Moments and saturation properties of eigenstates: Oscillator systems

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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.

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I. 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 nonassociative quantum mechanics that cannot be represented on a Hilbert space [1–3]. The latter arena has recently led to a new upper bound on the magnetic charge of elementary particles [4] 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 $\langle\cdot\rangle : \mathcal{A} \to \mathbb{C}$ 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 [5]: Any positive state obeys the Cauchy-Schwarz inequality

$$\langle\hat{a}^\dagger\hat{a}\rangle\langle\hat{b}^\dagger\hat{b}\rangle \geq |\langle\hat{a}^\dagger\hat{b}\rangle|^2 \tag{1}$$

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 parametrize a state by its basic expectation values $\langle\hat{x}_i\rangle$ and central moments

$$\Delta(x_1^{a_1}\cdots x_n^{a_n}) = \langle(\hat{x}_1 - \langle\hat{x}_1\rangle)^{a_1}\cdots(\hat{x}_n - \langle\hat{x}_n\rangle)^{a_n}\rangle_{\text{Weyl}} \tag{2}$$

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

$$\frac{\mathrm{d}\langle\hat{q}\rangle}{\mathrm{d}t} = \frac{\langle[\hat{q}, \hat{H}]\rangle}{i\hbar}, \qquad \frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t} = \frac{\langle[\hat{p}, \hat{H}]\rangle}{i\hbar} \tag{3}$$

we have

$$\frac{\mathrm{d}\Delta(q^2)}{\mathrm{d}t} = \frac{\mathrm{d}(\langle\hat{q}^2\rangle - \langle\hat{q}\rangle^2)}{\mathrm{d}t} = \frac{\langle[\hat{q}^2, \hat{H}]\rangle}{i\hbar} - 2\langle\hat{q}\rangle\frac{\mathrm{d}\langle\hat{q}\rangle}{\mathrm{d}t} \tag{4}$$

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 (3) and (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 [6] 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

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{q}^2. \tag{5}$$

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

$$\frac{\mathrm{d}\Delta(q^2)}{\mathrm{d}t} = 2\frac{\Delta(qp)}{m}, \tag{6}$$

$$\frac{\mathrm{d}\Delta(qp)}{\mathrm{d}t} = \frac{1}{m}\Delta(p^2) - m\omega^2\Delta(q^2), \tag{7}$$

$$\frac{\mathrm{d}\Delta(p^2)}{\mathrm{d}t} = -2m\omega^2\Delta(qp). \tag{8}$$

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)],

$$\langle\hat{H}\rangle = \frac{1}{2m}\Delta(p^2) + \frac{1}{2}m\omega^2\Delta(q^2) = \frac{1}{2}\hbar\omega, \tag{9}$$

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 (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 [7–10]. (See also [11,12] 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 [13–15] often makes explicit constructions of physical Hilbert spaces and wave functions untractable, while moment methods have been shown to present certain computational advantages [16–19]. And in nonassociative quantum mechanics, which plays a role in models with magnetic monopoles [20] or of certain flux compactifications in string theory [21–25], operators on wave functions (and therefore the usual definition of eigenvalues) are in general unavailable [23,26–29], but moments may still be used [4,30,31].

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 nonassociative example, see [32].) 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 [33]. 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 nonharmonic 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 [32]. Finally, our appendix presents an instructive finite-dimensional example given by a fermionic system.

II. 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,

$$\hat{H}\psi_\lambda = \lambda\psi_\lambda. \tag{10}$$

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

$$\langle \hat{O}(\hat{H} - \lambda\mathbb{I})\rangle_\lambda = \langle \psi_\lambda | \hat{O}(\hat{H} - \lambda\mathbb{I})\psi_\lambda\rangle = 0 \tag{11}$$

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 (11) for sufficiently many choices of $\hat{O}$, and (ii) the imposition of a condition that the expectation value in (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 (11) as a system of recurrence relations for moments of an eigenstate and impose positivity through (generalized) uncertainty relations. In an alternative derivation in Sec. II C we use generating functions and impose positivity more indirectly through continuity and boundedness conditions on a suitably defined object.

A. Notation

Equation (11) immediately implies that eigenstates of a self-adjoint $\hat{H}$ are stationary:

$$\frac{\mathrm{d}\langle \hat{O}\rangle_\lambda}{\mathrm{d}t} = \frac{\langle [\hat{O}, \hat{H}]\rangle_\lambda}{i\hbar} = \frac{\langle \hat{O}(\hat{H} - \lambda\mathbb{I})\rangle_\lambda - \langle \hat{O}^\dagger(\hat{H} - \lambda\mathbb{I})\rangle_\lambda^*}{i\hbar} = 0. \tag{12}$$

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

$$\hat{T}_{m,n} := (\hat{q}^m \hat{p}^n)_{\mathrm{Weyl}} \tag{13}$$

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 [34] for an explicit statement of the relevant reordering identity.

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

$$T_{m,n} := \langle \hat{T}_{m,n}\rangle. \tag{14}$$

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 [35]. More recently, a similar result has been developed from a different perspective in [36], providing a generalized uncertainty principle that imposes inequality constraints on higher moments. These results are key for our further constructions.

Consider the column vector, $\hat{\boldsymbol{\xi}}_J$, 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 $M_J = \langle \hat{\boldsymbol{\xi}}_J \hat{\boldsymbol{\xi}}_J{}^\dagger\rangle$ is positive semidefinite,

$$M_J = \langle \hat{\boldsymbol{\xi}}_J \hat{\boldsymbol{\xi}}_J{}^\dagger\rangle \geq 0 \tag{15}$$

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 [37], it is useful to bring this matrix to block diagonal form

$$M_J \to \begin{pmatrix} A_0 & & & \\ & A_1 & & \\ & & \ddots & \\ & & & A_{2J} \end{pmatrix} \tag{16}$$

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

$$L\begin{pmatrix} A & C^\dagger \\ C & B \end{pmatrix}L^\dagger = \begin{pmatrix} A & 0 \\ 0 & B - CA^{-1}C^\dagger \end{pmatrix} \tag{17}$$

to M_J, where

$$L = \begin{pmatrix} 1 & 0 \\ -CA^{-1} & 1 \end{pmatrix}. \tag{18}$$

This identity holds whenever the matrix on the left-hand side of Eq. (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

$$A_n \geq 0 \quad \text{for all } n \geq 0. \tag{19}$$

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

$$\langle \hat{T}_{m,n}(\hat{H} - \lambda \mathbb{I})\rangle_\lambda = 0 \tag{20}$$

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 (20) then implies recurrence relations for $T_{m,n}$ which depend on the system under consideration.

B. 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 (20) to solve for the moments in terms of the eigenvalue λ and then apply (15) to obtain information concerning the allowed values of λ (as yet unspecified). This combination is the basis of our new method.

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 (20) results in the following relations between the moments:

$$T_{m+2,n} + T_{m,n+2} = 2\lambda T_{m,n} + \frac{n(n-1)}{4}\hbar^2 T_{m,n-2} + \frac{m(m-1)}{4}\hbar^2 T_{m-2,n}, \tag{21}$$

$$nT_{m+1,n-1} = mT_{m-1,n+1} \tag{22}$$

which hold for all m, $n \geq 0$. Two constraints are obtained because (20)—defined without symmetric ordering of the product $\hat{T}_{m,n}\hat{H}$—has both real and imaginary parts. From (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 nonzero $m = 2j$ and $n = 2k$, we then define $S_{j,k}$ such that

$$T_{2j,2k} = \frac{(2j)!(2k)!}{j!k!}S_{j,k}. \tag{23}$$

For these coefficients, (22) implies the simple relation

$$S_{j+1,k} = S_{j,k+1}, \tag{24}$$

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

$$T_{2j,2k} = \frac{(2j)!(2k)!}{j!k!}\hbar^{j+k}b_{j+k}. \tag{25}$$

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

$$b_{j+k} = \frac{(j+k)!}{(2j+2k)!}a_{j+k}, \tag{26}$$

or

$$T_{2j,2k} = \frac{(2j)!(2k)!(j+k)!}{j!k!(2j+2k)!}\hbar^{j+k}a_{j+k}. \tag{27}$$

For instance,

$$T_{2j,0} = \hbar^j a_j \tag{28}$$

and

$$T_{2j,2} = \hbar^{j+1}\frac{a_{j+1}}{2j+1} \tag{29}$$

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

As a consequence of (21), the remaining coefficients, a_ℓ, are subject to a difference equation in a single independent variable:

$$a_{\ell+1} = \frac{\lambda\hbar^{-1}(2\ell+1)}{\ell+1}a_\ell + \frac{(2\ell+1)(2\ell)(2\ell-1)}{8(\ell+1)}a_{\ell-1}. \tag{30}$$

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 $2\hbar a_1 = T_{2,0} + T_{0,2} = 2\langle\hat{H}\rangle_\lambda = 2\lambda$), (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,

$$(\ell+1)b_{\ell+1} - \frac{\lambda}{2\hbar}b_\ell - \frac{1}{16}\ell b_{\ell-1} = 0, \tag{31}$$

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

$$\left(1 - \frac{1}{16}x^2\right)f'(x) = \frac{1}{2}\left(\frac{\lambda}{\hbar} + \frac{1}{8}x\right)f(x) \tag{32}$$

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

$$f(x) = \frac{(1+x/4)^{\lambda/\hbar-1/2}}{(1-x/4)^{\lambda/\hbar+1/2}}, \tag{33}$$

has the Taylor expansion

$$f(x) = \sum_{\ell=0}^{\infty}\left(\frac{-x}{4}\right)^\ell \frac{(\ell-\lambda/\hbar-1/2)!}{(-\lambda/\hbar-1/2)!\ell!} \times {}_2F_1(\lambda/\hbar+1/2, -\ell; \lambda/\hbar+1/2-\ell; -1) \tag{34}$$

and determines the b_ℓ in terms of hypergeometric functions.

2. Positivity

We now apply the generalized uncertainty principle (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 $\hat{\boldsymbol{\xi}}_J$ to form a new vector $\hat{\boldsymbol{\xi}}'_J$ and then taking

$$M'_J = \langle\hat{\boldsymbol{\xi}}'_J\hat{\boldsymbol{\xi}}'^{\dagger}_J\rangle. \tag{35}$$

In particular, consider the matrix M'_J formed by taking $\hat{\boldsymbol{\xi}}'_J$ 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

$$N_J = (J+1)(2J+1) \tag{36}$$

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

$$N'_J = 4J + 1 = N_J - J(2J-1) \tag{37}$$

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 nontrivial uncertainty relation. For $J = 1/2$, we have

$$M'_{1/2} = M_{1/2} = \left\langle\begin{pmatrix} 1 & \hat{q}/\sqrt{\hbar} & \hat{p}/\sqrt{\hbar} \\ \hat{q}/\sqrt{\hbar} & \hat{q}^2/\hbar & \hat{q}\,\hat{p}/\hbar \\ \hat{p}/\sqrt{\hbar} & \hat{p}\,\hat{q}/\hbar & \hat{p}^2/\hbar \end{pmatrix}\right\rangle \tag{38}$$

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

$$\det\begin{pmatrix} \langle\hat{q}^2\rangle & \langle\hat{q}\,\hat{p}\rangle \\ \langle\hat{p}\,\hat{q}\rangle & \langle\hat{p}^2\rangle \end{pmatrix} = T_{2,0}T_{0,2} - \left(T_{1,1} + \frac{1}{2}i\hbar\right)\left(T_{1,1} - \frac{1}{2}i\hbar\right) = T_{2,0}T_{0,2} - T_{1,1}^2 - \frac{\hbar^2}{4} \geq 0, \tag{39}$$

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

$$\hat{\boldsymbol{\xi}}'_1 = \begin{pmatrix} 1 \\ \hat{T}_{1,0}/\sqrt{\hbar} \\ \hat{T}_{0,1}/\sqrt{\hbar} \\ \hat{T}_{2,0}/\hbar \\ \hat{T}_{1,1}/\hbar \end{pmatrix} \tag{40}$$

which gives

$$M_1' = \left\langle \begin{pmatrix} 1 & \hat{T}_{1,0}/\sqrt{\hbar} & \hat{T}_{0,1}/\sqrt{\hbar} & \hat{T}_{2,0}/\hbar & \hat{T}_{1,1}/\hbar \\ \hat{T}_{1,0}/\sqrt{\hbar} & \hat{T}_{1,0}\hat{T}_{1,0}/\hbar & \hat{T}_{1,0}\hat{T}_{0,1}/\hbar & \hat{T}_{1,0}\hat{T}_{2,0}/\hbar^{3/2} & \hat{T}_{1,0}\hat{T}_{1,1}/\hbar^{3/2} \\ \hat{T}_{0,1}/\sqrt{\hbar} & \hat{T}_{0,1}\hat{T}_{1,0}/\hbar & \hat{T}_{0,1}\hat{T}_{0,1}/\hbar & \hat{T}_{0,1}\hat{T}_{2,0}/\hbar^{3/2} & \hat{T}_{0,1}\hat{T}_{1,1}/\hbar^{3/2} \\ \hat{T}_{2,0}/\hbar & \hat{T}_{2,0}\hat{T}_{1,0}/\hbar^{3/2} & \hat{T}_{2,0}\hat{T}_{0,1}/\hbar^{3/2} & \hat{T}_{2,0}\hat{T}_{2,0}/\hbar^{2} & \hat{T}_{2,0}\hat{T}_{1,1}/\hbar^{2} \\ \hat{T}_{1,1}/\hbar & \hat{T}_{1,1}\hat{T}_{1,0}/\hbar^{3/2} & \hat{T}_{1,1}\hat{T}_{0,1}/\hbar^{3/2} & \hat{T}_{1,1}\hat{T}_{2,0}/\hbar^{2} & \hat{T}_{1,1}\hat{T}_{1,1}/\hbar^{2} \end{pmatrix} \right\rangle \tag{41}$$

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

$$\hat{T}_{k,0}\hat{T}_{\ell,1} = \hat{T}_{k+\ell,1} - \frac{1}{2}ik\hbar\hat{T}_{k+\ell-1,0}, \tag{42}$$

$$\hat{T}_{k,1}\hat{T}_{\ell,1} = \hat{T}_{k+\ell,2} + \frac{1}{2}i(\ell-k)\hbar\hat{T}_{k+\ell-1,1} + \frac{1}{4}k\ell\hbar^2\hat{T}_{k+\ell-2,0}, \tag{43}$$

which follow from the general ordering equations given in [34] (or [37]). For fixed J, we can express the nonconstant components of $\hat{\boldsymbol{\xi}}_J' =: \hat{\xi}'$ as

$$\hat{\xi}_n' = \hbar^{-n/4} \cdot \begin{cases} \hat{T}_{n/2,0} & \text{if } n \text{ even} \\ \hbar^{1/4}\hat{T}_{(n-3)/2,1} & \text{if } n \text{ odd} \end{cases} \tag{44}$$

where $2 \le n \le 4J+1$. 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

$$\hat{M}_{mn}' = \hat{\xi}_m'\hat{\xi}_n'^{\dagger} = \hbar^{-(m+n)/4} \cdot \begin{cases} \hat{T}_{(m+n)/2,0} & \text{if } m,n \text{ even} \\ \hbar^{1/4}\hat{T}_{(m-3)/2,1}\hat{T}_{n/2,0} & \text{if } m \text{ odd and } n \text{ even} \\ \hbar^{1/4}\hat{T}_{m/2,0}\hat{T}_{(n-3)/2,1} & \text{if } m \text{ even and } n \text{ odd} \\ \hbar^{1/2}\hat{T}_{(m-3)/2,1}\hat{T}_{(n-3)/2,1} & \text{if } m,n \text{ odd} \end{cases}$$

$$= \hbar^{-(m+n)/4} \cdot \begin{cases} \hat{T}_{(m+n)/2,0} & \text{if } m,n \text{ even} \\ \hbar^{1/4}\hat{T}_{(m+n-3)/2,1} + \frac{1}{4}in\hbar^{5/4}\hat{T}_{(m+n-5)/2,0} & \text{if } m \text{ odd and } n \text{ even} \\ \hbar^{1/4}\hat{T}_{(m+n-3)/2,1} - \frac{1}{4}im\hbar^{5/4}\hat{T}_{(m+n-5)/2,0} & \text{if } m \text{ even and } n \text{ odd} \\ \hbar^{1/2}\hat{T}_{(m+n-6)/2,2} + \frac{n-m}{4}i\hbar^{3/2}\hat{T}_{(m+n-8)/2,1} + \frac{(m-3)(n-3)}{16}\hbar^{5/2}\hat{T}_{(m+n-10)/2,0} & \text{if } m,n \text{ odd} \end{cases} \tag{45}$$

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

$$M_{mn}' = \hbar^{-(m+n)/4} \cdot \begin{cases} T_{(m+n)/2,0} & \text{if } m,n \text{ even} \\ \frac{1}{4}in\hbar^{5/4}T_{(m+n-5)/2,0} & \text{if } m \text{ odd and } n \text{ even} \\ -\frac{1}{4}im\hbar^{5/4}T_{(m+n-5)/2,0} & \text{if } m \text{ even and } n \text{ odd} \\ \hbar^{1/2}T_{(m+n-6)/2,2} + \frac{1}{16}(m-3)(n-3)\hbar^{5/2}T_{(m+n-10)/2,0} & \text{if } m,n \text{ odd} \end{cases} \tag{46}$$

Some components M_{mn}' are zero for certain values of m and n, which can be seen by refining the parametrization 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

$$\hbar^{q+r} M'_{4q+\alpha,4r+\beta} = \begin{pmatrix} T_{2(q+r),0} & -iq\hbar T_{2(q+r-1),0} & 0 & 0 \\ ir\hbar T_{2(q+r-1),0} & T_{2(q+r-1),2} + (q-\frac{1}{2})(r-\frac{1}{2})\hbar^2 T_{2(q+r-2),0} & 0 & 0 \\ 0 & 0 & \hbar^{-1} T_{2(q+r+1),0} & -i(q+\frac{1}{2}) T_{2(q+r),0} \\ 0 & 0 & i(r+\frac{1}{2}) T_{2(q+r),0} & \hbar^{-1} T_{2(q+r),2} + qr\hbar T_{2(q+r-1),0} \end{pmatrix} \tag{47}$$

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 $q \geq 1$ and $r \geq 1$, while parts of these blocks make up the first three rows and columns of M'_J.) Using (28) and (29), we obtain the blocks

$$\hbar^{q+r} M'_{4q+\alpha,4r+\beta} = \begin{pmatrix} a_{q+r} & -iqa_{q+r-1} & 0 & 0 \\ ira_{q+r-1} & (2(q+r)-1)^{-1} a_{q+r} + (q-\frac{1}{2})(r-\frac{1}{2}) a_{q+r-2} & 0 & 0 \\ 0 & 0 & a_{q+r+1} & -i(q+\frac{1}{2}) a_{q+r} \\ 0 & 0 & i(r+\frac{1}{2}) a_{q+r} & (2(q+r)+1)^{-1} a_{q+r+1} + qra_{q+r-1} \end{pmatrix} \tag{48}$$

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

$$M'_1 = \begin{pmatrix} 1 & 0 & 0 & a_1 & 0 \\ 0 & a_1 & \frac{1}{2}i & 0 & 0 \\ 0 & -\frac{1}{2}i & a_1 & 0 & 0 \\ a_1 & 0 & 0 & a_2 & ia_1 \\ 0 & 0 & 0 & -ia_1 & \frac{1}{3}a_2 + \frac{1}{4} \end{pmatrix}. \tag{49}$$

It is block-diagonalized by identifying $C^\dagger$ in (17) with the vector $C_1^\dagger = (0, 0, a_1, 0)$:

$$L_1 M'_1 L_1^\dagger = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & a_1 & \frac{1}{2}i & 0 & 0 \\ 0 & -\frac{1}{2}i & a_1 & 0 & 0 \\ 0 & 0 & 0 & a_2 - a_1^2 & ia_1 \\ 0 & 0 & 0 & -ia_1 & \frac{1}{3}a_2 + \frac{1}{4} \end{pmatrix}. \tag{50}$$

Its determinant is equal to

$$\det(L_1 M'_1 L_1^\dagger) = \frac{1}{4}(\lambda/\hbar + 1/2)^2(\lambda/\hbar - 1/2)^2(\lambda/\hbar + 3/2)(\lambda/\hbar - 3/2) \tag{51}$$

using the solution $a_2 = \frac{3}{2}(\lambda^2/\hbar^2 + 1/4)$ of the recurrence relation (30).

3. Eigenvalues

For any J, we may block diagonalize M'_J as in Eq. (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

$$\det(A'_n) \geq 0 \tag{52}$$

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 (27) and (30). From explicit computations, we infer the general result

$$d_n = \det(A'_n) = \frac{1}{4^{n-1}} \prod_{k=1}^{n} (\lambda/\hbar - \alpha_k)(\lambda/\hbar + \alpha_k) \tag{53}$$

where $\alpha_k = (2k-1)/2$ are the odd half-integer multiples. [The polynomial (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 nonzero, 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 $\mathrm{sgn} d_{n+1} = -\mathrm{sgn} d_n$ 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

$$\lambda = \frac{1}{2}\hbar, \qquad \frac{3}{2}\hbar, \qquad \frac{5}{2}\hbar, \ldots \tag{54}$$

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 Sec. III, 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 (53).

C. 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, Eq. (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

$$L_\lambda(\gamma) = \langle \exp((1+\gamma)\hat{q}^2/\hbar)\rangle_\lambda. \tag{55}$$

For fixed λ, this function of γ is well defined for $\gamma \le -1$ because $\exp((1+\gamma)\hat{q}^2/\hbar)$ 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 [38].) 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 nonharmonic systems, including the standard hydrogen problem [32].

1. Recurrence relations

The moment expansion

$$\begin{aligned} L_\lambda(\gamma) &= \sum_{j=0}^{\infty} \hbar^{-j}\langle\hat{q}^{2j}\rangle_\lambda \frac{(1+\gamma)^j}{j!} \\ &= \sum_{j=0}^{\infty} a_j \frac{(1+\gamma)^j}{j!} \end{aligned} \tag{56}$$

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 (28). Using the recursion relation (30) for the a_j we obtain the differential equation

$$\begin{aligned} &3L_\lambda + 3(9+9\gamma+4\lambda/\hbar)L'_\lambda + 8(2+\lambda/\hbar \\ &\quad + \gamma(6+3\gamma+\lambda/\hbar))L''_\lambda + 4\gamma(1+\gamma)(2+\gamma)L'''_\lambda = 0 \end{aligned} \tag{57}$$

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

$$L_\lambda(\gamma) = \sum_{n=0}^{\infty} \alpha_{n,s}(-\gamma)^{-n-s} \tag{58}$$

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

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

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

$$L_\lambda(\gamma) = \sum_{n=0}^{\infty} A_n(-\gamma)^{-n-\frac{1}{2}} \tag{59}$$

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

$$\begin{aligned} &(1+2n)(1+2n-2\lambda/\hbar)A_n \\ &- 2(1+n)((3+3n-2\lambda/\hbar)A_{n+1} - (2+n)A_{n+2}) = 0. \end{aligned} \tag{60}$$

In the large-n limit, Eq. (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

$$\begin{aligned} L_\lambda(\gamma) &\approx \sum_{n=0}^{M-1} A_n(-\gamma)^{-n-\frac{1}{2}} \\ &\quad + \sum_{n=M}^{\infty} \left(c_1(-\gamma)^{-n-\frac{1}{2}} + 2^n c_2\left(-\gamma\right)^{-n-\frac{1}{2}}\right) \\ &= \sum_{n=0}^{M-1} A_n(-\gamma)^{-n-\frac{1}{2}} - (-\gamma)^{\frac{1}{2}-M}\left(\frac{c_1}{1+\gamma} + \frac{2^M c_2}{2+\gamma}\right) \end{aligned} \tag{61}$$

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

$$(2N-1)(2N-1-2\lambda/\hbar)A_{N-1} = 0 \tag{62}$$

from inserting $n = N-1$ in (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 (54).

2. Coefficients

Based on this result, the coefficients introduced in (59) 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 (59), we first write

$$\begin{aligned} A_n &= \frac{(-1)^{n+1}}{2\pi}\oint_{|z|=1} L_\lambda(z) z^{n-\frac{1}{2}} \mathrm{d}z \\ &= i(-1)^{n+1}\sum_{j=0}^{\infty}\frac{a_j}{2\pi j!}\int_0^{2\pi}(1+e^{i\theta})^j e^{i(n+1/2)\theta}\mathrm{d}\theta \\ &= i\sum_{j=0}^{\infty}\frac{a_j}{\pi j!}B(-1; n+1/2, j+1) \end{aligned} \tag{63}$$

using also (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

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

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

$$\begin{aligned} B\left(-1; n+\frac{1}{2}, j+1\right) &= \frac{(-1)^n}{2}\int_{-\pi}^{\pi}(1+e^{i\theta})^j e^{i(n+1/2)\theta}\mathrm{d}\theta \\ &\le \frac{(-1)^n}{2}\int_{-\infty}^{\infty} 2^j\exp(-j\theta^2/8 + ij\theta/2)e^{i(n+1/2)\theta}\mathrm{d}\theta + 2^j\pi\Delta_j \\ &= \sqrt{2\pi}(-1)^n\frac{2^j}{\sqrt{j}}\exp\left(-\frac{(1+j+2n)^2}{2j}\right) + 2^j\pi\Delta_j. \end{aligned} \tag{64}$$

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 (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

$$\begin{aligned} a_j &= \left(\frac{\mathrm{d}^j}{\mathrm{d}\gamma^j}L_\lambda(\gamma)\right)\Big|_{\gamma=-1} \\ &= \sum_{n=0}^{\infty}A_n\left(\frac{\mathrm{d}^j}{\mathrm{d}\gamma^j}(-\gamma)^{-n-\frac{1}{2}}\right)\Big|_{\gamma=-1} \\ &= (-1)^j\sum_{n=0}^{\infty}A_n\left(-n-\frac{1}{2}\right)^{(j)} \end{aligned} \tag{65}$$

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.

3. Probability density

The alternative method based on (55) allows a more direct derivation of the probability density of eigenstates compared with reconstruction from the moments of Sec. II B.

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 nonzero one. Its exact value will be fixed later by normalization. Running through the recursion relation (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 0th coefficient

A_0 using (60) for $n = 0$. After that, the recurrence terminates automatically: For $n = -1$ in (60), we obtain $A_{-1} = 0$ because of an overall factor of $(1 + n)$ in the second part of (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

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

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

$$L_{\lambda_4} = \frac{35 + 60\gamma + 42\gamma^2 + 12\gamma^3 + 3\gamma^4}{8(-\gamma)^{9/2}}. \tag{66}$$

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

$$L_\lambda(\gamma) = 2\int_0^\infty \exp\left(\frac{1+\gamma}{\hbar}x^2\right)P_\lambda(x)\mathrm{d}x \tag{67}$$

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

$$L_\lambda(-1 - \hbar t) = \int_0^\infty e^{-tu}\frac{P_\lambda(\sqrt{u})}{\sqrt{u}}\mathrm{d}u. \tag{68}$$

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

$$\begin{aligned} P_\lambda(x) &= \frac{x}{2\pi i}\lim_{T\to\infty}\int_{\delta-iT}^{\delta+iT} e^{tx^2}L_\lambda(-1-\hbar t)\mathrm{d}t \\ &= \sum_{n=0}^{N}\frac{x}{2\pi i}\lim_{T\to\infty}\int_{\delta-iT}^{\delta+iT} e^{tx^2}A_n(1+\hbar t)^{-n-\frac{1}{2}}\mathrm{d}t \\ &= \sum_{n=0}^{N}\frac{A_n n!(2x)^{2n}\exp(-x^2/\hbar)}{\sqrt{\pi}(2n)!\hbar^{n+\frac{1}{2}}}. \end{aligned} \tag{69}$$

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

$$\begin{aligned} P_{\lambda_4}(x) &= \frac{\exp(-x^2/\hbar)}{\sqrt{\pi\hbar}}\left(\frac{3}{8} - \frac{12}{8}\frac{2x^2}{\hbar} + \frac{42}{8}\frac{4x^4}{3\hbar^2} - \frac{60}{8}\frac{8x^6}{15\hbar^3} + \frac{35}{8}\frac{16x^8}{105\hbar^4}\right) \\ &= \frac{\exp(-x^2/\hbar)}{24\sqrt{\pi\hbar}}\left(3 - 12\frac{x^2}{\hbar} + 4\frac{x^4}{\hbar}\right)^2 = \frac{\exp(-x^2/\hbar)}{\sqrt{\pi\hbar}2^4 4!}H_4\left(\frac{x}{\sqrt{\hbar}}\right)^2 = |\psi_4(x)|^2. \end{aligned} \tag{70}$$

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 (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 [39]. However, they are based on ladder operators in Hilbert space and therefore require representations of the algebra of observables.

III. SATURATION OF INEQUALITIES

An interesting result that emerges from the solutions in Sec. II B 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 (53). 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 [40]. Moreover, it sharpens a saturation property found in [37], 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.

A. 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 $\hat{\boldsymbol{\xi}}_J{}'$ 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 (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 [6,41]. 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.

B. 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,

$$\hat{a} = \frac{1}{\sqrt{2\hbar}}(\hat{q} + i\hat{p}), \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2\hbar}}(\hat{q} - i\hat{p}). \tag{71}$$

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

$$\hat{f} = \hat{a}^n + \hat{a}^{\dagger n}, \qquad \hat{g} = \hat{a}^n - \hat{a}^{\dagger n}. \tag{72}$$

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

$$\langle \hat{f}^\dagger \hat{f}\rangle\langle \hat{g}^\dagger \hat{g}\rangle \geq |\langle \hat{f}^\dagger \hat{g}\rangle|^2 \tag{73}$$

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 nth inequality is saturated by any linear combination of the first n harmonic-oscillator eigenstates. For $n = 1$,

$$\langle \hat{q}^2\rangle\langle \hat{p}^2\rangle \geq \hbar^2/4 + \langle \hat{q}\,\hat{p}\rangle^2_{\text{Weyl}} \tag{74}$$

for $n = 2$,

$$\begin{aligned}(\langle \hat{p}^4\rangle + \langle \hat{q}^4\rangle - 2\langle \hat{p}^2\hat{q}^2\rangle_{\text{Weyl}} + \hbar^2)\left(\langle \hat{p}^2\hat{q}^2\rangle_{\text{Weyl}} + \frac{\hbar^2}{4}\right)\\ \geq \hbar^2(\langle \hat{p}^2\rangle + \langle \hat{q}^2\rangle)^2 + (\langle \hat{p}\hat{q}^3\rangle_{\text{Weyl}} - \langle \hat{p}^3\hat{q}\rangle_{\text{Weyl}})^2\end{aligned} \tag{75}$$

and for $n = 3$,

$$\begin{aligned}&\left(\frac{1}{9}\langle \hat{q}^6\rangle - \frac{2}{3}\langle \hat{p}^2\hat{q}^4\rangle_{\text{Weyl}} + \langle \hat{p}^4\hat{q}^2\rangle_{\text{Weyl}} + \hbar^2\langle \hat{q}^2\rangle + \hbar^2\langle \hat{p}^2\rangle\right)\left(\frac{1}{9}\langle \hat{p}^6\rangle - \frac{2}{3}\langle \hat{p}^4\hat{q}^2\rangle_{\text{Weyl}} + \langle \hat{p}^2\hat{q}^4\rangle_{\text{Weyl}} + \hbar^2\langle \hat{p}^2\rangle + \hbar^2\langle \hat{q}^2\rangle\right)\\ &\geq \hbar^2\left(\frac{\hbar^2}{3} + \frac{1}{2}\langle \hat{p}^4\rangle + \frac{1}{2}\langle \hat{q}^4\rangle + \langle \hat{p}^2\hat{q}^2\rangle_{\text{Weyl}}\right)^2 + \left(\frac{1}{3}\langle \hat{p}^5\hat{q}\rangle_{\text{Weyl}} + \frac{1}{3}\langle \hat{p}\hat{q}^5\rangle_{\text{Weyl}} - \frac{10}{9}\langle \hat{p}^3\hat{q}^3\rangle_{\text{Weyl}}\right)^2.\end{aligned} \tag{76}$$

Except for $n = 1$, there is no obvious relationship with minors of the matrices M'_J introduced in (35), which were found to be relevant for eigenstates in our previous analysis.

C. 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

$$(\sqrt{2\hbar}\hat{a})^n\psi = \alpha^n\psi. \tag{77}$$

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, $\hat{f} \coloneqq (2\hbar)^{n/2}(\hat{a}^n + \hat{a}^{\dagger n}) - \alpha^n$

and $\hat{g} := (2\hbar)^{n/2}(\hat{a}^n - \hat{a}^{\dagger n}) - \alpha^n$. In a state ψ that satisfies (77), we again obtain $\hat{f}\psi = -\hat{g}\psi$ and therefore

$$\langle \hat{f}^\dagger \hat{f}\rangle\langle \hat{g}^\dagger \hat{g}\rangle = \langle \hat{f}^\dagger \hat{g}\rangle\langle \hat{g}^\dagger \hat{f}\rangle = |\langle \hat{f}^\dagger \hat{g}\rangle|^2 \tag{78}$$

saturating (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

$$\begin{aligned}\langle \hat{f}^\dagger \hat{f}\rangle &= \langle 4\hat{q}^2 - 2(\alpha + \alpha^*)\hat{q} + |\alpha|^2\rangle \\ &= 4(\Delta q)^2 + \langle \hat{q}\rangle^2 + \langle \hat{p}\rangle^2,\end{aligned} \tag{79}$$

$$\langle \hat{g}^\dagger \hat{g}\rangle = 4(\Delta p)^2 + \langle \hat{q}\rangle^2 + \langle \hat{p}\rangle^2, \tag{80}$$

$$\begin{aligned}\langle \hat{f}^\dagger \hat{g}\rangle &= 4i\langle \hat{q}\,\hat{p}\rangle - 2(\alpha\langle \hat{q}\rangle + i\alpha^*\langle \hat{p}\rangle) + |\alpha|^2 \\ &= iC_{qp} - 2\hbar - \langle \hat{q}\rangle^2 - \langle \hat{p}\rangle^2,\end{aligned} \tag{81}$$

with the covariance $C_{qp} = \Delta(qp)$. The saturated uncertainty relation obtained immediately from (78) then takes the form

$$\begin{aligned}&(\Delta q)^2(\Delta p)^2 - C_{qp}^2 \\ &\quad + \frac{1}{4}(\langle \hat{q}\rangle^2 + \langle \hat{p}\rangle^2)((\Delta q)^2 + (\Delta p)^2 - \hbar) = \frac{1}{4}\hbar^2.\end{aligned} \tag{82}$$

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 (77) 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 (77) 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 $0 \le \ell < k$, the inner products

$$\begin{aligned}\langle kn + \ell|\alpha, k\rangle &= \frac{1}{\sqrt{(kn+\ell)!}}((\hat{a}^\dagger)^{kn+\ell}|0\rangle)^\dagger|\alpha, k\rangle \\ &= \frac{1}{(2\hbar)^{kn/2}}\frac{\alpha^{kn}}{\sqrt{(kn+\ell)!}}\langle 0|\hat{a}^\ell|\alpha, k\rangle \\ &= \frac{\alpha^{kn}}{(2\hbar)^{kn/2}}\frac{\sqrt{\ell!}}{\sqrt{(kn+\ell)!}}\langle \ell|\alpha, k\rangle \\ &=: \alpha^{kn}\frac{\sqrt{\ell!}}{\sqrt{(kn+\ell)!}}C_\ell\end{aligned} \tag{83}$$

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

$$\begin{aligned}|\alpha, k\rangle &= \sum_{m=0}^{\infty}\langle m|\alpha, k\rangle|m\rangle \\ &= \sum_{\ell=0}^{k-1} C_\ell\sqrt{\ell!}\sum_{n=0}^{\infty}\frac{\alpha^{kn}}{\sqrt{(kn+\ell)!}}|kn+\ell\rangle \\ &= \sum_{\ell=0}^{k-1} C_\ell\frac{\sqrt{\ell!}}{\alpha^\ell}\sum_{n=0}^{\infty}\frac{(\alpha\hat{a}^\dagger)^{kn+\ell}}{(kn+\ell)!}|0\rangle.\end{aligned} \tag{84}$$

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 kth root of unity $u_k = e^{2\pi i/k}$, it is possible to write our series as a superposition of exponential functions,

$$\sum_{n=0}^{\infty}\frac{(\alpha\hat{a}^\dagger)^{kn+\ell}}{(kn+\ell)!} = \frac{1}{k}\sum_{j=0}^{k-1}u_k^{-j\ell}\exp(u_k^j\alpha\hat{a}^\dagger) \tag{85}$$

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

$$\sum_{j=0}^{k-1}u_k^{-j\ell}\exp(u_k^j\alpha\hat{a}^\dagger) = \sum_{N=0}^{\infty}\frac{1}{N!}\left(\sum_{j=0}^{k-1}u_k^{j(N-\ell)}\right)(\alpha\hat{a}^\dagger)^N \tag{86}$$

implies the desired Eq. (85) because

$$\sum_{j=0}^{k-1}u_k^{j(N-\ell)} = \begin{cases} k & \text{if } N-\ell = kn \text{ for some integer } n \\ 0 & \text{otherwise}\end{cases} \tag{87}$$

thanks to properties of roots of unity, u_k.

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

$$\begin{aligned}|\alpha, k\rangle &= \sum_{\ell=0}^{k-1}C_\ell\frac{\sqrt{\ell!}}{\alpha^\ell}\frac{1}{k}\sum_{j=0}^{k-1}u_k^{-jl}\exp(u_k^j\alpha\hat{a}^\dagger)|0\rangle \\ &= \frac{1}{k}e^{\frac{1}{2}|\alpha|^2}\sum_{j=0}^{k-1}D_j|u_k^j\alpha\rangle\end{aligned} \tag{88}$$

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

$$D_j = \sum_{\ell=0}^{k-1}\frac{\sqrt{\ell!}}{\alpha^\ell}u_k^{-j\ell}C_\ell. \tag{89}$$

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 (88) 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 (88), 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 kth 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 [42], these generalized coherent states are the same as those introduced by Titulaer and Glauber in [33]; see also [43]. However, to the best of our knowledge, the relation to saturated uncertainty relations and energy eigenstates is new.

IV. ANHARMONIC OSCILLATORS

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

A. 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:

$$T_{m+2,n} + T_{m,n+2} - \frac{n(n-1)}{4} T_{m,n-2} - \frac{m(m-1)}{4} T_{m-2,n} - 2\lambda T_{m,n} + \epsilon\left(2\hat{T}_{m+4,n} - 3n(n-1)T_{m+2,n-2} + \frac{1}{8}n(n-1)(n-2)(n-3)T_{m,n-4}\right) = 0 \tag{90}$$

and

$$m\hat{T}_{m-1,n+1} = n\hat{T}_{m+1,n-1} + \epsilon(4n\hat{T}_{m+3,n-1} - n(n-1)(n-2)T_{m+1,n-3}). \tag{91}$$

Setting $n = 0$ in (90) and $n = 1$ in (91) while shifting m to $m + 1$, and combining to eliminate $T_{m,2}$ gives

$$\frac{(m+2)}{(m+1)} T_{m+2,0} - 2\lambda T_{m,0} - \frac{m(m-1)}{4} T_{m-2,0} + 2\epsilon\frac{(m+3)}{(m+1)} T_{m+4,0} = 0. \tag{92}$$

Then using (91) with n shifted to $n + 1$ and m to $m - 1$ results in

$$T_{m-2,n+2} = \frac{(n+1)}{(m-1)} T_{m,n} + \epsilon\left(4\frac{(n+1)}{(m-1)} T_{m+2,n} - \frac{(n+1)(n)(n-1)}{(m-1)} T_{m,n-2}\right). \tag{93}$$

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

$$T_{m,n} = \sum_k T^{(k)}_{m,n}\epsilon^k \tag{94}$$

and similarly for the eigenvalues,

$$\lambda = \sum_k \lambda_{(k)}\epsilon^k. \tag{95}$$

Using Eqs. (92)–(95), 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):

$$T^{(0)}_{\text{odd,odd}} = T^{(0)}_{\text{odd,even}} = T^{(0)}_{\text{even,odd}} = 0. \tag{96}$$

Then setting $m = 0$ and $n = 1$ in (91) gives $T^{(1)}_{1,0} = 0$. Using this and (92) with m odd gives $T^{(1)}_{\text{odd},0} = 0$. Taking $n = 0$ in (91) gives $T_{m,1} = 0$ at all orders in ϵ. Combining these two results with (93) implies that the rest of the odd moments vanish:

$$T^{(1)}_{\text{odd,odd}} = T^{(1)}_{\text{odd,even}} = T^{(1)}_{\text{even,odd}} = 0. \tag{97}$$

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 Sec. II, we find to first order in ϵ

$$\det(A'_1) = \left(\lambda_{(0)} - \frac{1}{2}\right)\left(\lambda_{(0)} + \frac{1}{2}\right) - \frac{1}{4}\epsilon\lambda_{(0)}(12\lambda^2_{(0)} - 8\lambda_{(1)} + 3) + O(\epsilon^2), \tag{98}$$

$$\det(A'_2) = \frac{1}{4}\left(\lambda_{(0)} - \frac{3}{2}\right)\left(\lambda_{(0)} - \frac{1}{2}\right)\left(\lambda_{(0)} + \frac{1}{2}\right)\left(\lambda_{(0)} + \frac{3}{2}\right) - \frac{1}{32}\epsilon\lambda_{(0)}(80\lambda^4_{(0)} - 32(\lambda_{(1)} + 4)\lambda^2_{(0)} + 40\lambda_{(1)} + 3) + O(\epsilon^2). \tag{99}$$

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

$$\det(A_1') = \epsilon\left(\lambda_{(1)} - \frac{3}{4}\right) + O(\epsilon^2), \tag{100}$$

$$\det(A_2') = \epsilon\left(\frac{3}{8} - \frac{1}{2}\lambda_{(1)}\right) + O(\epsilon^2). \tag{101}$$

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

$$E_0 = \frac{1}{2} + \frac{3}{4}\epsilon + O(\epsilon^2), \tag{102}$$

$$E_1 = \frac{3}{2} + \frac{15}{4}\epsilon + O(\epsilon^2) \tag{103}$$

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.

B. Commutator method

An alternative route to perturbated eigenvalues, which may sometimes be more feasible, proceeds by applying suitable commutator relationships. Following [7], 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

$$[\hat{H}, \hat{W}_1] = -i\hbar\frac{k-2}{m}\hat{q}^{k-3}\hat{p} - \hbar^2\frac{(k-2)(k-3)}{2m}\hat{q}^{k-4}, \tag{104}$$

$$[\hat{H}, \hat{W}_2] = -2i\hbar(k-1)\hat{q}^{k-2}(\hat{H} - V(\hat{q})) - \hbar^2\frac{(k-1)(k-2)}{2m}\hat{q}^{k-3}\hat{p} + i\hbar\hat{q}^{k-1}V'(\hat{q}). \tag{105}$$

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

$$0 = -2(k-1)E_n\langle\hat{q}^{k-2}\rangle_n + 2(k-1)\langle\hat{q}^{k-2}V(\hat{q})\rangle_n - \hbar^2\frac{(k-1)(k-2)(k-3)}{4m}\langle\hat{q}^{k-4}\rangle_n + \langle\hat{q}^{k-1}V'(\hat{q})\rangle_n. \tag{106}$$

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

$$0 = -2(k-1)E_n\langle\hat{q}^{k-2}\rangle_n - (k-1)(k-2)(k-3)\frac{\hbar^2}{4m}\langle\hat{q}^{k-4}\rangle_n + m\omega^2k\langle\hat{x}^k\rangle_n + 2\epsilon(k+1)\langle\hat{q}^{k+2}\rangle_n. \tag{107}$$

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

$$0 = m\omega^2\langle\hat{q}\rangle_n + 4\epsilon\langle\hat{q}^3\rangle_n, \tag{108}$$

$$0 = -2E_n + 2m\omega^2\langle\hat{q}^2\rangle_n + 6\epsilon\langle\hat{q}^4\rangle_n, \tag{109}$$

$$0 = -4E_n\langle\hat{q}\rangle_n + 3m\omega^2\langle\hat{q}^3\rangle_n + 8\epsilon\langle\hat{q}^5\rangle_n, \tag{110}$$

$$0 = -6E_n\langle\hat{q}^2\rangle_n - \frac{3\hbar^2}{2m} + 4m\omega^2\langle\hat{q}^4\rangle_n + 10\epsilon\langle\hat{q}^6\rangle_n. \tag{111}$$

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 (108), which implies $\langle\hat{q}^3\rangle_{n,0} = 0$ from (110), such that $\langle\hat{q}\rangle_{n,1} = 0$ from (108).

For even powers, $\langle\hat{q}^2\rangle_{n,0} = E_n/m\omega^2$ from (109) 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 (111). This value then appears in $\langle\hat{q}^2\rangle_{n,1} = -3\langle\hat{x}^4\rangle_{n,0}/m\omega^2$ from (109). We obtain some of the moments including $\hat{p}$ from (104) and (105). Setting $k = 4$ in (104) shows that $\langle\hat{q}\,\hat{p} + \hat{p}\,\hat{q}\rangle_n = 0$ in all energy eigenstates. Setting $k = 2$ in (105) and *not* using $\hat{H}|n\rangle = E_n$ implies

$$\langle\hat{p}^2\rangle_n = m\langle\hat{q}V'(\hat{q})\rangle_n = m^2\omega^2\langle\hat{q}^2\rangle_n + 4m\epsilon\langle\hat{q}^4\rangle_n, \tag{112}$$

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

$$\langle\hat{p}^2\rangle_{n,0} = m^2\omega^2\langle\hat{q}^2\rangle_{n,0} = mE_n, \tag{113}$$

$$\langle\hat{p}^2\rangle_{n,1} = m^2\omega^2\langle\hat{q}^2\rangle_{n,1} + 4m\langle\hat{q}^4\rangle_{n,0} = m\langle\hat{q}^4\rangle_{n,0}. \tag{114}$$

To first order in ϵ, we therefore compute

$$\langle\hat{q}^2\rangle_n = \langle\hat{q}^2\rangle_{n,0} + \epsilon\langle\hat{q}^2\rangle_{n,1} + O(\epsilon^2) = \frac{E_n}{m\omega^2} - \frac{9\epsilon}{8m^3\omega^6}(4E_n^2 + \hbar^2\omega^2) + O(\epsilon^2), \tag{115}$$

$$\langle\hat{p}^2\rangle_n = \langle\hat{p}^2\rangle_{n,0} + \epsilon\langle\hat{p}^2\rangle_{n,1} + O(\epsilon^2) = mE_n + \frac{3\epsilon}{8m\omega^4}(4E_n^2 + \hbar^2\omega^2) + O(\epsilon^2). \tag{116}$$

The uncertainty relation implies

$$\langle\hat{q}^2\rangle_n\langle\hat{p}^2\rangle_n = \frac{E_n^2}{\omega^2} - \frac{3\epsilon E_n}{4m^2\omega^6}(4E_n^2 + \hbar^2\omega^2) + O(\epsilon^2) \geq \frac{\hbar^2}{4}. \tag{117}$$

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

$$E_n \geq \frac{1}{2}\hbar\omega + \frac{3}{4}\frac{\epsilon\hbar^2}{m^2\omega^2} + O(\epsilon^2). \tag{118}$$

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.

V. 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 Sec. II, an algebraic derivation of eigenvalues imposes two conditions, Eq. (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 nonconstant 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 [32].

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 Sec. III 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 (11), or

$$\langle \hat{A}(\hat{H} - \lambda\mathbb{I})\rangle_\lambda = 0, \tag{119}$$

for an eigenstate $|\rangle_\lambda$ with eigenvalue λ, which has to be satisfied for all algebra elements $\hat{A}$. In particular, the definition is tailored 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 (119), we obtain the equation

$$\mathrm{Im}\langle \hat{q}(\hat{p} - \lambda\mathbb{I})\rangle = \frac{1}{2i}\langle[\hat{q}, \hat{p}]\rangle = \frac{1}{2}\hbar \tag{120}$$

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 (119) with $\hat{A} = \mathbb{I}$, and

$$\begin{aligned}\mathrm{Im}\langle \hat{q}\,\hat{p}(\hat{p}^2 - \lambda\mathbb{I})\rangle &= \frac{1}{2i}\langle[\hat{q}, \hat{p}^3] - \lambda[\hat{q}, \hat{p}]\rangle \\ &= \frac{1}{2}\hbar(3\langle\hat{p}^2\rangle - \lambda) = 0\end{aligned} \tag{121}$$

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,

$$\mathrm{Im}\langle \hat{q}(\hat{p}^2 - \lambda\mathbb{I})\rangle = \frac{1}{2i}\langle[\hat{q}, \hat{p}^2]\rangle = \hbar\langle\hat{p}\rangle = 0 \tag{122}$$

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

It is not surprising that an algebraic method 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 nonseparable Hilbert space may lead to a continuous set of eigenvalues for normalizable eigenstates. In this case, (119) 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 (1), 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 nonseparable 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 (119), unless it is strictly discrete. As a consequence, it remains an open question how the continuous spectrum could be defined in nonassociative quantum mechanics.

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APPENDIX: 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

$$[\hat{\xi}^\dagger,\hat{\xi}]_+ = \hbar, [\hat{\xi},\hat{\xi}]_+ = 0 = [\hat{\xi}^\dagger,\hat{\xi}^\dagger]_+. \tag{A1}$$

It generates a four-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

$$\hat{H} = \frac{1}{2}\omega(\hat{\xi}^\dagger\hat{\xi} - \hat{\xi}\hat{\xi}^\dagger) = \omega\hat{\xi}^\dagger\hat{\xi} - \frac{1}{2}\hbar\omega\mathbb{I} = \omega\hat{\xi}\hat{\xi}^\dagger + \frac{1}{2}\hbar\omega\mathbb{I}. \tag{A2}$$

1. Hilbert-space representation

For comparison, we briefly summarize the standard representation on a two-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

$$E_\pm = \pm\frac{1}{2}\hbar\omega. \tag{A3}$$

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

$$||\hat{\xi}|+\rangle||^2 = \langle\hat{\xi}^\dagger\hat{\xi}\rangle_+ = \frac{1}{\omega}\left(E_+ + \frac{1}{2}\hbar\omega\right) = \hbar, \tag{A4}$$

$$||\hat{\xi}|-\rangle||^2 = \langle\hat{\xi}\hat{\xi}^\dagger\rangle_- = \frac{1}{\omega}\left(-E_- - \frac{1}{2}\hbar\omega\right) = \hbar. \tag{A5}$$

A general state can be written as

$$|r,s\rangle = \cos r|-\rangle + e^{is}\sin r|+\rangle, \tag{A6}$$

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

$$\langle\hat{\xi}\rangle(r,s) = \frac{1}{2}\sqrt{\hbar}\sin(2r)e^{is} = \langle\hat{\xi}^\dagger\rangle(r,s)^*, \tag{A7}$$

$$\langle\hat{\xi}^\dagger\hat{\xi}\rangle(r,s) = \hbar\sin^2 r, \tag{A8}$$

$$\langle\hat{\xi}\hat{\xi}^\dagger\rangle(r,s) = \hbar\cos^2 r. \tag{A9}$$

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

$$\langle u|u\rangle = \langle\Delta\hat{\xi}^\dagger\Delta\hat{\xi}\rangle = \Delta(\xi^\dagger\xi) + \frac{1}{2}\hbar, \tag{A10}$$

$$\langle w|w\rangle = \langle\Delta\hat{\xi}\Delta\hat{\xi}^\dagger\rangle = -\Delta(\xi^\dagger\xi) + \frac{1}{2}\hbar, \tag{A11}$$

$$\langle u|w\rangle = \langle\Delta\hat{\xi}^\dagger\Delta\hat{\xi}^\dagger\rangle = 0 \tag{A12}$$

with the (graded) covariance

$$\begin{aligned}\Delta(\xi^\dagger\xi) &= \frac{1}{2}(\langle\hat{\xi}^\dagger\hat{\xi} - \hat{\xi}\hat{\xi}^\dagger\rangle - \langle\hat{\xi}\rangle^*\langle\hat{\xi}\rangle + \langle\hat{\xi}\rangle\langle\hat{\xi}\rangle^*) \\ &= \frac{1}{2}\langle\hat{\xi}^\dagger\hat{\xi} - \hat{\xi}\hat{\xi}^\dagger\rangle - \langle\hat{\xi}\rangle^*\langle\hat{\xi}\rangle.\end{aligned} \tag{A13}$$

Expanding $\Delta\hat{\xi}^\dagger\Delta\hat{\xi}$ in order to express equations such as (A10) 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

$$0 = |\langle u|w\rangle|^2 \le \langle u|u\rangle\langle w|w\rangle = -\Delta(\xi^\dagger\xi)^2 + \frac{1}{4}\hbar^2 \tag{A14}$$

and therefore

$$|\Delta(\xi^\dagger\xi)| \le \frac{1}{2}\hbar. \tag{A15}$$

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

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

$$\{\langle\hat{A}\rangle, \langle\hat{B}\rangle\}_+ = \frac{\langle[\hat{A},\hat{B}]_+\rangle}{i\hbar} \tag{A16}$$

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

$$\{\xi^*,\xi\}_+ = -i, \qquad \{\xi,\xi\}_+ = 0 = \{\xi^*,\xi^*\}_+ \tag{A17}$$

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 nonzero moment:

$$\begin{aligned}\Delta(\xi^\dagger\xi) &= \frac{1}{2}\langle\Delta\hat{\xi}^\dagger\Delta\hat{\xi} - \Delta\hat{\xi}\Delta\hat{\xi}^\dagger\rangle = \langle\Delta\hat{\xi}^\dagger\Delta\hat{\xi}\rangle - \frac{1}{2}\hbar \\ &= -\langle\Delta\hat{\xi}\Delta\hat{\xi}^\dagger\rangle + \frac{1}{2}\hbar,\end{aligned} \tag{A18}$$

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:

$$\dot{\xi} = \frac{\langle[\hat{\xi},\hat{H}]\rangle}{i\hbar} = -i\omega\xi \tag{A19}$$

implies $\xi(t) = \xi_0\exp(-i\omega t)$, or $r(t) = r_0$, $s(t) = s_0 - \omega t$ in the parameerization of (A6). 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,

$$0 = \langle \hat{H} - \lambda \mathbb{I} \rangle = \omega \langle \hat{\xi}^\dagger \hat{\xi} \rangle - \frac{1}{2}\hbar\omega - \lambda = -\omega \langle \hat{\xi}\hat{\xi}^\dagger \rangle + \frac{1}{2}\hbar\omega - \lambda, \tag{A20}$$

$$0 = \langle \hat{\xi}(\hat{H} - \lambda \mathbb{I}) \rangle = \left(\frac{1}{2}\hbar\omega - \lambda\right)\xi, \tag{A21}$$

$$0 = \langle \hat{\xi}^\dagger(\hat{H} - \lambda \mathbb{I}) \rangle = -\left(\frac{1}{2}\hbar\omega + \lambda\right)\xi^*, \tag{A22}$$

$$0 = \langle \hat{\xi}^\dagger \hat{\xi}(\hat{H} - \lambda \mathbb{I}) \rangle = \left(\frac{1}{2}\hbar\omega - \lambda\right)\langle \hat{\xi}^\dagger \hat{\xi} \rangle = \frac{\frac{1}{4}\hbar^2\omega^2 - \lambda^2}{\omega}, \tag{A23}$$

$$0 = \langle \hat{\xi}\hat{\xi}^\dagger(\hat{H} - \lambda \mathbb{I}) \rangle = -\left(\frac{1}{2}\hbar\omega + \lambda\right)\langle \hat{\xi}\hat{\xi}^\dagger \rangle = -\frac{\frac{1}{4}\hbar^2\omega^2 - \lambda^2}{\omega} \tag{A24}$$

using the first equation in the last step of (A23) and (A24). The last equation implies $\lambda_\pm = \pm\frac{1}{2}\hbar\omega$. For $\lambda_- = -\frac{1}{2}\hbar\omega$, (A21) implies $\xi = 0$ and (A23) implies $\langle \hat{\xi}^\dagger \hat{\xi} \rangle = 0$, so that $\langle \hat{\xi}\hat{\xi}^\dagger \rangle = \hbar$ from (A20). For $\lambda_+ = \frac{1}{2}\hbar\omega$, (A22) implies $\xi^* = 0$ and (A24) implies $\langle \hat{\xi}\hat{\xi}^\dagger \rangle = 0$, so that $\langle \hat{\xi}^\dagger \hat{\xi} \rangle = \hbar$ from (A20).

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.

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