

Article

Properties of Fluctuating States in Loop Quantum Cosmology

Martin Bojowald

Institute for Gravitation and the Cosmos, The Pennsylvania State University, 104 Davey Lab,
University Park, PA 16802, USA; bojowald@gravity.psu.edu

Received: 7 June 2019; Accepted: 16 July 2019; Published: 19 July 2019



Abstract: In loop quantum cosmology, the values of volume fluctuations and correlations determine whether the dynamics of an evolving state exhibits a bounce. Of particular interest are states that are supported only on either the positive or the negative part of the spectrum of the Hamiltonian that generates this evolution. It is shown here that the restricted support on the spectrum does not significantly limit the possible values of volume fluctuations.

Keywords: loop quantum cosmology; positive spectrum; fluctuations

1. Introduction

A solvable model [1] that captures basic features of classical and quantum cosmology is given by two canonical variables, Q and P with Poisson bracket $\{Q, P\} = 1$, and a one-parameter family of Hamiltonians, $H_\delta = |Q \sin(\delta P)|/\delta$ with $\delta \geq 0$. In the limit $\delta \rightarrow 0$, $H_0 = |QP|$ is quadratic up to the absolute value, and a system close to an upside-down harmonic oscillator is obtained. Since QP and therefore $\text{sgn}(QP)$ is preserved by equations of motion generated by the auxiliary Hamiltonian $H'_0 = QP$, the set of regular solutions (such that $QP \neq 0$) of the classical H_0 -system is given by the union of two disjoint sets: solutions of the H'_0 -system with initial values $Q(0), P(0)$ such that $\text{sgn}(Q(0)P(0)) = 1$, and solutions of the $-H'_0$ -system with initial values $Q(0), P(0)$ such that $\text{sgn}(Q(0)P(0)) = -1$. All classical solutions can therefore be obtained from a quadratic Hamiltonian.

For $\delta \neq 0$, $H_\delta = |\text{Im}J_\delta|/\delta$ is, up to the absolute value, linear in $J_\delta := Q \exp(i\delta P)$, whose real and imaginary parts, together with Q , are generators of the $\text{sl}(2, \mathbb{R})$ algebra

$$\{Q, \text{Re}J_\delta\} = -\delta \text{Im}J_\delta \quad , \quad \{Q, \text{Im}J_\delta\} = \delta \text{Re}J_\delta \quad , \quad \{\text{Re}J_\delta, \text{Im}J_\delta\} = \delta Q. \quad (1)$$

Again, introducing an auxiliary Hamiltonian $H'_\delta = \text{Im}J_\delta/\delta$, all regular solutions (such that $\text{Im}J_\delta \neq 0$) of the H_δ -system can be obtained from solutions of the $\pm H'_\delta$ -systems with suitable initial values.

In a simple cosmological interpretation, $|Q| = V/4\pi G$ is proportional to the volume V of an expanding or collapsing universe, while P is the (negative) Hubble parameter. According to the Friedmann equation of classical cosmology for flat spatial slices, which reads

$$P^2 = \frac{8\pi G}{3} \rho \quad (2)$$

in our canonical variables with the matter energy density ρ , $H_0 = |QP|$ can, up to a numerical factor, be interpreted as the momentum canonically conjugate to a free, massless scalar source ϕ , whose energy

density is $\rho = \frac{1}{2} p_\phi^2 / V^2$ with the momentum p_ϕ canonically conjugate to ϕ . In quantum cosmology, it is common to describe time dependence not with respect to a coordinate such as proper time, but rather with respect to one of the degrees of freedom of the model, such as ϕ [2]. Solutions $Q(\phi)$ and $P(\phi)$ of Hamilton’s equations of motion generated by $\pm H_0 \propto p_\phi$ therefore describe how Q and P change in relation to the “internal time” ϕ . If $\delta \neq 0$, H_δ can still be interpreted in this way, but only if the Friedmann equation is modified such that P^2 is replaced by $\sin^2(\delta P) / \delta^2$. This modification may be motivated by the appearance of holonomies in loop quantum gravity [3,4] and loop quantum cosmology [5], and is supposed to describe an implication of quantum geometry. (If a Taylor expansion of $\sin^2(\delta P) / \delta^2$ is used, higher-order terms in P , proportional to the Hubble parameter, can be interpreted as a specific form of higher-curvature corrections suggested by the theory.)

Replacing the unbounded function P^2 with a bounded function $\sin^2(\delta P) / \delta^2$, still proportional to the energy density of a matter source, suggests that the classical big-bang singularity, at which the energy density diverges, could be avoided by quantum-geometry effects [6]. Indeed, solutions for $Q(\phi)$ of equations of motion generated by $\pm H'_\delta$,

$$\frac{dQ}{d\phi} = \pm \text{Re}J_\delta(\phi) \quad , \quad \frac{d\text{Re}J_\delta}{d\phi} = \pm Q(\phi) \quad , \tag{3}$$

are superpositions of real exponential functions. If the condition $Q^2 - |J_\delta|^2 = 0$ is imposed, which ensures that P in the definition of J_δ is real, the equation

$$Q^2 - (\text{Re}J_\delta)^2 = (\text{Im}J_\delta)^2 = (\delta H'_\delta)^2 > 0 \quad , \tag{4}$$

which is by definition positive for regular solutions, implies that $Q(\phi)$ must be cosh-like and $\text{Re}J_\delta(\phi)$ sinh-like. The eternally collapsing behavior of the volume $Q(\phi)$ approaching zero if $\delta = 0$, $Q(\phi) = Q(0) \exp(\pm\phi)$, is then replaced by a “bounce” at the non-zero minimum of cosh.

The preceding argument ignores quantum fluctuations, which may be expected to be significant in a discussion of big-bang solutions. If $(\Delta Q)^2$ is large, it could conceivably change the balance of signs in Equation (4), in which $\langle \hat{Q}^2 \rangle = \langle \hat{Q} \rangle^2 + (\Delta Q)^2$ would take the place of Q^2 . For states with $(\Delta Q)^2 \geq (\delta H'_\delta)^2 + (\Delta \text{Re}J_\delta)^2$, the right-hand side of Equation (4), written for expectation values, is no longer positive, and $\langle \hat{Q} \rangle(\phi)$ would not be cosh-like. The possibility of such non-bouncing solutions in loop quantum cosmology has been demonstrated using canonical effective methods [7], in particular for small $\delta H'_\delta$ relevant for an understanding of generic spacelike singularities [8,9].

However, for quantum states, the absolute value in H_δ has to be treated with greater care than in the case of classical solutions. Solutions of quantum evolution generated by an operator \hat{H}_δ via a Schrödinger equation for wave functions can be expressed as superpositions of solutions of quantum evolution generated by an operator \hat{H}'_δ , provided the latter are supported solely on the positive or negative part of the spectrum of \hat{H}'_δ . (See Section 2.3 below for a demonstration.) This condition is a straightforward replacement of the classical restriction on initial values. However, it may have more significant ramifications, in particular when quantum fluctuations are taken into account that may be larger than the expectation value $\langle \hat{H}_\delta \rangle$, as required to change the signs in Equation (4). A state that is supported only on the positive part of the spectrum of \hat{H}'_δ and has an expectation value of $|\hat{H}'_\delta|$ close to zero may not have arbitrarily large fluctuations of \hat{H}'_δ . The question to be addressed in this paper is whether this restriction also limits the size of fluctuations of \hat{Q} .

2. Eigenstates

We first determine the spectra of \hat{H}'_0 and \hat{H}'_δ and then discuss relevant properties of states obtained from superpositions of their positive parts.

2.1. Eigenstates of \hat{H}'_0

We use the symmetric ordering

$$\hat{H}'_0 = \frac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q}) \tag{5}$$

to quantize $H'_0 = QP$ on the standard L^2 -Hilbert space. Eigenstates of this operator in the Q and P -representations are determined by the same type of first-order differential equation,

$$Q \frac{d\psi_\lambda(Q)}{dQ} + \frac{1}{2}\psi_\lambda(Q) = i\frac{\lambda}{\hbar}\psi_\lambda(Q) \tag{6}$$

in the Q -representation, and

$$P \frac{d\phi_\lambda(P)}{dP} + \frac{1}{2}\phi_\lambda(P) = -i\frac{\lambda}{\hbar}\phi_\lambda(P) \tag{7}$$

in the P -representation. For every λ , there are in each representation two orthogonal solutions $\psi_{\lambda\pm}(Q)$ and $\phi_{\lambda\pm}(P)$, respectively, given by

$$\psi_{\lambda+}(Q) = \begin{cases} 0 & \text{if } Q \leq 0 \\ c_{\lambda+}Q^{i\lambda/\hbar-1/2} & \text{if } Q > 0 \end{cases} \tag{8}$$

$$\psi_{\lambda-}(Q) = \begin{cases} c_{\lambda-}(-Q)^{i\lambda/\hbar-1/2} & \text{if } Q < 0 \\ 0 & \text{if } Q \geq 0 \end{cases} \tag{9}$$

$$\phi_{\lambda+}(P) = \begin{cases} 0 & \text{if } P \leq 0 \\ d_{\lambda+}P^{-i\lambda/\hbar-1/2} & \text{if } P > 0 \end{cases} \tag{10}$$

$$\phi_{\lambda-}(P) = \begin{cases} d_{\lambda-}(-P)^{-i\lambda/\hbar-1/2} & \text{if } P < 0 \\ 0 & \text{if } P \geq 0 \end{cases} \tag{11}$$

It is obvious that ψ_{λ_1+} and ψ_{λ_2-} are orthogonal to each other for any λ_1 and λ_2 , and so are ϕ_{λ_1+} and ϕ_{λ_2-} . Moreover,

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_{\lambda_1\pm}^*(Q)\psi_{\lambda_2\pm}(Q)dQ &= c_{\lambda_1\pm}c_{\lambda_2\pm} \int_0^{\infty} q^{i(\lambda_2-\lambda_1^*)/\hbar} \frac{dq}{q} \\ &= c_{\lambda_1\pm}c_{\lambda_2\pm} \int_{-\infty}^{\infty} \exp(ix(\lambda_2 - \lambda_1^*)/\hbar)dx \\ &= \begin{cases} 2\pi\hbar c_{\lambda_1\pm}c_{\lambda_2\pm}\delta(\lambda_2 - \lambda_1^*) & \text{if } \lambda_2 - \lambda_1^* \in \mathbb{R} \\ \infty & \text{otherwise} \end{cases} \end{aligned} \tag{12}$$

and

$$\begin{aligned}
 \int_{-\infty}^{\infty} \phi_{\lambda_1\pm}^*(P)\phi_{\lambda_2\pm}(P)dP &= d_{\lambda_1\pm}d_{\lambda_2\pm} \int_0^{\infty} p^{-i(\lambda_2-\lambda_1^*)/\hbar} \frac{dp}{p} \\
 &= d_{\lambda_1\pm}d_{\lambda_2\pm} \int_{-\infty}^{\infty} \exp(-iy(\lambda_2 - \lambda_1^*)/\hbar)dy \\
 &= \begin{cases} 2\pi\hbar d_{\lambda_1\pm}d_{\lambda_2\pm}\delta(\lambda_2 - \lambda_1^*) & \text{if } \lambda_2 - \lambda_1^* \in \mathbb{R} \\ \infty & \text{otherwise} \end{cases} \tag{13}
 \end{aligned}$$

where the substitutions $q = |Q|$, $x = \log q$, $p = |P|$ and $y = \log p$ have been used. For real λ , all eigenstates are delta-function normalizable, fixing the coefficients $c_{\lambda\pm} = 1/\sqrt{2\pi\hbar} = d_{\lambda\pm}$. The spectrum of \hat{H}'_0 is therefore real, continuous, and twofold degenerate.

2.2. Eigenstates of \hat{H}'_{δ}

For $\delta \neq 0$, the Hamiltonian is periodic in P with period $2\pi/\delta$. To be specific, we will assume that the basic operators are represented on a separable Hilbert space of square-integrable functions periodic in P , such that \hat{Q} has a discrete spectrum given by $\hbar\delta\mathbb{Z}$. Inequivalent representations, such as states which are periodic only up to a phase factor $\exp(i\epsilon)$, for which the spectrum of \hat{Q} is shifted by $\hbar\epsilon$, or non-separable Hilbert spaces as used often in loop quantum cosmology [10], would not change our results. In the Q -representation, our states therefore obey an ℓ^2 inner product such that

$$(\psi_1, \psi_2) = \sum_{n=-\infty}^{\infty} \psi_1(n\hbar\delta)^* \psi_2(n\hbar\delta). \tag{14}$$

We write \hat{H}'_{δ} as

$$\hat{H}'_{\delta} = \frac{\text{Im}\hat{J}_{\delta}}{\delta} = \frac{1}{2i\delta} (\hat{J}_{\delta} - \hat{J}_{\delta}^{\dagger}) = \frac{1}{2i\delta} (\hat{Q} \exp(i\delta\hat{P}) - \exp(-i\delta\hat{P})\hat{Q}). \tag{15}$$

Since $\exp(i\delta\hat{P})$ is a translation operator in the Q -representation, eigenstates of \hat{H}'_{δ} in this representation are determined by a difference equation

$$(Q + \hbar\delta)\psi_{\lambda}(Q + \hbar\delta) + 2i\delta\lambda\psi_{\lambda}(Q) - Q\psi_{\lambda}(Q - \hbar\delta) = 0 \tag{16}$$

where Q takes the values $n\hbar\delta$ with integer n . This equation with non-constant coefficients does not have straightforward solutions. It is, however, possible to show that eigenstates obey a similar twofold degeneracy as in the case of \hat{H}'_0 :

Lemma 1. For given λ , there are two orthogonal solutions $\psi_{\lambda\pm}$, one of which is supported on positive values of Q (and $Q = 0$), and one on negative values of Q . They are related by

$$\psi_{\lambda\pm}(Q) = \psi_{\lambda\mp}(-Q - \hbar\delta). \tag{17}$$

Proof. Let us first look for solutions such that $\psi_{\lambda+}(-\hbar\delta) = 0$. Using the Equation (16) for $Q = -\hbar\delta$, we obtain $\psi_{\lambda+}(-2\hbar\delta) = 2i(\lambda/\hbar)\psi_{\lambda+}(-\hbar\delta) = 0$. Moreover, if $\psi_{\lambda+}(-(n-1)\hbar\delta) = 0$ and $\psi_{\lambda+}(-n\hbar\delta) = 0$, using the equation for $Q = -n\hbar\delta$ shows that $\psi_{\lambda+}(-(n+1)\hbar\delta) = 0$. By induction, $\psi_{\lambda+}(Q) = 0$ for all integer $Q/\hbar\delta < 0$. However, if $\psi_{\lambda+}(0) \neq 0$ for such a solution, $\psi_{\lambda+}(\hbar\delta) = -2i(\lambda/\hbar)\psi_{\lambda+}(0) \neq 0$, using

Equation (16) for $Q = 0$. The solution therefore is not identically zero, and it is unique up to multiplication with a constant $\psi_{\lambda+}(0)$.

A similar line of arguments, starting with the assumption that $\psi_{\lambda-}(0) = 0$, implies that $\psi_{\lambda-}(Q) = 0$ for all integer $Q/\hbar\delta \geq 0$, while assuming $\psi_{\lambda-}(-\hbar\delta) \neq 0$ guarantees that the solution is not identically zero. Since the supports of any ψ_{λ_1+} and ψ_{λ_2-} are disjoint, the two states are orthogonal with respect to the inner product (14).

Substituting $-Q - \hbar\delta$ for Q in Equation (16), we obtain the equation

$$\begin{aligned} 0 &= -Q\psi_{\lambda}(-Q) + 2i\delta\lambda\psi_{\lambda}(-Q - \hbar\delta) + (Q + \hbar\delta)\psi_{\lambda}(-Q - 2\hbar\delta) = 0 \\ &= -Q\bar{\psi}(Q - \hbar\delta) + 2i\delta\lambda\bar{\psi}(Q) + (Q + \hbar\delta)\bar{\psi}(Q + \hbar\delta) \end{aligned} \tag{18}$$

equivalent to Equation (16). The definition $\bar{\psi}(Q) = \psi(-Q - \hbar\delta)$ introduced in the second line maps a function ψ supported on non-negative integers (times $\hbar\delta$) to a function $\bar{\psi}$ supported on negative integers (times $\hbar\delta$), and vice versa. Applied to solutions of Equation (16), it therefore maps $\psi_{\lambda\pm}$ to $\psi_{\lambda\mp}$. \square

In the P -representation, eigenstates of Equation (15) obey the first-order differential equation

$$\sin(\delta P) \frac{d\psi_{\lambda\pm}(P)}{dP} + \frac{1}{2}\delta \exp(i\delta P)\psi_{\lambda\pm}(P) = -i\frac{\lambda\delta}{\hbar}\psi_{\lambda\pm}(P). \tag{19}$$

This equation is solved by

$$\psi_{\lambda+}(P) = \begin{cases} 0 & \text{if } \pi \leq \delta P \leq 2\pi \\ \sqrt{\frac{\delta}{2\pi\hbar}} \frac{(\cot(\delta P/2))^{i\lambda/\hbar}}{\sqrt{\sin(\delta P)}} \exp(-i\delta P/2) & \text{if } 0 < \delta P < \pi \end{cases} \tag{20}$$

$$\psi_{\lambda-}(P) = \begin{cases} \sqrt{\frac{\delta}{2\pi\hbar}} \frac{(-\cot(\delta P/2))^{i\lambda/\hbar}}{\sqrt{-\sin(\delta P)}} \exp(-i\delta P/2) & \text{if } \pi < \delta P < 2\pi \\ 0 & \text{if } 0 \leq \delta P \leq \pi \end{cases}. \tag{21}$$

The substitution $x = \log|\cot(\delta P/2)|$ shows that these states are delta-function normalized. The spectrum therefore has the same properties as in the case of \hat{H}'_0 , being real, continuous, and twofold degenerate.

2.3. Existence of Positive-Energy Solutions with Large Fluctuations

For any δ , completeness of the eigenstates of a self-adjoint operator shows that any state $\psi(Q)$ has an expansion of the form

$$\psi(Q) = \frac{1}{\sqrt{2}} \left(\int_{-\infty}^{\infty} c_{\lambda+} \psi_{\lambda+}(Q) d\lambda + \int_{-\infty}^{\infty} c_{\lambda-} \psi_{\lambda-}(Q) d\lambda \right) \tag{22}$$

in terms of eigenstates of \hat{H}'_{δ} , for some $c_{\lambda\pm}$ normalized such that $\int_{-\infty}^{\infty} |c_{\lambda\pm}|^2 d\lambda = 1$. It evolves according to

$$\psi(Q, \phi) = \frac{1}{\sqrt{2}} \left(\int_{-\infty}^{\infty} c_{\lambda+} \exp(-i\lambda\phi/\hbar) \psi_{\lambda+}(Q) d\lambda + \int_{-\infty}^{\infty} c_{\lambda-} \exp(-i\lambda\phi/\hbar) \psi_{\lambda-}(Q) d\lambda \right). \tag{23}$$

The actual dynamics in our models of interest is generated by the Hamiltonian $\hat{H}_\delta = |\hat{H}'_\delta|$. This operator has the same eigenstates $\psi_{\lambda\pm}(Q)$, but with eigenvalues $|\lambda|$. Its spectrum is therefore four-fold degenerate and positive. Dynamical solutions in these models are given by

$$\psi(Q, \phi) = \frac{1}{\sqrt{2}} \left(\int_{-\infty}^{\infty} c_{\lambda+} \exp(-i|\lambda|\phi/\hbar) \psi_{\lambda+}(Q) d\lambda + \int_{-\infty}^{\infty} c_{\lambda-} \exp(-i|\lambda|\phi/\hbar) \psi_{\lambda-}(Q) d\lambda \right). \tag{24}$$

The decomposition $\psi(Q, \phi) = \frac{1}{\sqrt{2}} (N_- \psi_-(Q, \phi) + N_+ \psi_+(Q, \phi))$ with

$$\psi_-(Q, \phi) = \frac{1}{N_-} \left(\int_{-\infty}^0 c_{\lambda+} \exp(i\lambda\phi/\hbar) \psi_{\lambda+}(Q) d\lambda + \int_{-\infty}^0 c_{\lambda-} \exp(i\lambda\phi/\hbar) \psi_{\lambda-}(Q) d\lambda \right) \tag{25}$$

and

$$\psi_+(Q, \phi) = \frac{1}{N_+} \left(\int_0^{\infty} c_{\lambda+} \exp(-i\lambda\phi/\hbar) \psi_{\lambda+}(Q) d\lambda + \int_0^{\infty} c_{\lambda-} \exp(-i\lambda\phi/\hbar) \psi_{\lambda-}(Q) d\lambda \right), \tag{26}$$

where $N_-^2 = \int_{-\infty}^0 (|c_{\lambda+}|^2 + |c_{\lambda-}|^2) d\lambda$ and $N_+^2 = \int_0^{\infty} (|c_{\lambda+}|^2 + |c_{\lambda-}|^2) d\lambda$ such that $N_-^2 + N_+^2 = 2$, demonstrates the claim about solutions made in the introduction.

The decomposition into positive-energy solutions ψ_+ and negative-energy solutions ψ_- simply rewrites generic wave functions and does not restrict their fluctuations of Q or P . However, it is sometimes preferred [11] (although not required [12]) to discard negative-energy solutions and consider only positive-energy solutions ψ_+ (or vice versa, but no superpositions of solutions with opposite signs of the energy). A question of interest in quantum cosmology is whether this restriction in any way limits the possible magnitude of fluctuations of Q or P , which would then have consequences for bouncing or non-bouncing behavior according to Bojowald [7]. Using the spectral properties derived in the preceding section, we now show that this is not the case.

In particular, for potential non-bouncing behavior, we are interested in solutions with small $\langle \hat{H}_\delta \rangle$, such that

$$\delta^2 \langle \hat{H}_\delta \rangle^2 + \delta^2 (\Delta H_\delta)^2 \leq (\Delta Q)^2 - (\Delta \text{Re} J_\delta)^2. \tag{27}$$

If $\langle \hat{H}_\delta \rangle$ is small, given the positivity of the spectrum of \hat{H}_δ , the range of possible values of ΔH_δ seems to be limited because the state in the λ -representation can spread out only to one side of $\langle \hat{H}_\delta \rangle$. However, the twofold degeneracy of the spectrum of \hat{H}'_δ , of the specific form derived in the preceding section, in particular in Lemma 1, shows that there is no such limitation for fluctuations ΔQ even if $\langle \hat{Q} \rangle$ is required to be small: In order to construct a state, supported only on the positive part of the spectrum of \hat{H}'_δ , such that it has a small expectation value and large fluctuations of \hat{Q} , we choose some c_λ such that $\int_0^\infty |c_\lambda|^2 d\lambda = 1$, and define $\psi_{c+}(Q) = \int_0^\infty c_\lambda \psi_{\lambda+}(Q) d\lambda$. This state is supported on the positive part of the spectrum of \hat{H}'_δ , by construction, and has a certain expectation value $\langle \hat{Q} \rangle_{c+} > 0$ and fluctuations $\Delta_{c+} Q > 0$. Similarly, the state $\psi_{c-}(Q) = \int_0^\infty c_\lambda \psi_{\lambda-}(Q) d\lambda$, using the transformation in Equation (17), has expectation value $\langle \hat{Q} \rangle_{c-} = -\langle \hat{Q} \rangle_{c+} - \hbar\delta < 0$ and fluctuations $\Delta_{c-} Q = \Delta_{c+} Q > 0$. The state

$$\psi_c = \frac{1}{\sqrt{2}} \int_0^\infty c_\lambda \left(\alpha \psi_{\lambda+}(Q) + \sqrt{2 - \alpha^2} \psi_{\lambda-}(Q) \right) d\lambda, \tag{28}$$

with some $|\alpha| \leq \sqrt{2}$, then has expectation value

$$\langle \hat{Q} \rangle = \frac{1}{2} \left(\alpha^2 \langle \hat{Q} \rangle_{c+} + (2 - \alpha^2) \langle \hat{Q} \rangle_{c-} \right) = (\alpha^2 - 1) \langle \hat{Q} \rangle_{c+} - \frac{2 - \alpha^2}{2} \hbar\delta \tag{29}$$

and fluctuations given by

$$\begin{aligned}
 (\Delta Q)^2 &= \frac{1}{2} \left(\alpha^2 \langle \hat{Q}^2 \rangle_{c+} + (2 - \alpha^2) \langle \hat{Q}^2 \rangle_{c-} \right) - \langle \hat{Q} \rangle^2 \\
 &= (\Delta_{c+} Q)^2 + \frac{1}{2} \left(\alpha^2 \langle \hat{Q} \rangle_{c+}^2 + (2 - \alpha^2) \langle \hat{Q} \rangle_{c-}^2 \right) \\
 &\quad - (\alpha^2 - 1)^2 \langle \hat{Q} \rangle_{c+}^2 + (2 - \alpha^2)(\alpha^2 - 1) \hbar \delta \langle \hat{Q} \rangle_{c+} - \frac{(2 - \alpha^2)^2}{4} \hbar^2 \delta^2 \\
 &= (\Delta_{c+} Q)^2 + \alpha^2 (2 - \alpha^2) \left(\langle \hat{Q} \rangle_{c+} + \frac{1}{2} \hbar \delta \right)^2.
 \end{aligned} \tag{30}$$

For $\alpha \neq 1$, the result can also be written as

$$(\Delta Q)^2 = (\Delta_{c+} Q)^2 + \frac{\alpha^2 (2 - \alpha^2)}{(\alpha^2 - 1)^2} \left(\langle \hat{Q} \rangle + \frac{1}{2} \hbar \delta \right)^2 \tag{31}$$

using

$$(\alpha^2 - 1) \left(\langle \hat{Q} \rangle_{c+} + \frac{1}{2} \hbar \delta \right)^2 = \left(\langle \hat{Q} \rangle + \frac{1}{2} \hbar \delta \right)^2. \tag{32}$$

Since $\langle \hat{Q} \rangle_{c+}$ is not restricted by the positivity condition, ΔQ is unlimited even on states with small expectation value $\langle \hat{Q} \rangle$.

3. Moments

Since H'_0 is a function of Q and P , H'_0 -moments in a given state are related to Q and P -moments in the same state. There may therefore be restrictions on the magnitude of Q or P -fluctuations if a state is required to have small $\langle \hat{H}'_0 \rangle$ and small H'_0 -fluctuations. We will now demonstrate that Q and P -fluctuations are indeed restricted in such a state, but only if additional assumptions on the QP -covariance are made.

3.1. Relationships between Moments

Because \hat{H}'_0 is quadratic in \hat{Q} and \hat{P} , $\Delta H'_0$ is related to moments of up to fourth order in Q and P . In the following calculations, we use the notation of Tsobanjan [13], as in

Definition 1. Given a set of operators \hat{A}_i , $i = 1, \dots, n$, and integers $k_1, \dots, k_n \geq 0$ such that $\sum_i k_i \geq 2$, the moments of a state are

$$\Delta(A_1^{k_1} A_2^{k_2} \dots A_n^{k_n}) = \left\langle (\Delta \hat{A}_1)^{k_1} (\Delta \hat{A}_2)^{k_2} \dots (\Delta \hat{A}_n)^{k_n} \right\rangle_{\text{symm}}, \tag{33}$$

where $\Delta \hat{A}_i = \hat{A}_i - \langle \hat{A}_i \rangle$, all expectation values are taken in the given state, and the subscript “symm” indicates that all products of operators are taken in totally symmetric (or Weyl) ordering:

$$\langle \hat{O}_1 \dots \hat{O}_n \rangle_{\text{symm}} = \frac{1}{n!} \sum_{\sigma \in S_n} \left\langle \hat{O}_{\sigma(1)} \dots \hat{O}_{\sigma(n)} \right\rangle. \tag{34}$$

The following reordering relations are useful:

Lemma 2. For two operators \hat{Q} and \hat{P} such that $[\hat{Q}, \hat{P}] = i\hbar$,

$$\langle (\Delta\hat{Q})^2\Delta\hat{P} + 2\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} + \Delta\hat{P}(\Delta\hat{Q})^2 \rangle = 4\Delta(Q^2P) \tag{35}$$

$$\langle (\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q})^2 \rangle = 4\Delta(Q^2P^2) + \hbar^2. \tag{36}$$

Proof. Starting with the left-hand side of Equation (35), we write

$$\begin{aligned} 2\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} &= \frac{4}{3}\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} \\ &+ \frac{1}{3} \left((\Delta\hat{Q})^2\Delta\hat{P} - \Delta\hat{Q}[\Delta\hat{Q}, \Delta\hat{P}] \right) + \frac{1}{3} \left(\Delta\hat{P}(\Delta\hat{Q})^2 + [\Delta\hat{Q}, \Delta\hat{P}]\Delta\hat{Q} \right) \end{aligned}$$

such that

$$\begin{aligned} \langle (\Delta\hat{Q})^2\Delta\hat{P} + 2\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} + \Delta\hat{P}(\Delta\hat{Q})^2 \rangle &= \frac{4}{3} \langle (\Delta\hat{Q})^2\Delta\hat{P} + \Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} + \Delta\hat{P}(\Delta\hat{Q})^2 \rangle \\ &= 4\Delta(Q^2P) \end{aligned}$$

proves Equation (35).

On the left-hand side of Equation (36), we write

$$\begin{aligned} &\langle (\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q})^2 \rangle \\ &= \langle \Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{Q}(\Delta\hat{P})^2\Delta\hat{Q} + \Delta\hat{P}(\Delta\hat{Q})^2\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} \rangle \\ &= \frac{2}{3} \langle \Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q}\Delta\hat{P} + (\Delta\hat{Q})^2(\Delta\hat{P})^2 + \Delta\hat{Q}(\Delta\hat{P})^2\Delta\hat{Q} \\ &\quad + \Delta\hat{P}(\Delta\hat{Q})^2\Delta\hat{P} + (\Delta\hat{P})^2(\Delta\hat{Q})^2 + \Delta\hat{P}\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} \rangle \\ &+ \frac{1}{3} \langle \Delta\hat{Q}[\Delta\hat{P}, \Delta\hat{Q}]\Delta\hat{P} + \Delta\hat{Q}[(\Delta\hat{P})^2, \Delta\hat{Q}] + \Delta\hat{P}[(\Delta\hat{Q})^2, \Delta\hat{P}] + \Delta\hat{P}[\Delta\hat{Q}, \Delta\hat{P}]\Delta\hat{Q} \rangle \end{aligned}$$

using

$$\begin{aligned} \Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q}\Delta\hat{P} &= \frac{2}{3}\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q}\Delta\hat{P} + \frac{1}{3} \left((\Delta\hat{Q})^2(\Delta\hat{P})^2 + \Delta\hat{Q}[\Delta\hat{P}, \Delta\hat{Q}]\Delta\hat{P} \right) \\ \Delta\hat{Q}(\Delta\hat{P})^2\Delta\hat{Q} &= \frac{2}{3}\Delta\hat{Q}(\Delta\hat{P})^2\Delta\hat{Q} + \frac{1}{3} \left((\Delta\hat{Q})^2(\Delta\hat{P})^2 + \Delta\hat{Q}[(\Delta\hat{P})^2, \Delta\hat{Q}] \right) \\ \Delta\hat{P}(\Delta\hat{Q})^2\Delta\hat{P} &= \frac{2}{3}\Delta\hat{P}(\Delta\hat{Q})^2\Delta\hat{P} + \frac{1}{3} \left((\Delta\hat{P})^2(\Delta\hat{Q})^2 + \Delta\hat{P}[(\Delta\hat{Q})^2, \Delta\hat{P}] \right) \\ \Delta\hat{P}\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} &= \frac{2}{3}\Delta\hat{P}\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} + \frac{1}{3} \left((\Delta\hat{P})^2(\Delta\hat{Q})^2 + \Delta\hat{P}[\Delta\hat{Q}, \Delta\hat{P}]\Delta\hat{Q} \right). \end{aligned}$$

Evaluating the commutators and observing

$$\begin{aligned} \Delta(Q^2P^2) &= \frac{1}{6} \langle \Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q}\Delta\hat{P} + (\Delta\hat{Q})^2(\Delta\hat{P})^2 + \Delta\hat{Q}(\Delta\hat{P})^2\Delta\hat{Q} \\ &\quad + \Delta\hat{P}(\Delta\hat{Q})^2\Delta\hat{P} + (\Delta\hat{P})^2(\Delta\hat{Q})^2 + \Delta\hat{P}\Delta\hat{Q}\Delta\hat{P}\Delta\hat{Q} \rangle \end{aligned}$$

we obtain Equation (36). \square

Proposition 1. *If a state is such that it has a vanishing covariance $\Delta(QP) = \frac{1}{2}\langle\hat{Q}\hat{P} + \hat{P}\hat{Q}\rangle - \langle\hat{Q}\rangle\langle\hat{P}\rangle$ and zero skewness (third-order moments), then the relative fluctuations of \hat{Q} and \hat{P} are bounded from above by the relative fluctuation of $\hat{H} = \frac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q})$:*

$$\frac{(\Delta Q)^2}{\langle\hat{Q}\rangle^2} + \frac{(\Delta P)^2}{\langle\hat{P}\rangle^2} < \frac{(\Delta H_0')^2}{\langle\hat{H}_0'\rangle^2}. \tag{37}$$

Proof. Writing operators as $\hat{A} = \Delta\hat{A} + \langle\hat{A}\rangle$ in $\hat{H}_0' = \frac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q})$, we obtain

$$\begin{aligned} \langle\hat{H}_0'\rangle &= \frac{1}{2}\langle(\Delta\hat{Q} + \langle\hat{Q}\rangle)(\Delta\hat{P} + \langle\hat{P}\rangle) + (\Delta\hat{P} + \langle\hat{P}\rangle)(\Delta\hat{Q} + \langle\hat{Q}\rangle)\rangle \\ &= \frac{1}{2}\langle\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q}\rangle + \langle\hat{Q}\rangle\langle\hat{P}\rangle = \Delta(QP) + \langle\hat{Q}\rangle\langle\hat{P}\rangle. \end{aligned} \tag{38}$$

(Note that $\langle\Delta\hat{A}\rangle = 0$ for any \hat{A} .)

The derivation of the fluctuation $\Delta(H_0'^2)$ requires a longer calculation: We expand

$$\Delta(H_0'^2) = \langle\hat{H}_0'^2\rangle - \langle\hat{H}_0'\rangle^2 \tag{39}$$

$$= \frac{1}{4}\langle((\Delta\hat{Q} + \langle\hat{Q}\rangle)(\Delta\hat{P} + \langle\hat{P}\rangle) + (\Delta\hat{P} + \langle\hat{P}\rangle)(\Delta\hat{Q} + \langle\hat{Q}\rangle))^2\rangle \tag{40}$$

$$- \frac{1}{4}\langle(\Delta\hat{Q} + \langle\hat{Q}\rangle)(\Delta\hat{P} + \langle\hat{P}\rangle) + (\Delta\hat{P} + \langle\hat{P}\rangle)(\Delta\hat{Q} + \langle\hat{Q}\rangle)\rangle^2 \tag{41}$$

$$= \frac{1}{4}\langle(\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q} + 2\langle\hat{P}\rangle\Delta\hat{Q} + 2\langle\hat{Q}\rangle\Delta\hat{P} + 2\langle\hat{Q}\rangle\langle\hat{P}\rangle)^2\rangle \tag{42}$$

$$- \frac{1}{4}\langle(\langle\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q}\rangle + 2\langle\hat{Q}\rangle\langle\hat{P}\rangle)^2\rangle \tag{43}$$

$$= \frac{1}{4}\langle(\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q})^2\rangle \tag{44}$$

$$+ \frac{1}{2}\langle\hat{Q}\rangle\langle\Delta\hat{P}(\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q}) + (\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q})\Delta\hat{P}\rangle \tag{45}$$

$$+ \frac{1}{2}\langle\hat{P}\rangle\langle\Delta\hat{Q}(\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q}) + (\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q})\Delta\hat{Q}\rangle \tag{46}$$

$$+ \langle\hat{Q}\rangle\langle\hat{P}\rangle\langle\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q}\rangle + \langle\hat{Q}\rangle^2\langle(\Delta\hat{P})^2\rangle + \langle\hat{P}\rangle\langle(\Delta\hat{Q})^2\rangle \tag{47}$$

$$- \frac{1}{4}\langle\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q}\rangle^2. \tag{48}$$

Using Equation (36) in Equation (44), Equation (35) in Equation (46) and an analogous result in Equation (45), we obtain

$$\begin{aligned} \Delta(H_0'^2) &= \langle\hat{Q}\rangle^2\Delta(P^2) + \langle\hat{P}\rangle^2\Delta(Q^2) + 2\langle\hat{Q}\rangle\langle\hat{P}\rangle\Delta(QP) \\ &\quad + 2\langle\hat{P}\rangle\Delta(Q^2P) + 2\langle\hat{Q}\rangle\Delta(QP^2) + \Delta(Q^2P^2) + \frac{1}{4}\hbar^2 - \Delta(QP)^2. \end{aligned} \tag{49}$$

If $\Delta(QP) = 0$ and $\Delta(Q^2P) = 0 = \Delta(QP^2)$, we obtain

$$\frac{\Delta(H_0'^2)}{\langle\hat{H}_0'\rangle^2} = \frac{\Delta(Q^2)}{\langle\hat{Q}\rangle^2} + \frac{\Delta(P^2)}{\langle\hat{P}\rangle^2} + \frac{1}{4}\frac{\hbar^2 + 4\Delta(Q^2P^2)}{\langle\hat{Q}\rangle^2\langle\hat{P}\rangle^2} > \frac{\Delta(Q^2)}{\langle\hat{Q}\rangle^2} + \frac{\Delta(P^2)}{\langle\hat{P}\rangle^2}. \tag{50}$$

□

This result shows that a state with small relative H -fluctuations but large relative Q -fluctuations must have non-zero covariance or skewness.

3.2. Example

As shown in [14], the right-hand side of Equation (27) is strictly negative for a Gaussian state in Q . This inequality then cannot be fulfilled. The same paper showed that the right-hand side of Equation (27) is approximately zero for a state given by

$$\psi(Q) = \sqrt{\sqrt{\frac{2}{\pi}} \frac{\sigma}{\hbar Q}} \exp\left(-\sigma^2(\log(Q/\bar{Q}))^2/\hbar^2 + i(\bar{\lambda}/\hbar) \log(Q/\bar{Q})\right) \tag{51}$$

if $Q > 0$ and $\psi(Q) = 0$ otherwise, with constants $\bar{Q} > 0$, $\sigma > 0$ and $\bar{\lambda}$. We now demonstrate that such a state can be approximated by a state supported only on the positive part of the spectrum of \hat{H}'_0 , which then provides an example of how the restriction given by Proposition 1 can be overcome by states with non-zero covariance.

Let us choose a Gaussian

$$c_\lambda = \frac{N}{(2\pi)^{1/4} \sqrt{\sigma}} \exp\left(-\frac{(\lambda - \bar{\lambda})^2}{4\sigma^2} + \frac{i\bar{p}\lambda}{\hbar}\right) \tag{52}$$

for $\lambda > 0$ and $c_\lambda = 0$ otherwise, where

$$N^2 = \frac{2}{1 + \operatorname{erf}\left(\bar{\lambda}/(\sqrt{2}\sigma)\right)} \tag{53}$$

normalizes c_λ restricted to positive λ and is close to $N^2 \approx 1$ for $\bar{\lambda} \gg \sigma$, or $\Delta H'_0/\langle \hat{H}'_0 \rangle \ll 1$. Using the definition in Equation (28) with $\alpha = \sqrt{2}$, we consider the state $\psi_{c_+}(Q) = \int_0^\infty c_\lambda \psi_{\lambda_+}(Q) d\lambda$. The integral can be approximated by extending the integration over positive λ to all real λ , which is valid provided c_λ is negligible for $\lambda < 0$. Given Equation (52), the approximation can be used if the λ -variance σ is much less than the λ -expectation value, $\sigma \ll \bar{\lambda}$. The same condition allows us to approximate $N \approx 1$, and we obtain

$$\begin{aligned} \psi_{c_+}(Q) &= \int_0^\infty c_\lambda \psi_{\lambda_+}(Q) d\lambda \approx \int_{-\infty}^\infty c_\lambda \psi_{\lambda_+}(Q) d\lambda \\ &\approx \frac{1}{(2\pi)^{3/4} \sqrt{\sigma \hbar Q}} \int_{-\infty}^\infty \exp\left(-(\lambda - \bar{\lambda})^2/4\sigma^2 + i\lambda(\bar{p} + \log Q)/\hbar\right) d\lambda \end{aligned} \tag{54}$$

$$= \sqrt{\sqrt{\frac{2}{\pi}} \frac{\sigma}{\hbar Q}} \exp\left(-(\sigma^2/\hbar^2)(\bar{p} + \log Q)^2 + i(\bar{\lambda}/\hbar)(\bar{p} + \log Q)\right) \tag{55}$$

for $Q > 0$. Defining $\bar{Q} = \exp(-\bar{p})$, the result equals Equation (51).

The resulting state in Equation (54) shows that the $\log |Q|$ -variance is given by $\Delta \log |Q| = \hbar/(2\sigma)$, while the $\log |Q|$ -expectation value is $\langle \log |\hat{Q}| \rangle = -\bar{p}$. We can therefore maintain the condition $\bar{\lambda} \gg \sigma$, or $\Delta H'_0/\langle \hat{H}'_0 \rangle \ll 1$, for the approximation in Equation (54) to be valid, and choose a small $\langle \hat{Q} \rangle$ with large ΔQ .

According to Equation (37), this state must have non-zero covariance or skewness. We can easily confirm the former property by computing

$$\langle \hat{Q} \rangle = \sqrt{\frac{2}{\pi}} \frac{\sigma}{\hbar} \int_0^\infty \exp\left(-2(\sigma^2/\hbar^2)(\log(Q/\bar{Q}))^2\right) dQ = I_1 = \bar{Q} \exp(\hbar^2/8\sigma^2) \tag{56}$$

$$\langle \hat{P} \rangle = \sqrt{\frac{2}{\pi}} \frac{\sigma \bar{\lambda}}{\hbar} \int_0^\infty \frac{1}{Q^2} \exp\left(-2(\sigma^2/\hbar^2)(\log(Q/\bar{Q}))^2\right) dQ = \bar{\lambda} I_{-1} = \frac{\bar{\lambda}}{\bar{Q}} \exp(\hbar^2/8\sigma^2) \tag{57}$$

and

$$\frac{1}{2}\langle\hat{Q}\hat{P} + \hat{P}\hat{Q}\rangle = \text{Re}\langle\hat{Q}\hat{P}\rangle = \bar{\lambda}I_0 = \bar{\lambda}. \quad (58)$$

where we have used the integrals

$$I_a = \sqrt{\frac{2}{\pi}} \frac{\sigma}{\hbar} \int_{-\infty}^{\infty} e^{az} \exp(-2\sigma^2(z - \log \bar{Q})^2/\hbar^2) dz = \bar{Q}^a \exp(a^2\hbar^2/8\sigma^2) \quad (59)$$

for real a . Therefore,

$$\Delta(QP) = \bar{\lambda} \left(1 - \exp(\hbar^2/4\sigma^2)\right) < 0 \quad (60)$$

is non-zero, with $|\Delta(QP)|$ large for $\sigma \ll \hbar$, such that ΔQ can be large.

Funding: This research was funded by NSF grant number PHY-1607414.

Conflicts of Interest: The author declares no conflict of interest.

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