Quantum dynamics of gravitational massive shell

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The quantum dynamics of a self-gravitating thin matter shell in vacuum has been considered. The quantum Hamiltonian of the system is positive definite. Within a chosen set of parameters, the quantum shell bounces above the horizon. The considered quantum system does not collapse to the gravitational singularity of the corresponding classical system.

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 [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 a well-defined Hamiltonian description of the matter shell, we have decided to quantize that system to get insight into corresponding quantum dynamics. The present paper is devoted to the examination of such an issue.

The shell system is simple enough to be treated satisfactory at the classical level, and rich enough for the examination of various aspects of the corresponding quantum system. Recently, it was used for addressing the issue of the importance of the choice of time parameter at the 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 a 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. Section IV concerns the calculations of the matrix elements of quantum observables in a 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 $q \in \mathbb{R}_+ := \{x \in \mathbb{R} | x > 0\}$ 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

$$\dot{q} = \frac{\partial H}{\partial p}, \tag{2}$$

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$$\dot{p} = -\frac{\partial H}{\partial q}, \tag{3}$$

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) and (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

$$\dot{q} = \frac{\partial H}{\partial p} = \sinh(p)\sqrt{2q}\frac{\left(\cosh(p) - \sqrt{\frac{m^2}{2q} + \sinh^2(p)}\right)^2}{\sqrt{\frac{m^2}{2q} + \sinh^2(p)}}. \tag{5}$$

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 the considered isolated gravitational system at spatial infinity so that it is the ADM mass. It means, roughly speaking, that if the density of the 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 the considered gravitational system. The specific form of matter field may lead to the specific subspace Λ of the phase space $\Pi = \{(p,q)|p \in \mathbb{R}, q \in \mathbb{R}_+\}$, such that $H(p,q) > 0$ for $(p,q) \in \Lambda$. We call Λ the physical phase space.

Let us consider the case $m(q) := m = $ 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

$$H(p,q) = M \tag{6}$$

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 Eq. (6) [see also (4)] in the form

$$1 - \sqrt{\frac{2}{q}}M = \left(\cosh(p) - \sqrt{\frac{m^2(q)}{2q} + \sinh^2(p)}\right)^2, \tag{7}$$

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.

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

(i) for $M\sqrt{\frac{2}{q}} \geq \frac{m^2}{2q}$, i.e., $\sqrt{q} \geq \frac{m^2}{2\sqrt{2}M}$, the solution satisfies

$$\cosh(p) = \frac{2 - \frac{m^2}{2q} - M\sqrt{\frac{2}{q}}}{2\sqrt{1 - M\sqrt{\frac{2}{q}}}} =: f(q), \tag{8}$$

(ii) while for $M\sqrt{\frac{2}{q}} < \frac{m^2}{2q}$, i.e., $\sqrt{q} < \frac{m^2}{2\sqrt{2}M}$, it satisfies

$$\cosh(p) = -\frac{2 - \frac{m^2}{2q} - M\sqrt{\frac{2}{q}}}{2\sqrt{1 - M\sqrt{\frac{2}{q}}}} = -f(q). \tag{9}$$

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 $q = \frac{m^4}{8(m-M)^2}$ where $p = 0$. This is illustrated in Fig. 1. The plot for $p < 0$ is just a reflection by the q axis.

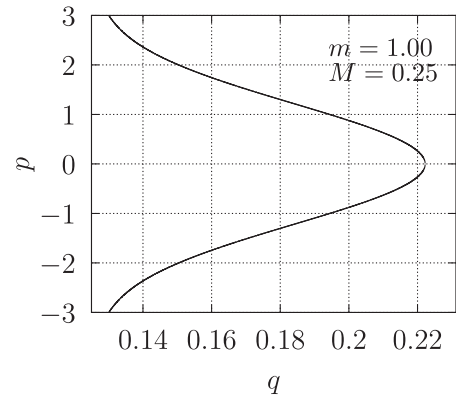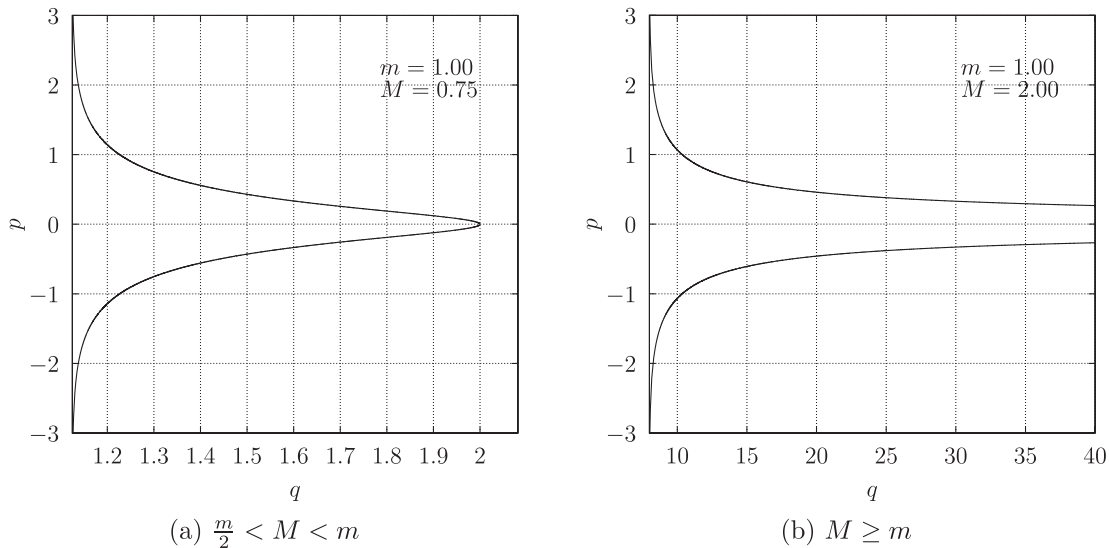FIG. 1.   Dust shell's trajectory with energy $H(p,q) = M < \frac{m}{2}$.

FIG. 2.   Dust shells' trajectories 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 $\sqrt{q} < \frac{m^2}{2\sqrt{2M}}$ 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 $q = \frac{m^4}{8(m-M)^2}$ where $p = 0$. This is illustrated in Fig. 2(a). 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 $q \to +\infty$. This is illustrated in Fig. 2(b).

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

$$H(0, q) < 0 \quad \text{for } q < m^2/8. \tag{10}$$

Since wee need to have $H(p, q) > 0$, the physical phase space Λ should be a subspace of the entire phase space Π. Some regions of Π, 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 [4,5].

The physical phase space of our gravitational system

$$\Pi := \{(p, q)|p \in \mathbb{R}, q \in \mathbb{R}_+\} \tag{11}$$

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

$$(p', q') \cdot (p, q) := (q'p + p', q'q), \tag{12}$$

with the unity (0,1) and the inverse

$$(p', q')^{-1} = \left(-\frac{p'}{q'}, \frac{1}{q'}\right). \tag{13}$$

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:

$$U(p, q)\psi(x) = e^{ipx}\psi(qx), \tag{14}$$

where[1] $\psi(x) = \langle x|\psi\rangle$ and $|\psi\rangle \in L^2(\mathbb{R}_+, d\nu(x))$.

We define the integrals over the affine group $\mathrm{G} = \mathrm{Aff}(\mathbb{R})$ as follows:

$$\int_{\mathrm{G}} d\mu(p, q) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dp \int_0^\infty \frac{dq}{q^2}. \tag{15}$$

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[1]We use Dirac's notation whenever we wish to deal with the abstract vector instead of functional representation of the vector.

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:

$$|p, q\rangle = U(p, q)|\Phi\rangle. \tag{16}$$

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 $L^2(\mathbb{R}_+, d\nu(x))$

$$\frac{1}{A_\Phi} \int_G d\mu(p, q)|p, q\rangle\langle p, q| = \mathbb{I}, \tag{17}$$

where the constant A_Φ can be determined by using any arbitrary, normalized vector $|f\rangle \in L^2(\mathbb{R}_+, d\nu(x))$ as follows:

$$A_\Phi = \int_G d\mu(p, q)\langle f|p, q\rangle\langle p, q|f\rangle = \int_0^\infty \frac{dq}{q^2}|\Phi(q)|^2. \tag{18}$$

B. Quantum observables

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

$$\mathcal{F} \ni f \to \hat{f} := \frac{1}{A_\Phi} \int_G d\mu(p, q)|p, q\rangle f(p, q)\langle p, q| \in \mathcal{A}, \tag{19}$$

where $\mathcal{F}$ is a vector space of real continuous functions on a phase space, and $\mathcal{A}$ 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 the Appendix we define an orthonormal basis (for any fixed value of the parameter $\alpha > -1$) of the unitary irreducible representation of the 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 $L_n^{(\alpha)}$ (see, e.g. [13]). For this purpose, it is convenient to restrict

the upper label α of the functions $L_n^{(\alpha)}(x)$ to any fixed integer. In this case, the generating function for the Laguerre polynomials reads

$$\frac{\exp(-\frac{xz}{1-z})}{(1-z)^{\alpha+1}} = \sum_{n=0}^\infty L_n^{(\alpha)}(x)z^n \quad \text{if } |z| < 1. \tag{20}$$

For calculation of the matrix elements of the operator (19), in the basis defined in the Appendix, 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:

$$\Phi^{(\alpha)}(x) := e_0^{(\alpha)}(x) = \sqrt{\frac{1}{\alpha!}} x^{\frac{1+\alpha}{2}} e^{-\frac{x}{2}}. \tag{21}$$

In this case one gets

$$\langle e_n^{(\alpha)}(x)|pq\rangle$$
$$= \sqrt{\frac{n!}{(n+\alpha)!\alpha!}} q^{\frac{1+\alpha}{2}} \int_0^\infty \frac{dx}{x} e^{ipx} x^{1+\alpha} e^{-\frac{q+1}{2}x} L_n^{(\alpha)}(x). \tag{22}$$

Let us define the function

$$\text{epq}(\alpha, p, q; z)$$
$$:= \sum_n \langle e_n^{(\alpha)}(x)|pq\rangle \left[\sqrt{\frac{n!}{(n+\alpha)!\alpha!}}\right]^{-\frac{1}{2}} z^n$$
$$= \left(\frac{\sqrt{q}}{1-z}\right)^{1+\alpha} \int_0^\infty dx\, x^\alpha \exp\left(-\left[\frac{q+1}{2} + \frac{z}{1-z} - ip\right]x\right). \tag{23}$$

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

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

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

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

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

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

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. 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 $Q \subset G = \text{Aff}(\mathbb{R})$, describes the localization of the system in the subspace Q of the phase space G.

The normalization condition

$$\hat{M}(G) = \frac{1}{A_\phi}\int_G d\mu(p,q)|p,q\rangle\langle p,q| = \hat{\mathbb{1}} \quad (29)$$

is required to get the so-called minimal probabilistic interpretation of quantum mechanics [14]:

$$\text{Prob}(Q, \Psi) = \langle\Psi|\hat{M}(Q)|\Psi\rangle, \quad (30)$$

which describes the probability of finding our system in Q, under the condition that this system is in the state Ψ.

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 the physical interpretation of the classical Hamiltonian, we quantize it

as a function restricted to the required region of the phase space by considering

$$\hat{H} = \frac{1}{A_\Phi}\int_G d\mu(p,q)|p,q\rangle\theta(H(p,q))H(p,q)\langle p,q|, \quad (31)$$

where θ 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 $(p', q') \notin \Omega$, then

$$\hat{H}|p',q'\rangle$$
$$= \frac{1}{A_\Phi}\int_\Omega d\mu(p,q)|p,q\rangle\theta(H(p,q))H(p,q)\langle p,q|p',q'\rangle$$
$$(32)$$

is usually a nonzero vector. This behavior is due to nonorthogonality of the states $|p, q\rangle$, i.e., the quantum phase space regions Ω and $G\backslash\Omega$ are not independent.

Another very important related problem is the quantization of the elementary observables (p, q). These observables represent the 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]:

$$\langle p, q|\hat{p}|p, q\rangle = p \quad \text{and} \quad \langle p, q|\hat{q}|p, q\rangle = q, \quad (33)$$

where

$$\hat{p} = \frac{1}{A_\Phi}\int_G d\mu(p,q)|p,q\rangle p\langle p,q| \quad \text{and}$$
$$\hat{q} = \frac{1}{A_\Phi}\int_G d\mu(p,q)|p,q\rangle q\langle p,q|. \quad (34)$$

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

$$\hat{H} = \frac{1}{A_\Phi}\int_G d\mu(p,q)|p,q\rangle\theta(H(p,q))H(p,q)\langle p,q|, \quad (35)$$

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

$$\langle\Psi\rangle = \frac{1}{A_\Phi} \int_G d\mu(p,q) |\Psi(p,q)|^2 \theta(H(p,q)) H(p,q) > 0. \tag{36}$$

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

$$i\frac{\partial}{\partial s}|\Psi(s)\rangle = \hat{H}|\Psi(s)\rangle, \tag{37}$$

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 the 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 $\frac{z}{1-z} = \frac{1}{1-z} - 1$ and $\frac{d}{dz}\frac{1}{1-z} = \frac{1}{(1-z)^2}$, we can simplify the expression for the basis element:

$$\langle e_n^{(1)}|pq\rangle = -\frac{q\sqrt{n+1}}{(n+1)!} \left[\frac{d^{n+1}}{dz^{n+1}} \int_0^\infty dx \right.$$
$$\left. \times \exp\left(-\left[\frac{q-1}{2} + \frac{1}{1-z} - ip\right]x\right)\right]_{|z=0} \tag{38}$$

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

$$f(z) = F(G(z)) = \exp(-G(z)x), \quad \text{where } G(z) = \frac{1}{1-z}. \tag{39}$$

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

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

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

$$B_{n,k}(z_1, z_2, ..., z_{n-k+1}) = \sum \frac{n!}{j_1! j_2! ... j_{n-k+1}!} \left(\frac{z_1}{1!}\right)^{j_1} \left(\frac{z_2}{2!}\right)^{j_2} ... \left(\frac{z_{n-k+1}}{(n-k+1)!}\right)^{j_{n-k+1}}, \tag{41}$$

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

$$j_1 + j_2 + \cdots + j_{n-k+1} = k, \tag{42}$$

$$j_1 + 2j_2 + 3j_3 + \cdots + (n-k+1)j_{n-k+1} = n. \tag{43}$$

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

$$G(0) = 1, \qquad G^m(0) = m!. \tag{44}$$

Therefore

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

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

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

where

$$L_{n,k} = (-1)^n \binom{n-1}{k-1} \frac{n!}{k!}, \qquad n \geq k \geq 1, \quad (47)$$

$$L_{0,0} = 1, \qquad L_{n,0} = 0, \qquad n \geq 1. \quad (48)$$

We extend the sum in (45) to $k = 0$ and obtain a formula valid for $n = 0$:

$$\frac{d^n}{dz^n} F(G(0)) = \sum_{k=0}^{n} (-1)^k |L_{n,k}| x^k e^{-x}. \quad (49)$$

In order to calculate $\langle e_n^{(1)} | pq \rangle$, we need to evaluate the integral

$$\int_0^\infty dx x^k \exp\left(-\left(\frac{q+1}{2} - \mathrm{i}p\right)x\right) = \frac{k!}{(\frac{q+1}{2} - \mathrm{i}p)^{k+1}}. \quad (50)$$

This integral directly follows from the Euler's integral formula (see for example Eq. (6.1.1) from [20]):

$$\Gamma(n) = z^n \int_0^\infty dx x^{n-1} e^{-zx} \quad \text{for } \Re(n) > 0, \ \Re(z) > 0. \quad (51)$$

In the formula above $\Gamma(z)$ is the Gamma function. Inserting this evaluation into (38) gives

$$\langle e_n^{(1)} | pq \rangle = \sqrt{n+1} \sum_{k=0}^{n+1} \frac{(-1)^{k+1} k!}{(n+1)!} |L_{n+1,k}| \frac{q}{(\frac{q+1}{2} - \mathrm{i}p)^{k+1}}. \quad (52)$$

We will define coefficients $E_{n,k}$:

$$E_{n,k} = \frac{(-1)^{k+1} k!}{n!} |L_{n,k}|. \quad (53)$$

Due to cancellation of terms, the coefficients have the following explicit form:

$$E_{n,k} = (-1)^{k-1} \binom{n-1}{k-1}, \qquad n \geq k \geq 1, \quad (54)$$

$$E_{0,0} = \frac{(-1)^{k-1} k!}{n!}, \qquad E_{n,0} = 0, \qquad n \geq 1. \quad (55)$$

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:

$$\langle e_n^{(1)} | pq \rangle = \sqrt{n+1} \sum_{k=1}^{n+1} (-1)^{k-1} \binom{n}{k-1} \frac{q}{(\frac{q+1}{2} - \mathrm{i}p)^{k+1}}. \quad (56)$$

We will change the summation variable into $k' = k - 1$ and obtain

$$\langle e_n^{(1)} | pq \rangle = \frac{q\sqrt{n+1}}{(\frac{q+1}{2} - \mathrm{i}p)^2} \sum_{k=0}^{n} \binom{n}{k} \frac{(-1)^k}{(\frac{q+1}{2} - \mathrm{i}p)^k}. \quad (57)$$

The last sum is the binomial expansion. Therefore

$$\langle e_n^{(1)} | pq \rangle = \frac{q\sqrt{n+1}}{(\frac{q+1}{2} - \mathrm{i}p)^2} \left(1 - \frac{1}{\frac{q+1}{2} - \mathrm{i}p}\right)^n$$

$$= q\sqrt{n+1} \frac{(\frac{q-1}{2} - \mathrm{i}p)^n}{(\frac{q+1}{2} - \mathrm{i}p)^{n+2}}. \quad (58)$$

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:

$$H_{nm} := \langle e_n^{(1)} | \hat{H} e_m^{(1)} \rangle$$

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

$$\times H(p,q) \langle e_m^{(1)} | pq \rangle^*. \quad (59)$$

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

$$H_{nm} := \frac{\sqrt{(n+1)(m+1)}}{2\pi} \int_0^\infty dq \int_{-\infty}^{+\infty} dp \, \theta(H(q,p)) H(q,p) \frac{(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} - \mathrm{i}p)^{n+2} (\frac{q+1}{2} + \mathrm{i}p)^{m+2}}. \quad (60)$$

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,

$$H_{nm} = \frac{\sqrt{(n+1)(m+1)}}{2\pi} \int_0^\infty dq \int_{-\infty}^{+\infty} dp \, \theta(H(q,p)) H(q,p) \frac{(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m (\frac{q+1}{2} + \mathrm{i}p)^{n-m}}{((\frac{q+1}{2})^2 + p^2)^{n+2}}. \quad (61)$$

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

$$H_{nm} = \frac{\sqrt{(n+1)(m+1)}}{2\pi} \int_0^\infty dq \int_{-\infty}^{+\infty} dp\, \theta(H(q,p)) H(q,p) \frac{((\frac{q-1}{2})^2 + p^2)^m (\frac{q^2-1}{4} + p^2 - \mathrm{i}p)^{n-m}}{((\frac{q+1}{2})^2 + p^2)^{n+2}}. \tag{62}$$

After expanding the expression $(\frac{q^2-1}{4} + p^2 - \mathrm{i}p)^{n-m}$ 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:

$$\Im H_{nm} = 0. \tag{63}$$

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 read as

$$p_{nm} := \frac{\sqrt{(n+1)(m+1)}}{2\pi} \int_0^\infty dq \int_{-\infty}^{+\infty} dp\, \frac{p(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} - \mathrm{i}p)^{n+2} (\frac{q+1}{2} + \mathrm{i}p)^{m+2}}. \tag{64}$$

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

$$p_{nm} := -\mathrm{i}\sqrt{(n+1)(m+1)} \int_0^\infty dq \mathrm{Res}\Big|_{p=-\mathrm{i}\frac{q+1}{2}} \left(\frac{p(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} - \mathrm{i}p)^{n+2} (\frac{q+1}{2} + \mathrm{i}p)^{m+2}} \right). \tag{65}$$

We will calculate now the residuum:

$$\begin{aligned}
\mathrm{Res}\Big|_{p=-\mathrm{i}\frac{q+1}{2}} \left(\frac{p(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} - \mathrm{i}p)^{n+2} (\frac{q+1}{2} + \mathrm{i}p)^{m+2}} \right) &= \mathrm{i}^{n+2} \frac{1}{(n+1)!} \frac{d^{n+1}}{dp^{n+1}} \left(\frac{p(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} + \mathrm{i}p)^{m+2}} \right) \\
&= \frac{\mathrm{i}^{n+2}}{(n+1)!} p \frac{d^{n+1}}{dp^{n+1}} \left(\frac{(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} + \mathrm{i}p)^{m+2}} \right) \Bigg|_{p=-\mathrm{i}\frac{q+1}{2}} \\
&\quad + \frac{\mathrm{i}^{n+2}}{n!} \frac{d^n}{dp^n} \left(\frac{(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} + \mathrm{i}p)^{m+2}} \right) \Bigg|_{p=-\mathrm{i}\frac{q+1}{2}}.
\end{aligned} \tag{66}$$

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

$$I(l,n,m,q) = \frac{1}{l!} \frac{d^l}{dp^l} \left(\frac{(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} + \mathrm{i}p)^{m+2}} \right) \Bigg|_{p=-\mathrm{i}\frac{q+1}{2}} \tag{67}$$

with $l = n$ or $l = n+1$. We will expand the derivative using a Leibnitz rule generalized to three factors:

$$I(l,n,m,q) = \frac{1}{l!} \sum_{\substack{k_1,k_2,k_3 \\ k_1+k_2+k_3=l}} \binom{l}{k_1,k_2,k_3} \frac{d^{k_1}}{dp^{k_1}} \left(\frac{q-1}{2} - \mathrm{i}p \right)^n \cdot \frac{d^{k_2}}{dp^{k_2}} \left(\frac{q-1}{2} + \mathrm{i}p \right)^m \frac{d^{k_3}}{dp^{k_3}} \left(\frac{q+1}{2} + \mathrm{i}p \right)^{-m-2} \Bigg|_{p=-\mathrm{i}\frac{q+1}{2}}, \tag{68}$$

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

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

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

Inserting this result into (68) gives

$$I(l, n, m, q) = \frac{1}{l!} \sum_{\substack{k_1, k_2, k_3 \\ k_1+k_2+k_3=l \\ k_1 \le n, k_2 \le m}} \binom{l}{k_1, k_2, k_3} \frac{n!}{(n-k_1)!} (-\mathrm{i})^{k_1} \left(\frac{q-1}{2} - \mathrm{i}p \right)^{n-k_1}$$

$$\cdot (\mathrm{i})^{k_2} \frac{m!}{(m-k_2)!} \left(\frac{q-1}{2} + \mathrm{i}p \right)^{m-k_2} (-\mathrm{i})^{k_3} \frac{(m+1+k_3)!}{(m+1)!} \left(\frac{q+1}{2} + \mathrm{i}p \right)^{-m-2-k_3} \Bigg|_{p=-\mathrm{i}\frac{q+1}{2}}. \tag{71}$$

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

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

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

$$I_1(n, m) = \int_0^\infty dq (q+1) I(n+1, n, m, q), \qquad I_2(n, m) = \int_0^\infty dq I(n, n, m, q). \tag{73}$$

In order to perform the integrals, we notice that they can be expressed in terms of the beta function

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

The first integral is

$$I_1(n, m) = (-1)^n (\mathrm{i})^{n+1} \sum_{\substack{k_1, k_2, k_3 \\ k_1+k_2+k_3=n+1 \\ k_1 \le n, k_2 \le m}} (-1)^{k_3} \binom{n}{k_1} \binom{m}{k_2} \binom{m+1+k_3}{k_3} B(m-k_2+1, k_2+k_3). \tag{75}$$

If $x, y \in \mathbb{N} - \{0\}$, the beta function takes the form

$$B(x, y) = \frac{(x-1)!(y-1)!}{(x+y-1)!}. \tag{76}$$

Inserting this property into Eq. (75) we get

$$I_1(n, m) = (-1)^n \mathrm{i}^{n+1} \sum_{\substack{k_1, k_2, k_3 \\ k_1+k_2+k_3=n+1 \\ k_1 \le n, k_2 \le m}} (-1)^{k_3} \binom{n}{k_1} \binom{m}{k_2} \binom{m+1+k_3}{k_3} \frac{(m-k_2)!(k_2+k_3-1)!}{(m+k_3)!}$$

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

$$= \frac{(-1)^n \mathrm{i}^{n+1}}{(n+1)(m+1)} \left(-(m+1) + \sum_{\substack{k_1, k_2, k_3 \\ k_1+k_2+k_3=n+1 \\ k_1 \le n+1, k_2 \le m}} (-1)^{k_3} \frac{(n+1)!}{k_1! k_2! k_3!} (m+1+k_3) \right). \tag{77}$$

The second integral is

$$
I_2(n,m) = (-1)^n(\mathtt{i})^n \sum_{\substack{k_1,k_2,k_3 \\ k_1+k_2+k_3=n \\ k_1 \le n, k_2 \le m}} (-1)^{k_3} \binom{n}{k_1}\binom{m}{k_2}
$$

$$
\times \binom{m+1+k_3}{k_3} \frac{(m-k_2)!(k_2+k_3)!}{(m+k_3+1)!}
$$

$$
= \frac{(-1)^n(\mathtt{i})^n}{m+1} \sum_{\substack{k_1,k_2,k_3 \\ k_1+k_2+k_3=n \\ k_1 \le n, k_2 \le m}} (-1)^{k_3} \frac{n!}{k_1!k_2!k_3!}. \tag{78}
$$

The matrix elements of the momentum operator can be expressed in terms of the functions $I_1(n,m)$ and $I_2(n,m)$:

$$
p_{nm} := \sqrt{(n+1)(m+1)}\, \mathtt{i}^{n+2}\left(-\frac{1}{2}I_1(n,m) - \mathtt{i}I_2(n,m)\right). \tag{79}
$$

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

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

$$
Z_{n,m} = \sum_{\substack{k_1,k_2,k_3 \\ k_1+k_2+k_3=n \\ k_1 \le n, k_2 \le m}} (-1)^{k_3} k_3 \frac{n!}{k_1!k_2!k_3!}. \tag{80}
$$

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

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

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

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

$$
= S_{n,m} + \frac{n!}{(n-m-1)!(m+1)!}
$$

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

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

In order to find the desired identity, we notice that

$$
S_{n,0} = \sum_{\substack{k_1,k_2,k_3 \\ k_1+k_2+k_3=n \\ k_1 \le n, k_2 = 0}} (-1)^{k_3} \frac{n!}{k_1!k_2!k_3!} = \sum_{\substack{k_1,k_3 \\ k_1+k_3=n}} (-1)^{k_3} \frac{n!}{k_1!k_3!} = \delta_{n,0}. \tag{83}
$$

Combining the results we get that

$$
S_{n,m} = \delta_{n,m} \quad \text{for } m \le n. \tag{84}
$$

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

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

$$
= Z_{n,m} + \binom{n}{m+1} \sum_{\substack{k_1,k_3 \\ k_1+k_3=n-m-1}} (-1)^{k_3} k_3 \binom{n-m-1}{k_3}
$$

$$
= \begin{cases} Z_{n,m}, & \text{if } m=n-1, \\ Z_{n,m}-n, & \text{if } m=n-2. \\ Z_{n,m}, & \text{if } m \le n-3. \end{cases} \tag{85}
$$

We can express the formula above using Kronecker delta:

$$
Z_{n,m+1} = Z_{n,m} - n\delta_{n,m+2}. \tag{86}
$$

The recurrence starts at $Z_{n,0}$:

$$
Z_{n,0} = \sum_{\substack{k_1,k_2,k_3 \\ k_1+k_2+k_3=n \\ k_1 \le n, k_2 = 0}} (-1)^{k_3} k_3 \frac{n!}{k_1!k_2!k_3!}
$$

$$
= \sum_{\substack{k_1,k_3 \\ k_1+k_3=n}} (-1)^{k_3} k_3 \binom{n}{k_3} = \begin{cases} 1, & \text{if } n=0, \\ -1, & \text{if } n=1. \\ 0, & \text{if } n \ge 2. \end{cases} \tag{87}
$$

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) $n \ge 2$. In this case $Z_{n,0} = 0$ and

$$
Z_{n,m+1} = Z_{n,m} - n\delta_{n,m+2}. \tag{88}
$$

As a result,

$$
Z_{n,m} = -n\delta_{n,m+1} - n\delta_{n,m}. \tag{89}
$$

Let us notice that the two cases can be written with one formula. For $n \ge 1$,

$$Z_{n,m} = -n\delta_{n,m+1} - n\delta_{n,m}. \tag{90}$$

Let us now go back to the expression for $I_1(n,m)$ and $I_2(n,m)$,

$$\begin{aligned}
I_1(n,m) &= \frac{(-1)^n \mathrm{i}^{n+1}}{(n+1)(m+1)} ((m+1)(S_{n+1,m}-1) + Z_{n+1,m}) \\
&= \frac{(-1)^n \mathrm{i}^{n+1}}{(n+1)(m+1)} ((m+1)(\delta_{n+1,m}-1) \\
&\quad - (n+1)\delta_{n+1,m+1} - (n+1\delta_{n+1,m}).
\end{aligned} \tag{91}$$

The second object is

$$I_2(n,m) = \frac{(-1)^n (\mathrm{i})^n}{m+1} S_{n,m} = \frac{(-1)^n (\mathrm{i})^n}{m+1} \delta_{n,m}. \tag{92}$$

We will combine the results to obtain the expression for the matrix elements of the momentum operator:

$$\begin{aligned}
p_{nm} &= \frac{\mathrm{i}}{\sqrt{(n+1)(m+1)}} \left(\frac{m+1}{2}(\delta_{n+1,m}-1) \right. \\
&\quad \left. - \frac{n+1}{2}\delta_{n+1,m+1} - \frac{n+1}{2}\delta_{n+1,m} + (n+1)\delta_{n,m} \right),
\end{aligned} \tag{93}$$

$$\begin{aligned}
p_{nm} &= \frac{\mathrm{i}}{\sqrt{(n+1)(m+1)}} \left(-\frac{m+1}{2} + \frac{n+1}{2}\delta_{n,m} \right. \\
&\quad \left. + \frac{m-n}{2}\delta_{n+1,m} \right).
\end{aligned} \tag{94}$$

Let us notice that we make the calculation for $m \leq n$ only. Therefore

$$p_{nm} = \frac{\mathrm{i}}{\sqrt{(n+1)(m+1)}} \left(-\frac{m+1}{2} + \frac{n+1}{2}\delta_{n,m} \right). \tag{95}$$

This means that

$$p_{nn} = 0, \qquad p_{nm} = -\frac{\mathrm{i}}{2}\sqrt{\frac{m+1}{n+1}} \quad \text{if } m < n. \tag{96}$$

2. The entries above the diagonal

For a cross-check, we will calculate the entries above the diagonal as well as $m > n$. In this case

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

$$= (1+1-1)^n = 1 \tag{97}$$

and

$$\begin{aligned}
Z_{n,m} &= \sum_{\substack{k_1,k_2,k_3 \\ k_1+k_2+k_3=n \\ k_1 \leq n, k_2 \leq m}} (-1)^{k_3} k_3 \frac{n!}{k_1!k_2!k_3!} \\
&= \sum_{\substack{k_1,k_2,k_3 \\ k_1+k_2+k_3=n \\ k_1 \leq n, k_2 \leq n}} (-1)^{k_3} k_3 \frac{n!}{k_1!k_2!k_3!} \\
&= x_3 \frac{\partial}{\partial x_3} (x_1 + x_2 - x_3)^n \Big|_{x_1=x_2=x_3=1} \\
&= -n(1+1-1)^n = -n.
\end{aligned} \tag{98}$$

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

$$p_{nm} = \frac{\mathrm{i}}{2}\sqrt{\frac{n+1}{m+1}} \quad \text{if } m > n. \tag{99}$$

This is consistent with the fact that the matrix p is Hermitian.

3. Summary

The calculations above show that

$$p_{nn} = 0, \qquad p_{nm} = -\frac{\mathrm{i}}{2}\sqrt{\frac{m+1}{n+1}} \quad \text{if } m < n,$$

$$p_{nm} = \frac{\mathrm{i}}{2}\sqrt{\frac{n+1}{m+1}} \quad \text{if } m > n. \tag{100}$$

D. The matrix elements of the coordinate operator

The matrix elements of the coordinate operator read as

$$\begin{aligned}
q_{nm} &:= \frac{\sqrt{(n+1)(m+1)}}{2\pi} \int_0^\infty dq \int_{-\infty}^{+\infty} dp \\
&\quad \times \frac{q(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} - \mathrm{i}p)^{n+2} (\frac{q+1}{2} + \mathrm{i}p)^{m+2}}.
\end{aligned} \tag{101}$$

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

$$\begin{aligned}
q_{nm} &:= -\mathrm{i}\sqrt{(n+1)(m+1)} \int_0^\infty dq\, q \mathrm{Res} \Big|_{p=-\mathrm{i}\frac{q+1}{2}} \\
&\quad \times \left(\frac{(\frac{q-1}{2} - \mathrm{i}p)^n (\frac{q-1}{2} + \mathrm{i}p)^m}{(\frac{q+1}{2} - \mathrm{i}p)^{n+2} (\frac{q+1}{2} + \mathrm{i}p)^{m+2}} \right).
\end{aligned} \tag{102}$$

We will calculate now the residuum:

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

$$=i^{n+2}\frac{1}{(n+1)!}\frac{d^{n+1}}{dp^{n+1}}\left(\frac{(\frac{q-1}{2}-ip)^n(\frac{q-1}{2}+ip)^m}{(\frac{q+1}{2}+ip)^{m+2}}\right). \quad (103)$$

The integral that we will need to calculate this time is

$$I_3(n,m)=\int_0^\infty dq\,qI(n+1,n,m,q). \quad (104)$$

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

$$q_{nm}=i^{n+1}\sqrt{(n+1)(m+1)}I_3(n,m). \quad (105)$$

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

$$I_3(n,m)=(-1)^n i^{n+1}\sum_{\substack{k_1,k_2,k_3\\k_1+k_2+k_3=n+1\\k_1\le n,k_2\le m}}(-1)^{k_3}\binom{n}{k_1}\binom{m}{k_2}\binom{m+1+k_3}{k_3}\int_0^\infty dq\,\frac{q^{m-k_2+1}}{(q+1)^{m+k_3+2}}$$

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

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

$$=\frac{(-i)^{n+1}}{(n+1)(m+1)}\left((m+1)-\sum_{\substack{k_1,k_2,k_3\\k_1+k_2+k_3=n+1\\k_1\le n+1,k_2\le m}}(-1)^{k_3}\frac{(n+1)!}{k_1!k_2!k_3!}(m+1-k_2)\right). \quad (106)$$

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

1. Diagonal terms

$$q_{nn}=\frac{1}{n+1}\left((n+1)-\sum_{\substack{k_1,k_2,k_3\\k_1+k_2+k_3=n+1\\k_1\le n+1,k_2\le n}}(-1)^{k_3}\frac{(n+1)!}{k_1!k_2!k_3!}(n+1-k_2)\right)$$

$$=\frac{1}{n+1}\left((n+1)-\sum_{\substack{k_1,k_2,k_3\\k_1+k_2+k_3=n+1\\k_1\le n+1,k_2\le n+1}}(-1)^{k_3}\frac{(n+1)!}{k_1!k_2!k_3!}(n+1-k_2)\right)$$

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

2. The terms above the diagonal

We will consider matrix elements q_{nm} for $m>n$. In this case,

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

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

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

3. Summary

Since q_{nm} is Hermitian, we have

$$q_{nm} = \sqrt{\frac{n+1}{m+1}} \quad \text{if } m \geq n,$$

$$q_{nm} = \sqrt{\frac{m+1}{n+1}} \quad \text{if } m < n. \tag{109}$$

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 behavior. 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 σ:

$$|\Psi\rangle = \frac{1}{N} \sum_i e^{-\frac{(E_i - M)^2}{2\sigma^2}} |E_i\rangle, \tag{110}$$

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

$$N^2 = \sum_i e^{-\frac{(E_i - M)^2}{\sigma^2}}. \tag{111}$$

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 cutoff in the matrix size. We choose the parameter σ such that all eigenvalues in the region are good approximations of the full eigenvalues. We will choose eigenvalues which converge when the cutoff 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 cutoff, $n < 1000$, $m < 1000$, and calculated the matrix elements H_{nm} using Eq. (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

$$q = e^{\pi \sinh(\tilde{q})}, \qquad p = \sinh(\pi \sinh(\tilde{p})) \tag{112}$$

and performing the integrals in the range $(-4, 4)$ using the open extended trapezoidal rule (Trapz structure from [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 the first $1000 - k$ rows and the 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 ith 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 plateau 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
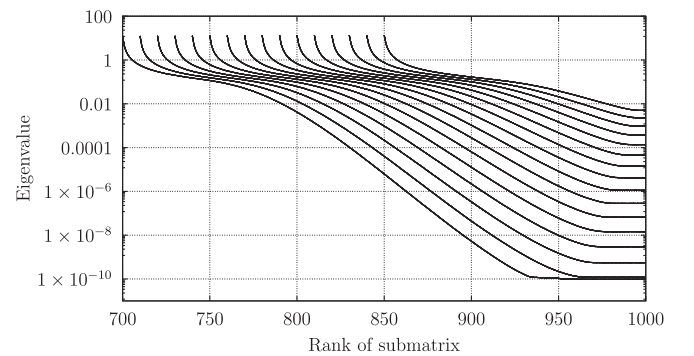

FIG. 3. The eigenvalues $E_i(k), i = 700, 710, \ldots, 850$ of the submatrices of $H(k)$. The eigenvalue $E_i(k)$ is the ith eigenvalue of the submatrix $H(k)$ (the eigenvalues are sorted in increasing order). Since the rank of $H(k)$ is equal to k, it follows that $i \leq k$ and the plot of $E_i(k)$ 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.

$M = 10^{-6}$ with standard deviation $\sigma = 10^{-7}$. This means that we considered a state

$$|\Psi(t)\rangle = \frac{1}{N}\sum_i e^{-\frac{(E_i-M)^2}{2\sigma^2} - \mathrm{i}E_i t}|E_i\rangle \tag{113}$$

and calculated the expectation values

$$\langle \hat{q}\rangle_t := \langle \Psi(t)\rangle \quad \text{and} \quad \langle \hat{p}\rangle_t := \langle \Psi(t)\rangle. \tag{114}$$

The calculations are performed in the $e_n^{(1)}$ basis. After finding the eigenvectors of $\hat{H}$, we calculated the components $\langle e_n^{(1)}\rangle$. 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 $\langle \hat{q}\rangle_t$ and $\langle \hat{p}\rangle_t$ for $m = 1.0, M = 2 \times 10^{-6}$, $\sigma = 10^{-7}$. The expectation value $\langle \hat{q}\rangle_t$ is bounded from below by approximately 0.006. The bounce, connecting contracting, and expanding branches, occurs well above the horizon $q_H = 2M^2 = 2 \times 10^{-12}$ 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 $q_{\max} = \frac{m^4}{8(m-M)^2} \approx \frac{1}{8}$. 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
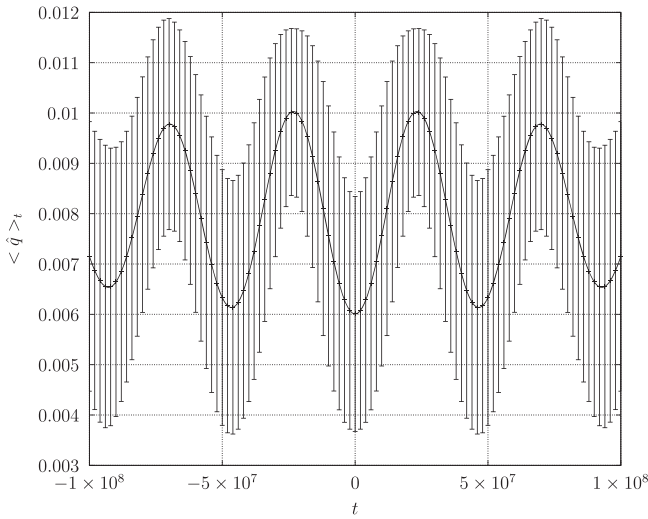

FIG. 4. Evolution of the expectation values of $\hat{q}$ in the coherent state peaked at energy $M = 10^{-6}$ with standard deviation $\sigma = 10^{-7}$. The expectation value is bounded from below by approximately 0.006 (0.037 if the error bars are taken into account). This is well above the horizon which in this case is at $q_H = 2M^2 = 2 \times 10^{-12}$. We interpret this as a quantum bounce above the horizon. As a result, the evolution has oscillatory character.

$\langle \hat{p}\rangle_t$ oscillates as a consequence of the oscillation of $\langle \hat{q}\rangle_t$. Indeed, such an effect is seen in Fig. 5.

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:

$$\begin{aligned}\langle \hat{q}\rangle_t &= \frac{1}{N^2}\sum_{i,j} e^{-\frac{(E_i-M)^2}{2\sigma^2} - \frac{(E_j-M)^2}{2\sigma^2}} e^{\mathrm{i}(E_i-E_j)t}\langle E_i|\hat{q}|E_j\rangle \\ &= \frac{1}{N^2}\sum_{i,j} e^{-\frac{(E_i-M)^2}{2\sigma^2} - \frac{(E_j-M)^2}{2\sigma^2}} \cos((E_i - E_j)t)\langle E_i|\hat{q}|E_j\rangle.\end{aligned} \tag{115}$$

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.

A similar analysis applies to $\langle \hat{p}\rangle_t$ 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 nonoscillatory functions could be achieved. In that case the sum in (115) is replaced by an integral and the resulting function may be nonoscillatory. A typical example of such behavior is a Fourier transform, which decomposes a nonoscillatory function into oscillatory modes. However, full spectral analysis is beyond the scope of this paper.
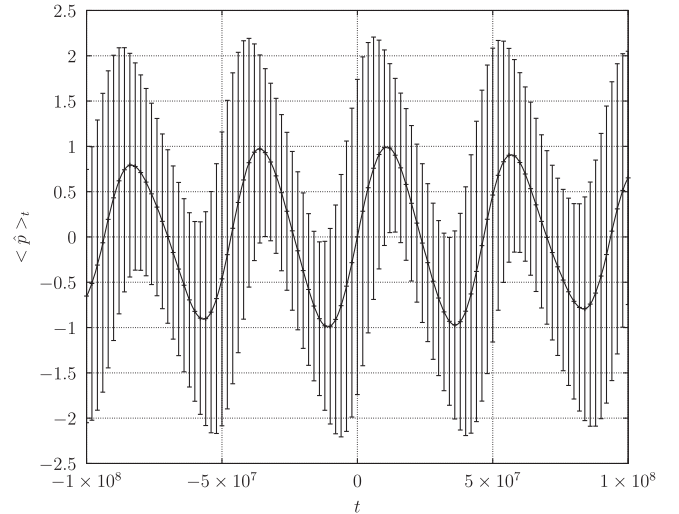

FIG. 5. Evolution of the expectation values of $\hat{p}$ in the coherent state peaked at energy $M = 10^{-6}$ with standard deviation $\sigma = 10^{-7}$. Let us notice that $\langle \hat{p}\rangle_t = 0$ when $\langle \hat{q}\rangle_t$ is extremal. Classically this happens only when q is maximal.

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 behavior 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-checks. The integrals involved in the expression of matrix elements of the Hamiltonian operator were calculationally demanding. This resulted in a rather limited size of the matrix and a 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 is 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 a 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 a 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 the positive part of the 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 the 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.

APPENDIX: ORTHONORMAL BASIS OF THE CARRIER SPACE

The basis of the Hilbert space $L^2(\mathbb{R}_+, d\nu(x))$, where $d\nu(x) \coloneqq dx/x$, is known to be [10]

$$e_n^{(\alpha)}(x) = \sqrt{\frac{n!}{\Gamma(n + \alpha + 1)}} e^{-x/2} x^{(1+\alpha)/2} L_n^{(\alpha)}(x), \quad \text{(A1)}$$

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 $\alpha > -1$).

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