\lambda_{(1)} \geq 3/4$ and $\lambda_{(1)} \leq 3/4$. Hence, $\lambda_{(1)} = 3/4$. Performing the same process with $\det(A'_2)$ and $\det(A'_3)$ using $\lambda_{(0)} = 3/2$ yields $\lambda_{(1)} = 15/4$.

Thus we have:

$$E_0 = \frac{1}{2} + \frac{3}{4}\epsilon + O(\epsilon^2) \tag{2.104}$$

$$E_1 = \frac{3}{2} + \frac{15}{4}\epsilon + O(\epsilon^2) \tag{2.105}$$

in agreement with the results from ordinary perturbation theory.

Note that at first order in ϵ, the energy eigenstates saturate the inequalities just as they did for the harmonic oscillator. Computations at higher order indicate that similar saturation results hold at each order in perturbation theory, although for higher orders in ϵ, one must go to higher n in order for $\det(A'_n) \geq 0$ to be saturated.

2.4.2 Commutator method

An alternative route to perturbated eigenvalues, which may sometimes be more feasible, proceeds by applying suitable commutator relationships. Following [17], we can derive recurrence relations for moments of energy eigenstates: We have $\langle n|[\hat{H}, \hat{W}]|n\rangle = 0$ for any operator $\hat{W}$, with eigenstates $|n\rangle$ of $\hat{H} = \frac{1}{2}m^{-1}\hat{p}^2 + V(\hat{q})$. Choosing $\hat{W}_1 = \hat{q}^{k-2}$ and $\hat{W}_2 = \hat{q}^{k-1}\hat{p}$, respectively, for some fixed k, we obtain

$$[\hat{H}, \hat{W}_1] = -i\hbar\frac{k-2}{m}\hat{q}^{k-3}\hat{p} - \hbar^2\frac{(k-2)(k-3)}{2m}\hat{q}^{k-4} \tag{2.106}$$

$$[\hat{H}, \hat{W}_2] = -2i\hbar(k-1)\hat{q}^{k-2}(\hat{H} - V(\hat{q})) - \hbar^2\frac{(k-1)(k-2)}{2m}\hat{q}^{k-3}\hat{p} + i\hbar\hat{q}^{k-1}V'(\hat{q})\,. \tag{2.107}$$

We combine these two equations (set equal to zero) and (divided by $i\hbar$) write

$$0 = -2(k-1)E_n\langle\hat{q}^{k-2}\rangle_n + 2(k-1)\langle\hat{q}^{k-2}V(\hat{q})\rangle_n - \hbar^2\frac{(k-1)(k-2)(k-3)}{4m}\langle\hat{q}^{k-4}\rangle_n + \langle\hat{q}^{k-1}V'(\hat{q})\rangle_n\,. \tag{2.108}$$

For a quartic anharmonicity, such that $V(q) = \frac{1}{2}m\omega^2q^2 + \epsilon q^4$, we have

$$0 = -2(k-1)E_n\langle\hat{q}^{k-2}\rangle_n - (k-1)(k-2)(k-3)\frac{\hbar^2}{4m}\langle\hat{q}^{k-4}\rangle_n + m\omega^2k\langle\hat{x}^k\rangle_n + 2\epsilon(k+1)\langle\hat{q}^{k+2}\rangle_n\,. \tag{2.109}$$

Starting with $k = 1$, the first four recurrence steps are:

$$\begin{aligned} 0 &= m\omega^2\langle\hat{q}\rangle_n + 4\epsilon\langle\hat{q}^3\rangle_n && (2.110)\\ 0 &= -2E_n + 2m\omega^2\langle\hat{q}^2\rangle_n + 6\epsilon\langle\hat{q}^4\rangle_n && (2.111)\\ 0 &= -4E_n\langle\hat{q}\rangle_n + 3m\omega^2\langle\hat{q}^3\rangle_n + 8\epsilon\langle\hat{q}^5\rangle_n && (2.112)\\ 0 &= -6E_n\langle\hat{q}^2\rangle_n - \frac{3\hbar^2}{2m} + 4m\omega^2\langle\hat{q}^4\rangle_n + 10\epsilon\langle\hat{q}^6\rangle_n\,. && (2.113) \end{aligned}$$

Assuming ϵ to be small and expanding $\langle\hat{q}^k\rangle_n = \sum_{j=0}^{\infty}\langle\hat{q}^k\rangle_{n,j}\epsilon^j$, we have $\langle\hat{q}\rangle_{n,0} = 0$ from (2.110), which implies $\langle\hat{q}^3\rangle_{n,0} = 0$ from (2.112), such that $\langle\hat{q}\rangle_{n,1} = 0$ from (2.110).

For even powers, $\langle\hat{q}^2\rangle_{n,0} = E_n/m\omega^2$ from (2.111) and $\langle\hat{q}^4\rangle_{n,0} = \frac{3}{2}E_n^2/m^2\omega^4 + \frac{3}{8}\hbar^2/m^2\omega^2$ from (2.113). This value then appears in $\langle\hat{q}^2\rangle_{n,1} = -3\langle\hat{x}^4\rangle_{n,0}/m\omega^2$ from (2.111). We obtain some of the moments including $\hat{p}$ from (2.106) and (2.107). Setting $k = 4$ in (2.106) shows that $\langle\hat{q}\hat{p} + \hat{p}\hat{q}\rangle_n = 0$ in all energy eigenstates. Setting $k = 2$ in (2.107) and *not* using $\hat{H}|n\rangle = E_n$ implies

$$\langle\hat{p}^2\rangle_n = m\langle\hat{q}V'(\hat{q})\rangle_n = m^2\omega^2\langle\hat{q}^2\rangle_n + 4m\epsilon\langle\hat{q}^4\rangle_n\,, \qquad (2.114)$$

the final equality for our anharmonic oscillator. Using the results for low orders of q-moments, we have

$$\begin{aligned} \langle\hat{p}^2\rangle_{n,0} &= m^2\omega^2\langle\hat{q}^2\rangle_{n,0} = mE_n && (2.115)\\ \langle\hat{p}^2\rangle_{n,1} &= m^2\omega^2\langle\hat{q}^2\rangle_{n,1} + 4m\langle\hat{q}^4\rangle_{n,0} = m\langle\hat{q}^4\rangle_{n,0}\,. && (2.116) \end{aligned}$$

To first order in ϵ, we therefore compute

$$\begin{aligned} \langle\hat{q}^2\rangle_n &= \langle\hat{q}^2\rangle_{n,0} + \epsilon\langle\hat{q}^2\rangle_{n,1} + O(\epsilon^2) && (2.117)\\ &= \frac{E_n}{m\omega^2} - \frac{9\epsilon}{8m^3\omega^6}(4E_n^2 + \hbar^2\omega^2) + O(\epsilon^2)\\ \langle\hat{p}^2\rangle_n &= \langle\hat{p}^2\rangle_{n,0} + \epsilon\langle\hat{p}^2\rangle_{n,1} + O(\epsilon^2) && (2.118)\\ &= mE_n + \frac{3\epsilon}{8m\omega^4}(4E_n^2 + \hbar^2\omega^2) + O(\epsilon^2)\,. \end{aligned}$$

The uncertainty relation implies

$$\langle\hat{q}^2\rangle_n\langle\hat{p}^2\rangle_n = \frac{E_n^2}{\omega^2} - \frac{3\epsilon E_n}{4m^2\omega^6}(4E_n^2 + \hbar^2\omega^2) + O(\epsilon^2) \geq \frac{\hbar^2}{4}\,. \qquad (2.119)$$

At zeroth order in ϵ, this implies $E_n \geq \frac{1}{2}\hbar\omega$. If we use an ϵ-expansion of $E_n = \sum_{j=0}^{\infty} E_{n,j}\epsilon^j$

at this stage, we obtain

$$E_n \geq \frac{1}{2}\hbar\omega + \frac{3}{4}\frac{\epsilon\hbar^2}{m^2\omega^2} + O(\epsilon^2)\,. \tag{2.120}$$

The present formulas indicate that neither the moments nor the uncertainty relations and bounds on eigenvalues are analytic in ω, such that we cannot take a $\omega \to 0$ limit for a single quartic potential.

2.5 Discussion

We have presented a new method that allowed us to rederive known results about energy eigenvalues using only properties of the algebra of observables. The results are therefore representation-independent, and the method can be applied to systems that do not have a Hilbert-space representation, for instance owing to violations of associativity. Even in standard, associative quantum mechanics, we have been able to derive new results related to how excited states saturate higher-order uncertainty relations, as well as connections between excited states and generalized coherent states.

As stated at the beginning of Section 2.2, an algebraic derivation of eigenvalues imposes two conditions, equation (2.11) as well as positivity of a state. The first condition, assuming some fixed eigenvalue λ, implies recurrence relations for moments of an eigenstate, or for expectation values of polynomials of basic operators. Depending on how these relations are set up, they may pose various challenges to finding sufficiently general solutions. In particular, if anharmonicity is introduced, independent recurrence relations in this system are more strongly coupled to one another, complicating the solution process.

Such difficulties can be addressed in two ways: First, a perturbative treatment may use solutions known for a less-coupled system to introduce approximate corrections for the more coupled one. We have demonstrated this option for anharmonic oscillators, which also by general methods require perturbation theory or numerical methods for a determination of eigenvalues. Secondly, it may be possible to rearrange the recurrence relations in a more suitable form that makes them solvable. There is no systematic method for decoupling recurrence relations with non-constant coefficients, as we are dealing with here. However, it may be possible to take some inspiration from other known properties of the given system and introduce convenient generating functions through expectation values of suitable operators. Here, we have demonstrated this method for the same harmonic oscillator used for the first method, but its broader applicability has

already been shown by a successful application to the standard hydrogen problem [40].

At the current stage of developments, the general range of applicability of algebraic methods to derive eigenvalues is far from being completely circumscribed. In addition to reorganizing recurrence relations by means of suitable expectation values as generating functions, we mention the possibility of using ladder-type operators for non-harmonic systems. Since our harmonic-oscillator example in Section 2.3 showed how properties of ladder operators may be related to saturation properties similar to those we found with our first method, such algebraic derivations may have a range of applicability beyond strictly harmonic or perturbative anharmonic systems, but a detailed extension requires further work.

We finally discuss the possibility that not only the tractability but even the overall applicability of our methods may be limited, depending on the Hamiltonian $\hat{H}$ whose eigenvalues are to be determined. To see this, we go back to the starting point of our method, given by the algebraic definition (2.11), or

$$\langle \hat{A}(\hat{H} - \lambda \mathbb{I})\rangle_\lambda = 0\,, \tag{2.121}$$

for an eigenstate $|\rangle_\lambda$ with eigenvalue λ, which has to be satisfied for all algebra elements $\hat{A}$. In particular, the definition is taylored to strict eigenstates which are normalizable since $\langle \mathbb{I}\rangle_\lambda$ must be finite for the equation to be meaningful for all $\hat{A}$ (including $\hat{A} = \mathbb{I}$). The method can therefore be used only for eigenvalues in the discrete part of the spectrum of $\hat{H}$.

If we try to work out the algebraic conditions for eigenstates in simple cases which are known to imply continuous spectra, we can easily find inconsistencies. For instance, taking $\hat{H} = \hat{p}$ as the momentum operator of a particle on the real line and $\hat{A} = \hat{q}$ in (2.121), we obtain the equation

$$\mathrm{Im}\langle \hat{q}(\hat{p} - \lambda \mathbb{I})\rangle = \frac{1}{2i}\langle [\hat{q}, \hat{p}]\rangle = \frac{1}{2}\hbar \tag{2.122}$$

while the eigenvalue condition for λ would require the left-hand side to equal zero.

For the free-particle Hamiltonian, $\hat{H} = \hat{p}^2$, we obtain $\langle \hat{p}^2\rangle - \lambda = 0$ from (2.121) with $\hat{A} = \mathbb{I}$, and

$$\mathrm{Im}\langle \hat{q}\hat{p}(\hat{p}^2 - \lambda \mathbb{I})\rangle = \frac{1}{2i}\langle [\hat{q}, \hat{p}^3] - \lambda [\hat{q}, \hat{p}]\rangle = \frac{1}{2}\hbar(3\langle \hat{p}^2\rangle - \lambda) = 0 \tag{2.123}$$

from $\hat{A} = \hat{q}\hat{p}$. Combining these two equations, only $\lambda = 0$ is allowed, such that $\langle \hat{p}^2\rangle = 0$.

However,

$$\mathrm{Im}\langle\hat{q}(\hat{p}^2-\lambda\mathbb{I})\rangle = \frac{1}{2i}\langle[\hat{q},\hat{p}^2]\rangle = \hbar\langle\hat{p}\rangle = 0 \tag{2.124}$$

then implies $(\Delta p)^2 = 0$, which is not consistent with Heisenberg's uncertainty relation.

It is not surprising that an algebraic methods for computing eigenvalues fails for operators that have a continuous spectrum in an irreducible representation on a separable Hilbert space (spanned by a countable basis) because the corresponding eigenfunctions require a generalized interpretation as distributions. However, it is possible for an operator to have a continuous spectrum with normalizable eigenfunctions if the Hilbert space is not separable or if the representation is not irreducible. (The set of eigenvalues by itself does not uniquely determine whether it is discrete or continuous because the real line can be equipped with discrete or continuous topologies.)

Since the algebraic condition for the spectrum is representation independent, an algebra that has a continuous family of inequivalent irreducible representations, or one that can be represented on a non-separable Hilbert space may lead to a continuous set of eigenvalues for normalizable eigenstates. In this case, (2.121) would be well-defined even if it permits a continuous range of values for λ. As an example, consider a particle moving on a circle. The corresponding algebra can be generated by three basic operators, $\hat{p}$, $\hat{S}$ and $\hat{C}$, with relations $[\hat{p},\hat{S}] = -i\hbar\hat{C}$, $[\hat{p},\hat{C}] = i\hbar\hat{S}$ and $[\hat{C},\hat{S}] = 0$. (The operators $\hat{S}$ and $\hat{C}$ quantize the sine and cosine of the angle.) This linear algebra has the Casimir element $\hat{K} = \hat{S}^2 + \hat{C}^2$ which we may require to equal $\hat{K} = \mathbb{I}$ as a further relation in the generated algebra. Our Hamiltonian is $\hat{H} = \hat{p}$.

The condition $\langle\hat{p}^{n-1}(\hat{H}-\lambda)\rangle = 0$ for $n \geq 1$ implies that $\langle\hat{p}^n\rangle = \lambda^n = \langle\hat{p}\rangle^n$, and therefore all central p-moments $\langle(\hat{p}-\langle\hat{p}\rangle)^n\rangle = 0$ vanish. More generally, it follows that $\langle\hat{A}(\hat{p}-\langle\hat{p}\rangle)\rangle = \langle\hat{A}(\hat{H}-\lambda)\rangle = 0$ for all $\hat{A}$. All generalized uncertainty relations are therefore identically satisfied because the lower bound in the Cauchy–Schwarz inequality (4.49), without loss of generality applied to an operator $\hat{b}$ that contains at least one factor of $\hat{p}-\langle\hat{p}\rangle$, is always zero for eigenstates. For any real λ, there is therefore an eigenstate with this eigenvalue.

This result is in agreement with Hilbert-space representations of the algebra, which are not unique up to unitary equivalence. Its inequivalent irreducible representations are labeled by a real number $0 \leq \epsilon < 1$, such that the momentum spectrum in the representation determined by ϵ is $\mathbb{Z}+\epsilon$. The direct sum of all inequivalent irreducible representations is a reducible representation of the algebra on a non-separable Hilbert space. In this reducible representation, which contains all inequivalent irreducible ones, the spectrum of $\hat{p}$ contains all real numbers λ as eigenvalues, but it is still discrete because

eigenfunctions of $\hat{p}$ are normalizable.

We have obtained the same result in our algebraic derivation, which is representation-independent and therefore implicitly takes into account all irreducible representations. Comparing with our first example of a continuous spectrum (the standard momentum operator for a particle on the real line), we see that the algebraic treatment correctly recognizes the important distinction between a continuous and discrete spectrum: For a continuous spectrum (particle on the real line), the algebraic equations have no consistent solution owing to a lack of normalizability of eigenfunctions. For a discrete spectrum (particle on a circle), the algebraic equations show that all real numbers may consistently be realized as eigenvalues. This distinction is subtle in algebraic form because it is usually based on properties of Hilbert-space representations, in particular on normalizability of eigenfunctions.

As these examples demonstrate, the spectrum cannot always be fully analyzed based on the algebraic condition (2.121), unless it is strictly discrete. As a consequence, it remains an open question how the continuous spectrum could be defined in non-associative quantum mechanics.

2.6 appendix

2.6.1 Eigenvalues in a fermionic system

It is instructive to compute eigenvalues in a fermionic system which has a finite-dimensional Hilbert space in its standard representation, making use only of the defining Grassmann algebra. For a finite number of fermions we have a finite-dimensional Hilbert space, in which our general method can easily be illustrated. This simplicity comes at the expense of requiring a careful discussion of anticommutation relations.

The single degree of freedom ξ included in the system we use here is subject to anticommutation relations

$$[\hat{\xi}^\dagger, \hat{\xi}]_+ = \hbar \quad , \quad [\hat{\xi}, \hat{\xi}]_+ = 0 = [\hat{\xi}^\dagger, \hat{\xi}^\dagger]_+ \,. \tag{2.125}$$

It generates a 4-dimensional unital $*$-algebra with vector-space basis given by $\mathbb{I}$, $\hat{\xi}$, $\hat{\xi}^\dagger$ and $\hat{\xi}^\dagger\hat{\xi}$. As a Hamiltonian, we choose

$$\hat{H} = \frac{1}{2}\omega(\hat{\xi}^\dagger\hat{\xi} - \hat{\xi}\hat{\xi}^\dagger) = \omega\hat{\xi}^\dagger\hat{\xi} - \frac{1}{2}\hbar\omega\mathbb{I} = \omega\hat{\xi}\hat{\xi}^\dagger + \frac{1}{2}\hbar\omega\mathbb{I} \,. \tag{2.126}$$

2.6.1.1 Hilbert-space representation

For comparison, we briefly summarize the standard representation on a 2-dimensional Hilbert space. Commutators of $\hat{\xi}$ and $\hat{\xi}^\dagger$ with $\hat{H}$ show that we can use the former as ladder operators: we have $[\hat{\xi}, \hat{H}] = \hbar\omega\hat{\xi}$. We define $|-\rangle$ such that $\hat{\xi}|-\rangle = 0$, and $|+\rangle$ as $\hat{\xi}^\dagger|-\rangle = \sqrt{\hbar}|+\rangle$. These two states are the only independent ones since $\sqrt{\hbar}\hat{\xi}^\dagger|+\rangle = (\hat{\xi}^\dagger)^2|-\rangle = 0$. The eigenstates of $\hat{H}$ are then given by $|\pm\rangle$ with eigenvalues

$$E_\pm = \pm\frac{1}{2}\hbar\omega\,. \tag{2.127}$$

The action of the ladder operators, $\hat{\xi}|+\rangle = \sqrt{\hbar}|-\rangle$ and $\hat{\xi}^\dagger|-\rangle = \sqrt{\hbar}|+\rangle$, follows from normalization of $|\pm\rangle$ and

$$||\hat{\xi}|+\rangle||^2 = \langle\hat{\xi}^\dagger\hat{\xi}\rangle_+ = \frac{1}{\omega}\left(E_+ + \frac{1}{2}\hbar\omega\right) = \hbar \tag{2.128}$$

$$||\hat{\xi}|-\rangle||^2 = \langle\hat{\xi}\hat{\xi}^\dagger\rangle_- = \frac{1}{\omega}\left(-E_- - \frac{1}{2}\hbar\omega\right) = \hbar\,. \tag{2.129}$$

A general state can be written as

$$|r,s\rangle = \cos r|-\rangle + e^{is}\sin r|+\rangle\,, \tag{2.130}$$

parameterizing all normalized states up to a phase. Expectation values in these states are given by

$$\langle\hat{\xi}\rangle(r,s) = \frac{1}{2}\sqrt{\hbar}\sin(2r)e^{is} = \langle\hat{\xi}^\dagger\rangle(r,s)^* \tag{2.131}$$

$$\langle\hat{\xi}^\dagger\hat{\xi}\rangle(r,s) = \hbar\sin^2 r \tag{2.132}$$

$$\langle\hat{\xi}\hat{\xi}^\dagger\rangle(r,s) = \hbar\cos^2 r\,. \tag{2.133}$$

States are subject to uncertainty relations, which will play a major role in our new method. Define $u = \Delta\hat{\xi}v$ and $w = \Delta\hat{\xi}^\dagger v$ for some state v, where $\Delta\hat{\xi} = \hat{\xi} - \langle\hat{\xi}\rangle_v$ with $\langle\hat{\xi}\rangle_v = \langle v|\hat{\xi}v\rangle$, and compute

$$\langle u|u\rangle = \langle\Delta\hat{\xi}^\dagger\Delta\hat{\xi}\rangle = \Delta(\xi^\dagger\xi) + \frac{1}{2}\hbar \tag{2.134}$$

$$\langle w|w\rangle = \langle\Delta\hat{\xi}\Delta\hat{\xi}^\dagger\rangle = -\Delta(\xi^\dagger\xi) + \frac{1}{2}\hbar \tag{2.135}$$

$$\langle u|w\rangle = \langle\Delta\hat{\xi}^\dagger\Delta\hat{\xi}^\dagger\rangle = 0 \tag{2.136}$$

with the (graded) covariance

$$\begin{aligned}\Delta(\xi^\dagger\xi) &= \frac{1}{2}\left(\langle\hat{\xi}^\dagger\hat{\xi} - \hat{\xi}\hat{\xi}^\dagger\rangle - \langle\hat{\xi}\rangle^*\langle\hat{\xi}\rangle + \langle\hat{\xi}\rangle\langle\hat{\xi}\rangle^*\right) \\ &= \frac{1}{2}\langle\hat{\xi}^\dagger\hat{\xi} - \hat{\xi}\hat{\xi}^\dagger\rangle - \langle\hat{\xi}\rangle^*\langle\hat{\xi}\rangle\,. \end{aligned} \tag{2.137}$$

Expanding $\Delta\hat{\xi}^\dagger\Delta\hat{\xi}$ in order to express equations such as (2.134) in terms of $\Delta(\xi^\dagger\xi)$ requires anticommutation relations not only between $\hat{\xi}$ and $\hat{\xi}^\dagger$ as provided by the original Grassmann algebra, but also between these operators and their expectation values. The equations shown here assume the convention that $\langle\hat{\xi}\rangle$ and $\langle\hat{\xi}^\dagger\rangle$ are Grassmann numbers which anticommute with each other and with $\hat{\xi}$ and $\hat{\xi}^\dagger$. (This convention is consistent with equations such as $\langle\hat{\xi}\xi^*\rangle = \xi\xi^*$ used in relating $\Delta\hat{\xi}^\dagger\Delta\hat{\xi}$ to $\Delta(\xi^\dagger\xi)$.)

The Cauchy–Schwarz inequality implies

$$0 = |\langle u|w\rangle|^2 \leq \langle u|u\rangle\langle w|w\rangle = -\Delta(\xi^\dagger\xi)^2 + \frac{1}{4}\hbar^2 \tag{2.138}$$

and therefore

$$|\Delta(\xi^\dagger\xi)| \leq \frac{1}{2}\hbar\,. \tag{2.139}$$

Both eigenstates of $\hat{H}$ saturate this inequality.

2.6.1.2 Algebra

Let us now proceed algebraically. We introduce a phase-space version of the fermion system by defining two Grassmann numbers, $\xi = \langle\hat{\xi}\rangle$ and $\xi^* = \langle\hat{\xi}^\dagger\rangle$. Any operator in the algebra $\mathcal{A}$ defines a function on the space of states on the algebra by evaluation, $A(\langle\cdot\rangle) := \langle\hat{A}\rangle$. The equation

$$\{\langle\hat{A}\rangle, \langle\hat{B}\rangle\}_+ = \frac{\langle[\hat{A},\hat{B}]_+\rangle}{i\hbar} \tag{2.140}$$

therefore defines a bracket on the space of states, which can be extended to arbitrary functions on states by using the (graded) Leibniz identity. Applied to our basic operators $\hat{\xi}$ and $\hat{\xi}^\dagger$, this bracket implies standard relations with anti-Poisson brackets

$$\{\xi^*, \xi\}_+ = -i \quad , \quad \{\xi, \xi\}_+ = 0 = \{\xi^*, \xi^*\}_+ \tag{2.141}$$

for basic expectation values. The bracket can be extended to an anti-Poisson bracket on moments of $\hat{\xi}$ and $\hat{\xi}^\dagger$ by using the Leibniz rule. As already stated, the basic expectation values anticommute with $\hat{\xi}$ and $\hat{\xi}^\dagger$.

There is only one non-zero moment:

$$\begin{aligned}\Delta(\xi^\dagger\xi) &= \frac{1}{2}\langle\Delta\hat{\xi}^\dagger\Delta\hat{\xi} - \Delta\hat{\xi}\Delta\hat{\xi}^\dagger\rangle = \langle\Delta\hat{\xi}^\dagger\Delta\hat{\xi}\rangle - \frac{1}{2}\hbar \\ &= -\langle\Delta\hat{\xi}\Delta\hat{\xi}^\dagger\rangle + \frac{1}{2}\hbar\,, \end{aligned} \tag{2.142}$$

using $\Delta\hat{\xi} := \hat{\xi} - \xi$ and $[\Delta\hat{\xi}^\dagger, \Delta\hat{\xi}]_+ = \hbar$. The dynamics now follows from the usual derivation given by a commutator with the Hamiltonian:

$$\dot{\xi} = \frac{\langle[\hat{\xi}, \hat{H}]\rangle}{i\hbar} = -i\omega\xi \tag{2.143}$$

implies $\xi(t) = \xi_0 \exp(-i\omega t)$, or $r(t) = r_0$, $s(t) = s_0 - \omega t$ in the parameterization of (2.130). Also, $\Delta(\bar{\xi}\xi)(t) = \Delta(\bar{\xi}\xi)(0)$ because $\Delta(\bar{\xi}\xi) = \omega^{-1}\hat{H} - |\xi|^2$ depends only on $\hat{H}$ and constants.

Assume now that we have an eigenstate of $\hat{H}$ with eigenvalue λ. In this state,

$$\begin{aligned} 0 &= \langle\hat{H} - \lambda\mathbb{I}\rangle = \omega\langle\hat{\xi}^\dagger\hat{\xi}\rangle - \frac{1}{2}\hbar\omega - \lambda \\ &= -\omega\langle\hat{\xi}\hat{\xi}^\dagger\rangle + \frac{1}{2}\hbar\omega - \lambda \qquad (2.144) \\ 0 &= \langle\hat{\xi}(\hat{H} - \lambda\mathbb{I})\rangle = \left(\frac{1}{2}\hbar\omega - \lambda\right)\xi \qquad (2.145) \\ 0 &= \langle\hat{\xi}^\dagger(\hat{H} - \lambda\mathbb{I})\rangle = -\left(\frac{1}{2}\hbar\omega + \lambda\right)\xi^* \qquad (2.146) \\ 0 &= \langle\hat{\xi}^\dagger\hat{\xi}(\hat{H} - \lambda\mathbb{I})\rangle = \left(\frac{1}{2}\hbar\omega - \lambda\right)\langle\hat{\xi}^\dagger\hat{\xi}\rangle \\ &= \frac{\frac{1}{4}\hbar^2\omega^2 - \lambda^2}{\omega} \qquad (2.147) \\ 0 &= \langle\hat{\xi}\hat{\xi}^\dagger(\hat{H} - \lambda\mathbb{I})\rangle = -\left(\frac{1}{2}\hbar\omega + \lambda\right)\langle\hat{\xi}\hat{\xi}^\dagger\rangle \\ &= -\frac{\frac{1}{4}\hbar^2\omega^2 - \lambda^2}{\omega} \qquad (2.148) \end{aligned}$$

using the first equation in the last step of (2.147) and (2.148). The last equation implies $\lambda_\pm = \pm\frac{1}{2}\hbar\omega$. For $\lambda_- = -\frac{1}{2}\hbar\omega$, (2.145) implies $\xi = 0$ and (2.147) implies $\langle\hat{\xi}^\dagger\hat{\xi}\rangle = 0$, so that $\langle\hat{\xi}\hat{\xi}^\dagger\rangle = \hbar$ from (2.144). For $\lambda_+ = \frac{1}{2}\hbar\omega$, (2.146) implies $\xi^* = 0$ and (2.148) implies $\langle\hat{\xi}\hat{\xi}^\dagger\rangle = 0$, so that $\langle\hat{\xi}^\dagger\hat{\xi}\rangle = \hbar$ from (2.144).

In this example, we have managed to compute all eigenvalues of the Hamiltonian using only the (anti-)commutator relationships. If we try the standard method of ladder operators in a system with an infinite-dimensional Hilbert space, it is well known that we need normalizability conditions in order to derive discrete eigenvalues. These conditions are available only for wave functions in the Hilbert space but do not have an analog in the algebra of observables. The main body of this paper shows how the new methods of using moments and uncertainty relations can produce the correct discrete spectra without an explicit normalizability condition even in systems with an infinite-dimensional Hilbert space.

Chapter 3
Small magnetic charges and monopole in non-associative quantum mechanics

Martin Bojowald, Suddhasattwa Brahma, Umut Büyükçam, Jonathan Guglielmon, Martijn van Kuppeveld

Weak magnetic monopoles with a continuum of charges less than the minimum implied by Dirac's quantization condition may be possible in non-associative quantum mechanics. If a weakly magnetically charged proton in a hydrogen atom perturbs the standard energy spectrum only slightly, magnetic charges could have escaped detection. Testing this hypothesis requires entirely new methods to compute energy spectra in non-associative quantum mechanics. Such methods are presented here, and evaluated for upper bounds on the magnetic charge of elementary particles.

In 1931, Dirac [52] showed that magnetic monopoles with charge g can be consistently described by wave functions provided the quantization condition $eg = N\hbar$ holds with half-integer N. Since the elementary electric charge e (or, rather, the fine structure constant) is small, the elementary magnetic charge is large. Therefore, there are strict limits on the possible magnetic charge of, say, a proton in a hydrogen nucleus because the strong magnetic charge would significantly alter the energy spectrum [53].

The aim of this letter is to point out and analyze the fact that Dirac's argument relies on properties of wave functions in a Hilbert space, and therefore implicitly assumes that quantum mechanics is associative. If the assumption of associativity is dropped, there is no Hilbert-space representation of the algebra of observables (which by necessicity would always be associative), but quantum mechanics may still be meaningful [5, 11, 14, 54].

Indeed, the existence of consistent non-associative algebras for magnetic charge densities has recently been demonstrated [33, 36–39]. Non-associative quantum mechanics can therefore be defined by replacing the operator product of observables with an abstract product, such that $\hat{a}_1(\hat{a}_2\hat{a}_3) \neq (\hat{a}_1\hat{a}_2)\hat{a}_3$ in general. States are defined as expectation-value functionals that assign complex numbers $\langle\hat{a}\rangle$ to algebra elements $\hat{a}$, subject to certain consistency conditions which make sure that uncertainty relations are respected. No wave functions appear in this formalism, and there is no analog of "single-valuedness" used crucially by Dirac. Without wave functions, Dirac's argument therefore loses its footing. Magnetic monopoles are then possible with small charges much less than the smallest non-zero value, $g_0 = \frac{1}{2}\hbar/e$, allowed by Dirac. It is conceivable that a small magnetic charge of the proton could have escaped detection in precision spectroscopy such as [55].

Here, we show that even a small magnetic charge of the nucleus would significantly shift the ground-state energy of a hydrogen atom. To the best of our knowledge, this is the first time that properties of energy spectra have been computed in non-associative quantum mechanics. We provide new methods to compute spectra in an algebraic manner, which may also be useful in other contexts.

Harmonic oscillator: We first demonstrate the new methods in an application to the harmonic oscillator in standard, associative quantum mechanics. We have two distinguished observables $\hat{q}$ and $\hat{p}$ with $[\hat{q},\hat{p}] = i\hbar$, and the quantum Hamiltonian $\hat{H} = \frac{1}{2}(\hat{p}^2/m + m\omega^2\hat{q}^2)$.

An eigenstate $|\psi_E\rangle$ of $\hat{H}$ with eigenvalue E obeys the equation $\hat{H}|\psi_E\rangle = E|\psi_E\rangle$, which implies

$$\langle\hat{a}(\hat{H} - E)\rangle_E = 0 \tag{3.1}$$

for the expectation value $\langle\cdot\rangle_E$ taken in $|\psi_E\rangle$, where $\hat{a}$ can be any polynomial in $\hat{q}$ and $\hat{p}$. We will first show that (3.1), which amounts to infinitely many equations given the freedom of choosing $\hat{a}$, allows one to compute the spectrum of $\hat{H}$ even if the eigenstates $|\psi_E\rangle$ are not known. In [56, 70], it has been shown how observables can be computed using algebraic relations between moments of a state. The methods used here are closely related to these papers but provide a new application to energy spectra. In this way, we will set up a method to compute eigenvalues without using wave functions or boundary conditions. The same method can then be applied to the Coulomb problem in non-associative quantum mechanics.

The demonstration is based on recurrence with respect to the degree of the polynomial $\hat{a}$ in $\hat{q}$ and $\hat{p}$. The ground-state energy can be obtained by elementary calculations as follows: First, $\hat{a} = \hat{1}$ (the identity operator) gives $E = \frac{1}{2}(\langle\hat{p}^2\rangle_E/m + m\omega^2\langle\hat{q}^2\rangle_E)$. For $\hat{a}$

not the identity, it is useful to refer to the equation

$$\langle[\hat{a},\hat{H}]\rangle_E = \langle\hat{a}\hat{H}\rangle_E - \overline{\langle\hat{a}^\dagger\hat{H}\rangle_E} = E\left(\langle\hat{a}\rangle_E - \overline{\langle\hat{a}^\dagger\rangle_E}\right) = 0 \tag{3.2}$$

with the complex conjugate $\bar{z}$ of a complex number z. In particular, $\langle[\hat{q},\hat{H}]\rangle_E = i\hbar\langle\hat{p}\rangle_E/m = 0$ from $\hat{a}=\hat{q}$ and $\langle[\hat{p},\hat{H}]\rangle_E = -i\hbar m\omega^2\langle\hat{q}\rangle_E = 0$ from $\hat{a}=\hat{p}$. From quadratic monomials, we obtain $\langle[\hat{q}^2,\hat{H}]\rangle_E = \frac{1}{2}i\hbar\langle\hat{q}\hat{p}+\hat{p}\hat{q}\rangle_E/m = 0$ and $\langle[\hat{q}\hat{p},\hat{H}]\rangle_E = i\hbar(\langle\hat{p}^2\rangle_E/m - m\omega^2\langle\hat{q}^2\rangle_E) = 0$. Therefore, any eigenstate has fluctuations obeying $\Delta_E p = m\omega\Delta_E q$, and zero covariance $0 = C^E_{qp} = \frac{1}{2}\langle\hat{q}\hat{p}+\hat{p}\hat{q}\rangle_E - \langle\hat{q}\rangle_E\langle\hat{p}\rangle_E$. From the condition for $\hat{a}=\hat{1}$, $(\Delta_E q)^2 = E/(m\omega^2)$ and $(\Delta_E p)^2 = mE$.

So far, we have computed moments of a bound state in terms of its energy value E. We obtain a restriction on E by making sure that the fluctuations we derived obey the uncertainty relation:

$$(\Delta_E q)^2(\Delta_E p)^2 - (C^E_{qp})^2 = \frac{E^2}{\omega^2} \geq \frac{\hbar^2}{4} \tag{3.3}$$

and therefore $E \geq \frac{1}{2}\hbar\omega$.

In order to evaluate all the conditions imposed on eigenstates by (3.1), we follow [43,44] and introduce the operators $\hat{T}_{m,n} := (\hat{q}^m\hat{p}^n)_{\rm Weyl}$ where m and n are non-negative integers, and the subscript indicates that the product is taken in the totally symmetric ordering. The Hamiltonian is a linear combination $\hat{H} = \frac{1}{2}(\hat{T}_{2,0}/m + m\omega^2\hat{T}_{0,2})$ of $\hat{T}_{2,0}$ and $\hat{T}_{0,2}$, and therefore (3.1) contains products of the form $\hat{T}_{m,n}\hat{T}_{m',n'}$. Using the basic commutation relation of $\hat{q}$ and $\hat{p}$, such products can always be rewritten as sums over individual $\hat{T}_{m'',n''}$ of order $m+n+m'+n'$ or less, as derived explicitly in [42]. The condition (3.1) is therefore equivalent to a recurrence relation for $\langle\hat{T}_{m,n}\rangle_E$ which is shown and discussed in more detail in our supplementary material. (This material also uses an algebraic notion of states [15] and makes contact with effective constraints [57, 58].)

In addition to higher-order moments $\langle\hat{T}_{m,n}\rangle_E$ of an eigenstate, we have higher-order uncertainty relations. They can be obtained just like Heisenberg's version, by applying the textbook derivation to integer powers of $\hat{q}$ and $\hat{p}$ or their products instead of just $\hat{q}$ and $\hat{p}$. A systematic procedure to organize these higher-order, or generalized, uncertainty relations has been given in [43, 44]. For our purposes, a subset of these relations is sufficient, which can be constructed as follows: We define $\hat{\xi}_J$ as the $2J$-dimensional column vector consisting of all $\hat{T}_{m,0}$ and $\hat{T}_{m-1,1}$ up to order $m = 2J$, where J is an integer or half-integer. According to the generalized uncertainty principle, the matrix $M_J = \langle\hat{\xi}_J\hat{\xi}_J^\dagger\rangle$ is positive semi-definite for all J, where the expectation value is taken element by element. For $J = 1/2$, we have Heisenberg's uncertainty principle because a

positive semi-definite matrix has a non-negative determinant.

As outlined in the supplementary material, positive semi-definiteness of M_J can be reduced to the conditions

$$\prod_{k=1}^{n}(E/\hbar\omega - \alpha_k)(E/\hbar\omega + \alpha_k) \geq 0 \tag{3.4}$$

for all integer $n \geq 1$, where $\alpha_k = (2k-1)/2$ are the odd half-integer multiples. Considered as functions of E for all n, these expressions have nodes at $\hbar\omega\alpha_k$ up to some maximum k that depends on the particular value of n. Between nodes, the functions are non-zero and alternate in sign. Moreover, sending n to $n+1$ causes the signs at fixed E to alternate. This behavior combined with the non-negativity of (3.4) implies that the only allowable values for E occur at the nodes. We can exclude negative values of E because we have already shown that $E \geq \frac{1}{2}\hbar\omega$. Thus, the only possible values for E are such that $E/\hbar\omega = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$ in agreement with the well-known eigenvalues of the harmonic oscillator.

Moreover, the arguments just given show that, for each eigenvalue $E_n = (n - \frac{1}{2})\hbar\omega$, there is a generalized uncertainty relation which restricts higher-order moments and is saturated by the corresponding excited state with energy E_n. This result generalizes the well-known statement that the ground state of the harmonic oscillator saturates Heisenberg's uncertainty relation. Also note that our derivation, based on expectation values, still applies if the state used is mixed, given by a density matrix. Since we obtain the usual energy spectrum of the harmonic oscillator, it follows that mixed states do not to enlarge the spectrum.

As another consequence, we obtain the full energy spectrum of the harmonic oscillator from the unfamiliar condition (3.1) on energy eigenvalues. This result serves as a proof of concept of the new algebraic method introduced here, which we now apply to the Coulomb problem. We will then be ready to generalize the results to non-associative quantum mechanics, where the usual methods of computing eigenvalues are not available.

Hydrogen: The hydrogen atom has the Hamiltonian $\hat{H} = \frac{1}{2}|\hat{p}|^2/m - \alpha\hat{r}^{-1}$ where $|\hat{p}|^2 = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2$ and $\hat{r}^2 = \hat{x}^2 + \hat{y}^2 + \hat{z}^2$. The position and momentum components are subject to the basic commutation relations $[\hat{x}, \hat{p}_x] = [\hat{y}, \hat{p}_y] = [\hat{z}, \hat{p}_z] = i\hbar$. For our purposes a different choice of distinguished observables,

$$\hat{r} \quad , \quad \hat{P} := \hat{r}|\hat{p}|^2 \quad , \quad \hat{Q} := \hat{x}\hat{p}_x + \hat{y}\hat{p}_y + \hat{z}\hat{p}_z \, , \tag{3.5}$$

is more useful. Closely related variables have been used, quite differently, to compute

hydrogen spectra in deformation quantization [59–61].

These operators have linear commutation relations

$$[\hat{r}, \hat{Q}] = i\hbar\hat{r} \quad , \quad [\hat{r}, \hat{P}] = 2i\hbar\hat{Q} \quad , \quad [\hat{Q}, \hat{P}] = i\hbar\hat{P}\,, \tag{3.6}$$

and there is a Casimir operator

$$\hat{K} = \frac{1}{2}(\hat{r}\hat{P} + \hat{P}\hat{r}) - \hat{Q}^2 \tag{3.7}$$

that commutes with $\hat{r}$, $\hat{P}$ and $\hat{Q}$. A direct calculation in terms of the position and momentum components in (4.6) shows that $\hat{K}$ is equal to the total angular momentum squared. We should keep in mind that not all the distinguished observables are self-adjoint. We do have $\hat{r}^\dagger = \hat{r}$, but $\hat{Q}^\dagger = \hat{Q} - 3i\hbar$ and

$$\hat{P}^\dagger = \hat{P} - 2i\hbar\hat{r}^{-1}\hat{Q} = \hat{P} - 2i\hbar\hat{Q}\hat{r}^{-1} - 2\hbar^2\hat{r}^{-1}\,. \tag{3.8}$$

As in our demonstration using the harmonic oscillator, we will be interested in expectation values of monomials in $\hat{r}$, $\hat{P}$ and $\hat{Q}$ evaluated in eigenstates that obey (3.1). We have another useful relationship between certain expectation values given by the virial theorem:

$$\alpha\langle\hat{r}^{-1}\rangle_E = 2E = -\frac{1}{m}\langle\hat{p}^2\rangle_E\,. \tag{3.9}$$

The procedure used for the harmonic oscillator does not directly apply to the Coulomb problem because the Hamiltonian is no longer quadratic, leading to highly coupled recurrence relations. We therefore reformulate the condition (3.1) in terms of a constraint linear in $\hat{P}$ and $\hat{r}$, introducing

$$\hat{C}_E = \hat{r}(\hat{H} - E) = \frac{1}{2m}\hat{P} - E\hat{r} - \alpha\,. \tag{3.10}$$

The condition on the spectrum of $\hat{H}$ then takes the form $\langle\hat{a}\hat{C}_E\rangle_E = 0$ for all polynomials $\hat{a}$ in $\hat{r}$, $\hat{r}^{-1}$, $\hat{P}$ and $\hat{Q}$. Unlike the Hamiltonian, $\hat{C}_E$ is not self-adjoint. It is still useful to apply commutator identities as in (3.2), but with a non-self-adjoint $\hat{C}_E$, there are additional terms: In an eigenstate such that $\langle\hat{a}\hat{C}_E\rangle_E = 0$ and $\langle\hat{a}^\dagger\hat{C}_E\rangle_E = 0$,

$$0 = \langle\hat{a}\hat{C}_E\rangle_E - \overline{\langle\hat{a}^\dagger\hat{C}_E\rangle_E} = \langle(\hat{a}\hat{C}_E - \hat{C}_E^\dagger\hat{a}\rangle_E\,. \tag{3.11}$$

With

$$\hat{C}_E^\dagger = \hat{C}_E - \frac{i\hbar}{m}\hat{r}^{-1}\hat{Q} = \hat{C}_E - \frac{i\hbar}{m}\hat{Q}\hat{r}^{-1} - \frac{\hbar^2}{m}\hat{r}^{-1} \tag{3.12}$$

using (4.10), we have

$$0 = \frac{\langle[\hat{a}, \hat{C}_E]\rangle_E}{i\hbar} + \frac{\langle\hat{Q}\hat{r}^{-1}\hat{a}\rangle_E}{m} - \frac{i\hbar\langle\hat{r}^{-1}\hat{a}\rangle_E}{m}\,. \tag{3.13}$$

For $\hat{a} = \hat{Q}$,

$$0 = \frac{\langle\hat{P}\rangle_E}{2m} + E\langle\hat{r}\rangle_E + \frac{\langle\hat{Q}^2\hat{r}^{-1}\rangle_E}{m} + \frac{\hbar^2}{m}\langle\hat{r}^{-1}\rangle_E\,. \tag{3.14}$$

If we replace $\hat{Q}^2$ using the Casimir operator $\hat{K}$, and $\langle\hat{P}\rangle_E$ using $\langle\hat{C}_E\rangle_E = 0$, we have $0 = 3\alpha + 4E\langle\hat{r}\rangle_E - K_\ell\langle\hat{r}^{-1}\rangle_E/m$. The eigenvalues $K_\ell = \ell(\ell+1)\hbar^2$ of $\hat{K}$ follow from angular-momentum quantization, and $\langle\hat{r}^{-1}\rangle_E$ is related to E by (4.23). With these ingredients and similar calculations for $\hat{a} = \hat{r}\hat{Q}$, we obtain

$$\langle\hat{r}\rangle_E = \frac{1}{2}\frac{K_\ell}{m\alpha} - \frac{3}{4}\frac{\alpha}{E}\,,\ \langle\hat{r}^2\rangle_E = \frac{3}{4}\frac{K_\ell}{mE} + \frac{5}{8}\frac{\alpha^2}{E^2} - \frac{1}{4}\frac{\hbar^2}{mE}\,. \tag{3.15}$$

In order to determine the allowed eigenvalues E, as before, we have to impose uncertainty relations. We are interested here in the ground state, for which we can focus on the lowest-order uncertainty relations, computed for our non-canonical operators $\hat{r}$, $\hat{P}$ and $\hat{Q}$ using the Cauchy–Schwarz inequality. There is only one non-trivial relation,

$$(\Delta_E r)^2 C^E_{\hat{Q}Q} \geq |C^E_{rQ} + \frac{1}{2}i\hbar\langle\hat{r}\rangle_E|^2\,, \tag{3.16}$$

with two covariances. Again using (3.13), we compute $\langle\hat{Q}\rangle_E = \frac{1}{2}i\hbar$ using $\hat{a} = \hat{r}$, $\langle\hat{r}\hat{Q} + \hat{Q}\hat{r}\rangle_E = i\hbar\langle\hat{r}\rangle_E$ using $\hat{a} = \hat{r}^2$. Finally, $\langle\hat{Q}^\dagger\hat{Q}\rangle_E = \langle\hat{Q}^2\rangle_E - 3i\hbar\langle\hat{Q}\rangle_E$ can be obtained using $\hat{K}$.

Inserting all the required moments and factorizing the resulting polynomial in E, (3.16) gives the condition

$$\ell^2(\ell+1)^2(\ell^2+\ell-1)\frac{1}{E}\left(E + \frac{1}{2}\frac{m\alpha^2}{\hbar^2(\ell+1)^2}\right)\left(E + \frac{1}{2}\frac{m\alpha^2}{\hbar^2\ell^2}\right)\left(E - \frac{1}{2}\frac{m\alpha^2}{\hbar^2(\ell^2+\ell-1)}\right) \geq 0\,. \tag{3.17}$$

It is saturated for all energy eigenvalues with maximal ℓ, for which

$$E_{\ell+1} = -\frac{m\alpha^2}{2\hbar^2(\ell+1)^2}\,. \tag{3.18}$$

Assuming the well-known degeneracy of the hydrogen spectrum, we obtain the full set of bound-state energies. As in the example of the harmonic oscillator, every eigenstate saturates an uncertainty relation, in this case (3.16).

Non-associative hydrogen: We are now in a position to derive our main result. In the presence of a magnetic central charge, we cannot use canonical momenta because they require a vector potential of the magnetic field $\vec{B}$. Instead, we generate an algebra using kinematical electron momenta, quantizing $p_i = m\dot{x}_i$. Their commutators are obtained by generalizing the case in which there is a vector potential $\vec{A}$ depending on $\vec{x}$, and canonical momenta are $\pi_i = p_i + eA_i$. Therefore,

$$[\hat{p}_j, \hat{p}_k] = i\hbar e \left(\widehat{\frac{\partial A_k}{\partial x_j}} - \widehat{\frac{\partial A_j}{\partial x_k}} \right) = i\hbar e \sum_{l=1}^{3} \epsilon_{jkl} \hat{B}^l \tag{3.19}$$

while $[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}$ is unchanged.

The final result depends only on $\vec{B}$ and therefore can be used to define the commutators $[\hat{p}_j, \hat{p}_k]$ also if $\nabla \cdot \vec{B} \neq 0$ in the presence of magnetic charges. A direct calculation shows that these commutators then no longer obey the Jacobi identity:

$$\begin{aligned} & [[\hat{p}_x, \hat{p}_y], \hat{p}_z] + [[\hat{p}_y, \hat{p}_z], \hat{p}_x] + [[\hat{p}_z, \hat{p}_x], \hat{p}_y] \\ = \;& i\hbar e \sum_{j=1}^{3} [\hat{B}^j, \hat{p}_j] = -\hbar^2 e \, \widehat{\mathrm{div}\vec{B}} \neq 0 \,. \end{aligned} \tag{3.20}$$

Even a single point-like monopole cannot be excised, as in Dirac's construction, if we consider weak charges that do not obey the quantization condition. However, a non-associative algebra generated by commuting $\hat{x}_i$ and non-commuting $\hat{p}_j$, with standard commutators between $\hat{x}_i$ and $\hat{p}_j$, is still meaningful [5, 11].

Another direct calculation shows that the commutators of $(\hat{r}, \hat{Q}, \hat{P})$ remain unchanged provided that $\vec{r} \times \vec{B} = 0$. This result, which relies on unexpected cancellations of the extra terms in commutators implied by (4.1), is crucial for the new application in this letter. In this case, $\vec{B} = g(\vec{r})\vec{r}$. For a static magnetic field, we have $\nabla \times \vec{B} = 0$, which implies that $g(r)$ is spherically symmetric. A monopole density $\nabla \cdot \vec{B} \neq 0$ then requires that $g(r) = Q_{\mathrm{m}}(r)/(4\pi r^3)$ with the magnetic charge

$$Q_{\mathrm{m}}(r) = 4\pi \int \nabla \cdot \vec{B}(r) r^2 \mathrm{d}r \tag{3.21}$$

enclosed in a sphere of radius r. For a single monopole at $r = 0$, $g(r) = g$ is constant.

The virial theorem relies only on algebraic properties and remains valid. With

monopole commutators for momentum components, however, the modified angular momentum $\hat{\vec{L}}' = \hat{\vec{L}} + eg\hat{\vec{r}}/\hat{r}$, not $\hat{\vec{L}}$ itself, satisfies the usual commutators of angular momentum [30, 62]. The Casimir of the algebra generated by $(\hat{r}, \hat{Q}, \hat{P})$ is still equal to $\hat{K} = \hat{\vec{L}}^2$, but in terms of the modified angular momentum it has an extra term:

$$\hat{K} = \hat{\vec{L}}^2 = \hat{\vec{L}}'^2 - e^2g^2\,. \tag{3.22}$$

For a single monopole at the center, the spectrum of $\hat{K}$ has a simple shift compared with the standard spectrum of $\hat{L}^2$, which is known to break the ℓ-degeneracy of the hydrogen spectrum [53]. Moreover, the allowed values of ℓ are restricted for non-zero g because $\hat{K}$, by definition, is positive, and so must be its eigenvalues. Therefore, $\ell = 0$ is not possible for $g \neq 0$, and larger ℓ may be ruled out as well for strong magnetic charges.

We will focus now on the range of weak magnetic charges given by

$$0 < \frac{eg}{\hbar} = N < \frac{1}{2}\,. \tag{3.23}$$

None of these values could be modeled by a Dirac monopole (they would not correspond to single-valued wave functions), but they can be considered if quantum mechanics is non-associative. Since the algebraic relations used to derive (3.17) are still applicable, we obtain conditions on the energy spectrum. The only difference is that the eigenvalues of $\hat{K}$ are now given by $K_\ell = \ell(\ell+1)\hbar^2 - e^2g^2$, which can be taken into account by replacing ℓ in (3.17) with

$$\tilde{\ell} = \sqrt{\left(\ell + \frac{1}{2}\right)^2 - \frac{e^2g^2}{\hbar^2}} - \frac{1}{2}\,. \tag{3.24}$$

For quantized magnetic charges, the corresponding eigenvalues for which the first parenthesis in (3.17) is zero are indeed included in the spectrum found in [53], but they no longer constitute the full spectrum.

For weak magnetic charges, positivity of $\hat{K}$ requires that the smallest possible ℓ is $\ell = 1/2$, which we use for the ground state. The corresponding $\tilde{\ell}$ is equal to

$$\tilde{\ell} = \sqrt{1 - N^2} - \frac{1}{2} \tag{3.25}$$

and lies in the range $\frac{1}{2}(\sqrt{3} - 1) < \tilde{\ell} < \frac{1}{2}$. This range does not come close to the integer values 0 or 1 which would amount to standard hydrogen eigenvalues. Therefore, even for weak magnetic monopoles the energy spectrum of hydrogen is strongly modified. The ground-state energy is discontinuous in the central magnetic charge as a consequence of

the positivity condition $K \geq 0$, which is the reason why even a small magnetic charge is not a simple perturbation of the usual hydrogen spectrum.

This result would seem to rule out any non-zero magnetic charge of the proton. However, from a purely experimental perspective, the smallest eigenvalue of the total angular momentum, used in our evaluation of $K \geq 0$, is zero only within some uncertainty. The angular momentum spectrum is very basic and hard to modify. For instance, the conservation law and its role played in parity considerations implies that, for a single component, it has the form of a ladder centered around zero. It is, however, conceivable that its values are washed out to within some δL^2. To estimate this quantity, we are not restricted to hydrogen-like systems because all energy levels depend in some way on the eigenvalues of $\hat{L}^2$. The best relative precision, of about $5 \cdot 10^{-19}$, is obtained for spectral lines used in atomic clocks [63]. In SI units, a non-zero upper bound

$$g \leq \frac{4\pi\epsilon_0\sqrt{\delta L^2}c^2}{e} \approx 4.7 \cdot 10^{-18}\text{Am} = 1.4 \cdot 10^{-9} g_{\text{Dirac}} \tag{3.26}$$

then follows from $K \geq 0$ and (4.83), where g_{Dirac} is the smallest magnetic charge allowed by Dirac.

For the proton, this bound is not as strong as existing ones [64, 65]. However, the bounds in [64, 65] are obtained by limiting the total magnetic charge of a macroscopic object, adding the individual charges of all electrons or nucleons. Our bound is obtained directly for a single proton. Moreover, the magnetic charge of the muon is more difficult to bound [65]. Our bound, on the other hand, also applies to a muon as the nucleus of muonium, and to antimatter such as the antiproton in antihydrogen [66, 67] or the positron in positronium [68].

If we directly apply hydrogen or muonium spectroscopy, with accuracies of $\Delta E/E \approx 4.5 \cdot 10^{-15}$ [55] and about 10^{-9} [69], respectively, we obtain weaker bounds: $g_{\text{proton}} \leq 9.5 \cdot 10^{-8} g_{\text{Dirac}}$ and $g_{\text{muon}} \leq 4.5 \cdot 10^{-5} g_{\text{Dirac}}$.

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Chapter 4
The ground state of non-associative hydrogen and upper bounds on the magnetic charge of elementary particles

Martin Bojowald, Suddhasattwa Brahma, Umut Büyükçam, Martijn van Kuppeveld

Formulations of magnetic monopoles in a Hilbert-space formulation of quantum mechanics require Dirac's quantization condition of magnetic charge, which implies a large value that can easily be ruled out for elementary particles by standard atomic spectroscopy. However, an algebraic formulation of non-associative quantum mechanics is mathematically consistent with fractional magnetic charges of small values. Here, spectral properties in non-associative quantum mechanics are derived, applied to the ground state of hydrogen with a magnetically charged nucleus. The resulting energy leads to new strong upper bounds for the magnetic charge of various elementary particles that can appear as the nucleus of hydrogen-like atoms, such as the muon or the antiproton.

4.1 Introduction

Eigenvalues and eigenstates can be defined and derived completely algebraically, without using a Hilbert-space representation of observables as operators. Such a formulation is important in particular in studies of non-associative algebras that cannot be represented on a Hilbert space. Physical examples can be found mainly in situations in which fractional magnetic charges may be present that do not obey Dirac's quantization condition [52],

which can be defined at the level of a non-associative algebra of observables even though no Hilbert-space representation exists [5, 11, 14, 54]. Magnetic monopole charges that obey Dirac's quantization condition are so large that they can easily be ruled out in elementary particles by atomic spectroscopy. While small non-zero magnetic charges may be compatible with observational bounds, they cannot obey the quantization condition and therefore require non-associative algebras of observables.

Non-associative products are obtained for magnetic monopoles as follows: In the presence of magnetic monopoles, the magnetic field has non-zero divergence and therefore cannot be described by a vector potential. The usual canonical momentum $\hat{\pi}_i = \hat{p}_i + e\hat{A}_i$ of a particle with electric charge e and mass m, where $\hat{p}_i = m\dot{\hat{x}}_i$ is the kinematical momentum, is then unavailable. However, it turns out that the commutator of two kinematical momenta,

$$[\hat{p}_j, \hat{p}_k] = [\hat{\pi}_j - e\hat{A}_j, \hat{\pi}_k - e\hat{A}_k] = i\hbar e\left(\widehat{\frac{\partial A_k}{\partial x_j}} - \widehat{\frac{\partial A_j}{\partial x_k}}\right) = i\hbar e\sum_{l=1}^{3}\epsilon_{jkl}\hat{B}^l \tag{4.1}$$

does not require a vector potential. (The usual bracket $[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}$ remains unchanged.) It can therefore be generalized to a point charge moving in the presence of a background magnetic charge, but it is not canonical and not even constant since the magnetic field is position dependent. The Jacobi identity is therefore not guaranteed to hold, and it is indeed violated as the calculation

$$[[\hat{p}_x, \hat{p}_y], \hat{p}_z] + [[\hat{p}_y, \hat{p}_z], \hat{p}_x] + [[\hat{p}_z, \hat{p}_x], \hat{p}_y] = i\hbar e\sum_{j=1}^{3}[\hat{B}^j, \hat{p}_j] = -\hbar^2 e\,\widehat{\mathrm{div}\vec{B}} \neq 0 \tag{4.2}$$

demonstrates. Since the assumption of an associative product would imply the Jacobi idenity for the commutator, magnetic monopoles are seen to require non-associative algebras of quantum observables [5, 11, 14, 54]. The basic commutators (4.1) together with an associator determined by (4.2) can be turned into a complete non-associative algebra by means of $*$-products [33, 36–39].

Purely algebraic derivations that do not make use of specific representations are usually more challenging than standard quantum mchanics, in particular if associativity cannot be assumed. As a consequence, such systems remain incompletely understood, and it remains to be seen whether they can be viable. Nevertheless, it has recently become possible to derive potential physical effects [56] and to use spectral results for new upper bounds on the possible magnetic charge of elementary particles [**?**]. The present paper presents details of the latter derivation as well as a discussion of new methods that

may be useful for further applications.

4.2 Associative algebra of the standard hydrogen atom

Modeled by a simple Coulomb potential, the hydrogen atom has the Hamiltonian

$$H = \frac{1}{2m}|p|^2 - \frac{\alpha}{r} \tag{4.3}$$

with constant α, where $|p|^2 = p_x^2+p_y^2+p_z^2$ and $r^2 = x^2+y^2+z^2$ in Cartesian coordinates. As operators, the position and momentum components are subject to the basic commutation relations

$$[\hat{x}, \hat{p}_x] = [\hat{y}, \hat{p}_y] = [\hat{z}, \hat{p}_z] = i\hbar\,, \tag{4.4}$$

and they are self-adjoint. These conditions define a so-called $*$-algebra, which, together with a quantum Hamiltonian $\hat{H}$, properties of angular momentum, and the virial theorem, will be the only ingredient in our derivation of spectral properties. We will not make use of operators that represent the observables on a Hilbert space of wave functions.

An eigenvalue is a property of an observable in the algebra together with a specific eigenstate. For a derivation of spectral properties we therefore need a notion of states on an algebra, bypassing the introduction of wave functions. Given a $*$-algebra $\mathcal{A}$, a quantum state [15] is defined as a positive linear functional $\omega\colon \mathcal{A} \to \mathbb{C}$ from the algebra to the complex numbers, such that $\omega(\hat{a}^*\hat{a}) \geq 0$ for all $a \in \mathcal{A}$. In addition, a state obeys the normalization condition $\omega(\hat{\mathbb{I}}) = 1$ where $\hat{\mathbb{I}} \in \mathcal{A}$ is the unit. The evaluation $\omega(\hat{a})$ is then the expectation value of $\hat{a} \in \mathcal{A}$, and moments such as $\omega(\hat{a}^n)$ for integer n define a probability distribution for measurements of the observable a if $\hat{a}$ is self-adjoint, $a^* = a$. Our aim is to derive properties of eigenvalues λ of a quantum Hamiltonian $\hat{H} \in \mathcal{A}$ for hydrogen through a suitable subset the moment conditions

$$\omega(\hat{a}(\hat{H} - \lambda)) = 0 \quad \text{for all} \quad \hat{a} \in \mathcal{A}\,. \tag{4.5}$$

We have to find a useful subset of $\hat{a} \in \mathcal{A}$ in order to make this derivation feasible.

4.2.1 Subalgebra for spherical symmetry

Instead of applying standard position and momentum components, spherical symmetry can be used to introduce a promising subset of algebra elements. A subalgebra of certain

spherically symmetric elements of $\mathcal{A}$ is generated by the three elements

$$\hat{r} \quad , \quad \hat{P} = \hat{r}|\hat{p}|^2 \quad , \quad \hat{Q} = \hat{x}\hat{p}_x + \hat{y}\hat{p}_y + \hat{z}\hat{p}_z - i\hbar\,. \tag{4.6}$$

Linear combinations of these generators form a 3-dimensional Lie algebra with basic relations

$$[\hat{r}, \hat{Q}] = i\hbar\hat{r} \quad , \quad [\hat{r}, \hat{P}] = 2i\hbar\hat{Q} \quad , \quad [\hat{Q}, \hat{P}] = i\hbar\hat{P}\,, \tag{4.7}$$

isomorphic to so$(2,1)$. (Closely related algebras have been used for derivations of the hydrogen spectrum in deformation quantization [59–61]. Our application of this algebra follows different methods, and our extension to non-associative hydrogen in the next section is completely new.) Its Casimir element is given by

$$\hat{K} := \frac{1}{2}(\hat{r}\hat{P} + \hat{P}\hat{r}) - \hat{Q}^2\,. \tag{4.8}$$

Using the definitions (4.6), $\hat{K}$ turns out to equal the square of angular momentum.

At this point, we can already see the main features of our new derivation, which consists of the following steps in the order of the next three subsections:

1. A Casimir element such as (4.8) is a powerful tool because it takes a constant value in a fixed irreducible representation. Physically, our Casimir is not new but identical with the square of angular momentum. Nevertheless, we will examine angular momentum in order to determine which of the standard properties are readily available in a completely algebraic derivation.

2. The standard hydrogen Hamiltonian $\hat{H}$ is not an element of our linear algebra because the Coulomb potential requires an inverse of $\hat{r}$, and $\hat{P}$ is not the correct kinetic energy. However, the basic variables $\hat{r}$ and $\hat{P}$ are such that the expression $\hat{r}\hat{H}$ is linear in our algebra generators. This observation by itself is not very helpful because $\hat{r}\hat{H}$ and $\hat{H}$ do not have the same eigenvalues. Nevertheless, it is a crucial step in our new strategy, combined with turning the Hamiltonian into a constraint equation: If we start with the constraint $\hat{H} - \lambda = 0$, encoded by the algebraic definition (4.5) of the spectrum, we replace it with the constraint $\hat{r}\hat{H} - \lambda\hat{r} = 0$, which is still linear in our basic generators. This step gives rise to several subtleties because we will have to employ methods from constrained systems, and even for non-self-adjoint constraints because we need the non-symmetric ordering $\hat{r}\hat{H}$ in the constraint in order to use $\hat{P}$ in our linear algebra. Once this step is completed, we

gain information about solutions of (4.5).

3. In the final step, we have to impose positivity of the state used in our solutions of (4.5). Instead of working directly with the basic positivity condition, we will evaluate uncertsinty relations which are derived from positivity. In this general form, there are many different versions of uncertainty relations because they depend on which basic operators one chooses as well as on the polynomial order in which they appear in moments. For our purposes, we do not need a complete analysis but rather have to find a suitable version of uncertainty conditions that gives us useful information about energy eigenvalues. Our main aim is to rule out a certain range of values that could be eigenenergies of non-associative hydrogen. The specific uncertainty relations we choose turn out to give us an interesting restriction by ruling out a large range of values. If there is another uncertainty relation that rules out more values, it would only strengthen our result without removing the bounds obtained here.

We will first explore the algebra and derive useful identities within it as well as in an extension that includes an inverse $\hat{r}^{-1}$. This inverse does not only appear in the Coulomb potential, where it can be evaded by using the constraint just described, but also, as it turns out, appears in the adjointness relation of $\hat{P}$. Since adjointness relations are essential for positivity conditions or uncertainty relations, we cannot avoid discussing a possible inclusion of $\hat{r}^{-1}$ in the algebra. The identities derived now for this purpose will be used in our main calculation.

The commutators (4.7) rely on $\hat{P}$ and $\hat{Q}$ being defined in the specific orderings shown in their definition (4.6), making them not self-adjoint. Completing the definition of a $*$-subalgebra, their adjointness relations can be derived from the basic commutators of Cartesian position and momentum components: In addition to $\hat{r}^* = \hat{r}$, we have

$$\hat{Q}^* = \hat{Q} - i\hbar\hat{\mathbb{I}} \tag{4.9}$$

and

$$\hat{P}^* = \hat{P} - 2i\hbar\hat{r}^{-1}\hat{Q} = \hat{P} - 2i\hbar\hat{Q}\hat{r}^{-1} - 2\hbar^2\hat{r}^{-1}\,. \tag{4.10}$$

At this point, we assume that the subalgebra generated by $\hat{r}$, $\hat{P}$ and $\hat{Q}$ is suitably extended such that it includes an inverse of $\hat{r}$ which, like $\hat{r}$, is also self-adjoint. The adjointness

relations imply the conditions

$$\mathrm{Im}\,\omega(\hat{Q}) = \frac{1}{2i}\omega(\hat{Q}-\hat{Q}^*) = \frac{1}{2}\hbar \tag{4.11}$$

and

$$\begin{aligned}\mathrm{Im}\,\omega(\hat{r}\hat{P}) &= \frac{1}{2i}\left(\omega(\hat{r}\hat{P})-\omega(\hat{P}^*\hat{r})\right) = \frac{1}{2i}\left(\omega(\hat{P}\hat{r}+2i\hbar\hat{Q})-\omega(\hat{P}\hat{r}-2i\hbar\hat{Q}-2\hbar^2\hat{\mathbb{I}})\right)\\ &= \hbar\omega(\hat{Q}+\hat{Q}^*) = 2\hbar\mathrm{Re}\,\omega(\hat{Q})\end{aligned} \tag{4.12}$$

for expectation values in any state ω on the algebra, in addition to $\mathrm{Im}\,\omega(\hat{r})=0$.

In deriving (4.10), we have made use of the commutator

$$[\hat{r},|\hat{p}|^2] = 2i\hbar\hat{r}^{-1}\hat{Q} = 2i\hbar(\hat{Q}-i\hbar\hat{\mathbb{I}})\hat{r}^{-1} \tag{4.13}$$

which is itself based on the commutator

$$[\hat{r}^{-1},\hat{Q}] = -i\hbar\hat{r}^{-1} \tag{4.14}$$

in the second step. These commutators can be computed easily in a position representation of momentum components in $\hat{p}$ and $\hat{Q}$, which then defines the extension of our algebra to one that includes $\hat{r}^{-1}$. Related useful commutators are

$$[\hat{Q},|\hat{p}|^2] = 2i\hbar\hat{r}^{-1}\hat{P} \tag{4.15}$$

$$[\hat{r}^{-1},|\hat{p}|^2] = 2i\hbar\hat{r}^{-3}(\hat{Q}+i\hbar) \tag{4.16}$$

$$[\hat{r}^{-1},\hat{P}] = 2i\hbar\hat{r}^{-2}(\hat{Q}+i\hbar) \tag{4.17}$$

and

$$[\hat{P}^*,\hat{P}] = -2i\hbar\hat{r}^{-1}\hat{Q}\hat{P}^* + 2i\hbar\hat{P}(\hat{Q}-i\hbar)\hat{r}^{-1} + 4\hbar^2\hat{r}^{-1}\hat{Q}(\hat{Q}-i\hbar)\hat{r}^{-1} \tag{4.18}$$

$$[\hat{P}^*,\hat{r}] = [\hat{r},\hat{P}]^* = -i\hbar\hat{r} \tag{4.19}$$

$$[\hat{P}^*,\hat{Q}] = -i\hbar\hat{P}^* = [\hat{P}^*,\hat{Q}^*]\,. \tag{4.20}$$

Adjointness relations require us to extend the algebra by an inverse of $\hat{r}$. Nevertheless, we will see that all moments required for a derivation of spectral properties can be derived using relations in the linear algebra because the expectation value $\omega(\hat{r}^{-1})$ is related to moments of polynomial expressions by the virial theorem, which states that for any

quantum Hamiltonian $\hat{H} = \frac{1}{2}m^{-1}\hat{p}^2 + \alpha\hat{r}^n$ with some integer n, the expectation values of kinetic and potential energy in a *stationary* state ω are related by

$$\omega(\hat{p}^2) = nm\alpha\omega(\hat{r}^n)\,. \tag{4.21}$$

Since all energy eigenstates are stationary, the theorem applies in our case. In addition, the eigenvalue condition $\omega(\hat{H} - \lambda) = 0$, as a special case of (4.5), implies a second condition for the same energy expectation values:

$$\frac{1}{2m}\omega(\hat{p}^2) + \alpha\omega(\hat{r}^n) = \lambda\,. \tag{4.22}$$

Therefore,

$$\omega(\hat{p}^2) = \frac{2nm\lambda}{n+2} \quad , \quad \alpha\omega(\hat{r}^n) = \frac{2\lambda}{n+2}\,. \tag{4.23}$$

For the Coulomb potential,

$$\omega(\hat{r}^{-1}) = \frac{2\lambda}{\alpha} \tag{4.24}$$

is strictly determined.

The proof of the virial theorem is brief and standard, but it is useful to display the key ingredients to demonstrate that no Hilbert-space representation is required. Since ω is stationary, we have

$$0 = \frac{\mathrm{d}\omega(\hat{Q})}{\mathrm{d}t} = -i\omega([\hat{x}\hat{p}_x + \hat{y}\hat{p}_y + \hat{z}\hat{p}_z, \hat{H}]) = \omega(m^{-1}|\hat{p}|^2 - n\alpha\hat{r}^n) \tag{4.25}$$

using $[\hat{p}_x, \hat{r}] = -i\widehat{\partial r/\partial x} = -i\hat{x}\hat{r}^{-1}$. This result proves the virial theorem not only for standard quantum mechanics but also for non-associative systems in the presence of magnetic monopoles: While some associativity is applied in computing the commutator in (4.25), none of the brackets (4.2) appear that would be modified for non-zero magnetic charge.

4.2.2 Angular momentum

We will use the familiar eigenvalues of angular momentum squared, which equal the eigenvalues of $\hat{K}$ defined in (4.8). The usual derivation of these eigenvalues is, to a large degree, algebraic, but it relies on applications of ladder operators on wave functions representing angular-momentum eigenstates. Such an application will no longer be available once we turn to non-associative hydrogen. We therefore provide here a complete

algebraic derivation of angular-momentum eigenvalues.

The relevant algebra in this derivation is the enveloping algebra $\mathcal{B}$ of the Lie algebra su(2), with self-adjoint generators $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$ such that

$$[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z \quad , \quad [\hat{J}_y, \hat{J}_z] = i\hbar\hat{J}_x \quad , \quad [\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y \, . \tag{4.26}$$

An angular-momentum eigenstate $\omega_{\iota,\mu}$ with eigenvalue ι of the square of angular momentum, $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$, and eigenvalue μ of the z-component $\hat{J}_z$ is a normalized and positive linear map from $\mathcal{B}$ to the complex numbers which obeys the conditions

$$\omega_{\iota,\mu}(\hat{a}(\hat{J}^2 - \iota)) = 0 \quad \text{and} \quad \omega_{\iota,\mu}(\hat{a}(\hat{J}_z - \mu)) = 0 \tag{4.27}$$

for all $\hat{a} \in \mathcal{B}$.

Although we will not apply the ladder operators $\hat{J}_\pm$ to wave functions, defined as usually as

$$\hat{J}_\pm = \hat{J}_x \pm \hat{J}_y \, , \tag{4.28}$$

they are still useful because they obey the identity

$$\begin{aligned} \hat{J}_-^N \hat{J}_+^N &= \hat{J}_-^{N-1}(\hat{J}^2 - \hat{J}_z^2 - \hat{J}_z)\hat{J}_+^{N-1} \\ &= \hat{J}_-^{N-1}\hat{J}_+^{N-1}(\hat{J}^2 - \hat{J}_z^2 - \hat{J}_z) + \hat{J}_-^{N-1}[(\hat{J}^2 - \hat{J}_z^2 - \hat{J}_z), \hat{J}_+^{N-1}] \\ &= \hat{J}_-^{N-1}\hat{J}_+^{N-1}\left(\hat{J}^2 - \hat{J}_z^2 - \hat{J}_z - 2(N-1)\hat{J}_z - (N-1)^2 - (N-1)\right) \end{aligned}$$

on $\mathcal{B}$ for any positive integer N. Similarly,

$$\hat{J}_+^N \hat{J}_-^N = \hat{J}_+^{N-1}\hat{J}_-^{N-1}\left(\hat{J}^2 - \hat{J}_z^2 + \hat{J}_z + 2(N-1)\hat{J}_z - (N-1)^2 - (N-1)\right) . \tag{4.29}$$

Evaluating these identities in an eigenstate, we find

$$\begin{aligned} \omega_{\iota,\mu}(\hat{J}_\mp^N \hat{J}_\pm^N) &= \omega_{\iota,\mu}(\hat{J}_\mp^{N-1}\hat{J}_\pm^{N-1})\left(\iota - (\mu \pm (N-1))^2 \mp (\mu \pm (N-1))\right) \\ &= \prod_{n=0}^{N-1}(\iota - (\mu \pm n)^2 \mp (\mu \pm n)) \end{aligned}$$

by iteration.

Since we have $\hat{J}_-^N \hat{J}_+^N = (\hat{J}_+^N)^*(\hat{J}_+^N)$ and $\hat{J}_+^N \hat{J}_-^N = (\hat{J}_-^N)^*(\hat{J}_-^N)$, positivity of $\omega_{\iota,\mu}$ implies

$$\prod_{n=0}^{N}(\iota - (\mu \pm n)^2 \pm (\mu \pm n)) \geq 0 \tag{4.30}$$

for all $N \geq 0$. The second term in each factor, $-(\mu \pm n)^2$, is a negative square which can grow arbitrarily negative. Therefore, only finitely many factors in the products (4.30) can be non-zero, such that, for some positive integers n_+ and n_-, we have

$$\iota - (\mu + n_+)^2 - (\mu + n_-) = 0 \quad \text{and} \quad \iota - (\mu - n_-)^2 + (\mu - n_-) = 0\,. \tag{4.31}$$

Solving these two equations implies that the eigenvalues are of the form

$$\iota = \left(\frac{n_- + n_+}{2}\right)\left(\frac{n_- + n_+}{2} + 1\right) \quad \text{and} \quad \mu = \frac{n_- - n_+}{2}\,, \tag{4.32}$$

which can be recognized as the familiar eigenvalues in finite-dimensional irreducible representations of su(2).

4.2.3 Eigenvalue constraint

We proceed with our derivation of energy eigenvalues. The Hamiltonian is not polynomial in basic observables of the linear algebra. However, some of the conditions (4.5) are defined on the linear algebra, provided $\hat{a}$ has at least one factor of $\hat{r}$ on its right. For instance, a single such factor, $\hat{a} = \hat{r}$, replaces the non-polynomial $\hat{H} - \lambda$ in (4.5) with the linear expression

$$\hat{C} := \hat{r}(\hat{H} - \lambda) = \frac{1}{2m}\hat{P} - \lambda\hat{r} - \alpha\,. \tag{4.33}$$

A subset of the spectrum conditions (4.5) can therefore be written in terms of $\hat{C}$ as the constraint equations

$$\omega(\hat{b}\hat{C}) = 0 \quad \text{for all} \quad \hat{b} \in \mathcal{A}\,. \tag{4.34}$$

These constraints might not be sufficient to obtain the full spectrum based on (4.5), but any condition on eigenvalues derived from (4.108) also applies to the full eigenvalues.

In what follows, we therefore replace the self-adjoint Hamiltonian $\hat{H}$ with a constraint operator $\hat{C}$ that, by definition, is *not* self-adjoint. Dealing with constraints that are not self-adjoint requires some care. In particular, while a self-adjoint constraint generates a gauge flow in much the same way as a self-adjoint Hamiltonian generates time evolution, there are additional terms in the relationship between the flow and the commutator with $\hat{C}$ when the constraint $\hat{C}$ is not self-adjoint.

For a self-adjoint Hamiltonian $\hat{H}$, a time-dependent state ω_t by definition evolves

according to

$$\frac{\mathrm{d}\omega_t(\hat{O})}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\omega_t(\exp(it\hat{H}/\hbar)\hat{O}\exp(-it\hat{H}/\hbar)) = \frac{\omega_t([\hat{O},\hat{H}])}{i\hbar} \tag{4.35}$$

for all $\hat{O} \in \mathcal{A}$. Similarly, defining the gauge flow generated by $\hat{C}$ through the (non-unitary) operator $\hat{F}_\epsilon = \exp(-i\epsilon\hat{C}/\hbar)$ a gauge-dependent state ω_ϵ flows according to

$$\frac{\mathrm{d}\omega_\epsilon(\hat{O})}{\mathrm{d}\epsilon} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\omega_\epsilon(\hat{F}_\epsilon^*\hat{O}\hat{F}_\epsilon) \tag{4.36}$$

because this condition implies that any state solving the constraint equation (4.108) is preserved by the flow: We then have

$$\omega(\hat{F}_\epsilon^*\hat{O}\hat{F}_\epsilon) = \omega(\hat{O}) \tag{4.37}$$

for all $\hat{O} \in \mathcal{A}$ if $\omega(\hat{b}\hat{C}) = 0$ for all $\hat{b} \in \mathcal{A}$. Infinitesimally, applying the flow operator implies a relationship,

$$\frac{\mathrm{d}\omega_\epsilon(\hat{O})}{\mathrm{d}\epsilon} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\omega_\epsilon(\exp(i\epsilon\hat{C}^*/\hbar)\hat{O}\exp(-i\epsilon\hat{C}/\hbar)) = \frac{\omega_\epsilon(\hat{O}\hat{C} - \hat{C}^*\hat{O})}{i\hbar}\,, \tag{4.38}$$

that is not directly related to the commutator of $\hat{O}$ and $\hat{C}$ because of the presence of a $\hat{C}^*$. In our specific case, we can use

$$\hat{C}^* = \hat{C} - \frac{i\hbar}{m}\hat{r}^{-1}\hat{Q} = \hat{C} - \frac{i\hbar}{m}\hat{Q}\hat{r}^{-1} - \frac{\hbar^2}{m}\hat{r}^{-1} \tag{4.39}$$

and arrive at

$$\frac{\mathrm{d}\omega_\epsilon(\hat{O})}{\mathrm{d}\epsilon} = \frac{\omega_\epsilon([\hat{O},\hat{C}])}{i\hbar} + \frac{\omega_\epsilon(\hat{Q}\hat{r}^{-1}\hat{O})}{m} - \frac{i\hbar\omega_\epsilon(\hat{r}^{-1}\hat{O})}{m}\,. \tag{4.40}$$

The constraint equations (4.108) play the same role as stationarity of eigenstates. Since every energy eigenstate ω is gauge invariant under the flow generated by $\hat{C}$, (4.40) implies that

$$\frac{\omega([\hat{O},\hat{C}])}{i\hbar} = -\frac{\omega((\hat{Q} - i\hbar\hat{\mathbb{I}})\hat{r}^{-1}\hat{O})}{m} \tag{4.41}$$

for any such state. Since $\hat{r}^{-1}$ appears on the right, these equations give us another way to derive moments involving $\hat{r}^{-1}$. For instance, for $\hat{O} = \hat{r}$, we obtain

$$\omega(\hat{Q}) = \frac{\omega([\hat{r},\hat{P}])}{2i\hbar} = \frac{m\omega([\hat{r},\hat{C}])}{i\hbar} = -\omega(\hat{Q} - i\hbar\hat{\mathbb{I}}) \tag{4.42}$$

from the basic commutators in the first step, the definition of $\hat{C}$ in the second step and an application of equation (4.41) in the last step. Thus,

$$\omega(\hat{Q}) = \frac{1}{2} i\hbar \,, \tag{4.43}$$

which is consistent with the reality condition (4.11) and in addition shows that $\mathrm{Re}\,\omega(\hat{Q}) = 0$ for stationary states.

In another example, choosing $\hat{O} = \hat{Q}$ and using the basic commutators, as well as (4.14), implies

$$\frac{1}{2m}\omega(\hat{P}) + \lambda\omega(\hat{r}) + \frac{1}{m}\omega(\hat{Q}^2\hat{r}^{-1}) - \frac{\hbar^2}{m}\omega(\hat{r}^{-1}) = 0 \,. \tag{4.44}$$

In this expression, The first term is given by

$$\frac{1}{2m}\omega(\hat{P}) = \lambda\omega(\hat{r}) + \alpha \tag{4.45}$$

using the constraint, $\omega(\hat{C}) = 0$. The factor of $\hat{Q}^2$ in the third moment can be eliminated by using the Casimir $\hat{K}$, such that

$$\begin{aligned} \hat{Q}^2\hat{r}^{-1} &= \left(-\hat{K} + \frac{1}{2}(\hat{r}\hat{P} + \hat{P}\hat{r})\right)\hat{r}^{-1} \\ &= -\hat{K}\hat{r}^{-1} + \frac{1}{2}[\hat{r}, \hat{P}]\hat{r}^{-1} + \hat{P} \\ &= -\hat{K}\hat{r}^{-1} + i\hbar\hat{Q}\hat{r}^{-1} + \hat{P} \,. \end{aligned} \tag{4.46}$$

The final appearance of $\hat{Q}$ in the second term of this new expression can be eliminated by applying (4.41) to $\hat{O} = \hat{\mathbb{I}}$: $i\hbar\omega(\hat{Q}\hat{r}^{-1}) = \hbar^2\omega(\hat{r}^{-1})$. Thus, equation (4.44) implies

$$3\alpha + 4\lambda\omega(\hat{r}) - \frac{K}{m}\omega(\hat{r}^{-1}) = 0 \tag{4.47}$$

with an eigenvalue $K = \hbar^2\ell(\ell+1)$ of $\hat{K}$ if we assume, as usual, that our eigenstate is simultaneously one of energy and angular momentum and then use the derivation given in Section 4.2.2. Using the virial theorem to replace $\omega(\hat{r}^{-1}) = 2\lambda/\alpha$, we obtain

$$\omega(\hat{r}) = -\frac{1}{2}\ell(\ell+1)\frac{\hbar^2}{m\alpha} - \frac{3}{4}\frac{\alpha}{\lambda} \tag{4.48}$$

for the radius expectation value. This equation gives the correct expression for the r-expectation value in all energy eigenstates in terms of the eigenvalue λ.

4.2.4 Uncertainty relations

So far, we have not obtained any restriction on the eigenvalues λ that may appear in (4.48). Such restrictions cannot be derived by using only the eigenmoment equation (4.5). In addition, we have to impose conditions that ensure that ω is positive (or "normalizable" in quantum-mechanics lingo). In order to keep the discussion more physically intuitive, we implement positivity through the equivalent conditions implied by uncertainty relations.

4.2.4.1 General derivation

To arrive at uncertainty relations, we follow standard results that imply the Cauchy–Schwarz inequality

$$\omega(\hat{a}^*\hat{a})\omega(\hat{b}^*\hat{b}) \geq |\omega(\hat{b}^*\hat{a})|^2 \tag{4.49}$$

for all $\hat{a}, \hat{b} \in \mathcal{A}$ and any state ω. The proof proceeds by defining a new algebra element $\hat{a}' := \hat{a}\exp(-i\arg\omega(\hat{b}^*\hat{a}))$, designed such that $|\omega(\hat{b}^*\hat{a})| = \omega(\hat{b}^*\hat{a}')$. This intermediate step allows us to rewrite the positivity condition as

$$\begin{aligned} 0 &\leq \omega\left(\left(\sqrt{\omega(\hat{b}^*\hat{b})}\hat{a}' - \sqrt{\omega(\hat{a}'^*\hat{a}')}\,\hat{b}\right)^*\left(\sqrt{\omega(\hat{b}^*\hat{b})}\hat{a}' - \sqrt{\omega(\hat{a}'^*\hat{a}')}\,\hat{b}\right)\right) \\ &= 2\omega(\hat{b}^*\hat{b})\omega(\hat{a}'^*\hat{a}') - \sqrt{\omega(\hat{b}^*\hat{b})\omega(\hat{a}'^*\hat{a}')}\left(\omega(\hat{a}'^*\hat{b}) + \omega(\hat{b}^*\hat{a}')\right) \\ &= 2\omega(\hat{b}^*\hat{b})\omega(\hat{a}'^*\hat{a}') - 2\sqrt{\omega(\hat{b}^*\hat{b})\omega(\hat{a}'^*\hat{a}')}|\omega(\hat{b}^*\hat{a})| \end{aligned} \tag{4.50}$$

and to conclude that

$$|\omega(\hat{b}^*\hat{a})| \leq \sqrt{\omega(\hat{a}^*\hat{a})}\sqrt{\omega(\hat{a}'^*\hat{a}')} = \sqrt{\omega(\hat{a}^*\hat{a})\omega(\hat{b}^*\hat{b})}\,.$$

Importantly, the result does not require associativity; see also [70].

Choosing $\hat{a} = \hat{O}_1 - \omega(\hat{O}_1)\hat{\mathbb{I}}$ and $\hat{b} = \hat{O}_2 - \omega(\hat{O}_2)\hat{\mathbb{I}}$ for self-adjoint $\hat{O}_1$ and $\hat{O}_2$, we compute the variances $\omega(\hat{a}^*\hat{a}) = (\Delta O_1)^2$, $\omega(\hat{b}^*\hat{b}) = (\Delta O_2)^2$ of O_1 and O_2, respectively, and $\omega(\hat{b}^*\hat{a}) = \Delta(O_1O_2) + \omega([\hat{O}_1, \hat{O}_2])$ is related to their covariance $\Delta(O_1O_2)$. In this way, the Cauchy–Schwarz inequality implies Heisenberg's uncertainty relation

$$(\Delta O_1)^2(\Delta O_2)^2 - \Delta(O_1O_2)^2 \geq \left(\sum_I C_{12}^I\omega(\hat{O}_I)\right)^2 \tag{4.51}$$

for any pair of observales O_1 and O_2 whose algebra elements $\hat{O}_1$ and $\hat{O}_2$ are two of the generators of a linear subalgebra of $\mathcal{A}$ with structure constants C_{IJ}^K: $[\hat{O}_1, \hat{O}_2] = \sum_I C_{12}^I\hat{O}_I$

with a summation range equal to the dimension of the subalgebra. According to (4.7), we can apply such an uncertainty relation to any pair of the generators $(\hat{r}, \hat{P}, \hat{Q})$. Some of our generators, $\hat{P}$ and $\hat{Q}$, are not self-adjoint. In such a case, according to the derivation shown here where $(\Delta O_1)^2$ results from $\omega(\hat{a}^*\hat{a})$, any variance of a self-adjoint expression should be replaced with the covariance of the algebra element and its adjoint, such as

$$\Delta(\bar{P}P) = \frac{1}{2}\omega(\hat{P}^*\hat{P} + \hat{P}\hat{P}^*) - |\omega(\hat{P})|^2 \,. \tag{4.52}$$

4.2.4.2 Relevant moments

We will apply these (generalized) uncertainty relations to pairs of algebra elements given by $\hat{r}$, $\hat{P}$ and $\hat{Q}$. An explicit evaluation in terms of the energy eigenvalue requires a derivation of the moments $\omega(\hat{r}^2)$, $\omega(\hat{P}^*\hat{P})$, $\omega(\hat{Q}^*\hat{Q})$, $\omega(\hat{r}\hat{P})$, $\omega(\hat{r}\hat{Q})$, and $\omega(\hat{Q}^*\hat{P})$. Also here, we can exploit (4.41) for different choices of $\hat{O}$, as well as (4.108) for various choices of $\hat{b}$.

We first compute one of the $\hat{Q}$-related moments. First, equation (4.41) evaluated for $\hat{O} = \hat{r}^2$ implies

$$\frac{\omega(\hat{r}\hat{Q} + \hat{Q}\hat{r})}{m} = \frac{\omega([\hat{r}^2, \hat{C}])}{i\hbar} = -\frac{\omega((\hat{Q} - i\hbar\hat{\mathbb{I}})\hat{r})}{m} = \frac{\omega(\hat{r}\hat{Q} - 2\hat{Q}\hat{r})}{m} \tag{4.53}$$

using the basic commutators (4.7) in the last step. Therefore,

$$\omega(\hat{Q}\hat{r}) = 0 \quad \text{and} \quad \omega(\hat{r}\hat{Q}) = \omega([\hat{r}, \hat{Q}]) = i\hbar\omega(\hat{r}) \,. \tag{4.54}$$

Together with (4.43), we arrive at

$$\Delta(rQ) = 0 \,. \tag{4.55}$$

For the $\hat{P}$-related moments, we apply (4.108) with $\hat{b}$ equal to the three linear generators $\hat{r}$, $\hat{Q}$ and $\hat{P}$ as well as the adjoint $\hat{P}^*$, giving us four equations,

$$\omega(\hat{r}^2) = \frac{1}{2m\lambda}\omega(\hat{r}\hat{P}) - \frac{\alpha}{\lambda}\omega(\hat{r}) \tag{4.56}$$

from $\hat{b} = \hat{r}$,

$$\omega(\hat{Q}\hat{P}) = i\hbar m\alpha \tag{4.57}$$

from $\hat{b} = \hat{Q}$ using $\omega(\hat{Q}\hat{r}) = 0$ as just derived,

$$\omega(\hat{P}^2) = 2m\lambda\omega(\hat{P}\hat{r}) + 2m\alpha\omega(\hat{P}) \tag{4.58}$$

from $\hat{b} = \hat{P}$, and

$$\begin{aligned}\omega(\hat{P}^*\hat{P}) &= 2m\lambda\omega(\hat{P}^*\hat{r}) + 2m\alpha\omega(\hat{P}^*) \\ &= 2m\lambda\omega(\hat{P}\hat{r}) + 2m\alpha\overline{\omega(\hat{P})} - 2m\lambda\hbar^2 \end{aligned} \tag{4.59}$$

from $\hat{b} = \hat{P}^*$ using (4.10) and (4.43). We apply gauge invariance (4.41) to $\hat{O} = \hat{r}\hat{Q}$, such that

$$\frac{1}{2m}\omega(\hat{r}\hat{P}) + \frac{2}{m}\omega(\hat{Q}^2) + \lambda\omega(\hat{r}^2) + \frac{1}{2m}\hbar^2 = 0\,. \tag{4.60}$$

In the last equation, we replace $\hat{Q}^2$ with the square of angular momentum and therefore $\hat{K}$, as before. Together with (4.56) as well as (4.48), we obtain

$$\omega(\hat{r}^2) = \frac{3}{4}\frac{\ell(\ell+1)\hbar^2}{m\lambda} + \frac{5}{8}\frac{\alpha^2}{\lambda^2} - \frac{1}{4}\frac{\hbar^2}{m\lambda} \tag{4.61}$$

which, like (4.48), is valid for all energy eigenstates in terms of λ. The remaining equations then allow us to solve for the $\hat{P}$-related moments

$$\omega(\hat{r}\hat{P}) = \frac{1}{2}\ell(\ell+1)\hbar^2 - \frac{1}{4}m\frac{\alpha^2}{\lambda} - \frac{1}{2}\hbar^2 \tag{4.62}$$

$$\omega(\hat{P}\hat{r}) = \frac{1}{2}\ell(\ell+1)\hbar^2 - \frac{1}{4}m\frac{\alpha^2}{\lambda} + \frac{1}{2}\hbar^2 \tag{4.63}$$

$$\omega(\hat{P}^*\hat{P}) = -\ell(\ell+1)m\lambda\hbar^2 + \frac{1}{2}m^2\alpha^2 - m\lambda\hbar^2\,. \tag{4.64}$$

The $\hat{Q}$-related moment $\omega(\hat{Q}\hat{P}) = i\hbar m\alpha$ is already determined by (4.57), which together with (4.9), (4.45) and (4.48) gives

$$\omega(\hat{Q}^*\hat{P}) = i\hbar\left(m\alpha - \omega(\hat{P})\right) = -i\hbar m\left(\alpha + 2\lambda\omega(\hat{r})\right) = i\hbar\left(\frac{1}{2}m\alpha + \frac{\lambda\ell(\ell+1)\hbar^2}{\alpha}\right)\,, \tag{4.65}$$

which is the second $\hat{Q}$-related moment relevant for uncertainty relations. The final moment, $\omega(\hat{Q}^*\hat{Q})$, is related to the square of angular momentum by

$$\omega(\hat{Q}^*\hat{Q}) = \omega(\hat{Q}^2) - i\hbar\omega(\hat{Q}) = -\omega(\hat{K}) + \frac{1}{2}\omega(\hat{r}\hat{P}+\hat{P}\hat{r}) - i\hbar\omega(\hat{Q}) = -\frac{1}{2}\ell(\ell+1)\hbar^2 - \frac{m\alpha^2}{4\lambda} + \frac{1}{2}\hbar^2\,, \tag{4.66}$$

using (4.62), (4.63) and (4.43).

We are now in a position to impose positivity of ω. Heisenberg's uncertainty relation for our variables include

$$(\Delta r)^2 \Delta(\bar{P}P) \geq |\Delta(rP) + i\hbar\omega(\hat{Q})|^2 \tag{4.67}$$

which is always saturated for our solutions, without restrictions on λ. In fact, the equality in this statement is implied by the eigenvalue constraint (4.108), such that $\omega(\hat{b}\hat{C}) = 0$ and $\omega(\hat{C}^*\hat{b}) = 0$ for any $\hat{b} \in \mathcal{A}$. Since $\hat{C}$ is linear in $\hat{P}$ and $\hat{r}$, any P in the moments in (4.67) can be replaced by an r as follows:

$$\begin{aligned} \Delta(rP) + i\hbar\omega(\hat{Q}) &= \frac{1}{2}\omega\left((\hat{r} - \omega(\hat{r}))(\hat{P} - \omega(\hat{P})) + (\hat{P} - \omega(\hat{P}))(\hat{r} - \omega(\hat{r}))\right) + \frac{1}{2}\omega([\hat{r}, \hat{P}]) \\ &= \omega\left((\hat{r} - \omega(\hat{r}))(\hat{P} - \omega(\hat{P}))\right) \approx 2m\lambda\omega\left((\hat{r} - \omega(\hat{r}))^2\right) \\ &= 2m\lambda(\Delta r)^2 \end{aligned} \tag{4.68}$$

and

$$\Delta(\bar{P}P) = \frac{1}{2}\omega\left((\hat{P}^* - \overline{\omega(\hat{r})})(\hat{P} - \omega(\hat{P})) + (\hat{P} - \omega(\hat{P}))(\hat{P}^* - \overline{\omega(\hat{r})})\right) \approx (2m\lambda)^2(\Delta r)^2 \tag{4.69}$$

where $\approx$ indicates equality on states obeying the constraint (4.108).

The remaining inequalities,

$$(\Delta r)^2 \Delta(\bar{Q}Q) \geq |\Delta(rQ) + \frac{1}{2}i\hbar\omega(\hat{r})|^2 \tag{4.70}$$

and

$$\Delta(\bar{Q}Q)\Delta(\bar{P}P) \geq |\Delta(\bar{Q}P) + \frac{1}{2}i\hbar\omega(\hat{P})|^2\,, \tag{4.71}$$

imply the the same condition on solutions of the constraint (4.108), but one that non-trivially restricts the values of λ.

4.2.5 Energy eigenvalues

We evaluate the inequality (4.70) explicitly, using a simplification implied by (4.55). For the variances on the left, we have

$$(\Delta r)^2 = \omega(\hat{r}^2) - \omega(\hat{r})^2 = \frac{3}{4}\frac{\ell(\ell+1)\hbar^2}{m\lambda} + \frac{5}{8}\frac{\alpha^2}{\lambda^2} - \frac{1}{4}\frac{\hbar^2}{m\lambda} - \left(\frac{1}{2}\ell(\ell+1)\frac{\hbar^2}{m\alpha} + \frac{3}{4}\frac{\alpha}{\lambda}\right)^2$$

$$= -\frac{\ell^2(\ell+1)^2\hbar^4}{4m^2\alpha^2} + \frac{\alpha^2}{16\lambda^2} - \frac{\hbar^2}{4m\lambda} \tag{4.72}$$

from (4.48) and (4.61), and

$$\Delta(\bar{Q}Q) = \omega(\hat{Q}^*\hat{Q}) - |\omega(Q)|^2 = -\frac{1}{2}\ell(\ell+1)\hbar^2 - \frac{m\alpha^2}{4\lambda} + \frac{1}{4}\hbar^2 \tag{4.73}$$

combining (4.66) and (4.43). Subtracting the right-hand side $\frac{1}{4}\hbar^2\omega(\hat{r})^2$ off (4.70), using $\Delta(rQ) = 0$ according to (4.55), we obtain the inequality

$$\frac{\ell^3(\ell+1)^3\hbar^6}{8m^2\alpha^2} + \frac{\ell^2(\ell+1)^2\hbar^4}{16m^2\alpha^2}\left(\frac{m\alpha^2}{\lambda} - 2\hbar^2\right) - \frac{\ell(\ell+1)\hbar^2}{32m\lambda^2}\left(m\alpha^2 + 2\hbar^2\lambda\right)$$
$$-\frac{m\alpha^4}{64\lambda^3} - \frac{\alpha^2\hbar^2}{16\lambda^2} - \frac{\hbar^4}{16m\lambda} \geq 0\,. \tag{4.74}$$

Upon multiplication with the positive λ^2, the left-hand side is given by λ^{-1} times a polynomial in λ of degree three, which can be factorized as

$$\frac{(\ell+1)^2\hbar^6}{8m^2\alpha^2\lambda}\left(\ell^2\lambda + \frac{1}{2}\frac{m\alpha^2}{\hbar^2}\right)\left(\lambda + \frac{1}{2}\frac{m\alpha^2}{\hbar^2(\ell+1)^2}\right)\left((\ell^2+\ell-1)\lambda - \frac{1}{2}\frac{m\alpha^2}{\hbar^2}\right) \geq 0\,. \tag{4.75}$$

The central parenthesis demonstrates that the inequality is saturated for any energy eigenvalue of the hydrogen problem with maximal angular momentum for a given quantum number n, such that $\ell = n-1$, using the standard expression

$$\lambda_n = -\frac{m\alpha^2}{2\hbar^2 n^2} = -\frac{m\alpha^2}{2\hbar^2(\ell+1)^2}\,. \tag{4.76}$$

Each degenerate energy level therefore contains a state that saturates an uncertainty relation, (4.70), even if it is highly excited. This surprising result extends an observation made in [**?**, 2] for the harmonic oscillator to the hydrogen problem.

4.2.6 Spectral conditions from uncertainty relations

The saturation result makes use of the known formula for energy eigenvalues of the hydrogen problem. Keeping in mind our aim to apply algebraic methods to the non-associative generalization of the problem in the presence of small magnetic charges, we are interested also in an independent derivation of spectral properties directly from the inequality (4.75). To this end, we first note that the left-hand side of this inequality approaches positive infinity for $\lambda \to -\infty$, while it has negative roots. In order to

demonstrate this result it is useful to split the discussion into two case, $\ell = 0$ and $\ell > 0$. In the first case, we can rewrite the inequality as

$$-\frac{\hbar^4}{16m^2\lambda}\left(\lambda + \frac{1}{2}\frac{m\alpha^2}{\hbar^2}\right)^2 \geq 0\,, \tag{4.77}$$

which eliminates all positive λ (where we have a continuous spectrum and therefore no normalizable states ω), and distinguishes the ground-state energy $\lambda = -\frac{1}{2}m\alpha^2/\hbar^2$ through a saturation condition. In the second case, the inequality written as

$$\frac{\ell^2(\ell+1)^2\hbar^6}{8m^2\alpha^2}\left(\lambda + \frac{1}{2}\frac{m\alpha^2}{\hbar^2\ell^2}\right)\left(\lambda + \frac{1}{2}\frac{m\alpha^2}{\hbar^2(\ell+1)^2}\right)\left(\ell^2+\ell-1-\frac{1}{2}\frac{m\alpha^2}{\hbar^2\lambda}\right) \geq 0 \tag{4.78}$$

has a final parenthesis which is always positive for negative λ. Therefore, it rules out any values of λ between the two roots given by the first two parentheses,

$$\lambda_1 = -\frac{1}{2}\frac{m\alpha^2}{\hbar^2\ell^2} \quad \text{and} \quad \lambda_2 = -\frac{1}{2}\frac{m\alpha^2}{\hbar^2(\ell+1)^2} \tag{4.79}$$

where $\lambda_1 < \lambda_2$. All intervals between the known degenerate eigenvalues are therefore eliminated. (An alternative derivation of this result not based on uncertainty relations is given in the Appendix.)

4.3 Non-associative hydrogen with small magnetic charge

A non-associative monopole algebra is not uniquely determined by basic commutators and associators such as (4.1) for a monopole system. Different versions can be classified via suitable star products that determine non-commutative and non-associative compositions of the basic position and momentum variables as formal power series in $\hbar$. To leading order, a direct calculation demonstrates that the commutators within the subset $\{\hat{r}, \hat{P}, \hat{Q}\}$ remain unchanged compared with the associative case, provided the background magnetic field obeys the condition

$$\vec{r} \times \vec{B} = 0\,. \tag{4.80}$$

In this case, therefore, corrections to our preceding results are at most perturbative in $\hbar$ multiplied by a number, such as the magnetic charge, that characterizes the strength of the magnetic field which appears in non-trivial commutators and associators of a monopole star product. Since we will be interested in weak magnetic charges, these

corrections will be small.

In order to determine how the magnetic charge appears, we further evaluate condition (4.80). In general, it implies that $\vec{B}(\vec{r}) = b(\vec{r})\vec{r}$ with some function $b(\vec{r})$. In the static case, we need $\nabla \times \vec{B} = 0$, which is fulfilled if and only if $b(r)$ is spherically symmetric. A monopole density $\mu(r) = \nabla \cdot \vec{B}$ then requires

$$b(r) = \frac{g(r)}{4\pi r^3} \tag{4.81}$$

with the magnetic charge

$$g(r) = 4\pi \int^r \mu(\tilde{r})\tilde{r}^2 \mathrm{d}\tilde{r} \tag{4.82}$$

enclosed in a sphere of radius r. For a single monopole at $r = 0$, $g(r)$ is constant, while $g(r)$ depends on r for a constant monopole density. We will assume that $g(r) = g$ is constant, which combined with the standard Coulomb potential implies that the hydrogen nucleus has magnetic charge g.

Given the magnetic field of a single monopole with magnetic charge g, according to [30, 62] the shifted angular momentum components $\hat{L}'_j = \hat{L}_j + eg\hat{x}_j\hat{r}^{-1}$ satisfy the usual commutators of angular momentum and therefore have the familiar spectrum. The Casimir of the algebra generated by $\hat{r}$, $\hat{P}$ and $\hat{Q}$ is still equal to $\hat{K} = \hat{L}^2$, but in terms of the modified angular momentum, it has an extra term:

$$\hat{K} = \hat{L}^2 = \hat{L}'^2 - e^2g^2\hat{\mathbb{I}}\,. \tag{4.83}$$

(For a monopole density with non-constant g, $\hat{K}$ and $\hat{L}'^2$ cannot be diagonalized simultaneously and an independent method would have to be used to find eigenvalues of $\hat{K}$.)

For a single monopole at the center, the spectrum of $\hat{K}$, according to (4.83) has a simple constant shift compared with the spectrum of $\hat{L}'^2$, which is known to break the degeneracy of the energy spectrum for magnetic monopoles that obey Dirac's quantization condition [53]. This condition, $eg = \frac{1}{2}\hbar$, implies a large value of the smallest non-zero magnetic charge because the electric fine structure constant is small. Dirac monopoles in a hydrogen nucleus would therefore be large perturbations that strongly modify the energy spectrum. They can easily be ruled out by standard spectroscopy. Dirac's quantization condition can be violated in non-associative quantum mechanics. Magnetic charges can then be small and might modify the energy spectrum sufficiently weakly to be phenomenologically viable. However, a derivation of eigenvalues in the non-associative

setting remained impossible for decades. Our methods from the preceding section can now be applied to this question.

We will focus on a range of small magnetic charges g characterized by the condition $0 < eg/\hbar < \frac{1}{2}$. As already noted, the commutators (4.7), the virial theorem and the Cauchy–Schwarz inequality all hold for a non-associative monopole algebra, at least up to higher-order terms in the star product. Specifically, corrections from the associator (4.2) or the commutator to real quantities are of the order $\hbar^2 eg$ or smaller. Second-order corrections in $\hbar$ and eg are therefore insensitive to the specific star product. To within this order, the only assumption that need be modified in our previous derivation of uncertainty relations is the spectrum of $\hat{K}$, which is no longer equal to the square of angular momentum but instead has the eigenvalues

$$K_\ell = \ell(\ell+1)\hbar^2 - e^2g^2\,. \tag{4.84}$$

It is convenient to parameterize the shift by replacing ℓ with a non-integer quantum number

$$\tilde{\ell} = \sqrt{\left(\ell+\frac{1}{2}\right)^2 - \frac{e^2g^2}{\hbar^2}} - \frac{1}{2}\,. \tag{4.85}$$

Substituting $\tilde{\ell}$ for ℓ in (4.75) then gives us conditions on energy eigenvalues of non-associative hydrogen. (Saturation conditions indeed give us correct eigenvalues according to [53], but since the usual degeneracy is broken, they do not give us the full spectrum.)

The range of ℓ is bounded by the fact that $\hat{K}$ is a positive operator (the components $\hat{L}_i$ being Hermitian [30,62]), such that the eigenvalues (4.84) cannot be negative. This condition rules out the quantum number $\ell = 0$, but for small magnetic charges the next possible value, $\ell = 1/2$, is allowed. We will assume this value for the ground state because (4.75) tells us that the smallest root of this equation is proportional to $-1/\ell^2$. The minimum energy eigenvalue is therefore obtained for the smallest possible ℓ. This value of ℓ implies

$$\tilde{\ell} = \sqrt{1 - \frac{e^2g^2}{\hbar^2}} - \frac{1}{2} \tag{4.86}$$

which lies in the range

$$\frac{1}{2}(\sqrt{3}-1) < \tilde{\ell} < \frac{1}{2}\,. \tag{4.87}$$

Since $\tilde{\ell} = 0$ is not possible, the uncertainty relation always rules out a range of energy eigenvalues between

$$\lambda_1 = -\frac{1}{2}\frac{m\alpha^2}{\hbar^2\tilde{\ell}^2} \tag{4.88}$$

and

$$\lambda_2 = -\frac{1}{2}\frac{m\alpha^2}{\hbar^2(\tilde{\ell}+1)^2}\,. \tag{4.89}$$

For any $\tilde{\ell}$ in the range (4.87), $\tilde{\ell} < 1$ while $\tilde{\ell}+1 > 1$. Therefore, a certain non-empty range around the usual hydrogen ground-state energy $-\frac{1}{2}m\alpha^2/\hbar^2$ is ruled out for any value of a small magnetic charge. We conclude that even a small magnetic charge would strongly modify the usual hydrogen spectrum and be incompatible with spectroscopic data. This strict exclusion is possible because the positivity of $\hat{K}$ implies a discontinuity of energy eigenvalues as functions of the magnetic charge g at $g = 0$.

4.4 Conclusions

Our derivations have produced the first results about spectral properties in a system of non-associative quantum mechanics. In particular, we have been able to demonstrate a discontinuity in the ground-state energy of hydrogen as a function of the magnetic charge of the nucleus. Addressing this question requires a continuous range of the magnetic charge around zero, which cannot be modeled by an associative treatment with Dirac monopoles for which the magnetic charge is quantized. Non-associative quantum mechanics is able to describe fractional magnetic charges of any value and is therefore a suitable setting for our question.

A Hilbert-space representation of an algebra by operators acting on wave functions is by necessity associative because for any ψ in the Hilbert space and operators $\hat{A}$, $\hat{B}$ and C we have

$$(\hat{A}\hat{B})\hat{C}\psi = \hat{A}\hat{B}\psi' = \hat{A}(\hat{B}\psi') = \hat{A}(\hat{B}\hat{C})\psi\,, \tag{4.90}$$

defining $\psi' = \hat{C}\psi$ in an intermediate step. Non-associative quantum mechanics can therefore not be represented on a Hilbert space, necessitating a purely algebraic derivation of properties of expectation values, moments, and eigenvalues. That such an algebraic treatment can indeed be used to derive a complete spectrum is demonstrated in [**?**, 2], in this case for the (associative) harmonic oscillator as a proof of principle. The algebraic treatment relies on uncertainty relations in order to impose positivity of states, replacing the more common normalizability conditions of Hilbert-space treatments. The new methods are therefore well-suited to finding unexpected saturation properties of eigenstates, even excited ones. As a new result of [**?**, 2], every eigenstate of the harmonic oscillator saturates a suitable uncertainty relation. Saturation results even extend to eigenstates of anharmonic systems in perturbative treatments.

Our application of related methods to non-associative hydrogen in the present paper have not resulted yet in a full energy spectrum because we focused on the ground state, deriving only one uncertainty relation explicitly. Nevertheless, a saturation result has been found for this state, indicating that the behavior seen in harmonic models might be extendable also to excited states of hydrogen. However, the dynamical algebra of hydrogen is more involved than the canonical algebra applicable to the harmonic oscillator, making a generic treatment of saturation results for hydrogen more complicated.

Our extension to non-associative hydrogen relied on several fortuitous algebraic properties of standard hydrogen that are not affected by introducing non-associativity of monopole type, given by a commutator (4.1) of kinematical momentum components with a magnetic field generated by a pointlike magnetic charge. For other non-associative algebras, or even a monopole algebra with a continuous magnetic charge distribution, the eigenvalue problem cannot yet be solved, presenting a challenging mathematical problem.

Our specific physical result demonstrates that the pursuit of these mathematical questions is worthwhile. We have found that the ground-state energy of hydrogen with a small magnetic nuclear charge g is significantly displaced from the usual value due to a discontinuity, even for infinitesimally small magnetic charge. Spectroscopy is therefore very sensitive to introducing a magnetic charge. In order to produce an upper bound on g consistent with observational data, we may, following [**?**], wash out the discontinuity implied by positivity of the non-associative angular momentum K because the eigenvalues of angular momentum squared are determined only within some δL^2 from a purely phenomenological viewpoint. In addition, a fundamental uncertainty in angular momentum could also be caused by an extended magnetic charge distribution in the nucleus, which would imply that $\hat{K}$ and $\hat{L}'^2$ no longer commute.

As an estimate of this uncertainty, we may use the value $5\cdot 10^{-19}$ given as the accuracy of recent atomic clocks [63], which rely on sharp spectral lines that would be affected by the same uncertainty δL^2 if angular momentum is not sharp. The inequality $K \geq 0$ for eigenvalues of $\hat{K}$, which must always hold because $\hat{K}$ is defined as a positive operator, then implies an upper bound

$$g \leq \frac{4\pi\epsilon_0\sqrt{\delta L^2}c^2}{e} \approx 4.7\cdot 10^{-18}\mathrm{Am} = 1.4\cdot 10^{-9} g_{\mathrm{Dirac}} \tag{4.91}$$

for the magnetic charge, written here in SI units. This upper bound is a small fraction of g_{Dirac}, the smallest non-zero magnetic charge allowed by Dirac's quantization condition in an associative treatment.

Magnetic charges of elementary particles have been bounded by various means. Using the proton as an example, interpreted here as the nucleus of hydrogen, our bound is not as strong as those found based on the total magnetic charge of a large number of nucleons in macroscopic objects [64, 65]. The large number of nucleons in macroscopic objects implies a strong magnification factor in the latter studies if their magnetic charges add up. However, this method is not available for those elementary particles that cannot be combined in stable macroscopic objects, such as unstable particles or antimatter. Some of them can nevertheless be used as substitutes of the nuclear proton in hydrogen-like atoms, with precision spectroscopic data being available in some cases such as muonium [69] or antihydrogen [66, 67]. For instance, muonium spectroscopy with a current accuracy of about 10^{-9} gives us an upper bound on the muon's magnetic charge of $g_{\text{muon}} \leq 4.5 \cdot 10^{-5} g_{\text{Dirac}}$, which is better than available upper bounds based on other methods.

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4.5 Appendix

4.5.1 Algebraic derivation of the associative hydrogen spectrum

It is instructive to derive the standard energy spectrum of an electric charge in a Coulomb potential by algebraic means, using the same subalgebra of observables generated by (4.6) as employed in the main text but imposing positivity of states not through uncertainty relations but, more indirectly, through convergence properties of certain expectation values expressed as power series. This derivation more closely resembles the standard derivation based on convergence properties of norms of wave functions, but it is still fully algebraic. However, it does not give rise to new saturation conditions of uncertainty relations, and it is more difficult to extend it to non-associative systems.

In addition to the basic commutators (4.7), we will make use of

$$[\hat{r}, \hat{C}] = \frac{i\hbar}{m} Q \quad \text{and} \quad [\hat{Q}, \hat{C}] = i\hbar \left(\frac{1}{2m} \hat{P} + \lambda \hat{r} \right) \tag{4.92}$$

with the constraint $\hat{C}$ defined in (4.33), as well as the expectation-value equation

$$\omega(\hat{b}\hat{P}) = 2m\omega\left(\hat{b}(\lambda\hat{r}+\alpha)\right) \tag{4.93}$$

for any $\hat{b} \in \mathcal{A}$, implied by the eigenvalue constraint (4.108). We will apply the invariance condition (4.41) in various ways, and use the operator (4.8) in the form

$$\hat{K} = \hat{r}\hat{P} - i\hbar\hat{Q} - \hat{Q}^2 \,. \tag{4.94}$$

4.5.1.1 Kramer's relation

Our first step is the algebraic derivation of a recurrence relation for expectation values of integer powers of $\hat{r}$ in energy eigenstates of hydrogen, known as Kramer's relation. To this end, we derive the commutators

$$[\hat{r}^n, \hat{Q}] = i\hbar n\hat{r}^n \quad , \quad [\hat{r}^n, \hat{P}] = 2in\hbar\hat{r}^{n-1}\hat{Q} + \hbar^2 n(n-1)\hat{r}^{n-1} \tag{4.95}$$

for integer n, using induction and being careful with taking commutators of powers because $[\hat{a},[\hat{a},\hat{b}]] = 0$ does not always hold for $\hat{a},\hat{b} \in \mathcal{A}$.

Second, invariance applied to $\hat{O} = m\hat{r}^s$ takes the form

$$\begin{aligned}
0 &= \frac{m}{i\hbar}\omega([\hat{r}^s,\hat{C}] + (\hat{Q}-i\hbar)\hat{r}^{s-1}) \\
&= \frac{1}{2i\hbar}\omega([\hat{r}^s,\hat{P}] + [(\hat{Q}-i\hbar),\hat{r}^{s-1}] + \hat{r}^{s-1}(\hat{Q}-i\hbar)) \\
&= s\omega(\hat{r}^{s-1}\hat{Q}) - \frac{i\hbar}{2}s(s-1)\omega(\hat{r}^{n-1}) - (s-1)i\hbar\omega(\hat{r}^{s-1}) + \omega(\hat{r}^{s-1}(\hat{Q}-i\hbar)) \\
&= \frac{s+1}{2}\omega(\hat{r}^{s-1}(2\hat{Q}-is\hbar)) \,,
\end{aligned}$$

such that

$$\omega(\hat{r}^{s-1}\hat{Q}) = \frac{1}{2}i\hbar s\omega(\hat{r}^{s-1}) \,. \tag{4.96}$$

Using this result, invariance applied to $\hat{O} = m\hat{r}^s\hat{Q}$ leads to

$$\begin{aligned}
0 &= \frac{m}{i\hbar}\omega([\hat{r}^s\hat{Q},\hat{C}] + (\hat{Q}-i\hbar)\hat{r}^{s-1}\hat{Q}) \\
&= \frac{1}{2i\hbar}\omega([\hat{r}^s,\hat{P}]\hat{Q}) + \frac{m}{i\hbar}\omega(\hat{r}^s[\hat{Q},\hat{C}]) + \omega([(\hat{Q}-i\hbar),\hat{r}^{s-1}]\hat{Q}) + \omega(\hat{r}^{s-1}(\hat{Q}-i\hbar)\hat{Q}) \\
&= s\omega(\hat{r}^{s-1}\hat{Q}^2) - \frac{i\hbar}{2}s(s-1)\omega(\hat{r}^{s-1}\hat{Q}) + \frac{1}{2}\omega(\hat{r}^s(\hat{P}+2m\lambda\hat{r})) - i\hbar(s-1)\omega(\hat{r}^{s-1}\hat{Q})
\end{aligned}$$

$$
\begin{aligned}
&+\omega(\hat{r}^{s-1}(\hat{Q}-i\hbar)\hat{Q}) \\
&= (s+1)\omega(\hat{r}^{s-1}\hat{Q}^2)+\frac{1}{2}\omega(\hat{r}^s\hat{P})+m\lambda\omega(\hat{r}^{s+1})-i\hbar\frac{s(s+1)}{2}\omega(\hat{r}^{s-1}\hat{Q}) \\
&= -(s+1)\omega(\hat{K}\hat{r}^{s-1})+(s+3/2)\omega(\hat{r}^s\hat{P})+m\lambda\omega(\hat{r}^{s+1})-i\hbar\frac{(s+2)(s+1)}{2}\omega(\hat{r}^{s-1}\hat{Q}) \\
&= -(s+1)\omega(\hat{K}\hat{r}^{s-1})+(s+3/2)\omega(\hat{r}^s\hat{P})+m\lambda\omega(\hat{r}^{s+1})+\hbar^2\frac{(s+2)(s+1)s}{4}\omega(\hat{r}^{s-1}) \qquad (4.97)
\end{aligned}
$$

Equation (4.93) then implies Kramer's relation

$$
0=\hbar^2(s+1)\left(\frac{s(s+2)}{4}-\ell(\ell+1)\right)\omega(\hat{r}^{s-1})+(2s+3)m\alpha\omega(\hat{r}^s)+2(s+2)m\lambda\omega(\hat{r}^{s+1}) \qquad (4.98)
$$

after inserting the standard angular-momentum eigenvalues of $\hat{K}$. Incidentally, invariance applied to $\hat{O}=\hat{r}^s\hat{P}$ results in an identity:

$$
\begin{aligned}
&\frac{m}{i\hbar}\omega([\hat{r}^s\hat{P},\hat{C}])+\omega((\hat{Q}-i\hbar)\hat{r}^{s-1}\hat{P}) \\
&= \frac{1}{2i\hbar}\omega([\hat{r}^s,\hat{P}]\hat{P})+\frac{m}{i\hbar}\omega(\hat{r}^s[\hat{P},\hat{C}])+\omega([(\hat{Q}-i\hbar),\hat{r}^{s-1}]\hat{P})+\omega(\hat{r}^{s-1}(\hat{Q}-i\hbar)\hat{P}) \\
&= 2m(s+1)\omega(\hat{r}^{s-1}\hat{Q}(\lambda\hat{r}+\alpha))-i\hbar ms(s+1)\omega(\hat{r}^{s-1}(\lambda\hat{r}+\alpha))+\omega(\hat{r}^s(2m\lambda\hat{Q})) \\
&= 2m\alpha(s+1)\omega(\hat{r}^{s-1}\hat{Q})+2m\lambda(s+1)\omega(\hat{r}^s(\hat{Q}-i\hbar))-i\hbar ms(s+1)\lambda\omega(\hat{r}^s) \\
&\quad -i\hbar m\alpha s(s+1)\omega(\hat{r}^{s-1})+2m\lambda\omega(\hat{r}^s\hat{Q})=0
\end{aligned}
$$

upon using (4.96).

4.5.1.2 Spectrum

Equipped with Kramer's relation, which we first shift down by one unit in s,

$$
0=\hbar^2 s\left(\frac{s^2-1}{4}-\ell(\ell+1)\right)\omega(\hat{r}^{s-2})+(2s+1)m\alpha\omega(\hat{r}^{s-1})+2(s+1)m\lambda\omega(\hat{r}^s)\,, \qquad (4.99)
$$

we can now set up a new recurrence relation. We first generalize Kramer's relation to

$$
0=\frac{\hbar^2}{4}\omega\left((\hat{r}f(\hat{r}))'''\right)-\hbar^2\ell(\ell+1)\omega(\hat{r}^{-1}f'(\hat{r}))+m\alpha\omega(2f'(\hat{r})+\hat{r}^{-1}f(\hat{r}))+2m\lambda\omega((\hat{r}f(\hat{r}))') \qquad (4.100)
$$

for any analytic function f, where derivatives of analytic functions of $\hat{r}$ are interpreted in the sense of formal power series.

Specializing $f(\hat{r})$ to $f_{s,k}(\hat{r}) = \hat{r}^s e^{-k\hat{r}}$ and defining

$$\kappa_s(k,\lambda) = \omega(\hat{r}^s e^{-k\hat{r}}) \tag{4.101}$$

then gives

$$\begin{aligned} 0 &= \hbar^2 s(-1-4\ell(1+\ell)+s^2)\kappa_{s-2}(k,\lambda) + (h^2 k(4\ell(1+\ell)-3s(1+s))+4m(1+2s)\alpha)\kappa_{s-1}(k,\lambda) \\ &\quad +(3\hbar^2k^2(1+s)+8m(\lambda(1+s)-k\alpha))\kappa_s(k,\lambda) - k(8m\lambda+k^2\hbar^2)\kappa_{s+1}(k,\lambda)\,. \end{aligned}$$

Again shifting s by defining $L_s(k,\lambda) = \kappa_{s-2}(k,\lambda)$, we rewrite the previous relation as the third-order linear differential equation

$$\begin{aligned} 0 &= \Big(\hbar^2 s(-1-4\ell(1+\ell)+s^2) - (h^2 k(4\ell(1+\ell)-3s(1+s))+4m(1+2s)\alpha)\partial_k \\ &\quad +(3\hbar^2k^2(1+s)+8m(\lambda(1+s)-k\alpha))\partial_k^2 + k(8m\lambda+k^2\hbar^2)\partial_k^3\Big)L_s(k,\lambda)\,. \end{aligned} \tag{4.102}$$

Since our $f_{s,k}(\hat{r})$ is a bounded operator for $k > 0$ and $s \geq 0$ with $\lim_{k\to\infty} f(\hat{r}) = \hat{0}$, any state should be such that $L_s(k,\lambda)$ is well-defined for all $k > 0$ and $s \geq 0$ with $\lim_{k\to\infty} L_s(k,\lambda) = 0$ for all λ. We also know that $L_s(k,\lambda)$ is well-defined for energy eigenstates at $k = 0$ as long as $s \geq 0$ is integer, because Kramer's relation together with the virial theorem provides finite numbers for expectation values of positive integer powers of $\hat{r}$. Under these conditions, we can perform a Laplace-like transformation and write

$$\begin{aligned} L_s(k,\lambda) &= \int_0^\infty a_{s,\lambda}(b,d)(k+d(s,\lambda))^{-b}\mathrm{d}b \\ &= \sum_{n=0}^{\infty}\int_0^1 a_{s,\lambda}(b+n,d)(k+d(s,\lambda))^{-n-b}\mathrm{d}b\,. \end{aligned} \tag{4.103}$$

In the first line, $a_{s,\lambda}(b,d)$ may be seen as the inverse Laplace transform of $L_s(e^t - d(s,\lambda))$ with respect to t. As we will see, it is convenient to introduce a free displacement $d(s,\lambda)$ on which the coefficients $a_{n,\lambda}$ will in general depend.

For further convenience, we now drop the explit dependences on s and λ from our notation. Comparing coefficients of the expansion (4.103) inserted in (4.102), we obtain the recurrence relation

$$C_3 a(b+n-3) + C_2 a(b+n-2) + C_1 a(b+n-1) + C_0 a(b+n) = 0 \tag{4.104}$$

with

$$C_3 = d(b+n-3)(b+n-2)(b+n-1)(d^2\hbar^2+8m\lambda) \tag{4.105}$$

$$C_2 = (b+n-2)(b+n-1)\Big(-3d^2\hbar^2(b+n-1-s)+8dm\alpha-8m(b+n-1+s)\Big) \tag{4.106}$$

$$\begin{aligned} C_1 = (b+n-1)\Bigg(&3d\hbar^2(b+n)(b+n+1)+d\hbar^2\Big(-4\ell(1+\ell)+3s(1+s)\Big)\\ &+(b+n)\Big(-6d\hbar^2(1+s)-8m\alpha\Big)+4m\alpha(1+2s)\Bigg) \end{aligned} \tag{4.107}$$

$$C_0 = -h^2(b+n-s)((b+n-s)^2-(2\ell+1)^2)\,. \tag{4.108}$$

By definition, the support of a as a function of b is bounded from below. If for a given solution $n_{\min}$ is the smallest integer such that $a(b+n_{\min})\neq 0$ while $a(b+n)=0$ for $n<n_{\min}$, the expression (4.108) shows that $n_{\min}+b-s=0$ or $|n_{\min}+b-s|-|2\ell+1|=0$. Using the fact that ℓ is an integer (since we are for now assuming the absence of a magnetic charge), b must be an integer. This result shows that $L_s(k,\lambda)$ allows an expansion as a Laurent series of the form

$$L_s(k,\lambda)=\sum_{n=0}^{\infty}A_{s,\lambda}(n)(k+d(s,\lambda))^{-n}\,. \tag{4.109}$$

(The original coefficients $a_{s,\lambda}(b,d)$ introduced in (4.103) are proportional to a Dirac comb of delta functions of b supported on the integers.)

The recurrence relation for $A_{s,\lambda}(n)$ can easily be obtained from (4.104) by absorbing b in n, ignoring the shift by b. The relation can be simplified further by making the choice $d=\sqrt{-8m\lambda}/\hbar$ for a given λ, such that the lowest-order term (at order $n-3$) drops out of the recurrence. We also choose $s=2\ell+2$ and obtain

$$\begin{aligned} 0 = {}& 2d(n-2)\Big(d\hbar^2(3+2\ell-n)+4m\alpha\Big)A(n-2)\\ &+\Big(d\hbar^2\Big(8\ell^2+\ell(26-12n)+3(n-3)(n-2)\Big)+4m\alpha(5+4\ell-2n)\Big)A(n-1)\\ &-\hbar^2(n-3-4\ell)(n-2-2l)A(n) \end{aligned} \tag{4.110}$$

after factoring out $b+n-1$. For very large n of either sign, this recursion takes the form $A(n)-3dA(n-1)+2d^2A(n-2)=0$, such that any non-zero asymptotic A_n behaves either as d^n or $(2d)^n$. However, these options would introduce a pole for $L_s(k,\lambda)$, either at $k=0$ or $k=d>0$, which cannot happen for well-defined states. Therefore, only finitely many $A(n)$ can be non-zero. According to the $A(n)$-term in (4.110), there is an

N_1 such that $A(n) = 0$ for $n < N_1$ because ℓ is an integer.

For the range of n where $A(n) \neq 0$ to be bounded from above, the first coefficient in (4.110) the latter condition requires

$$d = \frac{4m\alpha}{\hbar^2 \nu} \tag{4.111}$$

with some positive integer ν. Inserting this expression, we obtain

$$\begin{aligned} 0 \;\; = \;\; & 2(n+2\ell)(n-1-\nu)c_{n-2} \\ & -\left(n(3n-3-2\nu)+\nu-4\ell(1+\ell)\right)c_{n-1} \\ & +n(n-1-2\ell)c_n \end{aligned} \tag{4.112}$$

where

$$c_n = d^{-n} A_{n+2\ell+2}\,. \tag{4.113}$$

There is one final condition: as all these sequences are linear with recurrence relations that have integer coefficients (since ℓ is known to be an integer) we infer that, up to n-independent rescalings, for a given solution all the coefficients c_n are integer multiples of the same basic quantity, γ. Dividing the recurrence relation by γ, we have $0 = \nu c_{n-1}/\gamma$ `mod 2` for all n, because only a single term in the coefficients of (4.112) is not guaranteed to be even. As an overall factor of two could be absorbed into the definition of γ (and therefore c_{n-1}/γ may well be odd), we conclude that $\nu = 2N$, giving

$$\delta = \frac{2m\alpha}{\hbar^2 N} \tag{4.114}$$

and

$$\lambda = -\frac{m\alpha}{2\hbar^2 N}\,, \tag{4.115}$$

which is the known energy spectrum of hydrogen.

It is instructive to look at the detailed recurrence for the case of $\ell = 0$, which includes the ground state, such that $s = 2$. For $n = 0$ in (4.112), we obtain $c_{-1} = 0$. Choosing $n = 1$ in (4.112) then shows that $c_0 = 0$. For $n = 2$, we obtain a non-trivial relation that determines c_2 in terms of a free c_1:

$$c_2 = 3(1-\nu/2)c_1\,. \tag{4.116}$$

For $\nu = 2$, the smallest allowed value, $c_2 = 0$, which then implies $c_3 = 0$ at $n = 3$. With

two successive vanishing c_n, all the following c_n are zero. Since c_1 may be non-zero, there is a non-zero solution, as required for a non-zero expectation value of the positive operator $\hat{r}^2 e^{-k\hat{r}}$. A non-zero c_1 implies through (4.113) that A_3 is the only non-zero coefficient, such that

$$L_2(k,\lambda_0) \propto \left(k + \frac{2m\alpha}{\hbar^2}\right)^{-3} \tag{4.117}$$

using (4.109). According to its definition (4.101) as an expectation value, $L_2(k,\lambda_0) = \kappa_0(k,\lambda_0) = \omega_0(e^{-k\hat{r}})$ should be the ground-state expectation value of $e^{-k\hat{r}}$, which can easily be confirmed to be of the form (4.117) using the known ground-state wave function $\psi_0(r) \propto e^{-r/a}$ with the Bohr radius $a = \hbar^2/(m\alpha)$.

4.5.2 Generalization to hydrogen with a magnetic nuclear charge

Since most of the identities used in our new derivation of Kramer's relation hold true in the non-associative case with a pointlike magnetic monopole at the center, we can easily generalize this relation. We only have to adjust the spectrum of $\hat{K}$ using (4.84) in (4.97) and obtain

$$0 = \hbar^2(s+1)\left(\frac{s(s+2)}{4} - \ell(\ell+1) + e^2g^2/\hbar^2\right)\omega(\hat{r}^{s-1}) + (2s+3)m\alpha\omega(\hat{r}^s) + 2(s+2)m\lambda\omega(\hat{r}^{s+1}) \tag{4.118}$$

as a generalization of (4.98).

This equation takes the form

$$0 = \frac{\hbar^2}{4}\omega\left((\hat{r}f(\hat{r}))'''\right) - \hbar^2\left(\ell(\ell+1) - e^2g^2\right)\omega(\hat{r}^{-1}f'(\hat{r})) + m\alpha\omega(2f'(\hat{r}) + \hat{r}^{-1}f(\hat{r})) + 2m\lambda\omega((\hat{r}f(\hat{r}))') \tag{4.119}$$

as a differential equation replacing (4.119), which in turn implies the equation

$$\begin{aligned} 0 \;=\; & \Big(\hbar^2 s(s^2 - 1 - 4(\ell(\ell+1) - e^2g^2/\hbar^2)) \\ & -(4m\alpha(2s+1) + k(4\ell(\ell+1) - 4e^2g^2/\hbar^2 - 3s(s+1)))\partial_k \\ & +(8m(s+1) - 8km\alpha + 3k^2(1+s)\hbar^2)\partial_k^2 + k(8m\lambda + k^2)\hbar^2\partial_k^3\Big)L_s(k,\lambda) \end{aligned}$$

instead of (4.102).

The recurrence relation (4.104) still holds with the same C_3 and C_2, while C_1 and C_0 are replaced by

$$
\begin{aligned}
C_1' &= (b+n-1)\Big(3d\hbar^2(b+n)(b+n+1)+d\hbar^2\Big(-4\ell(1+\ell)+-4e^2g^2/\hbar^2+3s(1+s)\Big)\\
&\quad +(b+n)\Big(-6d\hbar^2(1+s)-8m\alpha\Big)+4m\alpha(1+2s)\Big)\\
C_0' &= -h^2(b+n-s)((b+n-s)^2-(2\ell+1)^2+4e^2g^2/\hbar^2)\,.
\end{aligned}
$$

The same choice $d=\sqrt{-8m\lambda}/\hbar$ as in the derivation of (4.110) can be used to reduce the equation to second order, and it has the same large-n behavior as before. The sequence of a_n therefore still has only finitely many non-zero elements, which is again the case if $b-s$ is an integer because the coefficient $b+n-s$ in the last term of the recurrence relation has not changed. However, there is now a second possibility if b and s are such that $(b+n-s)^2=(2\ell+1)^2-4e^2g^2/\hbar^2$ for some integer n. This condition can provide new solutions and a more complicated spectrum.

The last coefficient, $(b+n-s)^2-(2\ell+1)^2+4e^2g^2/\hbar^2$, no longer factorizes. Setting $b=0$ as before, we therefore obtain a relation,

$$
\begin{aligned}
0 &= 2d(n-2)(n-1)\Big(-4m\alpha+d(-1+n-s)\hbar^2\Big)a_{n-2}\\
&\quad +(n-1)\Big(-4m\alpha(2s+1)-3dn(1+n)\hbar^2+d(4\ell(\ell+1)-4e^2g^2/\hbar^2-3s(1+s))\hbar^2\\
&\quad +n(8m\alpha+6d(1+s)\hbar^2)\Big)a_{n-1}\\
&\quad +(n-s)\left((n-s)^2-(2\ell+1)^2+4e^2g^2/\hbar^2\right)\hbar^2a_n\,,
\end{aligned}
$$

in which the coefficient $n-1$ does not cancel out as before (for $s=2\ell+2$) because the last coefficient no longer factorizes in the same way. In the previous section we have already indicated several steps in the derivation of the standard hydrogen spectrum that would no longer hold if ℓ (or the effective $\tilde{\ell}$ in (4.86) if $g\neq 0$) is not an integer.

More specifically, we again now look at the case of $\ell=0$ or $s=2$, comparing with the discussion at the end of the preceding section. Now, choosing $n=1$ implies a non-trivial condition, given by $a_1=0$, because we are no longer able to factor our $n-1$. With this value, $n=2$ is then identically satisfied. At this stage, we have the same behavior as before, with a single coefficient (a_1 here corresponding to c_{-1} before) required to be zero.

At $n = 3$, we obtain a linear relationship between a_2 and a_3, specifically

$$2(m\alpha - de^2g^2)a_2 = e^2g^2a_3\,. \tag{4.120}$$

The previous equation, $c_0 = 0$, would correspond to $a_2 = 0$, which is implied only if $g = 0$, while $a_3 = 0$ may be implied for suitable quantized charges such that e^2g^2 is an integer, given the value of d. For generic magnetic charges g, and in particular for small ones such that $0 \neq e^2g^2/\hbar^2 \ll 1$, a_2 and a_3 are not independent. It is then impossible to make the recurrence end with a non-zero expectation value of $e^{-k\hat{r}}$, which is a contradiction. As in the main text, we see that the quantum number $\ell = 0$ is ruled out for weak magnetic charges.

Chapter 5
Discussion

In this thesis we've been able to adequately describe the physics of several quantum systems without needing to refer to the existence of a Hilbert space. While there is a limit on how widely applicable these techniques are, as mentioned in the discussion in chapter 2, we nonetheless found new relationships between energy eigenstates and uncertainty relationships, and by avoiding a Hilbert space formulation, we were able to describe non-Dirac monopoles. The surprisingly non-continuous way in which magnetic charge deformed the spectrum of the angular momentum operators then allowed us to place new bounds on the magnetic charge of a muon.

Several open questions remain however:

- Are there systems beyond the harmonic oscillator whose spectrum can be found with the methods used in Chapter 2? The primary properties of the harmonic oscillator we used to get this spectrum was the fact that we had access to a sequence of self-adjoint operators ($\hat{T}_{i,j}$), whose products had an easy enough expansion in terms of thos same self-adjoint operators, and from which we could easily construct the Hamiltonian. There is no a priori reason to think this should only hold for the harmonic oscillator.

- One can wonder whether further constraints on magnetic charges can be given from data concerning cosmological particle production or from scattering amplitudes of collisions in particle colliders. Unfortunately, finding an unambiguous relativistic field theory for theories admit both electric and magnetic charge is difficult, as we prove in appendix A that these theories can't be Poincaré invariant.

- There is some difficulty in interpreting what nonassociativy in our operator algebra means in a practical sense. The noncommutativity that distinguishes the $C*$

algebras of quantum theories with the abelian algebras of classical physics can be sloganized into the statement that the order of measurements changes their outcome. In the ordinary conception of time however, there should not be a difference between a sequence of processes that goes as "(A and then B) and then C" versus the sequence "A and then (B and C)". Starting with an associative product we can get nonassociativity in the composition of processes by having a certain probability of swapping the two arguments of the multiplication ($a \star b = pa \cdot b + (1-p)b \cdot a$), or on the algebra of, say, 1 second long processes by doing both tasks in the correct order, but at twice the speed. I.e.:

$$(U_2 \star U_1)(t) = \begin{cases} U_1(2t) : t \in [0, \frac{1}{2}] \\ U_2(2t-1) \cdot U_1(1) : t \in [\frac{1}{2}, 1]. \end{cases}$$

Whether these two scenarios exhaust all physically relevant non-associative systems is neither known nor obvious.

Appendix B contains some notes on transition probabilities that might be useful in getting the first steps in how this nonassociativity works on an operational level.

Appendix A
Magnetic Charges and Field theory

In order to see whether a field theory with both electric and magnetic charges is compatible with special relativity, we must show that it has energy- and momentum densities h and d_i, respectively a scalar- and vector field, both local in the fields [1], which satisfy the following Poisson-brackets:

$$\left\{H(\bar{M}), H(\bar{N})\right\} = D_i(\bar{M}\partial^i\bar{N} - \bar{N}\partial^i\bar{M}) \tag{A.1}$$

$$\left\{H(\bar{M}), D_i(\bar{V}^i)\right\} = H(\bar{V}^i\partial_i\bar{M}) \tag{A.2}$$

$$\left\{D_i(\bar{V}^i), D_j(\bar{W}^j)\right\} = D_i(\bar{W}^j\partial_j\bar{V}^i - \bar{W}^j\partial_j\bar{V}^i); \tag{A.3}$$

where

$$H(\bar{M}) = \int h\bar{M}\mathrm{d}^3x$$
$$D_i(\bar{V}^i) = \int d_i\bar{V}^i\mathrm{d}^3x$$

and we restrict ourselves to smearing scalarfields $\bar{M}$ and $\bar{N}$ with vanishing Hessian and smearing vector fields $\bar{V}^i$ and $\bar{W}^i$ that are Killing[2].

For any theory that couples the electromagnetic field to other matter fields with just

[1] That is, the value of these quantities at any given point depends only on the value of the physical fields at that point and a finite number of their derivatives.

[2] This gives us a subset of Dirac's hypersurface deformation algebra [71] which is isomorphic to the Poincaré algebra. If the algebra closes for arbitrary scalar functions and vector fields the theory is not just Lorentz-invariant, but fully diffeomorphism invariant.

electric charge, we can write down the following momentum density[3]

$$d_i = \epsilon_{ijk} E^j B^k + p_i + eA_i + \ldots, \tag{A.4}$$

keeping only the lowest order terms in field strength and electric charge. Here E^i is the electric field, B^i the magnetic, p_i is the momentum density of all the other fields, e is a local charge density and A_i is a vectorpotential of B^i, whose curl equals the divergence-free part of B^i. This satisfies the relations above with the only nonzero Poisson brackets being given by [4]

$$\left\{E^i(x), B^j(y)\right\} = \frac{1}{2}\epsilon^{ijk}\left(\frac{\partial}{\partial x^k} - \frac{\partial}{\partial y^k}\right)\delta^{(3)}(x-y) \tag{A.5}$$

$$\{p_i(x), p_j(y)\} = p_{[i,j]}(x)\delta^{(3)}(x-y) \tag{A.6}$$

$$\{p_i(x), e(y)\} = e_{,i}(x)\delta^{(3)}(x-y) \tag{A.7}$$

and the two usual constraints

$$C_E = E^i_{,i} + e + \ldots \approx 0 \tag{A.8}$$

$$C_B = B^i_{,i} + \ldots \approx 0. \tag{A.9}$$

Using the duality transformation that rotates electric to magnetic fields and likewise for charges [72], we then see that the momentum density of a theory with only magnetic charges has to be of the form

$$d_i = \epsilon_{ijk} E^j B^k + p_i + mZ_i + \ldots, \tag{A.10}$$

where m is now the magnetic charge density and Z_i the vector potential for E_i. This leads to the additional bracket

$$\{p_i(x), m(y)\} = m_{,i}(x)\delta^{(3)}(x-y) \tag{A.11}$$

[3]Throughout we will assume all fields fall off rapidly enough for us to neglect boundary terms.

[4]Note that B.5 may look somewhat unorthodox, but follows from the usual fact that the electric field is the canonical conjugate of the vectorpotential and the fact that the longitudonal part of the magnetic field purely depends on the other matter fields.

with the constraints

$$C_E = E^i_{,i} + \ldots \approx 0 \tag{A.12}$$

$$C_B = B^i_{,i} - m + \ldots \approx 0. \tag{A.13}$$

Combining this into a single a theory of both electric and magnetic charges then gives the following general expression for the momentum density and constraints

$$d_i = \epsilon_{ijk} E^j B^k + p_i + eA_i + mZ_i + \ldots \tag{A.14}$$

$$C_E = E^i_{,i} + e + \ldots \approx 0 \tag{A.15}$$

$$C_B = B^i_{,i} - m + \ldots \approx 0, \tag{A.16}$$

with the additional requirement that $\{C_E(x), C_B(y)\} \approx 0$, as we don't want to over-constrain the system. This leads to the relation

$$\{e(x), m(y)\} = 0. \tag{A.17}$$

With these brackets we then find

$$\begin{aligned}
0 &= \left\{D_i(\bar{V}^i), D_j(\bar{W}^j)\right\} - D_i(\bar{W}^j \partial_j \bar{V}^i - \bar{W}^j \partial_j \bar{V}^i) \\
&= \int \bar{V}^i(x)\bar{W}^j(y)\Big(e(x)m(y)\left\{A_i(x), Z_j(y)\right\} + e(x)m(y)\left\{Z_i(x), A_j(y)\right\}\Big)\mathrm{d}^3x\mathrm{d}^3y \\
&= \int \left(\bar{V}^i(x)\bar{W}^j(y) - \bar{W}^i(x)\bar{V}^j(y)\right) e(x)m(y)\left\{A_i(x), Z_j(y)\right\}\mathrm{d}^3x\mathrm{d}^3y \\
&= \int \left(\bar{V}^i(x)\bar{W}^j(y) - \bar{W}^i(x)\bar{V}^j(y)\right) e(x)m(y)\left\{A_i(x), E^k(z)\right\}\epsilon_{jkm}\frac{d}{dz^m}\frac{1}{4\pi|y^i - z^i|}\mathrm{d}^3x\mathrm{d}^3y\mathrm{d}^3z \\
&= \int \left(\bar{V}^i(x)\bar{W}^j(y) - \bar{W}^i(x)\bar{V}^j(y)\right) e(x)m(y)\epsilon_{jim}\frac{d}{dx^m}\frac{1}{4\pi|y^i - x^i|}\mathrm{d}^3x\mathrm{d}^3y
\end{aligned}$$

However, for general independent electric and magnetic charge densities this last term does not vanish, forcing us to conclude that theories with both types of charges can't be compatible with special relativity[5]

[5]as this argument involves only the momentum densities, it turns out mixed charges aren't even compatible with Galilean relativity. One interesting thing to note is this integral *does* vanish when $\bar{V}^i = \epsilon^{ijk}v_j x_k$, $\bar{W}^i = \epsilon^{ijk}w_j x_k$ and when $m = g\delta^{(3)}(x)$. This implies that there is a well defined notion of angular momentum around point-like magnetic charges, which is what we've used in Chapters 3 and 4.

Appendix B
Probabilities in nonassociative quantum mechanics

B.1 Projections onto eigenspaces

In associative quantum mechanics, transition amplitudes are defined using the Hermitian innerproduct on the given Hilbert space, or by taking the trace of the product of two density matrices. In non-associative quantum mechanics we no longer have direct access to this machinery, so we have to be a bit more careful in how we find transition probabilities.

The Born rule tells us that after measuring an observable H, the probability of finding value E is given by the expectation of the projection onto that eigenspace.

For simplicity, assume H is a Hermitian operator. We're looking for a linear map $P_{H,E}$ on the algebra of operators such that for all operators X we have

$$H \star P_{H,E}(X) = P_{H,E}(X) \star H = E P_{H,E}(X)$$

We construct this map by first projecting on the commutant of H with a map P_H, after which we can pick the correct eigenvalue with what is in essence a Fourier transform.

B.1.1 Making the map P_H

First define the (linear) evolution map $evol_{H,t}$ as follows:

$$evol_{H,0}(X) \;=\; X$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}evol_{H,t}(X) &= iH \star evol_{H,t}(X) - ievol_{H,t}(X) \star H \\ &= i(L_H - R_H)evol_{H,t}(X)\end{aligned}$$

Where L_H is the linear map from left multiplication by H, and R_H is a similar map by right multiplication. We can always get this map as a series expansion in t:

$$evol_{H,t}(X) = \sum_{n=0}^{\infty} \frac{(it(L_H - R_H))^n}{n!} X$$

We then define P_H as the zero mode of this map:

$$P_H = \oint_0 \frac{dw}{2\pi i} \int_0^{\infty} \exp(-wt) evol_{H,t}(X) \mathrm{d}t$$

where we use some analytical continuation to perform the contour integral around a point arbitrarily close to 0.

This map commutes with H as we have

$$\begin{aligned}H \star P_H(X) - P(X) \star H &= i(L_H - R_H)P_H(X) \\ &= \oint_0 \frac{dw}{2\pi i} \int_0^{\infty} \exp(-wt) i(L_H - R_H) evol_{H,t}(X) \mathrm{d}t \\ &= \oint_0 \frac{dw}{2\pi i} \int_0^{\infty} \exp(-wt) (\frac{\mathrm{d}}{\mathrm{d}t} evol_{H,t}(X)) \mathrm{d}t \\ &= \oint_0 \frac{dw}{2\pi i} (X - w \int_0^{\infty} \exp(-wt) \sum_{n=0}^{\infty} \frac{(it(L_H - R_H))^n}{n!} X \mathrm{d}t \\ &= 0\end{aligned}$$

B.1.2 Picking out the correct eigenvalue

To project onto only one eigenvalue, we can perform a similar trick of picking out the correct mode. We define $P_{H,E}$ as follows: $\mathrm{P}_{H,E}(X) = \oint_E \frac{dz}{2\pi i} \int_0^{\infty} \exp(-zs) exp(iL_H s, P_H(X)) \mathrm{d}s$ where the exponent in this formula is defined as the solution to

$$\begin{aligned}exp(0, X) &= X \\ \frac{\mathrm{d}}{\mathrm{d}s} exp(iL_H s, X) &= iH \star exp(iL_H s, X)\end{aligned}$$

$$= \quad iL_H exp(iL_H s, X)$$

The fact that this satisfies the equations we want an operator to satisfy follows a similar line as we saw with P_H.

B.2 Transition probabilities

The Born rule in our formalism becomes

$$Prob(\omega, H, E) = \omega(P_{H,E}(1))$$

and after this measurement we end with the state $\omega_{H,E}$ defined by

$$\omega_{H,E}(X) = \frac{\omega(P_{H,E}(X))}{\omega(P_{H,E}(1))}$$

In associative quantum mechanics, the transition probability of going from an eigenstate of an operator A with eigenvalue a, to an eigenstate of an operator B with eigenvalue b by measuring B, is the same as vice versa:

$$Prob(|A,a\rangle \rightarrow |B,b\rangle) = \quad \|\langle B,b|A,a\rangle\|^2 = \quad \|\langle A,a|B,b\rangle\|^2 = \quad Prob(|B,b\rangle \rightarrow |A,a\rangle)$$

This boils down to the statement that for each state ω, each set of operators A and B and each set of eigenvalues a and b

$$\omega(P_{A,a}(P_{B,b}(1)))\omega(P_{B,b}(1)) = \omega(P_{B,b}(P_{A,a}(1)))\omega(P_{A,a}(1))$$

Whether this equation holds in general is an open question.

B.3 Examples

B.3.1 Finite dimensional Hilbert-space

Expanding any operator in terms of the eigen-basis of H (assuming discrete, unique eigenvalues) we get

$$X \quad = \quad \sum_{a,b} X_{ab} E_a E_b$$

$$
\begin{aligned}
evol_{H,t}(X) &= \sum_{a,b} X_{ab} e^{i(E_a - E_b)t} E_a E_b \\
P_H(X) &= \sum_{a} X_{aa} E_a E_a \\
P_{H,E_i}(X) &= X_{ii} E_i E_i
\end{aligned}
$$

B.3.2 Sedenions

The (complexified) sedenions, which result from applying the Cayley–Dickson construction to the octonions, are an interesting finite dimensional toy model for the quantum mechanics of the monopole models in chapter 3 and 4, as this algebra is also not alternative. Explicit computation of the projectors above shows that

- each self-adjoint operator has 2 eigenstates.
- The transition amplitudes are symmetric per equation 1, even for nonzero operators whose product vanishes.
- there is no longer have a resolution of the identity: the projections onto eigenspaces don't sum to 1.
- For each state ω there is a density matrix ρ_ω such that

  $$\omega(X) = Tr(\rho L_X) \qquad\qquad = Tr(\rho R_X),$$

  but the eigenstates of self-adjoint operators are never pure ($Tr(\rho^2) \neq 1$).

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Vita

Martinus van Kuppeveld

Martinus G.D.K. "Martijn" van Kuppeveld was born in Druten, the Netherlands on the 26th of August, 1994. They obtained a double Bachelor degree in Mathematics / Physics and Astronomy at the Radboud University in Nijmegen in 2015, and, through the Perimeter Scholars International program, a Master of Science from the University of Waterloo in 2016.
Since then, Martijn has worked under the supervision of Martin Bojowald at the Pennsylvania State University, resulting in the following publications:

- *"Small Magnetic Charges and Monopoles in Nonassociative Quantum Mechanics"*, M. Bojowald, S. Brahma, U. Büyükçam, J. Guglielmon, and M. van Kuppeveld, Physical Review Letters 121 201602, 2018

- *"Moments and saturation properties of eigenstates"*, M. Bojowald, J. Guglielmon, and M. van Kuppeveld, Physical Review Letters D 103 126005, 2021

- *"The ground state of non-associative hydrogen and upper bounds on the magnetic charge of elementary particles"*, M. Bojowald, S. Brahma, U. Büyükçam, and M. van Kuppeveld, Physical Review Letters D 104 105009, 2021