Loop quantum gravity with optimal control path integral, and application to black hole tunneling

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Abstract
This paper presents a novel path integral formalism for Einstein’s theory of gravitation from the viewpoint of optimal control theory. Despite its close connection to the well-known variational principle of physicists, optimal control turns out to be more general. Within this context, a Lagrangian which is different from the Einstein-Hilbert Lagrangian is defined. Einstein’s field equations are recovered exactly with variations of the new action functional. The quantum theory is obtained using Ashtekar variables and the loop scalar product. As an illustrative example, the tunneling process of a black hole into another black hole or into a white hole is investigated with a toy model.

Keywords Loop quantum gravity · Optimal control · Path integral · Transition of geometry

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1 Introduction

The Lagrangian and Hamiltonian formulation of general relativity is a long-standing problem that has been solved mostly in the sixties by Dirac, Arnowit, Deser, Misner [1–3], and in the eighties by Ashtekar [4] for the connection formulation. Most of the scientific research on this branch of physics has followed the path sketched by these papers (see [5] for a historical review). The problem could have been considered closed, but remaining technical difficulties encountered in quantum gravity (such as the difficulty to determine properly determine the Hamiltonian operator in Loop Quantum Gravity (LQG) [6–8], or the difficulties encountered with spinfoam [9–16]) leads us to think that maybe, this is not the end of the story, and a novel starting point is required. For example, we can change the variational principle, as suggested by C. Cremaschini, M. Tessarotto in Refs. [17–20].

Independently of this context, a Lagrangian and Hamiltonian formalism for optimal control problems has been developed during the second half of the 20th century, by Bellman, Pontryagin, and their collaborators [21, 22]. Since, Optimal Control Theory (OCT) has been one of the most successful theories of mathematics, with applications in engineering, aerospace [23], robotics, finance, quantum technologies [24, 25]... Despite its close connection to the well-known variational principle used in classical physics, optimal control has a few small differences that allow us to tackle more general situations [26]. In particular, it can handle dynamical problems without a natural canonical adjoint state of the generalized coordinates. Recently, several papers have outlined the precise relationship between OCT and classical/quantum physics [26–30]. As an example, one can explain how quantum mechanics can be understood through stochastic optimization on space-times [31, 32].

Following the idea that a novel approach is required to solve quantum gravity dynamics, the issue is explored using the optimal control formalism. The first step is to express (classical) general relativity dynamics in a suitable form. This can be performed using any variables in 3+1 formalism. Then, a Lagrangian and a Hamiltonian can be defined over an extended configuration space. It turns out that the corresponding path integral propagator takes a very simple form. However, optimal control does not give us a natural way to construct quantum gravitational states. Thus, we employ Ashtekar variables and the LQG scalar product for that purpose. As an illustrative example, we consider a toy model of black hole tunneling. This hypothetical quantum effect [33, 34] has been studied recently in the context of LQG in order to shed light on Planck stars [35, 36].

This article is structured as follows, in Sect. 2 the connection between optimal control and physical systems is reviewed. In Sect. 3 the path integral is defined and analyzed with the harmonic oscillator. In Sects. 4 and 5 we apply the theory to general relativity expressed in Ashtekar variables and the path integral is derived. The application to black hole tunneling is considered in Sect. 6. Finally, a conclusion is made in Sect. 7.
2 Lagrangian and Hamiltonian in OCT

This first section is devoted to a concise presentation of the Lagrangian and the Hamiltonian formalism in optimal control theory \[22, 23\]. The case of the harmonic oscillator is considered as an example. Additional technical details concerning the relations between standard physics and optimal control can be found in Ref. \[26\].

We consider a physical system described by the real variable \(x \in \mathbb{C}\) (a classical state that belongs to the configuration space) whose dynamics are governed by the first-order differential equation:

\[
\dot{x} = f(x, u(t), t).
\]

\(u(t)\) is a time-dependent control field, an input of the system that must be determined. A standard optimal control problem is to determine \(u\) in order to transform \(x\) from an initial state \(x_0\) to a target state \(x_t\) while minimizing one or several constraints, such as the time of the transformation, the energy consumption,... To solve this problem, a Lagrangian and a Hamiltonian are constructed, by analogy with classical mechanics. For a given control problem, we define the cost function:

\[
C = \int_0^t dt' f_0(x, u, t').
\]  

(1)

Extremums of \(C\) are found using the calculus of variations. However, to take into account the constraints imposed by the system dynamics, we introduce another dynamical constraint with the use of a Lagrange multiplier. We define:

\[
S = \int_0^t dt' (f_0(x, u, t') + px(\dot{x} - f(x, u, t')) + pu).
\]  

(2)

which can be assimilated to the physical action, and \(\mathcal{L}_{OC} = f_0(x, u, t') + px(\dot{x} - f(x, u, t')) + pu\) is the system Lagrangian in the extended configuration space \(\mathcal{C}'\) defined by the vector \((x, u, px, pu)\). Here, \(pu\) is a Lagrange multiplier for the control field. For a constrained control field, \(pu\) must be multiplied by a function of \(u, \dot{u}, \) or any parameter that specifies the constraints on the control field. For simplicity, we consider here an unconstrained control. Extremals of this action, with fixed boundaries, are described by Euler-Lagrange’s equation, \(\partial_X \mathcal{L}_{OC} - \dot{d}_t (\partial_{\dot{X}} \mathcal{L}_{OC}) = 0\), with \(X \in \{x, u, px, pu\}\). For the system above, one obtains:

\[
\dot{x} = f(x, u, t)
\]  

(3)

\[
\dot{px} = \partial_x (f_0 - px f)
\]  

(4)

\[
0 = \partial_u (f_0 - px f)
\]  

(5)

\[
pu = 0
\]  

(6)

We can also define the Pontryagin Hamiltonian:

\[
H_{OC} = px \dot{x} + pu \dot{u} - \mathcal{L}_{OC}
\]  

(7)

Where \(pu\) must be set to zero in order to satisfy Eq. (6). Hamilton’s equations \(\partial_X H_{OC} = -\dot{P}\) and \(\partial_P H_{OC} = \dot{X}\), \(X \in \{x, u\}\) and \(P \in \{px, pu\}\) gives us again the equation of motions. From Hamilton equation, one also obtains:
\[
\frac{\partial H_{OC}}{\partial u} = \frac{\partial}{\partial u}(p_x f - f_0) = 0.
\] (8)

This corresponds to Pontryagin Maximum Principle for an unconstrained control field. Note that contrary to classical mechanics, the Hamiltonian is a function on \( C' = (x, u, p_x, p_u) \), and the Lagrangian is a function of \( (x, \dot{x}, u, \dot{u}, p_x, p_u, \dot{p}_x, \dot{p}_u) \).

If initial and final states are sub-manifolds of \( C \), the calculation of the first-order variation of \( S \) gives us also the so-called transversality condition:

\[
[p_x \delta x]_0 = 0
\] (9)

with \( \delta x \) a variation of the system position. In the following, we do not discuss this case further, because it does not impact the path integral.

As an example, we consider the case of a harmonic oscillator, described by the following equations of motion:

\[
\dot{x} = \frac{p}{m}; \quad \dot{p} = -kx.
\] (10)

where \( x \) gives the position of the oscillator of mass \( m \), and \( p \) is its momentum. \( k \) is the spring constant. The configuration space is the phase space \( C = (x, p) \). To define the optimal control Lagrangian and Hamiltonians, we define the extended configuration space \( C' = (x, p, \chi, \pi) \), where \( \chi \) and \( \pi \) are assimilated to the respective adjoint states of \( x \) and \( p \). With this system, there is no control field and no additional constraints on the system dynamics. Then, the Lagrangian simply read:

\[
\mathcal{L}_{OC} = \chi \left( \dot{x} - \frac{p}{m} \right) + \pi \left( \dot{p} + kx \right),
\] (11)

and the Hamiltonian is:

\[
H_{OC} = \chi \frac{p}{m} - k\pi x.
\] (12)

using Hamilton’s equations, we can deduce dynamical equations for the adjoint states:

\[
\dot{\pi} = \frac{\chi}{m}; \quad \dot{\chi} = -k\pi.
\] (13)

They are the same as equations (10). If we impose as initial conditions \( \pi(0) = x(0)/2 \) and \( \chi(0) = p(0)/2 \), the Hamiltonian becomes:

\[
H_{OC} = \frac{1}{2} \left( \frac{p^2}{m} + kx^2 \right).
\] (14)

This is the system’s Hamiltonian in classical mechanics. With the optimal control approach, we have another description of the system’s time evolution in terms of variations of a scalar function. Because the extended configuration space \( C' \) is bigger than the phase space, there are many possible trajectories. However, they are all identical when they are projected on \( \tilde{C} \). Only trajectories given by the equations (10) are physically possible. We shall now discuss the definition of the path integral.
3 Path integral

Given a classical system described by the optimal control problem described in Sect. 2, we can switch to a quantum theory by introducing a path integral. Note that this is unrelated to stochastic optimal control, where path integrals are also used.

The path integral of the optimal control problem is formally given by [26]:

\[
\hat{W} = \int Dx Dp_x e^{i \int_0^t L_{OC} dt'}.
\]  

(15)

Here, \( x \) refers to the classical state, and \( p_x \) to its adjoint state in \( C' \). Since the control field is treated as a position coordinate, we do not include it in the equations. It is straightforward to recover the case with an explicit control field. If the control is classical, we do not integrate over the control variables.

The path integral (15) can be computed explicitly using standard methods [37, 38]. To ensure a well-defined path integral, time is discretized, such that the formal definition becomes:

\[
\hat{W} = N \int \prod_t dx^{(t)} dp^{(t)}_x e^{i \sum_t \Delta t (f_0^{(t)} + p_x^{(t)}(x^{(t)} - f^{(t)}))},
\]  

(16)

where \( N = (\sqrt{2\pi})^{-d} \) is a normalization coefficient, \( \dot{x}^{(t)}, f_0^{(t)}, \) and \( f^{(t)} \) are functions of the system state at other time steps: \( x^{(t-1)}, p^{(t-1)}, x^{(t-2)}, p^{(t-2)}, \) etc. For example, if one discretizes derivatives with an Euler method, we have \( \dot{x}^{(t)} = \frac{1}{\Delta t} (x^{(t)} - x^{(t-1)}) \).

We remark in Eq. (16) that the adjoint state is used only once, at each time step. Then, the integration over \( p_x^{(t)} \) is simple:

\[
\hat{W} = N \int \prod_t dx^{(t)} \delta_0 (\Delta t (\dot{x}^{(t)} - f^{(t)})) e^{i \sum_t \Delta t f_0^{(t)}}.
\]  

(17)

The adjoint state concentrates the possible paths along classical trajectories. There is only one Dirac distribution per \( x^{(t)} \), then, Eq. (17) is well defined. Additionally, it is a simple propagator of the system dynamics, as we can expect in the original theory of Feynman.

A simple application can be made using the harmonic oscillator. The quantum state is a function \( \psi(x, p) \). If at time \( t = 0 \) the system is in the state \( \psi(x^{(0)}, p^{(0)}) \), at time \( \Delta t \) we have from Eq. (17):

\[
\int dx^{(0)} dp^{(0)} \delta_0 \left( x^{(1)} - x^{(0)} - \Delta t \frac{p^{(0)}}{m} \right) \delta_0 \left( p^{(1)} - p^{(0)} + \Delta t k x^{(0)} \right) |\psi(x^{(0)}, p^{(0)})| \\
= \left( 1 + \frac{k \Delta t^2}{m} \right) |\psi\left( \frac{m x^{(1)} - \Delta t p^{(1)}}{m + k \Delta t^2}, \frac{m p^{(1)} + k \Delta t x^{(1)}}{m + k \Delta t^2} \right)|. 
\]  

(18)
To be consistent with the first-order approximation, we have $\Delta t^2 \simeq 0$. Then, the last equation becomes:

$$\left| \psi \left( x^{(1)} - \frac{\Delta t}{m} p^{(1)}, p^{(1)} + k \Delta t x^{(1)} \right) \right|. \tag{19}$$

It is therefore obvious that the propagator has the following property:

$$\hat{W}(t) \left| \psi(x, p) \right\rangle = \left| \psi(\hat{W}^{-1}(t)x(t), \hat{W}^{-1}(t)p(t)) \right\rangle, \tag{20}$$

where $\hat{W}^{-1}(t) X$ denotes the inverse flow of $X$.

With this formalism, solving the time evolution of the wave function is a trivial problem once the flow of the classical state is known. This can be solved analytically for the simplest systems, but otherwise, numerical integrations must be employed.

At this point, the main question concerns the consistency of this theory with the standard quantum harmonic oscillator \cite{39}. The standard quantum Hamiltonian operator is (in $\hbar$ units): $\hat{H} = \omega \hat{a}^\dagger \hat{a}$, with eigenvalues $\omega n$ and eigenstates $|n\rangle$. To make the relation with the path integral, we shall introduce the coherent state $|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$. A straightforward calculation of the evolution operator $\hat{U}$ applied to an arbitrary coherent state $|\alpha_0\rangle$ gives:

$$e^{-i t \hat{H}} |\alpha_0\rangle = |\alpha_0 e^{-i \omega t}\rangle. \tag{21}$$

Then,

$$|\alpha(t)\rangle = \hat{U}(t)|\alpha_0\rangle = |\alpha_0 e^{-i \omega t}\rangle. \tag{22}$$

In this equation, $\alpha$ is the classical counterpart of the annihilation operator $\hat{a}$. It is related to $x$ and $p$ by the relation:

$$\alpha = \frac{i}{\sqrt{2\omega m}} p + \sqrt{\frac{k}{2\omega}} x, \tag{23}$$

and it follows the classical equations of motion \cite{39}:

$$\frac{d\alpha}{dt} = -i \omega \alpha. \tag{24}$$

The solution of this equation is simply $\alpha(t) = e^{-i \omega t} \alpha_0$. From these definitions, it is clear that $|\alpha\rangle$ corresponds to a state $|\psi(x, p)\rangle$ with the mapping $(x, p) \rightarrow \alpha$. Moreover, we have $\alpha_0 = e^{i \omega t} \alpha(t)$, which corresponds to $\hat{W}^{-1}(t) \alpha(t)$ in Eq. (20). Contrary to Eq. (22), the initial state is used to parametrize the system time evolution, and not the final state. It turns out that the path integral propagator of the optimal control formalism (of the harmonic oscillator) is equivalent to the standard evolution operator.

Also, the path integral must encode the scalar product between two coherent states. From now, nothing tells us what the scalar product is. This issue can be solved with a terminal cost, which does not influence the dynamics. In OCT, the terminal cost
is usually the distance between the final state and the target state (see [40] for an application of OCT to controlled quantum systems). It is a measure of distance in the configuration space. The terminal cost for the harmonic oscillator can be inferred as follows: the scalar product between two coherent states is

\[ \langle \alpha | \beta \rangle = \exp \left( -|\alpha|^2/2 - |\beta|^2/2 + \alpha^* \beta \right), \]

and the probability is:

\[ |\langle \alpha | \beta \rangle|^2 = \exp \left( |\alpha|^2 - |\beta|^2 + 2\Re(\alpha^* \beta) \right) = \exp(-|\alpha - \beta|^2). \]

This is the exponential of the square distance between \( \alpha \) and \( \beta \).

Therefore, the terminal cost can be defined as:

\[ S_T = i(-|\alpha|^2/2 - |\beta|^2/2 + \alpha^* \beta) = i \log \langle \alpha | \beta \rangle, \]  

with \( \alpha, \beta \), defined by Eq. (23).

## 4 Optimal control formulation of general relativity

In the previous section, a simple path integral was derived using optimal control theory. The idea is to proceed similarly for the theory of general relativity.

Contrary to the standard approach, the idea is not to assume a Lagrangian similar to the Einstein-Hilbert Lagrangian, but a new Lagrangian is constructed from Einstein’s field equations with an optimal control approach. As a rough guide, the theoretical proposal must be computationally efficient (at least, by using state-of-the-art numerical methods in quantum mechanics and relativity).

Einstein’s field equations (in the vacuum) are generally written as [3]:

\[ R_{\mu\nu} + g_{\mu\nu} \left( \Lambda - \frac{1}{2} R \right) = 0. \]  

(26)

\( R_{\mu\nu} \) is the Ricci tensor, calculated using the metric tensor \( g_{\mu\nu} \). \( \Lambda \) is the cosmological constant, and \( R = R_{\mu\nu} g^{\mu\nu} \). Written in this covariant form, it is not easy to work with Einstein’s field equations because there is no explicit notion of evolution. There are redundancies in the variables, and some gauge degrees of freedom must be chosen in order to make explicit calculations. In order to make an easier link with state-of-the-art canonical quantum gravity (i.e., the standard loop approach), we introduce Ashtekar variables \( E_a^i \) and \( A_a^i \) [4, 6, 9, 41, 42]. However, the following theory is sufficiently flexible to use any set of variables, such as ADM variables, or any other variables introduced in numerical relativity [43–45].

To derive Ashtekar variables, it is necessary to express the metric with a tetrad field:

\[ g_{\mu\nu} = e_\mu^I e_\nu^J \eta_{IJ}, \]  

(27)

with \( \eta_{IJ} \) the Minkowski metric, and \( e_\mu^I \) the tetrad. In the following, we use the signature \((-+, +, +, +)\). The next step is to decompose the tetrad as follows [42]:

\[ e_\mu^I = \left( \begin{array}{c} N \\ e_a^i N^a \end{array} \right). \]  

(28)
with \( N, N^a \) the lapse function and the shift vectors, which are gauge degrees of freedom. \( e_i^a \) is the triad. Finally, we define the “gravitational electric field”:

\[
E_i^a = \det (e_i^b) e_i^a, \tag{29}
\]

and the extrinsic curvature:

\[
k_a^i = \frac{e^{bi}}{2N} \left( \partial_t (e_i^b e_j^k) \delta_{jk} + D_a (\nu_0) \right). \tag{30}
\]

The operator \( D_a \) is the covariant derivative of the three metric. To complete the definition of Ashtekar variables, we introduce the gravitational potential:

\[
A^i_a = \omega^i_a + \beta k^i_a, \tag{31}
\]

where \( \omega^i_a = \omega^i_{ab} e^b_j \) is the triad spin connection and \( \beta \) is a real parameter (it is also possible to define the theory with a complex parameter). Dynamics of \( E_i^a \) and \( A^i_a \) are given by first-order differential equations. For conciseness, we present here the differential equations for \( \Lambda = 0 \), and in the gauge \( N = 1, N_a = 0 \) (the differential equations, in the complex case, can be found in \([46, 47]\)).

\[
\dot{E}_i^a = \frac{1}{\beta \sqrt{\det (E_i^a)}} \left( A_j^b - \omega^j_b \right) (E_j^b E_i^a - E_i^b E_j^a) \tag{32}
\]

\[
\dot{A}^i_a = \frac{1}{2\beta \sqrt{\det (E_i^a)}} E_j^b e^{ijk} F_{abk} \tag{33}
\]

We have introduced \( F_{abk} = F_i^a \delta_{ik} \) the curvature two-forms of \( A^i_a \). In the following, the explicit formula of each time derivative is of little interest. We only require their existence, such that the Cauchy problem in general relativity is well-posed. In addition to these dynamical equations, the gravitational field must verify some constraints:

\[
C_0 = \mathcal{E}_{a\Sigma} + E_i^a E_j^b e^{ijk} F_{abk} - \frac{2(\beta^2 + 1)}{\beta^2} E_i^a E_j^b (A_i^a - \omega_i^a) (A_j^b - \omega_j^b) = 0, \tag{34}
\]

\[
C_i = D_a E_i^a = 0, \tag{35}
\]

\[
C_a = - F_i^a E_i^b = 0. \tag{36}
\]

We introduced \( \mathcal{E}_{a\Sigma} \), which is a possible surface contribution to the system energy \([48]\). Equations (32), (33) (36), (35), and (34) must be verified at each point of the space-time manifold. Hence, we have to consider this fact in the construction of the action functional.

In order to obtain a well-defined variational principle that is compatible with optimal control theory, we propose the following construction: we choose a finite number of \( N \) points in a 3D-hypersurface \( \Sigma \) of the space-time manifold. They define a network in \( \Sigma \), noted \( X_N \). A sequence of networks is defined by increasing successively the
number of points such that \( X_N < X_{N+1} \) (the first \( N \) points of \( X_{N+1} \) are identical to the points of \( X_N \), and the point \( N + 1 \) is a new point in the network). At each point of \( X_N \), we have a couple \((E^a_i, A^i_a)\) whose evolution is parametrized by the time variable \( t \). For this set of points, the following action is defined:

\[
S_N = \sum_{n=1}^{N} \int_{t_0}^{t_f} dt \, P^i_a(x_n)(\dot{E}^a_i(x_n) - G^a_i(x_n))
+ \Pi^i_a(x_n)(\dot{A}^i_a(x_n) - F^i_a(x_n)) + \lambda^A(x_n)C_A(x_n).
\]  

(37)

where \( G \) and \( F \) are given respectively by the right side of (32), and (33), \( P^i_a, \Pi^i_a \), and \( \lambda^A \) are adjoint states, and the index \( A \) takes the values \((i, a, 0)\).

When the number of points covers \( \Sigma \) sufficiently well, such that the covariant derivative \( \mathcal{D}_a \) can be computed using the field variables of the neighborhood points (with finite differences, for example), we can define a continuous action functional on \( \Sigma \). Let \( P_\Sigma X_N \) be a partition of \( \Sigma \) such that each cell is unequivocally associated with a single point of \( X_N \). Let \( V_N = \max_{\sigma \in P_\Sigma X_N} (\text{Vol}(\sigma)) \), with \( \text{Vol} \) the Lebesgue measure. When \( \lim_{N \to \infty} V_N = 0 \) and when the discretized versions of \( \dot{E}^a_i, \dot{A}^i_a, G^a_i, F^i_a, C_A \) converge in measure to the continuous versions, we define the action of the full space-time manifold:

\[
S = \lim_{N \to \infty} S_N.
\] 

(38)

and we have:

\[
S = \int_{t_0}^{t_f} dt \int_{\Sigma} d^3 x \, P^i_a(x)(\dot{E}^a_i(x) - G^a_i(x))
+ \Pi^i_a(x)(\dot{A}^i_a(x) - F^i_a(x)) + \lambda^A(x)C_A(x).
\] 

(39)

Note that the adjoint states written in Eq. (39) are in fact proportional to the ones in Eq. (37) by a factor \( \text{Vol}(\sigma)^{-1} \), in order to use functional derivatives in Euler-Lagrange equations instead of partial derivatives. Moreover, the field variables are densitized quantities, and therefore, an integration weight \( \det(e^i_a) \) is implicit in Eq. (39).

From (39), we can determine the equation of motions. If, we assume fixed boundaries (i.e., \( E^a_i \) and \( A^i_a \) cannot change at \( t_0 \) and \( t_f \)), the Euler-Lagrange equation gives us:

\[
\dot{E}^a_i(x) = G^a_i(x)
\]

(40)

\[
\dot{P}^i_a(x) = P^i_a(x) \frac{\partial G^b_j}{\partial E^a_i}(x) + \Pi^j_b(x) \frac{\partial F^i_a}{\partial E^a_i}(x) - \lambda^A \frac{\partial C_A}{\partial E^a_i}(x)
\]

(41)

\[
\dot{A}^i_a(x) = F^i_a(x)
\]

(42)

\[
\dot{\Pi}^i_a(x) = P^j_b(x) \frac{\partial G^b_j}{\partial A^i_a}(x) + \Pi^j_b(x) \frac{\partial F^i_a}{\partial A^i_a}(x) - \lambda^A \frac{\partial C_A}{\partial A^i_a}(x)
\]

(43)

\[
C_A(x) = 0.
\]

(44)
where we recover exactly Eq.s (32), (33), (34), (36), (35). If the boundaries are not fixed, we are not free to choose arbitrarily the initial and final adjoint states, and they must verify the transversality condition (see Eq. (9)).

Interestingly, $P^i_t$ and $\Pi^a_i$ depend on $E^a_i$ and $A^i_t$, but not reciprocally. Hence, classical dynamics of the gravitational state are not affected by the adjoint states. For the same reason, classical dynamics of $P^i_t$ and $\Pi^a_i$ do not affect the path integral. However, fluctuations of the adjoint states allow us (via the Euler-Lagrange equation) to determine how the gravitational field evolves, thus it can have an interesting impact on the canonical quantization. A few preliminary results in this direction are given in Appendix A.

4.1 The gravitational terminal cost: the quantum scalar product

The next step is to provide the terminal cost that encodes the distance in the space of physical solutions. There is a liberty of choice for this definition, but there are also many physical constraints, imposed by covariance and gauge invariance. For this study we use the well-developed scalar product between two coherent spin-network states [9, 49–53]. This allows us to make an explicit link with loop quantum gravity.

The usual approach is to define a spin-network state that describes a classical discretized manifold, by using complexifier coherent states. To each node of the spin-network, we associate a cell of the discretized manifold. A link of the network corresponds to the boundary between two cells. Usually, we work with simplicial manifold. In such a case, a node of the spin network is 4-valent (it has four links), and it is associated with a tetrahedron. In this paper, we prefer to work with 6-valent nodes, in order to describe hexahedrons. This choice simplifies the link with the classical geometry, defined by a metric tensor. Then, the classical manifold is discretized using hexahedrons, and the dual graph is used to define the spin-network. To each link of the network, we associate two quantities:

- The holonomy of the Ashtekar connection between the centers of each hexahedron, respectively noted $x_s$ and $x_t$ for the source and the target points:

$$U_l(x_s, x_t) = \mathbb{P} \exp \left( \frac{i}{2} \int_{x_s}^{x_t} A^j_t(x) \hat{i} t_a(x) dx \right) \approx \exp \left( \frac{i}{2} A^j_t(x_s) \hat{i} t_a(x_s) L \right),$$

(45)

with $\mathbb{P}$ the path-ordering operator, $\hat{i}$ the Pauli matrices, $t_a$ the unit tangent covector to the link, and $L$ the length of the path.

- The second quantity is the integral of the “electric” field over the surface dual to the link:

$$X^i = \int_{S} \tilde{E}^i_a dS^a \approx U_l(x_l, x_s) \left[ E^i_a(x_l) n^a S \right] U_l^{-1}(x_l, x_s).$$

(46)

The tilde above $E^i_a$ denotes the fact that it is defined by the parallel transport of the electric field to the starting point $x_s$ of the link [49]. In the approximated version of this quantity, this is achieved by an holonomy $U_l(x_l, x_s)$, where $x_l$ is
the intersection point between the path associated with the link and the surface. $n^\alpha$ is the normal vector of the surface with area $S$.

From these two quantities, we define the following $SL(2, \mathbb{C})$ matrix [49]:

$$g_l = \exp \left( \frac{1}{2} X^i \hat{\sigma}_i \right) U_l.$$  \hspace{1cm} (47)

The matrices associated with the links are used to parameterize the coherent state. The state is defined in a two-step procedure. First, we define a function called “heat kernel”:

$$K^\zeta_{gl}(U_l) = \sum_{j_i \in \mathbb{N}/2} e^{-\zeta j_i (j_i + 1)/2 d_{j_i}} \text{Tr}^j (g_l^{-1} U_l),$$  \hspace{1cm} (48)

with $d_{j_i} = 2 j_i + 1$, $\text{Tr}^j$ is the trace of the spin-$j_i$ representation, and $\zeta$ is a parameter defining the coherent state. Semi-classical properties are obtained when $\zeta \to 0$. The second step is to take the product over the links of the heat kernel function and to make the state gauge-invariant at the nodes. This is achieved with an integral over $SU(2)$ at each node:

$$\psi^\zeta_{[g_l]}(U_1, ..., U_{NL}) = \int_{SU(2)^{NN}} \prod_{c=1}^{NN} dh_c \prod_{l=1}^{NL} K^\zeta_{h_a g_l h_b^{-1}}(U_l)$$

(49)

where we have assumed that the spin network has $N_N$ nodes and $N_L$ links. In the integral, an $SU(2)$ element $h_c$ is associated with the node $c$. For convenience, we note $h_a$ the $SU(2)$ element of the source node, and $h_b$ the $SU(2)$ element of the target node. The notation $[g_l]$ is used to specify that the state is gauge-invariant.

When $\zeta \to 0$, the coherent state has a Gaussian-like distribution over the spins $j_i$. The center of the Gaussian tends to infinity when $\zeta \to 0$. Then, for a sufficiently small $\zeta$, we can make a large $j$-approximation of the state. We review here the main idea of the approximation, but additional details can be found in [53]. The idea is to rewrite the $SL(2, \mathbb{C})$ matrices $g_l$ defined in Eq. (47) using a Cartan decomposition $g_l = u_l e^{r_j \sigma_z/2} v_i^{-1}$, with $r_l \in \mathbb{R}_+$ and $u_l, v_l \in SU(2)$. Then, the heat kernel defined in Eq. (48) can be rewritten as:

$$K^\zeta_{h_a g_l h_b^{-1}}(U_l) = \sum_{j_i \in \mathbb{N}/2} e^{-\zeta j_i (j_i + 1)/2 d_{j_i}} \text{Tr}^j (h_a g_l^{-1} h_b^{-1} U_l)$$

$$= \sum_{j_i \in \mathbb{N}/2} e^{-\zeta j_i (j_i + 1)/2 d_{j_i}} \sum_{mnl} D^{jl}_{mn}(h_a u_l) D^{jl}_{nl}(e^{r_j \sigma_z/2}) D_{lm}^{jl}(v_i^{-1} h_b^{-1} U_l)$$

(50)

In the large spin limit, we have $D^{jl}_{nl}(e^{r_j \sigma_z/2}) \approx e^{r_j} \vert j \rangle \langle j \vert$ (since $r \sigma_z/2$ is a real diagonal matrix, the Wigner matrix is characterized by an ensemble of exponentials, which are
dominated by the largest eigenvalue).

\[
K_{h_a g} (U_l) \approx \sum_{j_i \in \mathbb{N}/2} e^{-\zeta j_i (j_i+1)/2} d_{j_i} D_{j_i}^j (v_l^{-1} h_b^{-1} U_l h_a u_l)
\]  

(51)

By introducing this equation into Eq. (49), we deduce:

\[
\psi (U_1, \ldots, U_{N_L}) \approx \sum_{j_i} \prod_{l=1}^{N_L} e^{-\zeta j_i (j_i+1)/2} d_{j_i} e^{r_l j_i} \Psi_{j_i, u_l, v_l} (U_l),
\]  

(52)

where \( \Psi_{j_i, u_l, v_l} (U_l) \) is the intrinsic coherent state [9, 53]. Compared to the usual notation used in the literature, a slightly different convention is used. The phase factor of each link is included in the matrices \( u_l \) and \( v_l \). This simplifies the numerical calculations. Moreover, the notation \( \sum_{j_i} \prod_{l=1}^{N_L} \) must be understood as follows: for a given network, the state is given by a sum of terms labeled by the spin numbers associated with the links of the network (hence the notation \( \sum_{j_i} \)), and for a given set of spin numbers, its contribution to the sum is a product of terms associated with the links (hence the notation \( \prod_{l=1}^{N_L} \)).

Finally, we can define the scalar product between two gauge-invariant complexifier coherent states:

\[
\left\langle \psi_{g_1} \mid \psi_{g_1}' \right\rangle = \int_{SU(2)^N} dU_l \psi_{g_1}^* \left( U_1, \ldots, U_{N_L} \right) \psi_{g_1}^* \left( U_1, \ldots, U_{N_L} \right).
\]  

(53)

For additional details on gauge-invariant complexifier coherent states, we refer to [49–52]. Based on these definitions, and following the idea introduced near Eq. (25), we define the terminal cost:

\[
S_T = i \log \left( \frac{\left\langle \psi_{g_1} \mid \psi_{g_1}' \right\rangle}{\sqrt{\left\langle \psi_{g_1} \mid \psi_{g_1} \right\rangle \left\langle \psi_{g_1} \mid \psi_{g_1} \right\rangle}} \right).
\]  

(54)

Similarly to the terminal cost of the harmonic oscillator, Eq. (54), the terminal cost of Eq. (54) is also related to the distance between two states, but in a more subtle way: the scalar product \( \left\langle K_{g_1} \mid K_{g_1}' \right\rangle \) is related to the \( SL(2, \mathbb{C}) \) geodesic lengths between \( g_l \) and \( g_l' \) [49].

As a final remark, we note that it is also possible to consider the reduced gravitational state of a small portion of space. Reduced states play a key role in open quantum systems. They are also a relevant quantity to consider in experiments. A precursory study of such a state is given in the appendix C.
5 Optimal control path integral of general relativity

We can now construct a path integral for the gravitational field using the optimal control formalism. For that purpose, we have to include the action $S_{tot} = S_T + S$ in a path integral. There is, however, a subtle point concerning the constraints $C_A$. They are non-dynamical and there is no associated state propagation. If these constraints are kept in the action, and if we integrate over $\lambda^A$, we obtain seven additional Dirac distributions, and hence the path integral is a divergent generalized function (see e.g., [54] for an introduction concerning generalized non-linear functions). This divergence is, however, non-physical and it is only the result that these constraints are considered on the same level as dynamical constraints. To avoid such a problem, we transform these constraints in a specific integration measure (see [55] for a similar discussion in the spinfoam setting):

$$\hat{W} = \int \mathcal{D} E^a_i(x) \mathcal{D} A^i_a(x) \mathcal{D} \Pi^a_i(x) \mathcal{D} P^i_a(x) \mathbb{I}_{|C_A|=0}(E^a_i, A^i_a) e^{-iS'} ,$$

(55)

where $S'$ is given by $S' = S_T + S$, with $\lambda^A = 0$, and $\mathbb{I}_{|C_A|=0}(E^a_i, A^i_a)$ is the indicator function such that $\mathbb{I}_{|C_A|=0}(E^a_i, A^i_a) = 1$ if all constraints $C_A = 0$ are verified, and $\mathbb{I}_{|C_A|=0}(E^a_i, A^i_a) = 0$ otherwise. If we work with an approximation of the space-time manifold, we could use a weaker version of the constraint, such as $|C_A| < \varepsilon$.

After the discretization, the path integral (55) becomes.

$$\hat{W} \propto \int \prod_{x,t} d E^a_i(x,t) d A^i_a(x,t) d \Pi^a_i(x,t) d P^i_a(x,t)$$

$$\times \mathbb{I}_{|C_A|=0}(E^a_i(x,t), A^i_a(x,t)) e^{-iS_{lattice}} .$$

(56)

This integral has exactly the same form as (17). Then, the integration over $\Pi^a_i(x,t)$ and $P^i_a(x,t)$ leaves us with:

$$\hat{W} = \int \prod_{x,t} d \mu(E^a_i(x,t) d A^i_a(x,t)) e^{-iS_T}$$

$$\times \delta_0(\Delta t[E^a_i(x,t) - G^a_i])$$

$$\times \delta_0(\Delta t[A^i_a(x,t) - F^i_a])$$

(57)

with,

$$d \mu(E^a_i(x,t) d A^i_a(x,t)) = d E^a_i(x,t) d A^i_a(x,t) \mathbb{I}_{|C_A|=0}(E^a_i(x,t), A^i_a(x,t)).$$

(58)

Surprisingly, Eq. (57) has a similar structure as spinfoams transition amplitudes [9, 10, 56]: $\int_G \prod_{e=1}^N dU_e \prod_f \delta(\prod_{e \in f} U_e)$, with $G$ the gauge group of the theory, $U_e \in G$ is the holonomy associated with the edge $e$ of the spinfoam graph, and $f$ is a face, composed of several edges. However, the optimal control formalism offers a
straightforward implementation of the cosmological constant, which can be induced in the theory with a modification of Eq. (33), and thus, a modification in the definition of \( F_a^I \). This is a non-trivial point in spinfoam theory which usually requires the use of a deformed algebra [9].

From the material presented in Sect. 3, we easily deduce that the propagator \( \hat{W} \) propagates semi-classical states, and returns the scalar product between two semi-classical states:

\[
\langle E'(t), A'(t) \mid \hat{W} (t) \mid E(0), A(0) \rangle = \exp^{-iS_{T}(E'(t), A'(t), \hat{W}_t^{-1}E(t), \hat{W}_t^{-1}A(t))}
\]

The propagation of an arbitrary quantum state is possible with a mapping between coherent states and another basis of quantum states (e.g., spin-network states).

The theory presented here above has a strong similitude with the propagation of a standard quantum field in the Hamiltonian framework. The propagator propagates a classical solution over time, without any changes in the classical dynamics. For example, consider an electromagnetic wave, such as a plane wave. The Schrödinger equation propagates the plane wave (by multiplying the solution with a factor \( e^{i\omega t} \)) exactly as Maxwell’s equations do. A similar thing happens for any solution of Maxwell’s equations. Once a classical solution is known, it is possible to define the corresponding coherent state, and other non-classical states [39]. Here, the same thing happens for a classical solution of Einstein’s equations.

The main difficulty of the approach is therefore to solve Einstein’s field equations. This is a very arduous task in 4D, even in numerical relativity [43]. The only thing we can do (for the moment) is to find a set of solutions sufficiently large in order to describe some relevant physical effects with good accuracy. This can give us a landscape of possible quantum effects, and we can estimate some physical observables. The obvious drawback of this approach is that nothing guarantees that an important classical solution is missing in the calculations.

To fix the idea, we can work with the following inclusion of sets:

\[
C' \supset C \supset C \supset C,
\]

with \( C \) the ensemble of a solution of Einstein’s equations, and \( C \) the ensemble of known solutions of \( C \). This set can be used to define a subset of the quantum Hilbert space.

At this stage, one can ask where quantum mechanics is hidden. Is this formalism restricted to describe only semi-classical states? In fact, no, and all non-classical effects are described by the terminal cost that represents the scalar product between quantum states.

### 6 Application to black hole tunneling

As an illustrative application, we consider the problem of the transition of geometry from a black hole (B.H.) towards another black hole or towards a white hole (W.H.). This effect is usually called black hole tunneling in the spinfoam formalism [33–36].
For this paper we consider a simple toy model for which the effect is given by the transition amplitude between two geometries. Hence, we have to evaluate Eq. (59) between two B.H. (or W.H.) states.

For that purpose, we choose \( C \) to be the ensemble of Schwarzschild geometries labeled by the Schwarzschild radius \( r_S \), the sign \( s \) of the extrinsic curvature [33], and a time \( \tau \). We present the calculations in Lemaitre coordinates, but other coordinate systems can be used as well. With these coordinates the line element is:

\[
ds^2 = -d\tau^2 + \frac{r_S}{r} d\rho^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2,
\]

with,

\[
r = \left( \frac{3}{2} (\rho - \tau) \right)^{2/3} r_S^{1/3}.
\]

The extrinsic curvature \( K_{ab} \) for a \( \tau = \text{Cst} \) hypersurface is given by a diagonal matrix:

\[
K_{ab} = \frac{2sr^2}{3(\rho - \tau)} \begin{pmatrix}
2/9 (\rho - \tau)^2, & -1, & -\sin^2 \theta
\end{pmatrix}.
\]

We are then able to determine the “gravitational electric field”:

\[
E_i^a = \sin \theta \cdot \begin{pmatrix}
2/9 (\rho - \tau)^2, & \sqrt{rr_S}, & \sqrt{rr_S} \csc^2 \theta
\end{pmatrix},
\]

with \( \csc \theta \) the cosecant function, and the Ashtekar connection:

\[
A^a_i = \begin{pmatrix}
\frac{s\beta r_S}{2r} & 0 & 0 \\
0 & -\frac{s\beta r_S}{\sqrt{rr_S}} & -1 \\
-\frac{1}{2} \sin(2\theta)\csc \theta & \frac{1}{2} ((\csc \theta)^{-1} + \sin \theta) - \frac{s\beta \sqrt{rr_S}}{\sqrt{r_s} \csc^2 \theta}
\end{pmatrix}
\]

In the following, we use the standard value \( \beta = 1.2 \). From these classical variables, we need to construct quantum states. Following the Sect. 4, we discretize the space-like submanifolds at \( \tau = \text{Cst} \) by a set of \( N \) points of coordinates \( (\rho, \theta, \phi) \) in \( ]\tau, \infty[ \times [0, \pi] \times [0, 2\pi[ \), for which we attach a couple \( (A^i_a, E^a_i) \). Note that the singularity is removed for a given network \( X_N \), but it is recovered when \( N \to \infty \) (because diagonal elements of \( A^i_a \) diverge when \( \rho \to \tau \)).

It has been argued for a long time that black hole singularities are removed in loop quantum gravity with a bounce. Recent studies [57] suggest that this may be a non-physical effect that breaks covariance. Since then, it has been imagined that the singularity is avoided during the collapse (with, for example, a signature change). Hence, to solve the singularity problem completely, one should have a clear understanding of black holes formations. From this point of view, a Schwarzschild black hole is not only a “steady-state” geometry, but an approximated “steady-state” geometry. Therefore, the quantum states considered in this paper are only the approximation of real black hole quantum states. They can be used only for a first look at the quantum phenomenology. Also, the quantum interaction with matter fields may play a key role.

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role in the definition of a realistic black hole state. This issue is not considered in the following.

To evaluate the probability transition, we have to deal with spin-networks with an infinite number of nodes, and we have to sum over an infinite number of spin labels. In practice, we have to restrict the analysis to a very small number of nodes, and to sum over the most relevant graphs. By increasing both the number of graphs and the number of nodes, we can extrapolate the result and deduce qualitative limit properties. Details concerning the numerical methods used to evaluate the scalar product between two coherent states are given in Appendix B. The networks considered in this paper are given in Table 1. In all cases, nodes have 6 links. Due to the network truncation, they may not be explicitly connected to other nodes. While the first two graphs are rather obvious choices to increase step-by-step the complexity of the spin-network, a comment on the third case seems necessary. Eq. (52) tells us that the state is a product of terms associated with nodes and links. As an approximation, we can neglect all other entities surrounding a given region of the network, but we can also consider several unconnected regions. Then, we simply have to take the product of all the amplitudes associated with these regions. With this trick, we can explore a larger portion of space, where the gravitational field has very different strengths. Note that the coordinates \((\rho, \theta, \phi)\) of the nodes are kept fixed. We make this assumption in order to simplify the analysis of the transition probability when the size of the spin-network grows.

In addition to these considerations, we have to choose a value of \(\zeta\) (the parameter defining the coherent state). The semi-classical limit is obtained for \(\zeta \to 0\). In this limit, the state is distributed over many different graphs with very large spins. This may render the numerical calculations extremely difficult. Then, it is necessary to choose the largest value of \(\zeta\) as possible. With this issue in mind, we have fixed \(\zeta = 1/\sqrt{2}\), and we have adapted the size of the discretization grid in order to obtain \(r_l \approx 1.7\). This gives us a maximum of \(e^{-\xi j_l (j_l+1)/2}d_j e^{r l_j}\) around \(j_l = 2\). All the data required to reconstruct the boundary state are given in the online version of the code [58].

Figures 1 and 2 show examples of transition probability, for respectively a B.H. to B.H. transition, and a B.H. to W.H. transition. These transitions are given by \(|\langle +, r_S, 0 | +, 500, 0 \rangle|^2\) and \(|\langle -, r'_S, 0 | +, r_S, 0 \rangle|^2\). In the first case, the initial black hole has a radius \(r_S/(2l_P) = 500\) (with \(l_P\) the Planck length), and the radius of the final black hole is allowed to change. In the second case, the radius is not necessarily identical for both the initial and final states, and the sign of the extrinsic curvature \(s\) is changed. In these examples, the time is fixed to \(\tau = 0\).

The oscillations observed in the single graph case (orange curves in the Figs. 1 and 2) can be easily understood with Eq. (51), where the Wigner D-matrices are
Fig. 1 B.H. to B.H. transition probability from $|+, 500, 0\rangle$ to $|+, r_S, 0\rangle$ for different spin-network configurations. 

- **a** Single node spin-network.
- **b** Spin-network with two nodes connected by one link.
- **c** Ensemble of unconnected nodes.

For the subfigures a, and b, each curve corresponds to a different number of graphs which are taken into account in the evaluation of the scalar product. The graphs are selected in order to keep only the ones with the largest contributions. As an example, for the subfigure a, the orange curve is computed with $\{j_l\} = \{2, 2, 2, 2, 2, 2\}$, and the blue curve is computed with $\{j_l\} = \{2, 2, 2, 2, 2, 2\}, \{2, 3, 2, 2, 2, 2\}, \ldots$. For the subfigure c, we keep only the graph with the highest contribution, which means that the orange curve of (a) is the same as the orange curve of (c).

Oscillating function whose argument depends on $E_i^\alpha$ and $A_i^\alpha$. Explicit calculations are lengthy, but we can easily see that we are not restricted to a unique period of oscillation of Eq. (51). When we increase the number of graphs that are taken into account in the estimation of the scalar product, we observe a kind of interference between the graphs (see the blue and yellow curves). The fluctuations depend on the approximation scheme (because the results depend on the spin-network). This is a consequence of the very poor approximation of the scalar product. Hence, we consider only the limit that arises from the data. We observe that all the small fluctuations are suppressed when the number of nodes or the number of graphs is increased. This gives a transition probability extremely peaked around the initial state. While it is not shown explicitly in this paper, similar results have been observed for the transition between several time slices. Finally, we arrive at the conclusion:

$$
|\langle s', r'_S, \tau' | s, r_S, \tau \rangle|^2 = \begin{cases} 
\delta_{ss'}\|\{r'_S\}\|\{\tau'\}, & r_s \neq 0 \\
\|\{0\}\|\{r'_S\}, & r_s = 0
\end{cases}
$$

(63)

When $r_S = 0$, black hole ($s = +$) and the white hole ($s = -$) solutions are identical. In this latter case, the system is also time invariant.
Fig. 2 Panels a to c are the same as Fig. 1, but for the transition of geometry between a black hole state $|+, r_s, 0\rangle$ to a white hole state $|-, r_s, 0\rangle$. Panel d shows the transition probability between the states $|+, r'_s, 0\rangle$ and $|+, r_s, 0\rangle$ for a single node spin-network. The scalar product is evaluated using the 16 graphs with the largest weights.

With Eq. (63), the tunneling effect is impossible or at least extremely improbable. However, such a phenomenon could be enhanced by the interaction with matter. During the black hole formation, we might have a strong entanglement with the matter field that produces a kind of “squeezed” gravitational state. This state might have a large spreading and it can make possible a kind of tunneling. This issue can be addressed only with an accurate modeling of the B.H. formation that takes into account the quantum interaction between the gravitational field and matter fields. This issue is investigated in [59] with the framework of Loop Quantum Cosmology, and several key ingredients could be adapted to the approach of this paper.

7 Conclusion

The aim of this paper is to present a novel path integral formalism in general relativity, based on the framework of optimal control theory. Using an extended configuration space of classical variables, we are able to construct a new Lagrangian for the gravitational field. Variations of the action functional with respect to the adjoint variables

\[ \frac{\partial}{\partial \lambda} S = 0 \]

1 Here, “squeezed” is used by analogy with a situation of quantum electrodynamics, where the coherent interaction of an atomic system with a mode of the electromagnetic field tends to create squeezed states of light.
give (in standard optimal control theory) a set of admissible optimal trajectories. Here, this corresponds to the set of space-time satisfying Einstein’s field equations.

The time discretization of the dynamical system allows us to define rigorously the propagator. The physical scalar product of the Hilbert space is implemented in the theory using a terminal cost that describes a measure of distance in the space of classical solutions. This cost is analogous to the one introduced in optimal control theory to relax the target state constraint. The formalism is flexible enough to define the propagator with any set of classical variables expressed in a 3+1 formalism, but we provide explicit calculations with Ashtekar variables. This allows us to define the terminal cost with the LQG scalar product.

As an example, the tunneling problem of a black hole is investigated using a subset of the Hilbert space generated by Schwarzschild geometries. The transition probability from a black hole towards another black hole, or towards a white hole is estimated numerically. The calculations suggest that such transitions are impossible (or at least, extremely improbable), but additional mechanisms coming from the interaction with matter fields may change the result.

The theory presented in this paper is only at an early stage, and many points are left unexplored. Future studies shall focus on the connection between the Pontryagin Hamiltonian for the gravitational field and the ADM Hamiltonian. It must also be clarified the role that Pontryagin Hamiltonian can play in the canonical quantization. Also, a clearer link with Oeck’s general boundary formalism [60] could be interesting. Finally, we point out that the coupling with matter fields can be straightforward with the formalism of this paper. We have not discussed this topic since it must be addressed simultaneously with decoherence and quantum measurements.

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Data Availability The code used for the numerical computations of this paper is available at [58]. All data generated or analysed during this study are included in this published article and in the numerical code.

Appendix A Hamiltonian operator

This appendix contains some preliminary results concerning the canonical quantization using the Optimal Control Hamiltonian. The main ideas are first introduced using the harmonic oscillator, and the case of the gravitational field is considered in a second step.

Given a function $F \in \mathcal{C}'$, its time derivative is given by the Poisson-bracket:

$$d_t F = \{F, H_{OC}\},$$

(A1)

with,

$$\{F, H_{OC}\} = \sum_i \frac{\partial F}{\partial x^i} \frac{\partial H_{OC}}{\partial p_{x^i}} - \frac{\partial F}{\partial p_{x^i}} \frac{\partial H_{OC}}{\partial x^i}.$$  

(A2)

The quantum state is assumed to be a function on $\mathcal{C}$. Then, the Poisson-bracket is reduced to $\{\psi, H_{OC}\} = \sum_i \frac{\partial \psi}{\partial x^i} \frac{\partial H_{OC}}{\partial p_{x^i}}$. Moreover, the Hamiltonian in the optimal
control framework is of the form: \( H_{OC} = \sum_i p_{x^i} f^i \), where \( f^i = \dot{x}^i \). Then, the quantization rule \( p_{x^i} \rightarrow i\partial_{x^i} \) allows us to define a Hamiltonian operator \( \hat{H}_{OC} = i f^i \partial_{x^i} \), such that:

\[
d_t \psi = -i \hat{H}_{OC} \psi. \tag{A3}
\]

Precisely, for the harmonic oscillator, we have:

\[
\hat{H}_{OC} = i \left( \frac{p}{m} \partial_x - kx \partial_p \right) \tag{A4}
\]

This operator is equivalent to the standard Hamiltonian operator in the holomorphic representation \cite{39}:

\[
\hat{H} = \omega \alpha \partial_{\alpha} \tag{A5}
\]

with \( \alpha \) defined by Eq. (23). An explicit calculation gives us: \( d_t \alpha = -i \hat{H}_{OC} \alpha = -i \hat{H} \alpha \), and more generally, for any holomorphic function \( \psi: \hat{H}_{OC} \vert \psi(\alpha) \rangle = \hat{H} \vert \psi(\alpha) \rangle \). The optimal control Hamiltonian allowed us to construct straightforwardly the Hamiltonian operator in the holomorphic representation of the harmonic oscillator. We shall proceed similarly with the gravitational field. From the results of Sect. 4 the Hamiltonian is:

\[
H_{OC}(x) = P_i^a(x) G_i^a(x) + \Pi_i^a(x) F_i^a(x) - \lambda A(x) C_A(x), \tag{A6}
\]

and the corresponding Hamiltonian operator is given by:

\[
\hat{H}_{OC}(x) = i \left( G_i^a(x) \frac{\partial}{\partial E_i^a(x)} + F_i^a(x) \frac{\partial}{\partial A_i^a(x)} - C_A(x) \frac{\partial}{\partial C_A(x)} \right). \tag{A7}
\]

Assuming that \( \vert \psi \rangle \) does not depend explicitly on \( C_A \), the part \( C_A \partial_{C_A} \) vanishes in \( \hat{H}_{OC} \). Using operations on the loop space, it is possible to transform \( \hat{H}_{OC} \) into an operator on loop quantum states (like in Refs. \cite{6, 46}). Similarly to other canonical quantization approaches, cautions must be taken (e.g., with the regularization of the operators on the lattice), but the link between coherent spin-networks and classical geometries can provide a welcome simplification. A detailed study of this Hamiltonian operator is left for another study.

**Appendix B Numerical methods**

Spin networks are objects with many degrees of freedom and the evaluation of the scalar product between different coherent spin-network states can be challenging. In this appendix, we provide several details concerning the numerical methods employed for the calculations.
In the following, all computation times are given for a single core clocked at 3.3 GHz. Numerical calculations are made using Mathematica.

The numerical algorithm used for the calculation is based on several key ingredients. First of all, the scalar product is evaluated using an approximation derived in the large \( j \)-limit. Using similar computation steps as the ones between (50) and (52), we can derive an approximated expression for the scalar product between two heat kernels:

\[
\left( K_{h_a g}^{\xi} h_b^{-1} \right) = \sum_{j} \sum_{l} e^{-\xi j_{(j_l+1)} d_j} T_{r_l}^{j_l} \left( h_b g_l^{j_{l+1}} a h_{l}^{j_{l}} h_{l}^{j_{l}} g_{l}^{j_{l}} \right)
\]

\[
\approx \sum_{j} \sum_{l} e^{-\xi j_{(j_l+1)} d_j} e^{(r_l+r_{l})j_{l}} D_{j_l}^{j_{l}} \left( v_l^{j_{l}} h_{b}^{j_{l}} h_{b} v_l \right) D_{j_{l+1}}^{j_{l+1}} \left( v_l^{j_{l+1}} h_{l}^{j_{l+1}} a u_l^{j_{l+1}} \right)
\]

(B8)

where \( h_a, h_b, h_a', h_b' \) are SU(2) matrices associated with the nodes which are used to produce gauge invariant states, and \( g_l \), \( g_l' \) are rewritten using a Cartan decomposition \( g_l = u_l e^{r_l z} v_l^\dagger \), with \( r_l \in \mathbb{R}_+ \) and \( u_l, v_l \in SU(2) \).

In the last line, we observe that \( u \) and \( v \) are separated into different Wigner matrices. We are left with a product of terms, each one being associated with different nodes. Now, if we consider the complete gauge coherent state, we have:

\[
\left\langle \psi_{[r]}^{\xi} \right| \psi_{[\xi]}^{\xi} \right\rangle = \int_{SU(2)^{2N}} d h_a d h_a' \prod_{a=1}^{N} \prod_{l=1}^{N_L} e^{-\xi j_{(j_l+1)} e^{(r_l+r_{l})j_{l}}} d_j D_{j_l}^{j_{l}} \left( w_l^{j_{l}} h_{a}^{j_{l}} a w_l \right)
\]

(B9)

where \( w_l \) corresponds to \( u_l \) or \( v_l \), depending on the orientation of the link. Then, the scalar product is a sum of terms labeled by all possible combinations of \( j_l \). For each term, we have a link contribution \( e^{-\xi j_{(j_l+1)} e^{(r_l+r_{l})j_{l}}} d_j \), and a node contribution given by the integral of a product of functions \( D_{j_l}^{j_{l}} \). This integral can be computed numerically using the following scheme:

1. For each matrix \( g_l \) defining \( \psi_{[r]}^{\xi} \) and \( \psi_{[\xi]}^{\xi} \), determine \( u_l, v_l, r_l \) such that \( g_l = u_l e^{r_l z} v_l^\dagger \). This can be achieved easily using the build-in diagonalization function of Mathematica: Eigensystem. When a matrix of \( SL(2, C) \) is diagonalized numerically, the algorithm returns the matrix of eigenvectors \( P \) in the form of a matrix of SU(2), and the eigenvalues are returned in the form \( (e^{z/2}, e^{-z/2}) \), \( z \in \mathbb{C} \), but if the matrix to diagonalize is a pure boost, we have \( z \in \mathbb{R} \). Using the fact that \( g_l = H_l U_l \), with \( H_l \) defined in (47) and \( U_l \) defined in (45), we can decompose \( g_l \) as follows: \( u = P^\dagger, r = z, v^\dagger = P U_l \), where \( P \) and \( z \) are deduced from the diagonalization of \( H_l \).

2. The second step is to determine the set of values \( j_l \) such that \( \prod_{l} e^{-\xi j_{(j_l+1)} e^{(r_l+r_{l})j_{l}}} d_j \) is sufficiently high. This allows us to reduce considerably the number of terms in the final evaluation of the spin networks. In practice, many terms have a weight of zero or a negligible weight. The procedure that allows us to select the most relevant graphs is discussed below.
3. Compute the node amplitudes

$$\int_{SU(2)^2} dh_a dh'_a \prod_l D^{ji}_{jl} (w^+_l h_a w'_l)^j.$$  

Because $SU(2)$ is a compact Lie group, $\int f(hh')dh = \int f(h^+)dh = \int f(h)dh$. Then, we can drop an integral, and we are left with:

$$\int_{SU(2)} dh_a \prod_l D^{ji}_{jl} (w^+_l h_a w'_l)^j = \int_0^{4\pi} d\psi \int_0^\pi d\theta \int_0^{2\pi} d\phi \sin(\theta)$$  

$$\times \prod_l \left[ (w^+_l h_a(\psi,\theta,\phi) w'_l)^j \right]^{2jl}.$$  

(B10)

In the second line we have introduced the matrix element $(1,1)$ of $w^+_l h_a w'_l$, and the Euler angles $(\psi, \theta, \phi)$ of $h_a$. Two options are available. The first option provides an exact result (up to the numerical precision). The idea is to expand

$$\sin \theta \prod_l \left[ (w^+_l h_a w'_l)^j \right]^{2jl}$$

into a polynomial of the form:

$$\sum_{k,l,m,\ldots} c_{klmnop} \cos^k \frac{\psi}{2} \sin^l \frac{\psi}{2} \cos^m \frac{\theta}{2} \sin^n \frac{\theta}{2} \cos^o \frac{\phi}{2} \sin^p \frac{\phi}{2}$$

with $c_{klmnop} \in \mathbb{C}$. This step can be performed with repeated uses of the function $CoefficientList$. Then, an exact evaluation is possible with the identities:

$$2 \int_0^{2\pi} \cos^n \psi \sin^m \psi d\psi = (1 + (-1)^n)(1 + (-1)^{n+m}) \frac{\Gamma((m + 1)/2)\Gamma((n + 1)/2)}{\Gamma((m + n + 2)/2)}$$

$$2 \int_0^{\pi/2} \cos^n \theta \sin^m \theta d\theta = \frac{\Gamma((m + 1)/2)\Gamma((n + 1)/2)}{\Gamma((m + n + 2)/2)}$$

$$2 \int_0^{\pi} \cos^n \phi \sin^m \phi d\phi = (1 + (-1)^n) \frac{\Gamma((m + 1)/2)\Gamma((n + 1)/2)}{\Gamma((m + n + 2)/2)}.$$  

The other method is based on a “brute force” numerical integration using the function $NIntegrate$ with the method $MultiPeriodic$. This method is specifically designed for the integration of highly oscillating functions. The two methods are compared in Fig. 3. The exact method is particularly efficient for small values of $j_l$, but the computation time increases exponentially. On another side, the numerical estimation with $NIntegrate$ has a stable computation time and a small error $\lesssim 10^{-6}$ (the error is defined by the distance between the approximated result and the exact one). We observe that the exact method is faster for $\langle j \rangle = \sum_{l=1}^6 j_l/6 < 2$. Then, we can adjust the integration scheme as a function of $\langle j \rangle$.

As outlined above in this section, all labeled graphs do not contribute equivalently in a coherent state. It can be sufficient to compute the scalar product using only a small
number of graphs. This can reduce the accuracy of the computation, but this gives us qualitative behaviors. We describe below a list of properties that allows us to select the relevant graphs.

- The integration over $SU(2)$ at each node induces a selection rule for the different spin numbers. For the 6-valent intertwiner, we have the following condition: $\sum_l j_l \in \mathbb{N}$.
- For an arbitrary configuration, we can decompose each $j_l$ into an integer part and a half-integer part: $j_l = n_l + \delta_l$ with $n_l \in \mathbb{N}$, and $\delta_l = 0$ or $1/2$. If all spins in the graph have integer values, the sum of the spins at each node is an integer, and thus it is a valid graph. Non-trivial cases are given when there are $\delta_l \neq 0$. In fact, the validity of the graph depends only on the set of $\delta_l$, but not on the values of $n_l$.

Hence, we can first determine the set of valid graphs with $j_l = \delta_l$, and then we can generate all other graphs by adding to these solutions an integer $n_l$ to each $j_l$.

### Appendix C Reduced gravitational states

The quantum state $|\psi\rangle$ is an idealized concept that is, in practice, experimentally not accessible. Rather than $|\psi\rangle$, we may have access to the reduced density matrix of the system (and the reduced density matrix may not be a pure state of the form $|\psi\rangle \langle \psi|$). The reduced state consists of the density matrix describing the state of “everything” where we have made a partial trace over all degrees of freedoms that do not describe the system of interest.

The density matrix for spin network states can be defined as follows. For any set of spin networks, we can define $\rho(U_1, \ldots, U_{NL}) = \sum_i \psi_i (U_1, \ldots, U_{NL}) |i(U_1, \ldots, U_{NL})\rangle \langle i(U_1, \ldots, U_{NL})|$ where $|i\rangle$ is a spin-network, function of $NL$ variables $U_l \in SU(2)$. Then, a density matrix is simply given by:

$$\rho(U_1, \ldots, U_{NL}, U'_1, \ldots, U'_{NL}) = \sum_{i,i'} c_{i,i'} |i(U_1, \ldots, U_{NL})\rangle \langle i'(U'_1, \ldots, U'_{NL})|,$$  \hspace{1cm} (C11)

such that $\sum_i c_{ii} = 1$. Since nodes and links describe geometric quantities, we can define the partial trace over space degrees of freedoms by integrating over $SU(2)$ for...
Fig. 4 An illustrative example of sub-graph induced by the partial trace over the links of a spin-network (for simplicity, only the links and nodes surrounding the interesting area are shown). The part of the graph in the gray area corresponds to the entities eliminated by the partial trace. The result is then a sub-graph with the node $n_0$, and links $l_1, ..., l_6$

each link outside the region of interest:

$$\rho_S = \int_{SU(2)^{N_L-N'_L}} dU_l \delta(U_l.U_l^{-1}) \rho(U_1, ..., U_{N_L}, U'_1, ..., U'_{N_L}). \quad (C12)$$

Note that the integration over $U'_l$ is in fact hidden in the definition of $\langle i |$. The result of this partial trace leads to a kind of spin-network with links connected to a single node. Hence, we are forced to work with a new kind of state defined on open graphs. These states are called below sub-spin-networks. The idea is illustrated in Fig. 4.

Equation (52) allows us to derive an approximated reduced density matrix of a gravitational state $\rho = |\psi^{\xi}_{[s]}\rangle \langle \psi^{\xi}_{[s]}|$. Using the partial trace defined in Eq. (C12), we deduce:

$$\rho_S = \sum_{j_l,j'_l} c(\{j_l\}, \{j'_l\}) \prod_{l,l'} e^{-\zeta(j_l(j_l+1)/2} d_{j_l} e^{-\zeta j'_l(j'_l+1)/2} d_{j'_l} e^{\gamma_{j_l} j'_l} e^{-\gamma_{j'_l}} \langle \Psi_{j_l,u_l,v_l} | \langle \Psi_{j'_l,u'_l,v'_l} |, \quad (C13)$$

with $c(\{j_l\}, \{j'_l\})$, a term that depends on all the $j_l$ of a given graph (here, $l$ runs over all the links of the sub-network). This can be viewed as a coefficient measuring the
Fig. 5  Numerical estimation of $c(\{j_l\}, \{j'_l\})$ for a 1-node reduced density matrix. We show only the sign of the coefficient (0 or 1, given respectively by white or blue pixels). While it is easy to deduce if a coefficient is different from 0, it is, however, very difficult to estimate its exact value (the convergence of the Monte-Carlo methods is very slow). Based on our numerical observation we conjecture that, for the case presented here, they are almost all identical. Calculations are made using $r = 1.5$ and a set of 46 graphs with spin numbers $j_l$ in the range $[\frac{3}{2}, \frac{5}{2}]$

coherence between two graphs. Its value depends on the links and nodes amplitudes of the region of the graph which is traced out.

Under several assumptions we can estimate these coefficients for a given reduced state. We explore briefly the case illustrated in Fig. 4, for a reduced density matrix of a single 6-valent node. We assume that the central node is a part of a bigger graph with 6 other nodes, and 30 other links. This is still a sub-graph of a hypothetical larger graph, but we assume that the coefficients depend mostly on the nearest neighbors. They are estimated by first choosing a finite set of sub-graphs with link labels $\{j_1, ..., j_6\}$. For each couple of sub-graphs, we generate randomly the spin-numbers of the rest of the graph (i.e., the values of the 30 other $j_l$), and we compute the amplitude $\prod_{k=1}^{30} e^{-\zeta j_k(j_k+1)} d_{j_k} e^{2r_k j_k} \langle \Psi_{j_k,u_k,v_k} | \Psi_{j_k,u_k,v_k} \rangle$. Without an explicit knowledge of the state in the traced region, we fix $r_k = r$, with $r$ a chosen value, and we assume $\langle \Psi_{j_k,u_k,v_k} | \Psi_{j_k,u_k,v_k} \rangle = 1$ or 0 if the configuration is non-physical (the sum of the $j_l$ at each node must be an integer). This may be improved by introducing a more realistic estimation of $\langle \Psi_{j_k,u_k,v_k} | \Psi_{j_k,u_k,v_k} \rangle$, for example, by using a random number with a specific probability distribution. The coefficients are deduced by summing the amplitude of many (ideally an infinite number) of random graphs. Finally, the result is normalized, to obtain $\text{Tr}(\rho_S) = 1$. 
An example of coefficients is given in Fig. 5. Due to the non-zero diagonal elements and the sparse structure of non-diagonal elements, we see that the reduced density matrix is in a mixed state. Using the fact that the sum of the \( j_i \) at each node must be an integer, we can show that the statistical mixture is induced by half-integer spins while some of the coherence is kept by integer spins. The reduced density matrix formalism may be interesting to compute mean values of observable, but it is not well adapted to the problem studied in Sect. 6. The probability transition of mixed states must be computed using the quantum fidelity, and this quantity is difficult to compute with coherent states.

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