Quantum dynamics of gravitational massive shell

Andrzej Góźdź,¹,* Marcin Kisielowski,²,† and Włodzimierz Piechocki²,‡

¹Institute of Physics, Maria Curie-Skłodowska University,
pl. Marii Curie-Skłodowskiej 1, 20-031 Lublin, Poland
²Department of Fundamental Research,
National Centre for Nuclear Research,
Pasteura 7, 02-093 Warszawa, Poland

(Dated: February 8, 2023)
Abstract
The quantum dynamics of a self-gravitating thin matter shell in vacuum has been consid-
ered. Quantum Hamiltonian of the system is positive definite. Within chosen set of pa-
rameters, the quantum shell bounces above the horizon. Considered quantum system
does not collapse to the gravitational singularity of the corresponding classical system.

CONTENTS

I. Introduction 3

II. Classical dynamics 4

III. Quantum level 7
   A. Affine coherent states 8
   B. Quantum observables 9
   C. Quantum dynamics 10

IV. Matrix elements of quantum observables 12
   A. New expression for the basis elements 13
   B. The matrix elements of the Hamiltonian operator 15
   C. The matrix elements of the momentum operator 16
      1. Entries below and on the diagonal 19
      2. The entries above the diagonal 21
      3. Summary 22
   D. The matrix elements of the coordinate operator 22
      1. Diagonal terms 24
      2. The terms above the diagonal 24
      3. Summary 24

V. Evolution of quantum observables 25
   A. Gaussian state 25
   B. Eigenvalues convergence 26
   C. Evolution of the observables 26
   D. Oscillatory character of the evolution 29

andrzej.gozdz@umcs.lublin.pl
marcin.kisielowski@gmail.com
wlodzimierz.piechocki@ncbj.gov.pl
I. INTRODUCTION

The dynamics of a self-gravitating thin matter shell is one of the simplest models describing gravitational collapse of an isolated gravitational system. In the case of a spherically symmetric shell in vacuum, a satisfactory Hamiltonian description of that dynamics has been found; see the paper [1] and references therein. By shell in vacuum one means a thin matter shell with a region of flat Minkowski space in the interior and the Schwarzschild geometry in the exterior of the shell. The global Hamiltonian of that system is explicitly time independent and is a function of two canonically conjugated phase space variables. That Hamiltonian is equal to the Arnowit-Deser-Misner (ADM) mass at spacial infinity. Having well defined Hamiltonian description of matter shell, we have decided to quantize that system to get insight into corresponding quantum dynamics. Present paper is devoted to the examination of such an issue.

The shell system is simple enough to be treated satisfactory at classical level, and rich enough for the examination of various aspects of corresponding quantum system. Recently, it was used for addressing the issue of the importance of the choice of time parameter at quantum level [2]. It was shown that quantum theories of the shell for different choices of time are not unitarily equivalent.

We have found that our quantum Hamiltonian is positive definite which supports its classical property. Within chosen set of parameters describing our system, the quantum shell bounces above the horizon that is in contrast to the classical case. It means that due to quantum effects our quantum system does not collapse to gravitational singularity.

The paper is organized as follows: In Sec. II we present the solution to Hamilton’s dynamics restricting considerations to the subspace of phase space for which the Hamiltonian is positive definite. In Sec. III we recall the coherent states quantization method applied in this paper. Sec. IV concerns the calculations of the matrix elements of quantum observables in specific basis of considered Hilbert space. That includes the operator of Hamiltonian and operators of canonical variables. The quantum evolution of the system is presented in Sec. V. We conclude in Sec. VI.
In the following we choose \( G = c = 1 = \hbar \) except where otherwise noted.

II. CLASSICAL DYNAMICS

For self-consistency of the present paper, we recall the main results of Ref. [1]. Next, we present the solution to the classical dynamics.

The canonical structure of the phase space of the system “shell+gravity” is given by
\[
\omega = dp \wedge dq, \tag{1}
\]
where \( q \in \mathbb{R}_+ := \{ x \in \mathbb{R} \mid x > 0 \} \) is the configuration variable representing the proper volume of the shell, and \( p \in \mathbb{R} \) is the momentum representing the hyperbolic angle between the surfaces of constant time on both sides of the shell.

Hamilton’s dynamics reads
\[
\begin{align*}
\dot{q} &= \frac{\partial H}{\partial p}, \tag{2} \\
\dot{p} &= -\frac{\partial H}{\partial q}, \tag{3}
\end{align*}
\]
where the Hamiltonian is defined to be
\[
H(p, q) := \sqrt{\frac{q}{2}} \left[ 1 - \left( \cosh(p) - \sqrt{\frac{m^2(q)}{2q} + \sinh^2(p)} \right)^2 \right], \tag{4}
\]
and where \( m(q) \) represents the total rest mass of the matter (energy) of the shell and plays the role of the constitutive equation for the matter field of the shell. The dots over \( q \) and \( p \) in (2)–(3) denote time derivatives, where the time variable is the Schwarzschild time \( t \) measured at spatial infinity. Since \( H \) is time independent, the total energy of the entire system is conserved.

Making use of (2)–(4) we can determine if the shell’s size increases or decreases with time. It follows that
\[
\dot{q} = \frac{\partial H}{\partial p} = \sinh(p) \sqrt{\frac{2q}{m^2}} (\cosh(p) - \sqrt{\frac{m^2}{2q} + \sinh^2(p)})^2 \sqrt{\frac{m^2}{2q} + \sinh^2(p)}. \tag{5}
\]
Therefore the sign of \( \dot{q} \) is dictated (up to singularities where the right-hand-side vanishes) by \( \sinh(p) \). This means that for positive \( p \) the shell grows \( \dot{q} \geq 0 \) and for negative \( p \) the shell shrinks \( \dot{q} \leq 0 \).
Any canonical transformation of the system (1)–(4) leads to the physically equivalent system. The advantage of the present choice of the phase space variables is their clear physical interpretation.

The Hamiltonian function (4) is equal to the total energy of considered isolated gravitational system at spatial infinity so that it is the ADM mass. It means, roughly speaking, that if the density of considered matter field is positive, the ADM mass must be positive (see, [3] and references therein). This may impose the restriction on the phase space of considered gravitational system. The specific form of matter field may lead to the specific subspace \( \Lambda \) of the phase space \( \Pi = \{ (p, q) \mid p \in \mathbb{R}, q \in \mathbb{R}_+ \} \), such that \( H(p, q) > 0 \) for \( (p, q) \in \Lambda \). We call \( \Lambda \) the physical phase space.

Let us consider the case \( m(q) := m = \text{const} \) which corresponds to the dust matter. Since the Hamiltonian is time independent, the energy is conserved. For each value of the Schwarzschild mass \( M > 0 \), the curve
\[
H(p, q) = M
\]
is the shell's trajectory in the phase-space. Let us notice, that the Hamiltonian is an even function of \( p \) and therefore it is enough to look for solutions with positive momentum \( p > 0 \). Rewriting the equation (6) (see also (4)) in the form
\[
1 - \sqrt{\frac{2}{q}} M = \left( \cosh(p) - \sqrt{\frac{m^2(q)}{2q} + \sinh^2(p)} \right)^2,
\]
we immediately notice that \( q > 2M^2 \). This condition says that the proper volume \( q \) is bounded from below so that reflects the fact that the shell is outside the event horizon of the exterior Schwarzschild solution.

The equation (6) can be solved for \( p \) as a function of \( q \) and \( M \). It can be checked by substitution that

- for \( M \sqrt{\frac{2}{q}} \geq \frac{m^2}{2q} \), i.e., \( \sqrt{q} \geq \frac{m^2}{\sqrt{2}M} \), the solution satisfies:
\[
\cosh(p) = \frac{2 - \frac{m^2}{2q} - M \sqrt{\frac{2}{q}}}{2 \sqrt{1 - M \sqrt{\frac{2}{q}}}} =: f(q),
\]

- while for \( M \sqrt{\frac{2}{q}} < \frac{m^2}{2q} \), i.e., \( \sqrt{q} < \frac{m^2}{\sqrt{2}M} \), it satisfies:
\[
\cosh(p) = -\frac{2 - \frac{m^2}{2q} - M \sqrt{\frac{2}{q}}}{2 \sqrt{1 - M \sqrt{\frac{2}{q}}}} = -f(q).
\]
At the first glance, it may seem that for \( 0 \leq M < \frac{m}{2} \) both relations (8) and (9) are relevant and that there is a discontinuity at \( q = \frac{m^2}{2\sqrt{2}M} \). However, it turns out that in this case for \( \sqrt{q} \geq \frac{m^2}{2\sqrt{2}M} \) the function \( f(q) \) takes only values smaller than 1 and therefore the only relevant relation is (9). The function \(-f(q)\) decreases from \(+\infty\) at \( 2M^2 \) to \(-1\) at \(+\infty\). This means that \( p(q) \) decreases from \(+\infty\) at \( q = 2M^2 \) until \( q = \frac{m^4}{8(\sqrt{m-M})^2} \) where \( p = 0 \). This is illustrated on figure 1. The plot for \( p < 0 \) is just a reflection by the \( q \) axis.

Figure 1: Dust shell’s trajectory with energy \( H(p,q) = M < \frac{m}{2} \).

For \( M = \frac{m}{2} \) the function \( f(q) \) takes only values smaller than 1 and therefore there is no solution.

If \( M > \frac{m}{2} \), we have \( \sqrt{q} < \frac{m^2}{2\sqrt{2}M} \) so the function \( f(q) \) is fully determined by the relation (8). The case \( M > \frac{m}{2} \) splits further into two other cases:

1. \( \frac{m}{2} < M < m \): In this case the function \( f(q) \) decreases from \(+\infty\) at \( q = 2M^2 \), reaches a minimal value smaller than 1 and grows asymptotically to 1 as \( q \) goes to \(+\infty\). This means that \( p(q) \) decreases from \(+\infty\) at \( q = 2M^2 \) until \( q = \frac{m^4}{8(\sqrt{m-M})^2} \) where \( p = 0 \). This is illustrated on figure 2a. The plot for \( p < 0 \) is just a reflection by the \( q \) axis.

2. \( M \geq m \): In this case the function \( f(q) \) decreases from \(+\infty\) at \( q = 2M^2 \) to 1 at \(+\infty\). This means that \( p(q) \) decreases from \(+\infty\) at \( q = 2M^2 \) to 0 at \( q \rightarrow +\infty \). This is illustrated on figure 2b.
Let us examine the issue of the positive definiteness of $H(p,q)$. For $p = 0$, Eq. (4) reads $H(0,q) = m - m^2/\sqrt{8q}$ so that we have

$$H(0,q) < 0 \text{ for } q < m^2/8.$$  

(10)

Since we need to have $H(p,q) > 0$, the physical phase space $\Lambda$ should be a subspace of the entire phase space $\Pi$. Some regions of $\Pi$, for instance defined by (10), may lead to the breaking of this condition.

III. QUANTUM LEVEL

The affine coherent states quantization applied in this article is based on the formalism presented in our papers [4] and [5].

The physical phase space of our gravitational system

$$\Pi := \{(p,q) \mid p \in \mathbb{R}, q \in \mathbb{R}_+\},$$  

(11)

can be identified with the affine group $G \equiv \text{Aff}(\mathbb{R})$, by defining the multiplication law as follows

$$(p',q') \cdot (p,q) := (q'p + p', q'q).$$  

(12)
with the unity \((0, 1)\) and the inverse
\[
(p', q')^{-1} = (-\frac{p'}{q'}, \frac{1}{q'}) .
\] (13)

### A. Affine coherent states

The affine group has two, nontrivial, inequivalent irreducible unitary representations \([6–8]\). Both are realized in the Hilbert space \(\mathcal{H} = L^2(\mathbb{R}_+, d\nu(x))\), where \(d\nu(x) := dx/x\) is an invariant measure on the multiplicative group \((\mathbb{R}_+, \cdot)\). In what follows we choose the one defined by the following action
\[
U(p, q)\psi(x) = e^{ipx}\psi(qx) ,
\] (14)

where \(\psi(x) = \langle x|\psi \rangle\) and \(|\psi\rangle \in L^2(\mathbb{R}_+, d\nu(x))\).

We define the integrals over the affine group \(G = \text{Aff}(\mathbb{R})\) as follows
\[
\int_G d\mu(p, q) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dp \int_0^{+\infty} dq \frac{1}{q^2} .
\] (15)

Fixing the normalized vector \(|\Phi\rangle \in L^2(\mathbb{R}_+, d\nu(x))\), called the fiducial vector, we can define a continuous family of affine coherent states \(|p, q\rangle \in L^2(\mathbb{R}_+, d\nu(x))\) as follows
\[
|p, q\rangle = U(p, q)|\Phi\rangle .
\] (16)

The irreducibility of the representation, used to define the coherent states (16), enables making use of Schur’s lemma [9], which leads to the resolution of the unity in \(L^2(\mathbb{R}_+, d\nu(x))\)
\[
\frac{1}{A_{\Phi}} \int_G d\mu(p, q)|p, q\rangle\langle p, q| = \mathbb{I} ,
\] (17)

where the constant \(A_{\Phi}\) can be determined by using any arbitrary, normalized vector \(|f\rangle \in L^2(\mathbb{R}_+, d\nu(x))\) as follows
\[
A_{\Phi} = \int_G d\mu(p, q) \langle f|p, q\rangle\langle p, q|f\rangle = \int_0^{+\infty} dq \frac{1}{q^2} |\Phi(q)|^2 .
\] (18)

\(^1\) We use Dirac’s notation whenever we wish to deal with abstract vector, instead of functional representation of the vector.
B. Quantum observables

Using the resolution of the identity (17), we define the quantization of a classical observable \( f \) as follows \[ 11 \]

\[
F \ni f \rightarrow \hat{f} := \int_G d\mu(p,q) f(p,q) \langle p,q | \in A ,
\]

(19)

where \( F \) is a vector space of real continuous functions on a phase space, and \( A \) is a vector space of operators (quantum observables) acting in the Hilbert space \( L^2(\mathbb{R}_+, d\nu(x)) \). It is clear that (19) defines a linear mapping and the observable \( \hat{f} \) is a symmetric operator. Self-adjointness of \( \hat{f} \) is an open problem as symmetricity does not assure self-adjointness so that further examination is required [12].

In Appendix A we define an orthonormal basis (for any fixed value of the parameter \( \alpha > -1 \)) of the unitary irreducible representation of considered affine group. This basis can be used in concrete calculations. To make these calculations feasible, we use the technics of generating functions for generalized Laguerre polynomials \( L^{(\alpha)}_n \) (see, e.g. [13]). For this purpose, it is convenient to restrict the upper label \( \alpha \) of the functions \( L^{(\alpha)}_n(x) \) to any fixed integer. In this case, the generating function for the Laguerre polynomials reads:

\[
\frac{\exp(-xz)}{(1-z)^{\alpha+1}} = \sum_{n=0}^{\infty} L^{(\alpha)}_n(x) z^n \text{ if } |z| < 1 .
\]

(20)

For calculation of the matrix elements of the operator (19), in the basis defined in App. A, one needs to calculate the overlaps between the coherent state vectors and the vectors of this orthonormal basis. To perform these calculations explicitly, we choose the fiducial vector for our coherent states as follows

\[
\Phi^{(\alpha)}(x) := e^{(\alpha)}_0(x) = \sqrt{\frac{1}{\alpha!}} \frac{1}{z^\frac{1+\alpha}{2}} e^{-\frac{x}{2}}.
\]

(21)

In this case one gets

\[
\langle e^{(\alpha)}_n(x)|pq \rangle = \sqrt{\frac{n!}{(n+\alpha)!\alpha!}} q^{\frac{1+\alpha}{2}} \int_0^\infty dx x^{\frac{1+\alpha}{2}} e^{-\frac{x}{2} - \frac{ip}{z}} L^{(\alpha)}_n(x).
\]

(22)

Let us define the function

\[
epq(\alpha, p, q; z) := \sum_n \langle e^{(\alpha)}_n(x)|pq \rangle \left[ \sqrt{\frac{n!}{(n+\alpha)!\alpha!}} \right]^{-\frac{1}{2}} z^n,
\]

\[
epq(\alpha, p, q; z) = \left( \frac{\sqrt{q}}{1-z} \right)^{1+\alpha} \int_0^\infty dx x^{\alpha} \exp \left( - q + \frac{1}{2} - \frac{z}{1-z} - ip \right) x .
\]

(23)
The required overlaps turn out to be defined by the derivatives of these functions calculated at $z = 0$ as follows

$$\langle e_n^{(\alpha)}(x)|pq \rangle = \frac{1}{\sqrt{\alpha!n!(n + \alpha)!}} \left[ \frac{d^n}{dz^n} e^{pq(\alpha, p, q; z)} \right]_{|z=0}. \quad (24)$$

Using exactly the same method, the matrix elements of the operator (19) are found to be

$$\langle e_n^{(\alpha)}|\hat{f}|e_{n'}^{(\alpha)} \rangle = \frac{1}{A_\Phi} \frac{1}{\sqrt{\alpha!n!(n + \alpha)!\alpha!n'!(n' + \alpha)!}} \cdot \left[ \frac{\partial^n}{\partial z_1^n} \frac{\partial^{n'}}{\partial z_2^{n'}} \int_{\text{Aff}(\mathbb{R})} d\mu(p, q) e^{pq(\alpha, p, q; z_1)} f(p, q) e^{pq(\alpha, p, q; z_2)^*} \right]_{|z_1=z_2=0}. \quad (25)$$

The simplest basis, satisfying required conditions, is obtained by taking $\alpha = 1$. In this case, the function $e^{pq(1, p, q; z)}$ reads:

$$e^{pq(1, p, q; z)} = \frac{q}{(1 - z)^2} \left( q + \frac{1}{2} + \frac{z}{1 - z} - ip \right)^{-2}. \quad (26)$$

C. Quantum dynamics

The mapping (19) applied to the classical Hamiltonian (4) reads

$$\hat{H}_{\text{unbounded}} = \frac{1}{A_\Phi} \int_G d\mu(p, q) |p, q \rangle H(p, q) \langle p, q|. \quad (27)$$

However, our classical analysis applies only to the region of phase space for which $H(p, q) > 0$.

An important problem is introducing constraints into the integral quantization approach. This quantization is based on deformation of quantum measure represented by a set of positive self-adjoint operators determining the operator valued measure (POV). They are considered as generalization of more standard self-adjoint quantum observables [14].

In our case the set of operators

$$\hat{M}(Q) := \frac{1}{A_\Phi} \int_G d\mu(p, q) |p, q \rangle \chi_Q(g) \langle p, q|,$$  \quad (28)

where $\chi_Q(g) = 1$ if $g \in Q$ and 0 otherwise, and where $Q \subset G = \text{Aff}(\mathbb{R})$, describe the localization of the system in the subspace $Q$ of the phase space $G$.  

10
The normalization condition
\[ \hat{M}(G) = \frac{1}{A} \int_G d\mu(p, q) |p, q\rangle \langle p, q| = \mathbf{1} \]  

(29)
is required to get the so called minimal probabilistic interpretation of quantum mechanics [14]:
\[ \text{Prob}(Q, \Psi) = \langle \Psi | \hat{M}(Q) | \Psi \rangle , \]
which describes the probability of finding our system in \( Q \), under condition that this system is in the state \( \Psi \).

On the other hand, to construct the condition (29) one needs to integrate over the whole group manifold and the representation (16) has to be irreducible. This excludes the possibility of using a smaller region \( \Omega \subset G \) of the phase space to fulfill the classical constraint, where \( \Omega = \{(p, q) : H(p, q) > 0\} \).

To have a consistent quantization method, the only possibility of quantizing any observable restricted to a smaller region of the phase space is to quantize it over the whole phase space, represented in this approach by the group \( G \).

Following these requirements, to keep physical interpretation of the classical Hamiltonian, we quantize it as a function restricted to the required region of the phase space by considering:
\[ \hat{H} = \frac{1}{A} \int_G d\mu(p, q) |p, q\rangle \theta(H(p, q)) H(p, q) \langle p, q| , \]

(31)
where \( \theta \) is the Heaviside theta function.

An important feature of the operator \( \hat{H} \) is that it acts in a nontrivial way on the whole phase space. Let \( (p', q') \not\in \Omega \), then
\[ \hat{H}|p', q'\rangle = \frac{1}{A} \int_\Omega d\mu(p, q) |p, q\rangle \theta(H(p, q)) H(p, q) \langle p, q|p', q'\rangle \]

(32)
is usually a non-zero vector. This behavior is due to non-orthogonality of the states \( |p, q\rangle \), i.e., the quantum phase space regions \( \Omega \) and \( G \setminus \Omega \) are not independent.

Another very important problem related is the quantization of the elementary observables \( (p, q) \). These observables represent position of the system in the quantum full phase space \( G \). The corresponding quantum operators \( (\hat{p}, \hat{q}) \) should satisfy the following consistency conditions [15]:
\[ \langle p, q|\hat{p}|p, q\rangle = p \quad \text{and} \quad \langle p, q|\hat{q}|p, q\rangle = q , \]

(33)
where
\[ \hat{p} = \frac{1}{A} \int_G d\mu(p, q) |p, q\rangle p(p, q) \quad \text{and} \quad \hat{q} = \frac{1}{A} \int_G d\mu(p, q) |p, q\rangle q(p, q) . \]

(34)
Satisfying (33) is possible only when the operators are defined on the entire phase space $G$. The consistency conditions support the physical interpretation of the POV measure (28).

The above analysis allow us to be consistent and to quantize the restricted form of the Hamiltonian $H$ and unrestricted form of the elementary observables $(p, q)$.

We will restrict to this region of a phase space by considering:

$$\hat{H} = \frac{1}{A_\Phi} \int_G d\mu(p, q) |p, q\rangle \theta(H(p, q)) H(p, q) |p, q\rangle,$$

(35)

where $\theta$ is the Heaviside theta function. Let us notice that the operator $\hat{H}$ is positive definite. Indeed, for any state $|\Psi\rangle$ we have:

$$\langle \Psi | \hat{H} \Psi \rangle = \frac{1}{A_\Phi} \int_G d\mu(p, q) |\Psi(p, q)\rangle^2 \theta(H(p, q)) H(p, q) > 0.$$

(36)

The quantum evolution of our gravitational system is defined by the Schrödinger equation:

$$i \frac{\partial}{\partial s} |\Psi(s)\rangle = \hat{H} |\Psi(s)\rangle,$$

(37)

where $|\Psi\rangle \in L^2(\mathbb{R}_+, d\nu(x))$, and where $s$ is an evolution parameter of the quantum level.

In general, the parameters $t$ of the classical level and $s$ are different. To get the consistency between the classical and quantum levels we postulate that $t = s$, which defines the time variable at both levels. This way we support the interpretation that Hamiltonian is the generator of classical and corresponding quantum dynamics.

IV. MATRIX ELEMENTS OF QUANTUM OBSERVABLES

In this section we calculate the matrix elements for the operators $\hat{H}, \hat{q},$ and $\hat{p}$. The matrix elements of $\hat{H}$ are calculated numerically using (60). We calculate the matrix elements of $\hat{q}$ and $\hat{p}$ analytically. The computations are based on a new formula for the basis elements $e_{m}^{(1)}$ that we derive in the first subsection. The results of this section are used in Sec. V to find an evolution of the quantum observables.
A. New expression for the basis elements

In what follows, we use the basis with $\alpha = 1$. Since $\frac{1}{z^2} = \frac{1}{(1-z)^2}$, we can simplify the expression for the basis element:

$$\langle e^{(1)}_n | pq \rangle = -q \sqrt{n+1} \frac{d^{n+1}}{dz^{n+1}} \int_0^\infty dx \exp \left( -\left[ \frac{q-1}{2} + \frac{1}{1-z} - ip \right] x \right) \Big|_{z=0}$$

The technical problem is now to calculate $\frac{d^n}{dz^n} f(z)$, where $f(z)$ is a composite function:

$$f(z) = F(G(z)) = \exp \left( -G(z)x \right), \text{ where } G(z) = \frac{1}{1-z}.$$

We will use the Faa di Bruno’s formula [16, 17]:

$$\frac{d^n}{dz^n} F(G(z)) = \sum_{k=1}^n F^{(k)}(G(z)) \cdot B_{n,k}(G'(z), G''(z), \ldots, G^{(n-k+1)}(z)),$$  \hspace{1cm} (40)

where $B_{n,k}(x_1, \ldots, x_{n-k+1})$ are Bell polynomials [17, 18]. In the formula above we denote by $F^{(k)}$ the k-th derivative of $F$. The Bell polynomial $B_{n,k}(z_1, z_2, \ldots, z_{n-k+1})$ is given by

$$B_{n,k}(z_1, z_2, \ldots, z_{n-k+1}) = \sum_{j_1, j_2, \ldots, j_{n-k+1} \in \mathbb{N}} \frac{n!}{j_1! j_2! \cdots j_{n-k+1}!} \left( \frac{z_1}{1!} \right)^{j_1} \left( \frac{z_2}{2!} \right)^{j_2} \cdots \left( \frac{z_{n-k+1}}{(n-k+1)!} \right)^{j_{n-k+1}},$$  \hspace{1cm} (41)

where the sum is over all sequences $j_1, \ldots, j_{n-k+1} \in \mathbb{N}$ such that

$$j_1 + j_2 + \ldots + j_{n-k+1} = k,$$
$$j_1 + 2j_2 + 3j_3 + \ldots + (n-k+1)j_{n-k+1} = n.$$  \hspace{1cm} (42, 43)

We are interested only in derivatives at $z = 0$, therefore in equation (40) we should put $z = 0$. Let us notice that

$$G(0) = 1, \quad G^{(m)}(0) = m!.$$  \hspace{1cm} (44)

Therefore

$$\frac{d^n}{dz^n} F(G(0)) = \sum_{k=1}^n (-1)^k x^k e^{-x} B_{n,k}(1!, 2!, \ldots, (n-k+1)!).$$  \hspace{1cm} (45)

The coefficient $B_{n,k}(1!, 2!, \ldots, (n-k+1)!)$ can be expressed in terms of the Lah number [17, 19]:

$$B_{n,k}(1!, 2!, \ldots, (n-k+1)!) = |L_{n,k}|.$$  \hspace{1cm} (46)

13
where
\[ L_{n,k} = (-1)^n \binom{n-1}{k-1} \frac{n!}{k!}, \quad n \geq k \geq 1, \] (47)
\[ L_{0,0} = 1, \quad L_{n,0} = 0, \quad n \geq 1. \] (48)

We extend the sum in (45) to \( k = 0 \) and obtain a formula valid for \( n = 0 \):
\[ \frac{d^n}{dz^n} F(G(0)) = \sum_{k=0}^{n} (-1)^k |L_{n,k}| x^k e^{-x}. \] (49)

In order to calculate \( \langle e^{(1)}_n |pq \rangle \), we need to evaluate the integral
\[ \int_0^\infty dx \, x^k \exp \left( -\left( \frac{q+1}{2} - ip \right) x \right) = \frac{k!}{(q+1/2 - ip)^{k+1}}. \] (50)

This integral directly follows from the Euler’s integral formula (see for example equation 6.1.1 from [20]):
\[ \Gamma(n) = z^n \int_0^\infty dx \, x^{n-1} e^{-zx}, \quad \text{for } \Re(n) > 0, \, \Re(z) > 0. \] (51)

In the formula above \( \Gamma(z) \) is the Gamma function. Inserting this evaluation into (38) gives:
\[ \langle e^{(1)}_n |pq \rangle = \sqrt{n+1} \sum_{k=1}^{n+1} \frac{(-1)^{k+1} k!}{(n+1)!} \frac{q}{(q+1/2 - ip)^{k+1}} |L_{n+1,k}|. \] (52)

We will define coefficients \( E_{n,k} \):
\[ E_{n,k} = \frac{(-1)^{k+1} k!}{n!} |L_{n,k}|. \] (53)

Due to cancellation of terms, the coefficients have the following explicit form:
\[ E_{n,k} = (-1)^{k-1} \binom{n-1}{k-1}, \quad n \geq k \geq 1, \] (54)
\[ E_{0,0} = \frac{(-1)^{k-1} k!}{n!}, \quad E_{n,0} = 0, \quad n \geq 1. \] (55)

Let us notice, that in our formulas we need only the coefficients with \( n \geq 1 \). Since, \( E_{n,0} = 0 \) for \( n \geq 1 \), we can assume that \( k \geq 1 \). The formula (52) takes now a more compact form:
\[ \langle e^{(1)}_n |pq \rangle = \sqrt{n+1} \sum_{k=1}^{n+1} (-1)^{k-1} \binom{n}{k-1} \frac{q}{(q+1/2 - ip)^{k+1}}. \] (56)
We will change the summation variable into $k' = k - 1$ and obtain:

$$\langle e^{(1)}_n|pq \rangle = \frac{q \sqrt{n+1}}{(q+\frac{1}{2} - ip)^2} \sum_{k=0}^{n} \binom{n}{k} \frac{(-1)^k}{(q+\frac{1}{2} - ip)^k}.$$

(57)

The last sum is the binomial expansion. Therefore

$$\langle e^{(1)}_n|pq \rangle = q \sqrt{n+1} \left(1 - \frac{1}{(q+\frac{1}{2} - ip)^2}\right)^n = q \sqrt{n+1} \left(\frac{q-1 - ip}{q+\frac{1}{2} - ip}\right)^{n+2}.$$  

(58)

B. The matrix elements of the Hamiltonian operator

The new expression for the basis elements that we found in the previous section allows us to calculate the matrix elements of the Hamiltonian:

$$H_{nm} := \langle e^{(1)}_n|\hat{H}e^{(1)}_m \rangle = \frac{1}{A_{\Phi}} \int_{G} d\mu(p,q) \langle e^{(1)}_n|pq \rangle \theta(H(q,p))H(p,q)\langle e^{(1)}_m|pq \rangle^*.$$  

(59)

After applying the formula (58) to the equation above, we obtain:

$$H_{nm} := \frac{\sqrt{(n+1)(m+1)}}{2\pi} \int_{0}^{\infty} dq \int_{-\infty}^{+\infty} dp \theta(H(q,p))H(q,p) \frac{(q-i p)^n (q+\frac{1}{2} + ip)^m}{(q+\frac{1}{2} - ip)^{n+2} (q+\frac{1}{2} + ip)^{m+2}}.$$  

(60)

Since $\hat{H}$ is hermitian, it is enough to calculate the lower triangular part of the matrix, i.e. $H_{nm}$ for $n \geq m$. In this case:

$$H_{nm} = \frac{\sqrt{(n+1)(m+1)}}{2\pi} \int_{0}^{\infty} dq \int_{-\infty}^{+\infty} dp \theta(H(q,p))H(q,p) \frac{(q-i p)^n (q+\frac{1}{2} + ip)^m (q+\frac{1}{2} + ip)^{n-m}}{((q+\frac{1}{2})^2 + p^2)^{n+2}}.$$  

(61)

In order to calculate the real and the imaginary part of the matrix, we write the Hamiltonian in the form

$$H_{nm} = \frac{\sqrt{(n+1)(m+1)}}{2\pi} \int_{0}^{\infty} dq \int_{-\infty}^{+\infty} dp \theta(H(q,p))H(q,p) \frac{((q+\frac{1}{2})^2 + p^2)^m (q^2 + p^2 - ip)^{n-m}}{((q+\frac{1}{2})^2 + p^2)^{n+2}}.$$  

(62)

After expanding the expression $(q^2 + p^2 - ip)^{n-m}$ in powers of $i$, we notice that the real part of the integrant is an even function in $p$ and the imaginary part is an
odd function in $p$. As a result, the imaginary part of $H_{nm}$ vanishes:

$$\Im H_{nm} = 0.$$  \hfill (63)

We conclude that $H_{nm}$ is a real symmetric matrix. We will calculate the matrix elements by evaluating the integrals over $q$ and $p$ numerically.

The diagonal elements $H_{nn}$ are positive since the integrand of (62) is a positive function of the variables $q$ and $p$.

### C. The matrix elements of the momentum operator

The matrix elements of the momentum operator:

$$p_{nm} := \sqrt{(n+1)(m+1)} \int_0^\infty dq \int_{-\infty}^{+\infty} dp \frac{p \left( \frac{q-1}{2} - ip \right)^n \left( \frac{q-1}{2} + ip \right)^m}{\left( \frac{q+1}{2} - ip \right)^{n+2} \left( \frac{q+1}{2} + ip \right)^{m+2}}.$$  \hfill (64)

The integral over $p$ can be done using a contour method. We take the sunset contour in the lower half plane and obtain

$$p_{nm} := -i \sqrt{(n+1)(m+1)} \int_0^\infty dq \text{Res}_{p=-\frac{1}{2}+i} \left( \frac{p \left( \frac{q-1}{2} - ip \right)^n \left( \frac{q-1}{2} + ip \right)^m}{\left( \frac{q+1}{2} - ip \right)^{n+2} \left( \frac{q+1}{2} + ip \right)^{m+2}} \right).$$

We will calculate now the residuum:

$$\text{Res}_{p=-\frac{1}{2}+i} \left( \frac{p \left( \frac{q-1}{2} - ip \right)^n \left( \frac{q-1}{2} + ip \right)^m}{\left( \frac{q+1}{2} - ip \right)^{n+2} \left( \frac{q+1}{2} + ip \right)^{m+2}} \right) =$$

$$= i^{n+2} \frac{1}{(n+1)!} \left. dp^{n+1} \left( \frac{p \left( \frac{q-1}{2} - ip \right)^n \left( \frac{q-1}{2} + ip \right)^m}{\left( \frac{q+1}{2} - ip \right)^{n+2} \left( \frac{q+1}{2} + ip \right)^{m+2}} \right) \right|_{p=-\frac{1}{2}+i} +$$

$$+ \frac{i^{n+2}}{n!} d^n \left( \frac{\left( \frac{q-1}{2} - ip \right)^n \left( \frac{q-1}{2} + ip \right)^m}{\left( \frac{q+1}{2} - ip \right)^{n+2} \left( \frac{q+1}{2} + ip \right)^{m+2}} \right) \bigg|_{p=-\frac{1}{2}+i}. \hfill (65)$$

Let us notice that the two terms in the last line are proportional to expressions of the form:

$$I(l, n, m, q) = \frac{1}{l!} \left. dp^l \left( \frac{\left( \frac{q-1}{2} - ip \right)^n \left( \frac{q-1}{2} + ip \right)^m}{\left( \frac{q+1}{2} - ip \right)^{n+2} \left( \frac{q+1}{2} + ip \right)^{m+2}} \right) \right|_{p=-\frac{1}{2}+i}. \hfill (67)$$
with $l = n$ or $l = n + 1$. We will expand the derivative using a Leibnitz rule generalized to three factors:

$$I(l, n, m, q) = \frac{1}{l!} \sum_{k_1, k_2, k_3} \binom{l}{k_1, k_2, k_3} \frac{d^{k_1}}{dp^{k_1}} \left( \frac{q - 1}{2} - ip \right)^n \cdot \frac{d^{k_2}}{dp^{k_2}} \left( \frac{q - 1}{2} + ip \right)^m \frac{d^{k_3}}{dp^{k_3}} \left( \frac{q + 1}{2} + ip \right)^{-m-2} \bigg|_{p=-\frac{q+1}{2}}. \quad (68)$$

where $(k_1, k_2, k_3) = \frac{n}{k_1 k_2 k_3}$. The derivatives of power functions can be calculated and give ($j, k \in \mathbb{Z}, j \geq 0, k \geq 0$):

$$\frac{d^k}{dx^k} x^j = \begin{cases} \binom{j}{j-k} \cdot x^{j-k}, & \text{for } j \geq k, \\ 0, & \text{for } j < k, \end{cases} \quad (69)$$

$$\frac{d^k}{dx^k} x^{-j} = (-1)^k \binom{j+k-1}{j-1} \cdot x^{-j-k}. \quad (70)$$

Inserting this result into (68) gives:

$$I(l, n, m, q) = \frac{1}{l!} \sum_{k_1, k_2, k_3} \binom{l}{k_1, k_2, k_3} \frac{n!}{(n-k_1)!} (-1)^{k_1} \left( \frac{q - 1}{2} - ip \right)^{n-k_1} \cdot \frac{m!}{(m-k_2)!} (-1)^{k_2} \left( \frac{q - 1}{2} + ip \right)^m \cdot \left( \frac{q + 1}{2} + ip \right)^{-m-k_3} \bigg|_{p=-\frac{q+1}{2}}. \quad (71)$$

After evaluating at $p = -i \frac{q+1}{2}$ we get:

$$I(l, n, m, q) = (-1)^n \binom{l}{n} \sum_{k_1, k_2, k_3} (-1)^{k_3} \binom{n}{k_1} \binom{m}{k_2} \binom{m+1+k_3}{k_3} \frac{q^{m-k_2}}{(q+1)^{m+k_3+2}}. \quad (72)$$

In order to find the expression for the matrix elements of the momentum operator, we need to evaluate 2 integrals:

$$I_1(n, m) = \int_0^\infty dq \ (q+1) I(n+1, n, m, q), \quad I_2(n, m) = \int_0^\infty dq \ I(n, n, m, q). \quad (73)$$
In order to perform the integrals, we notice that they can be expressed in terms of the beta function

\[ B(x, y) = \int_0^\infty dt \frac{t^{x-1}}{(1 + t)^{x+y}}, \quad \text{for } \Re(x) > 0, \Re(y) > 0. \quad (74) \]

The first integral is:

\[ I_1(n, m) = (-1)^n \frac{n!}{(n+1)!} \sum_{k_1, k_2, k_3} (-1)^{k_3} \binom{n}{k_1} \binom{m}{k_2} \binom{m + 1 + k_3}{k_3} B(m-k_2+1, k_2+k_3). \quad (75) \]

If \( x, y \in \mathbb{N} \setminus \{0\} \), the beta function takes the form:

\[ B(x, y) = \frac{(x-1)!(y-1)!}{(x+y-1)!}. \quad (76) \]

Inserting this property into equation (75) we get:

\[ I_1(n, m) = (-1)^n \frac{n!}{(n+1)!} \sum_{k_1, k_2, k_3} (-1)^{k_3} \binom{n}{k_1} \binom{m}{k_2} \binom{m + 1 + k_3}{k_3} \frac{(m-k_2)!(k_2 + k_3 - 1)!}{(m+k_3)!} = \]

\[ = (-1)^n \frac{n!}{(n+1)(m+1)!} \sum_{k_1, k_2, k_3} (-1)^{k_3} \frac{(n+1)!}{k_1! k_2! k_3!} (m+1+k_3) = \]

\[ = (-1)^n \frac{n!}{(n+1)(m+1)} \left( -(m+1) + \sum_{k_1, k_2, k_3} (-1)^{k_3} \frac{(n+1)!}{k_1! k_2! k_3!} (m+1+k_3) \right). \quad (77) \]

The second integral is:

\[ I_2(n, m) = (-1)^n \frac{n!}{m+1} \sum_{k_1, k_2, k_3} (-1)^{k_3} \binom{n}{k_1} \binom{m}{k_2} \binom{m + 1 + k_3}{k_3} \frac{(m-k_2)!(k_2 + k_3)!}{(m+k_3+1)!} = \]

\[ = (-1)^n \frac{n!}{m+1} \sum_{k_1, k_2, k_3} (-1)^{k_3} \frac{n!}{k_1! k_2! k_3!}. \quad (78) \]
The matrix elements of the momentum operator can be expressed in terms of the functions $I_1(n, m)$ and $I_2(n, m)$:

$$p_{nm} := \sqrt{(n+1)(m+1)}i^{n+2} \left(-\frac{1}{2}I_1(n, m) - iI_2(n, m)\right)$$  \hfill (79)

1. Entries below and on the diagonal

We will look for a compact formula for the matrix elements. To this end we will find expressions for

$$S_{nm} = \sum_{k_1, k_2, k_3} (-1)^{k_3} \frac{n!}{k_1!k_2!k_3!}, \quad Z_{nm} = \sum_{k_1, k_2, k_3} (-1)^{k_3} k_3 \frac{n!}{k_1!k_2!k_3!}.$$  \hfill (80)

We will find $S_{nm}$ and $Z_{nm}$ recursively. In this derivation we will rely on the following identity holding for any polynomial $P$ of degree smaller than $n$:

$$\sum_{k=0}^{n} (-1)^k \binom{n}{k} P(k) = 0.$$  \hfill (81)

Let us consider first $S_{nm}$. From the definition, it is clear that

$$S_{n,m+1} = S_{n,m} + \sum_{k_1, k_2, k_3} (-1)^{k_3} \frac{n!}{k_1!k_2!k_3!} =$$

$$= S_{n,m} + \frac{n!}{(n-m-1)!(m+1)!} \sum_{k_1, k_3} (-1)^{k_3} \binom{n-m-1}{k_1} \frac{n!}{k_1!k_3!} =$$

$$= \begin{cases} S_{n,m} + 1, & \text{if } m = n - 1, \\ S_{n,m}, & \text{if } m < n - 1. \end{cases}$$  \hfill (82)

In order to find the desired identity, we notice that

$$S_{n,0} = \sum_{k_1, k_2, k_3} (-1)^{k_3} \frac{n!}{k_1!k_2!k_3!} = \sum_{k_1, k_3} (-1)^{k_3} \frac{n!}{k_1!k_3!} = \delta_{n,0}.$$  \hfill (83)
Combining the results we get that:

\[ S_{n,m} = \delta_{n,m} \text{ for } m \leq n. \]  

(84)

The second sum will be calculated in completely similar manner. We have the following recurrence:

\[
Z_{n+1,m} = Z_{n,m} + \sum_{k_1, k_2, k_3 \leq n, k_1 + k_2 + k_3 = n} (-1)^{k_3} \frac{n!}{k_1! k_2! k_3!} =
\]

\[
= Z_{n,m} + \left( \frac{n}{m+1} \right) \sum_{k_1, k_3 \leq n, k_1 + k_3 = n - m - 1} (-1)^{k_3} \binom{n-m-1}{k_3} =
\]

\[
\begin{cases} 
Z_{n,m}, & \text{if } m = n - 1, \\
Z_{n,m} - n, & \text{if } m = n - 2, \\
Z_{n,m}, & \text{if } m \leq n - 3.
\end{cases}
\]  

(85)

We can express the formula above using Kronecker delta:

\[
Z_{n+1,m} = Z_{n,m} - n\delta_{n,m+2}.
\]  

(86)

The recurrence starts at \( Z_{n,0} \):

\[
Z_{n,0} = \sum_{k_1, k_2, k_3 \leq n, k_1 + k_2 + k_3 = n} (-1)^{k_3} \frac{n!}{k_1! k_2! k_3!} = \sum_{k_1, k_3 \leq n, k_1 + k_3 = n} (-1)^{k_3} \binom{n}{k_3} = \begin{cases} 
1, & \text{if } n = 0, \\
-1, & \text{if } n = 1, \\
0, & \text{if } n \geq 2.
\end{cases}
\]  

(87)

In our study, we will only need to consider the following two cases.

1. \( n = 1 \). In this case \( Z_{1,0} = -1 \) and \( Z_{1,1} = -1 \).

2. \( n \geq 2 \). In this case \( Z_{n,0} = 0 \) and

\[
Z_{n+1,m} = Z_{n,m} - n\delta_{n,m+2}.
\]  

(88)

As a result,

\[
Z_{n,m} = -n\delta_{n,m+1} - n\delta_{n,m}.
\]  

(89)
Let us notice that the two cases can be written with one formula. For \( n \geq 1 \):
\[
Z_{n,m} = -n\delta_{n,m+1} - n\delta_{n,m}.
\] (90)

Let us now go back to the expression for \( I_1(n,m) \) and \( I_2(n,m) \).
\[
I_1(n,m) = \frac{(-1)^n i^{n+1}}{(n+1)(m+1)} (m+1)(S_{n+1,m} - 1) + Z_{n+1,m} = \frac{(-1)^n i^{n+1}}{(n+1)(m+1)} ((m+1)(\delta_{n+1,m} - 1) - (n+1)\delta_{n+1,m+1} - (n+1)\delta_{n+1,m}).
\] (91)

The second object is:
\[
I_2(n,m) = \frac{(-1)^n i^n}{m+1} S_{n,m} = \frac{(-1)^n i^n}{m+1} \delta_{n,m}.
\] (92)

We will combine the results to obtain the expression for the matrix elements of the momentum operator:
\[
p_{nm} = \frac{i}{\sqrt{(n+1)(m+1)}} \left( \frac{m+1}{2} (\delta_{n+1,m} - 1) - \frac{n+1}{2} \delta_{n+1,m+1} - \frac{n+1}{2} \delta_{n+1,m} + (n+1)\delta_{n,m} \right).
\] (93)

\[
p_{nm} = \frac{i}{\sqrt{(n+1)(m+1)}} \left( -\frac{m+1}{2} + \frac{n+1}{2} \delta_{n,m} + \frac{m-n}{2} \delta_{n+1,m} \right).
\] (94)

Let us notice that we make calculation for \( m \leq n \) only. Therefore
\[
p_{nm} = \frac{i}{\sqrt{(n+1)(m+1)}} \left( -\frac{m+1}{2} + \frac{n+1}{2} \delta_{n,m} \right).
\] (95)

This means that:
\[
p_{nn} = 0, \quad p_{nm} = -\frac{i}{2} \frac{\sqrt{m+1}}{n+1} \text{ if } m < n.
\] (96)

2. The entries above the diagonal

For a cross-check, we will calculate the entries above the diagonal as well \( m > n \). In this case
\[
S_{n,m} = \sum_{k_1, k_2, k_3} (-1)^{k_3} \frac{n!}{k_1! k_2! k_3!} = \sum_{k_1, k_2, k_3} (-1)^{k_3} \frac{n!}{k_1! k_2! k_3!} = (1 + 1 - 1)^n = 1
\] (97)
and

\[ Z_{n,m} = \sum_{k_1+k_2+k_3 = n, k_1 \leq n, k_2 \leq m} (-1)^{k_3} k_3 \frac{n!}{k_1!k_2!k_3!} = \sum_{k_1+k_2+k_3 = n, k_1 \leq n, k_2 \leq m} (-1)^{k_3} k_3 \frac{n!}{k_1!k_2!k_3!} = \]

\[ = x_3 \frac{\partial}{\partial x_3} (x_1 + x_2 - x_3)^n |_{x_1 = x_2 = x_3 = 1} = -n(1 + 1 - 1)^n = -n. \] (98)

Inserting the formulas into \( I_1(n, m), I_2(n, m) \) and into \( p_{nm} \) afterwards, we get:

\[ p_{nm} = \frac{i}{2} \sqrt{\frac{n + 1}{m + 1}} \text{ if } m > n. \] (99)

This is consistent with the fact that the matrix \( p \) is hermitian.

3. Summary

The calculations above show that

\[ p_{nn} = 0, \quad p_{nm} = -\frac{i}{2} \sqrt{\frac{m + 1}{n + 1}} \text{ if } m < n, \quad p_{nm} = \frac{i}{2} \sqrt{\frac{n + 1}{m + 1}} \text{ if } m > n. \] (100)

D. The matrix elements of the coordinate operator

The matrix elements of the coordinate operator:

\[ q_{nm} := \sqrt{(n+1)(m+1)} \int_{0}^{\infty} dq \int_{-\infty}^{+\infty} dp \frac{q^{\frac{1}{2}}}{(q^{\frac{1}{2}} - ip)^{n+2}} \frac{(q^{\frac{1}{2}} + ip)^m}{(q^{\frac{1}{2}} + ip)^{m+2}}. \] (101)

The integral over \( p \) can be done using a contour method. We take the sunset contour in the lower half plane and obtain

\[ q_{nm} := -i \sqrt{(n+1)(m+1)} \int_{0}^{\infty} dq \text{ Res}_{p=-\frac{1+i}{2}} \frac{(q^{\frac{1}{2}} - ip)^n}{(q^{\frac{1}{2}} + ip)^{n+2}} \frac{(q^{\frac{1}{2}} + ip)^m}{(q^{\frac{1}{2}} + ip)^{m+2}}. \] (102)

We will calculate now the residuum:

\[ \text{Res}_{p=-\frac{1+i}{2}} \left( \frac{(q^{\frac{1}{2}} - ip)^n}{(q^{\frac{1}{2}} + ip)^{n+2}} \frac{(q^{\frac{1}{2}} + ip)^m}{(q^{\frac{1}{2}} + ip)^{m+2}} \right) = \]

\[ = i^{n+2} \frac{1}{(n+1)!} \frac{d^{n+1}}{dp^{n+1}} \left( \frac{(q^{\frac{1}{2}} - ip)^n}{(q^{\frac{1}{2}} + ip)^{n+2}} \frac{(q^{\frac{1}{2}} + ip)^m}{(q^{\frac{1}{2}} + ip)^{m+2}} \right). \] (103)
The integral that we will need to calculate this time is

\[ I_3(n, m) = \int_0^\infty dq \, q I(n + 1, n, m, q). \]  

(104)

With this integral, we can express the matrix elements of the coordinate operator in the following form:

\[ q_{nm} = i^{n+1} \sqrt{(n + 1)(m + 1)} I_3(n, m). \]  

(105)

As previously, we can express the integral \( I_3(n, m) \) as a sum.

\[
I_3(n, m) = (-1)^n i^{n+1} \sum_{k_1, k_2, k_3 \atop k_1 + k_2 + k_3 = n+1 \atop k_1 \leq n, k_2 \leq m} (-1)^{k_3} \binom{n}{k_1} \binom{m}{k_2} \binom{m + 1 + k_3}{k_3} \int_0^\infty dq \, q^{m-k_2+1} (q + 1)^{m+k_3+2} =
\]

\[
= (-1)^n i^{n+1} \sum_{k_1, k_2, k_3 \atop k_1 + k_2 + k_3 = n+1 \atop k_1 \leq n, k_2 \leq m} (-1)^{k_3} \binom{n}{k_1} \binom{m}{k_2} \binom{m + 1 + k_3}{k_3} \frac{(m - k_2 + 1)!(k_2 + k_3 - 1)!}{(m + k_3 + 1)!} =
\]

\[
= -\frac{(-1)^n i^{n+1}}{(n+1)(m+1)} \sum_{k_1, k_2, k_3 \atop k_1 + k_2 + k_3 = n+1 \atop k_1 \leq n, k_2 \leq m} (-1)^{k_3} \frac{(n+1)!}{k_1!k_2!k_3!} (m + 1 - k_2) =
\]

\[
= \frac{(-1)^{n+1}}{(n+1)(m+1)} \left( (m+1) - \sum_{k_1, k_2, k_3 \atop k_1 + k_2 + k_3 = n+1 \atop k_1 \leq n+1, k_2 \leq m} (-1)^{k_3} \frac{(n+1)!}{k_1!k_2!k_3!} (m + 1 - k_2) \right). \tag{106}
\]

This time we will consider separately the terms on the diagonal and above the diagonal (and we will not calculate the terms below diagonal.)
1. Diagonal terms

\[ q_{nn} = \frac{1}{n+1} \left( (n+1) - \sum_{k_1,k_2,k_3} (-1)^{k_3} \frac{(n+1)!}{k_1!k_2!k_3!}(n + 1 - k) \right) = \]

\[ = \frac{1}{n+1} \left( (n+1) - \sum_{k_1,k_2,k_3} (-1)^{k_3} \frac{(n+1)!}{k_1!k_2!k_3!}(n + 1 - k) \right) = \]

\[ = \frac{1}{n+1} \left( (n+1) - (n+1)(1 + 1 - 1)^{n+1} + x_2 \frac{\partial}{\partial x_2} (x_1 + x_2 - x_3)^{n+1} \bigg|_{x_1=x_2=x_3=1} \right) = 1. \quad (107) \]

2. The terms above the diagonal

We will consider matrix elements \( q_{nm} \) for \( m > n \). In this case:

\[ q_{nm} = \frac{1}{\sqrt{(n+1)(m+1)}} \left( (m+1) - \sum_{k_1,k_2,k_3} (-1)^{k_3} \frac{(n+1)!}{k_1!k_2!k_3!}(m + 1 - k) \right) = \]

\[ = \frac{1}{\sqrt{(n+1)(m+1)}} \left( (m+1) - (m+1)(1 + 1 - 1)^{n+1} + x_2 \frac{\partial}{\partial x_2} (x_1 + x_2 - x_3)^{n+1} \bigg|_{x_1=x_2=x_3=1} \right) = \]

\[ = \sqrt{\frac{n+1}{m+1}}. \quad (108) \]

3. Summary

Since \( q_{nm} \) is hermitian, we have

\[ q_{nm} = \sqrt{\frac{n+1}{m+1}} \text{ if } m \geq n, \quad q_{nm} = \sqrt{\frac{m+1}{n+1}} \text{ if } m < n. \quad (109) \]
V. EVOLUTION OF QUANTUM OBSERVABLES

In what follows, we consider the quantum evolution corresponding to the classical case with $M < \frac{m}{2}$, where $m$ is the total rest mass of the shell. Classically, the shell reaches the horizon $q_H = 2M^2$ after an infinite time (of an observer at spatial infinity), as it is illustrated in Fig. 1.

Remarkably, our quantum model experiences a different behaviour. In a finite time, the quantum shell reaches a minimum size and after a bounce, which is above the horizon, it expands until it reaches a maximum size. More precisely, in our quantum model we choose a state peaked at energy $M$. One needs to remember that the energy of the system is conserved during the time evolution given by the Schrödinger equation. We diagonalize the quantum Hamiltonian numerically. Due to technical limitations of our numerical procedure we can study the model for small values of $M$ only. We calculate the quantum evolution of the expectation values of the operators $\hat{q}$ and $\hat{p}$. We notice that the expectation values $\langle q \rangle_t$ and $\langle p \rangle_t$ are periodic functions of time $t$.

A. Gaussian state

We choose a state peaked at energy $M$ with standard deviation $\sigma$:

$$|\Psi\rangle = \frac{1}{N} \sum_i e^{-\frac{(E_i - M)^2}{2\sigma^2}} |E_i\rangle,$$

(110)

where $|E_i\rangle$ is the eigenstate of the Hamiltonian operator with the eigenvalue $E_i$ and $N$ is the normalization constant:

$$N^2 = \sum_i e^{-\frac{(E_i - M)^2}{2\sigma^2}}.$$

(111)

In practical calculations we limit the sum to the region $[M - 4\sigma \sqrt{2 \ln(10)}, M + 4\sigma \sqrt{2 \ln(10)}]$. With this choice, at the end of the interval the exponential factor is $-\frac{(E_i - M)^2}{2\sigma^2} = e^{-16\ln(10)} = 10^{-16}$, which is approximately equal to the machine precision for double accuracy used in our calculations. We introduce a cut-off in the matrix size. We choose the parameter $\sigma$ such that all eigenvalues in the region are good approximations of the full eigenvalues. We will choose eigenvalues which converge when the cut-off is increased. The precise definitions will be given in the next section.
B. Eigenvalues convergence

In order to find the Gaussian states and their evolution, we look for some of the eigenvalues and eigenvectors of the Hamiltonian operator. We considered a cut-off: \( n < 1000, m < 1000 \) and calculated the matrix elements \( H_{nm} \) using equation (60). We calculated the integrals numerically using the DE rules for infinite range integrals as they are described in [21]. This amounts to making a change of variables

\[
q = e^{\pi \sinh(\tilde{q})}, \quad p = \sinh(\pi \sinh(\tilde{p}))
\]

and performing the integrals in the range \([-4, 4]\) using the open extended trapezoidal rule ([21]). We perform the integral over \( q \) first and afterwards we perform the integral over \( p \).

We look for convergence of the eigenvalues. Let us consider a family of submatrices \( H(k), k = 1, \ldots, 1000 \), where each matrix \( H(k) \) is obtained from the Hamiltonian matrix \( H \) by removing first \( 1000 - k \) rows and first \( 1000 - k \) columns. In particular \( H(1000) = H \) and \( k \) is the rank of the matrix \( H(k) \). Let us order the eigenvalues of \( H(k) \) in the increasing order and let us denote by \( E_i(k), i \leq k \) the \( i \)-th eigenvalue of \( H(k) \). We look for convergence of the eigenvalues \( E_i(k) \) as we increase \( k \). The plot 3 shows that eigenvalues \( E_i \) for \( 700 \leq i \leq 850 \) converge. Each of the eigenvalues stabilizes, which is reflected by the plateaux on the plot of \( E_i \) as a function of \( k \).

C. Evolution of the observables

We calculated the evolution of the expectation values of the operators \( \hat{q} \) and \( \hat{p} \) in a coherent state peaked at energy \( M = 10^{-6} \) with standard deviation \( \sigma = 10^{-7} \). This means that we considered a state:

\[
| \Psi(t) \rangle = \frac{1}{N} \sum_i e^{-\frac{(E_i - M)^2}{2\sigma^2} - 4 E_i t} | E_i \rangle
\]

and calculated the expectation values

\[
< \hat{q} >_t := ( \Psi(t) | \hat{q} \Psi(t) \rangle \quad \text{and} \quad < \hat{p} >_t := ( \Psi(t) | \hat{p} \Psi(t) \rangle.
\]

The calculations are performed in the \( e_n^{(1)} \) basis. After finding the eigenvectors of \( \hat{H} \), we calculated the components \( (e_n^{(1)} | \Psi(t) \rangle \). Afterwards, we used the formulas (109) and (100) for the matrix elements of \( \hat{q} \) and \( \hat{p} \) in the \( e_n^{(1)} \) basis.

We calculated \( < \hat{q} >_t \) and \( < \hat{p} >_t \) for \( m = 1.0, M = 2 \cdot 10^{-6}, \sigma = 10^{-7} \). The expectation value \( < \hat{q} >_t \) is bounded from below by approximately 0.006. The
Figure 3: The eigenvalues $E_i(k), i = 700, 710, \ldots, 850$ of the submatrices of $H(k)$. The eigenvalue $E_i(k)$ is the $i$-th eigenvalue of the sub-matrix $H(k)$ (the eigenvalues are sorted in the increasing order). Since the rank of $H(k)$ is equal $k$, it follows that $i \leq k$ and the plot of $E_i(k)$ starts at $k = i$. For each $i$ we connected the values $E_i(k)$ with a line in order to guide the eye, i.e. each line represents one eigenvalue $E_i$.

bounce, connecting contracting and expanding branches, occurs well above the horizon $q_H = 2M^2 = 2 \cdot 10^{-12}$ and at finite time as measured by an observer at spatial infinity. We recall that in the corresponding classical case the shell falls onto the horizon at an infinite time. The value $\langle \hat{q} \rangle_t$ is also bounded from above by approximately 0.01, which is smaller than the classical maximal size of the shell $q_{\text{max}} = \frac{m^3}{8(s(m-M))^2} \approx \frac{1}{8}$. It is clear that $\langle \hat{q} \rangle_t$ must oscillate as illustrated by Fig. 4.

Since the classical variable $p$ is the measure of the angle between the surfaces of constant time on both sides of the shell, it is reasonable to expect that the expectation value $\langle \hat{p} \rangle_t$ oscillates as a consequence of the oscillation of $\langle \hat{q} \rangle_t$. Indeed, such an effect is seen in Fig. 5.
Figure 4: Evolution of the expectation values of $\hat{q}$ in the coherent state peaked at energy $M = 10^{-6}$ with standard deviation $\sigma = 10^{-7}$. The expectation value is bounded from below by approximately 0.006 (0.037 if the error bars are taken into account). This is well above the horizon which in this case is at $q_H = 2M^2 = 2\cdot10^{-12}$. We interpret this as a quantum bounce above the horizon. As a result, the evolution has oscillatory character.
Figure 5: Evolution of the expectation values of $\hat{p}$ in the coherent state peaked at energy $M = 10^{-6}$ with standard deviation $\sigma = 10^{-7}$. Let us notice that $\langle \hat{p} \rangle_t = 0$ when $\langle \hat{q} \rangle_t$ is extremal. Classically this happened only when $q$ is maximal.

D. Oscillatory character of the evolution

The oscillatory character of the evolution is related to our choice of the Gaussian state. This can be shown by the following calculation:

$$< \hat{q} >_t = \frac{1}{N^2} \sum_{i,j} e^{-(E_i - M)^2 / 2\sigma^2} \sum_{i,j} e^{-(E_j - M)^2 / 2\sigma^2} e^{i(E_i - E_j)t} \langle E_i | \hat{q} | E_j \rangle =$$

$$= \frac{1}{N^2} \sum_{i,j} e^{-(E_i - M)^2 / 2\sigma^2} \sum_{i,j} e^{-(E_j - M)^2 / 2\sigma^2} \cos((E_i - E_j)t) \langle E_i | \hat{q} | E_j \rangle. \quad (115)$$
In the formula above, we used the fact that the eigenvectors $|E_i\rangle$ have real components in the $e_n^{(1)}$ basis and the fact $q_{nm} = q_{mn}$, $q_{nm} \in \mathbb{R}$. Let us recall that in our numerical calculations we limited the sum to finite number of terms. Therefore the resulting function is oscillatory as a finite sum of cosine functions.

Similar analysis applies to $<\hat{p}>_t$ giving trigonometric series.

We expect an oscillatory character if the spectrum is purely discrete. If the spectrum turns out to be continuous, we expect that non-oscillatory functions could be achieved. In that case the sum in (115) is replaced by an integral and the resulting function may be non-oscillatory. A typical example of such behaviour is a Fourier transform, which decomposes non-oscillatory function into oscillatory modes. However, full spectral analysis is beyond the scope of this paper.

VI. CONCLUSIONS

We used the coherent state quantization technique to investigate a quantum model of a massive shell. We developed the new mathematical tools: we found a closed formula for the basis elements $e_n^{(1)}$, and for the matrix elements of the operators $\hat{q}$ and $\hat{p}$ in this basis. We studied the spectrum of the quantum Hamiltonian operator numerically in the case $m = 1.0$. We truncated the operator spectrum and observed that some of the eigenvalues stabilize as we increase the truncation.

Using calculated eigenstates, we built a Gaussian state peaked at energy $M = 10^{-6}$. We investigated the evolution of the expectation values of $\hat{q}$ and $\hat{p}$ in the Gaussian state and observed that the quantum shell bounces well above the horizon. This leads to an oscillatory behaviour of the system which is in contrast with the classical solution where the shell collapses and reaches the Schwarzschild horizon $q_H = 2M^2$ in infinite time (as measured by an observer at infinity). The oscillatory character of the evolution may be traced back to our construction of the Gaussian state. More detailed analysis of this phenomenon needs a careful study of the spectral properties of the Hamiltonian operator.

Our analysis of the quantum Hamiltonian is based on a series of numerical experiments. The analytical analysis seems to be out of range. According to these experiments it seems that this Hamiltonian, in the investigated region, up to accuracy of our calculations (double accuracy) has a continuous spectrum.

We realize that the research presented in this paper is not a complete analysis. We developed the necessary tools and showed that this research direction may lead to interesting results. In particular, the results concerning oscillatory behaviour of the quantum system and the quantum origin of a bounce above the horizon require independent cross-check. The integrals involved in the expression of matrix elements of the Hamiltonian operator were calculationally demanding. This resulted in rather
limited size of the matrix and small value of eigenvalues which can be reliably calculated. More efficient numerical integration methods are needed in order to study the model in more details. An advantage of our approach is that the quantum Hamiltonian $\hat{H}$ we consider is positive definite, which is generally true and independent on the chosen set of parameters.

The issue of the positivity of both classical and quantum Hamiltonians are of special interest. At the classical level, it can be realized by restricting the phase space. The quantum level is more demanding. In our integral quantization method there is a one-to-one correspondence between the phase space points and the space of coherent states. However, we cannot follow the classical procedure of choosing the subspace of all coherent states to obtain positivity of quantum Hamiltonian. The reason is that such procedure would violate the mathematical consistency of the integral quantization and its physical interpretation as deformation of POV measure which results in problems with the probabilistic interpretation of this approach. Therefore, in the integral defining the mapping of a classical observable into quantum observable one cannot restrict the region of integration, but one can restrict the integrant by taking $\theta(H)H$ instead of $H$. This way one obtains the quantum Hamiltonian $\hat{H}$ which still acts on the full Hilbert space but it is positively defined because our quantization procedure maps positive functions on the phase space into positive operators. Similar logic has been used, for instance, in the paper [22] within loop quantum gravity, where the dynamics is defined by a square root of positive part of quantum gravitational scalar constraint operator.

To use this procedure consequently, the position and momentum quantum observables have to be defined on the whole Hilbert space. They determine physical meaning of the coherent states as quantum counterparts of the configuration space points. Our procedure is consistent with treating the operators $\hat{M}(Q)$, see Eq. (28), as the POV measure.

ACKNOWLEDGMENTS

We would like to thank Jacek Jezierski, Jerzy Kijowski, and Daniele Malafarina for helpful discussions. This work was partially supported by the National Science Centre, Poland grant No. 2018/28/C/ST9/00157.
Appendix A: Orthonormal basis of the carrier space

The basis of the Hilbert space $L^2(\mathbb{R}_+, d\nu(x))$, where $d\nu(x) := dx/x$, is known to be \[10\]
\[ e_n^{(\alpha)}(x) = \sqrt{\frac{n!}{\Gamma(n + \alpha + 1)}} e^{-x/2} x^{(1+\alpha)/2} L_n^{(\alpha)}(x), \quad (A1) \]
where $L_n^{(\alpha)}$ is the Laguerre function and $\alpha > -1$. One can verify that $\int_0^\infty e_n^{(\alpha)}(x)e_m^{(\alpha)}(x)d\nu(x) = \delta_{nm}$ so that $e_n^{(\alpha)}(x)$ is an orthonormal basis (for any fixed value of the parameter $\alpha > -1$).

---

[1] J. Kijowski, G. Magli, and D. Malafarina, “New derivation of the variational principle for the dynamics of a gravitational spherical shell”, Phys. Rev. D 74, 084017 (2006).
[2] C. Vaz, “Proper time quantization of a thin shell”, arXiv:2205.06867 [gr-qc].
[3] J. Jezierski and J. Kijowski, “Positivity of total energy in general relativity”, Phys. Rev. D 36, 1041 (1987).
[4] A. Góźdź, W. Piechocki and G. Plewa, “Quantum Belinski-Khalatnikov-Lifshitz scenario”, Eur. Phys. J. C 79, 45 (2019).
[5] A. Góźdź, W. Piechocki, and T. Schmitz, “Dependence of the affine coherent states quantization on the parametrization of the affine group”, Eur. Phys. J. Plus 136, 18 (2021).
[6] I. M. Gel’fand and M. A. Naĭmark, “Unitary representations of the group of linear transformations of the straight line”, Dokl. Akad. Nauk. SSSR 55, 567 (1947).
[7] E. W. Aslaksen and J. R. Klauder, “Unitary Representations of the Affine Group”, J. Math. Phys. 9, 206 (1968).
[8] E. W. Aslaksen and J. R. Klauder, “Continuous Representation Theory Using Unitary Affine Group”, J. Math. Phys. 10, 2267 (1969).
[9] A. O. Barut and R. Rączka, Theory of group representations and applications (PWN, Warszawa, 1977).
[10] J. P. Gazeau and R. Murenzi, “Covariant affine integral quantization(s),” J. Math. Phys. 57, 052102 (2016).
[11] H. Bergeron and J. P. Gazeau, “Integral quantizations with two basic examples,” Annals Phys. 344, 43 (2014).
[12] M. Reed and B. Simon, *Methods of Modern Mathematical Physics* (San Diego, Academic Press, 1980), Vols I and II. III B

[13] G. B. Arfken, H. J. Weber, F. E. Harris, *Mathematical Methods for Physicists: A Comprehensive Guide* (Academic Press, Oxford, 2011). III B

[14] P. Busch, P. J. Lahti and P. Mittelstaedt, *The Quantum Theory of Measurement*, second Rev. Edition, Springer-Verlag, Berlin Heidelberg, 1996, ISBN 3-540-61355-2. III C, III C

[15] A. Góźdź, A. Pędrak, and W. Piechocki, “Ascribing quantum system to Schwarzschild spacetime with naked singularity”, Class. Quantum Grav. 39, 145005 (2022). III C

[16] F. Faà di Bruno, “Note sur une nouvelle formule du calcul différentiel,” Quart. J. Math., 1 (1855) pp. 359-360. IV A

[17] Bell polynomial. Encyclopedia of Mathematics. URL: http://encyclopediaofmath.org/index.php?title=Bell_polynomial&oldid=46007 IV A, IV A, IV A

[18] E.T. Bell, “Exponential polynomials,” Ann. of Math., 35 (1934) pp. 258-277. IV A

[19] I. Lah, “Eine neue Art von Zahlen, ihre Eigenschaften und Anwendung in der mathematischen Statistik,” Mitteil. Math. Statist., 7 (1955) pp. 203-216 IV A

[20] M. Abramowitz and I. A. Stegun, eds. *Handbook of mathematical functions with formulas, graphs, and mathematical tables* (US Government printing office, 1964), Vol. 55. IV A

[21] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, Brian, *Numerical Recipes: The Art of Scientific Computing* (Cambridge University Press, 2007). V B, V B

[22] T. Pawlowski and A. Ashtekar, “Positive cosmological constant in loop quantum cosmology”, Phys. Rev. D 85, 064001 (2012). VI
