The physical hamiltonian 
in non-perturbative quantum gravity

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Abstract

A quantum Hamiltonian which evolves the gravitational field according  
to time as measured by constant surfaces of a scalar field is defined through 
a regularization procedure based on the loop representation, and is shown  
to be finite and diffeomorphism invariant. The problem of constructing  
this Hamiltonian is reduced to a combinatorial and algebraic problem which  
involves the rearrangements of lines through the vertices of arbitrary graphs.  
This procedure also provides a construction of the Hamiltonian constraint  
as a finite operator on the space of diffeomorphism invariant states as well  
as a construction of the operator corresponding to the spatial volume of the  
universe.

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One of the main problems of nonperturbative quantum gravity has been how to realize physical time evolution in the absence of a fixed background spacetime geometry \[1\]. One solution to this problem, which has been often discussed, is to use a matter degree of freedom to provide a physical clock \[2\], and represent evolution as change with respect to it. In this letter we show that it is possible to explicitly implement this proposal in the full theory of quantum general relativity, using the nonperturbative approach \[3, 4, 5\] based on the Ashtekar variables \[6\] and the loop representation \[7, 8\]. In particular, we use a scalar field as a clock as suggested in several recent papers \[9, 10\], and we show that it is possible to construct the hamiltonian operator \(\hat{H}\) that gives the evolution in this clock time.

We construct the hamiltonian operator \(\hat{H}\) by using regularization techniques recently introduced for generally covariant theories \[4, 11, 12, 13\]. The main technical result that we obtain is that the operator \(\hat{H}\), although constructed through a regularization procedure that breaks diffeomorphism invariance, is nevertheless diffeomorphism invariant, background independent and (as we have argued elsewhere \[3, 4, 12, 13\] is implied by these conditions) finite. It follows that \(\hat{H}\) is well defined on the space \(\mathcal{V}\) of the spatially diffeomorphism invariant states of the gravitational field. Since this space \(\mathcal{V}\), which we call the knot space, is spanned by the basis given by the generalized knot classes \[7\] (diffeomorphism equivalence classes of finite sets of loops in \(\Sigma\), the three-dimensional space manifold), \(\hat{H}\) is represented by an infinite dimensional matrix in knot space. We present here a procedure for computing all the matrix elements of the hamiltonian \(\hat{H}\) in knot space. This procedure is purely combinatorial and algebraic. Thus, our main result is the reduction of the problem of computing the physical evolution of the quantum gravitational field with respect to a clock to a problem in graph theory and combinatorics.

We begin by introducing the scalar field \(T(x)\), whose three-surfaces of constant values may be taken, under appropriate circumstances, to represent time \[8, 10\]. If we denote its conjugate momentum by \(\pi(x)\), the Hamiltonian constraint has, classically, the form,

\[
C(x) = \frac{1}{\mu} \pi^2 + \frac{1}{2} \tilde{q}^{ab} \partial_a T \partial_b T + C_{grav} \tag{1}
\]

where \(\mu\) is a constant with dimensions of energy density, necessary so that \(T\) have dimensions of time. The gravitational contribution has the standard form \[6\]

\[
C_{grav} = \epsilon_{ijk} \tilde{E}^{ai} \tilde{E}^{bj} F_{ik} + \Lambda q = C_{Einst} + \Lambda q \tag{2}
\]
where $q = \det(q_{ab})$, $\Lambda$ is the cosmological constant, and all other symbols have the usual meaning in the Ashtekar formalism [6]. We then restrict the freedom of choosing the time coordinate by fixing the gauge $\partial_a T = 0$. It is not difficult to show [10] that this implies that the lapse is $N(x) = a/\pi(x)$ for some constant $a$ and that all of the infinite number of hamiltonian constraints $C(x)$ turn out to be gauge fixed, except one, which is an integral over the three manifold $\Sigma$:

$$\int_\Sigma \frac{C}{\pi} = (2\mu)^{-\frac{1}{2}} \int_\Sigma \pi + \int_\Sigma \sqrt{-C_{grav}} = 0. \quad (3)$$

This gauge fixing commutes with the generators of spatial diffeomorphisms, which may be imposed exactly on the $T = constant$ surfaces. If we go over to the quantum theory the diffeomorphism invariant states are then of the form $\Psi[\{\alpha\}, T]$, where $\{\alpha\}$ indicates a generalized knot class, namely a diffeomorphism equivalence class of (multiple) loops $\alpha$, and the real number $T$ is the constant value of the time. These states then satisfy a Schroedinger-like equation

$$i\hbar \frac{d\Psi}{dT} = \sqrt{2\mu} \hat{H} \Psi \quad (4)$$

where $\hat{H}$ is the quantum operator corresponding to the observable

$$H = \int_\Sigma \sqrt{-C_{grav}}. \quad (5)$$

We now proceed to construct the quantum operator $\hat{H}$. We regularize the integral by writing it as a limit of a sum, and, in addition, we regularize each operator product according to the techniques developed in refs. [4, 11, 12, 13]. We write

$$\hat{H} = \lim_{L \to 0, A \to 0, \delta \to 0} \sum_I L^3 \sqrt{-C^{L,\delta, A}_{Einst I}} - \Lambda q^L_I \quad (6)$$

where we have divided the spatial manifold $\Sigma$ into cubes of size $L$ according to an arbitrary set of fixed euclidean coordinates, and the sum is over these cubes, labeled $I$. The quantities $\delta$ and $A$ are parameters involved in the regularization of the Einstein term. The order in which the limits have to be taken is a crucial part of the definition of the quantum operator: we specify this order below. The Einstein term in detail is

$$C^{L,\delta, A}_{Einst I} = \frac{1}{2L^3 A} \int_{\text{cube } I} d^3x \int d^3y \int d^3z \frac{f^\delta(x,y)f^\delta(x,z)}{\sqrt{-C^{L,\delta, A}_{Einst I}}} \sum_{\hat{a} < \hat{b}} \left[ \hat{T}^{\hat{a}\hat{b}} \gamma_{xyz} \circ \gamma_{x\hat{a}\hat{b}}^A(y,z) + \hat{T}^{\hat{a}\hat{b}} \gamma_{xyz} \circ \gamma_{x\hat{a}\hat{b}}^{A-1}(y,z) \right] \quad (7)$$
where \( f^\delta(x, y) = \frac{2}{4\pi^2} \Theta(\delta - |x - y|) \) regulates the distributional products (\( \Theta \) is the step function). \( \hat{T}^{ab} \) is defined in [4, 7, 11]. \( \gamma_{xyz} \) is a zero area curve running from \( x \) to \( y \) to \( z \) and back and \( \gamma_{x\hat{a}\hat{b}} \) is a circle based at \( x \) in the \( \hat{a}\hat{b} \) plane with area \( A \), all defined with respect to the arbitrary euclidean coordinates. This operator depends on three regularization scales, \( \delta, A \) and \( L \). It is straightforward to check that the classical expression corresponding to (6,7) reproduces (5) when the limits are taken.

Let us now study the action of (7) on a loop state \( \Psi[\alpha] \). First, we notice that for fixed \( L \) and \( A \) the limit \( \delta \to 0 \) is zero unless there is an intersection or kink in the \( I \)'th cube. In these cases, let us label the \( n \) lines going into the intersection point, \( p \), as \( \alpha_i, i = 1, ..., n \). We then have, using the explicit forms of the operator \( \hat{T}^{ab} \) [3, 4, 7],

\[
\hat{C}^{L,\delta,A}_{\text{Einst}} I \Psi[\alpha] = \frac{l_{Pl}^4}{AL^3} \sum_{i<j\leq n} X(I, i, j, \delta) \sin(\theta_{ij}) \sum_r (-1)^r \left[ \Psi[(\alpha \ast_i \ast_j \gamma_{p}^A \dot{\alpha}_i(p)\dot{\alpha}_j(p))] + \Psi[(\alpha \ast_i \ast_j \gamma_{p}^{-1} \dot{\alpha}_i(p)\dot{\alpha}_j(p))] \right],
\]

where

\[
X(I, i, j, \delta) = \int_{\text{cube} I} d^3x \int ds \int dt f^\delta(x, \alpha_i(s)) f^\delta(x, \alpha_j(t)),
\]

\( l_{Pl} \) is the Planck length, for simplicity we have chosen a parametrization such that \( |\dot{\alpha}_i^a(s)| = 1 \), and \( \ast_i \) indicates the action of a "grasp" [4] on the line \( \alpha_i \). The angle \( \theta_{ij} \) is the angle between the \( i \)'th and \( j \)'th tangent vectors at the intersection point \( p \) and \( \gamma_{p}^A \dot{\alpha}_i(p)\dot{\alpha}_j(p) \) is a loop based at \( p \) in the \( \dot{\alpha}_i(p)\dot{\alpha}_j(p) \) plane, with area \( A \). This loop, and the \( \sin(\theta_{ij}) \) factor, appear because we have used the identity

\[
\sum_{\hat{a}<\hat{b}} v^\hat{a} w^\hat{b} \left[ \Psi[\alpha ** \gamma_{x\hat{a}\hat{b}}^A] + \Psi[\alpha ** \gamma_{x\hat{a}\hat{b}}^{-1}] \right] = |\vec{v}| |\vec{w}| \sin(\theta_{\vec{v}\vec{w}}) \left[ \Psi[\alpha ** \gamma_{x\vec{v}\vec{w}}^A] + \Psi[\alpha ** \gamma_{x\vec{v}\vec{w}}^{-1}] \right]
\]

which is true for every two vectors \( \vec{v} \) and \( \vec{w} \), with an angle \( \theta_{\vec{v}\vec{w}} \) between them, because its classical counterpart expressed in terms of traces of holonomies is true, to order \( A \), for all connections, and we require that all such identities be satisfied in the loop representation [5].

An explicit calculation then shows that for \( \delta \ll L \), we have \( X(I, i, j, \delta) = 4\pi^2 / \sin(\theta_{ij}) \delta \), so that the angular dependence in (8) cancels. This cancellation is the first "fortunate accident" that makes it possible to define a diffeomorphism invariant operator.
Assuming that $L$ has been taken small enough so that there is at most one intersection per cube, we then have
\[
\hat{C}_{\text{Einst}} I \Psi[\alpha] = \frac{4\pi^2 P_I}{\delta AL^3} \mathcal{O}_I^A \Psi[\alpha] + O(\delta^2/A) + O(\delta/L)
\] (11)
where the operator $\mathcal{O}_I^A$ is zero unless there is an intersection in the box $I$, in which case it is given by
\[
\mathcal{O}_I^A \Psi[\alpha] = \sum_{i<j} \sum_r (-1)^r \left[ \Psi[(\alpha *^j_\gamma p_{\alpha_i}(p) \delta_{ij}(p))^r] + \Psi[(\alpha *^j_\gamma p_{\alpha_i}(p) \delta_{ij}(p))^{-r}] \right]
\] (12)
and is sensitive only to diffeomorphism invariant features of the intersection: the rooting of the lines through it and the linear dependences of the tangent vectors at the intersection. The effect of the operator is to add a loop of area $A$ (measured by the fictitious background metric) based at the intersection point in each plane made by each pair of tangent vectors at the intersection, and then sum over rearrangements of the rooting through the intersection.

Let us now discuss the finiteness and the diffeomorphism invariance of the operator. As far as finiteness is concerned, the problem is to show that the limits $\delta \to 0$, $A \to 0$ and $L \to 0$ can be taken, respecting the conditions assumed namely $\delta \ll L$ and $\delta^2 \ll A$, so that the resulting operator in (6) is finite. We can accomplish this task if we pose $L = \kappa \delta$ and $A = \kappa^3 \delta^2$ and take first the limit $\delta \to 0$ at fixed $\kappa$, followed by the limit $\kappa \to \infty$. This limit exists and is finite because up to terms of order $\kappa^{-1}$ the powers of $\delta$ and $\kappa$ coming from the operator and from the volume $L^3$ outside the square root in the sum (6) cancel. This cancellation is the second "fortunate accident" that makes the present construction possible.

As the dependence on the regularization parameters cancels, we may go on to discuss the diffeomorphism invariance of the operator. Let us assume that $\Psi[\alpha]$ is a diffeomorphism invariant state, so that $\Psi[\alpha] = \Psi[\phi \circ \alpha]$ for all $\phi \in Diff_0(\Sigma)$. To zeroth order in $\kappa^{-1}$ and $\delta$, the action of $\mathcal{O}_I^A$ is diffeomorphism covariant, in the sense that $\mathcal{O}_I^A \Psi[\phi \circ \alpha] = \mathcal{O}_I^A \Psi[\phi \circ \alpha]$, the reason being the following. For fixed $\alpha$, and for small enough $\delta$ the action of the operator becomes independent of $\delta$, because the added loop doesn’t link any other component of $\alpha$. More precisely, for each given $\alpha$ and $\kappa$, there is a $\delta_0$ such that for all $\delta < \delta_0$ there is a diffeomorphism $\phi_{\delta}$ such that $\mathcal{O}_I^{(\kappa^3 \delta^2)} \Psi[\alpha] = \mathcal{O}_I^{(\kappa^3 \delta^2)} \Psi[\phi_{\delta} \circ \alpha] + O(\kappa^{-1}) = \mathcal{O}_I^{(\kappa^3 \delta^2)} \Psi[\alpha] + O(\kappa^{-1})$; the last equality following from the diffeomorphism invariance of $\Psi$. It follows
that on the diffeomorphism invariant states the limit exists trivially because close to \( \delta = 0 \) we have that \( \mathcal{O}_I^{(\kappa^3 \delta^2)} \Psi[\alpha] \) is constant in \( \delta \) (provided that the intersection remains in the box as the box is scaled down). Moreover, the only effect on \( \mathcal{O}_I^{(\kappa^3 \delta^2)} \Psi[\alpha] \) of a diffeomorphism on \( \alpha \) is, (up to errors of order \( \delta \) and \( \kappa^{-1} \)), to possibly take the intersection outside the box. This is because in the limit the action of the operator (adding a small loop, which doesn’t link anything, in the planes defined by the pairs of tangent vectors, and rearranging the rootings at the intersection) is well defined on the diffeomorphism equivalence classes of loops. Thus, the effect of a diffeomorphism on \( \alpha \) can be simply compensated by moving the box accordingly. The result is that we have defined an operator which is different from zero only if the box \( I \) contains an intersection, is finite, and transforms covariantly under diffeomorphisms. From this, we obtain below a genuinely diffeomorphism invariant operator simply by summing over all the boxes.

Next, the determinant of the three metric is regulated as

\[
\hat{q}_I^I = \frac{1}{10L^6} \sum_{\hat{a} \leq \hat{b} \leq \hat{c}} \int_{I\hat{a}} d^2 S_a(\sigma_1) \int_{I\hat{b}} d^2 S_b(\sigma_2) \int_{I\hat{c}} d^2 S_c(\sigma_3) \hat{T}^{abc}(\sigma_1, \sigma_2, \sigma_3)
\]

(13)

where the integrals are over the faces of the cube, which we labelled as \( I\hat{a} \), summing both front and back, and \( d^2 S_a = \epsilon_{abc} d^2 S^{bc} \) is the area element of the \( \hat{a} \)th face of the \( I \)th cube\(^1\). From the fact that as \( L \to 0 \) we have \( T^{abc}(\sigma_1, \sigma_2, \sigma_3) = \epsilon^{abc} q \), the correct classical limit is assured. At the same time, this sum leads (see [11]) to the diffeomorphism covariant quantum action

\[
\hat{q}_I^I \Psi[\alpha] = \frac{I^6}{10L^6} \sum_{\hat{a} \leq \hat{b} \leq \hat{c}} \sum_{i,j,k} I[I\hat{a}, \alpha_i]I[I\hat{b}, \alpha_j]I[I\hat{c}, \alpha_k] \quad \mathcal{W} \Psi[\alpha] + O(L)
\]

(14)

where \( I[I\hat{a}, \alpha_i] \) is the intersection number between the \( \hat{a} \)th face of the \( I \)th cube and the \( i \)th line coming into the intersection and \( \mathcal{W} \) is the (diffeomorphism covariant) linear operator that rearranges the rooting through the intersection according to the grasp defined by \( \hat{T}^{abc} \), and is zero if there is no intersection in the box.

Let us now put these results together. If we define the operator \( \mathcal{M}_I \) by

\[
L^6 \left[ \hat{q}_I^{(\kappa \delta), \delta, (\kappa^3 \delta^2)} + \Lambda \hat{q}_I^I \right] \Psi[\alpha] = \mathcal{M}_I \Psi[\alpha] + O(\kappa^{-1}) + O(\delta),
\]

(15)

\(^1\)This definition is different from the one given in [4], which is not diffeomorphism invariant.
then we have found that when the $I$'th box contains an intersection

$$\mathcal{M}_I = \lim_{\delta \to 0} \left[ 4\pi^2 l_{Pl}^4 \mathcal{O}_I^{4\delta^2} + l_{Pl}^6 \Lambda \sum_{\hat{a} \leq \hat{b} \leq \hat{c}} \sum_{i,j,k} J[\hat{a},\alpha_i]J[\hat{b},\alpha_j]J[\hat{c},\alpha_k] \mathcal{W} \right] + O(\kappa^{-1})$$

To complete the definition of the operator $\hat{H}$ we have to take the square root and then take the limits. Since the only non–vanishing terms in the sum in (6) come when there is an intersection in the box, the sum reduces to a sum over the intersections of $\alpha$. We label these intersections with the index $i$. This sum is now genuinely diffeomorphism invariant. For each term, the square root is equal to the square root of $\mathcal{M}_i = \mathcal{M}_{I(i)}$, where, for every $\delta$ and $\kappa$, $I(i)$ is the box in which there is the intersection $i$, plus terms that vanish as $\delta \to 0$ for all fixed $\kappa$. The limit $\delta \to 0$ may then be taken, and, if $\Psi$ is a diffeomorphism invariant state, the result is, according to the argument given above, diffeomorphism invariant up to terms of order $\kappa^{-1}$. The limit $\kappa \to \infty$ may then be taken, and the result is the diffeomorphism invariant operator

$$\hat{H} \Psi[\alpha] = \sum_i [\mathcal{M}_i]^{\frac{1}{2}} \Psi[\alpha], \quad (17)$$

where the sum is now over all the intersections $i$ of $\alpha$.

The action indicated by (17) is finite and diffeomorphism invariant. It remains to describe the form of the operator $\mathcal{M}$ and the meaning of its square root. To do this it is convenient to choose a basis for the diffeomorphism invariant bra states of the form $< m_1, ..., m_n; \mathcal{K}_P; a_1, ..., a_n >$. This refers to a graph with $n$ intersections with $2m_i$, $i = 1, ..., n$ lines entering each one. The discrete infinite dimensional index $\mathcal{K}_P$ labels the knotting and linking of a nonintersecting link class with $P$ ordered open ends (a tangle), which are joined to the intersections; here $P = \sum_i 2m_i$. Given a knot with $P$ open lines attached to $n$ intersection, we can still have diffeomorphism inequivalent knots, by varying the rooting, and/or the linear dependences among the tangent vectors, at each intersection. These inequivalent knots span a subspace of the state space, which we denote as $\mathcal{S}[\mathcal{K}_P, m_1, ..., m_n]$. This subspace is isomorphic to the tensor product of a linear space $V_i$ for every intersection $i$. $V_i$ is spanned by the basis vectors labelled by $a_i$. If there are four or less distinct tangent vectors at the point of intersection $V_i$ is finite dimensional, as the only diffeomorphism invariant information is
contained in the rooting and in the possible coincidences of three or more tangent vectors in planes. However, if there are five or more distinct lines entering the intersection, the diffeomorphism equivalence classes form a finite dimensional configuration space which in general is not discrete\footnote{Contrary to what has been implied by the authors previously.}, because in general the diffeomorphism equivalence classes of loops with intersections are also labelled by continuous parameters.

The operator $M_i$ then has the form of an infinite dimensional matrix

$$< m_1, ..., m_n, K_P, a_1, ..., a_n | M_i =$$
$$= < m_1, ..., m_i, ..., m_n, \tilde{K}_P, a_1, ..., a_i, ..., a_n | [M_i]_{a_i m_i K_P}$$

The term coming from $\det(q)$ is diagonal in the indices $m_i$ and $K_P$, because it only rearranges the lines at the intersection. The Einstein term is non-vanishing only in the first upper diagonal in these indices: more precisely, it has the form $\delta^{m_i+1}_{\tilde{m}_i} \delta_{K_P}^ {\tilde{K}_P+2}$, times a matrix in the $a_i$ space. This is because its action is to add a new loop, not linking anything, for every pair of the $2m_i$ tangent vectors, the added loop being in the plane defined by the two tangents, followed by the rearrangement of the rooting through the intersection. This structure gives $M_i$ a relatively simple ”block diagonal and upper-diagonal” form

$$[M_i]_{\tilde{a}_i \tilde{m}_i \tilde{K}_P} = \delta^{m_i}_{\tilde{m}_i} \delta_{K_P}^ {\tilde{K}_P} [M_i^q]_{\tilde{a}_i} + \delta^{m_i+1}_{\tilde{m}_i} \delta_{K_P}^{\tilde{K}_P+2} [M_i^{\text{Einst}}]_{\tilde{a}_i}$$

where $K_P^{\cup+2}$ is the $P+2$ tangle that is gotten from the $P$ tangle $K$ by adding a simple loop which links nothing else in $K$.

The explicit computation of the blocks $[M_i^q]_{\tilde{a}_i}$ and $[M_i^{\text{Einst}}]_{\tilde{a}_i}$ is a tedious but straightforward exercise in three dimensional geometry and combinatorics, defined by the rearranging of rooting through the intersection produced by the grasps of loop operators $\hat{T}_{ab}$ and $\hat{T}_{abc}$. In the computation one must take into account the standard spinor identities of the loop representation \footnote{Contrary to what has been implied by the authors previously.}: if the definition is consistent, the operator should commute with these identities. The remaining problem is to compute the square root of a block diagonal and upper-diagonal infinite dimensional matrix. A technique is under development to accomplish this order by order in the number of lines coming into each intersection.

In summary, the main result reported in this work is the discovery of a regularization procedure that provides the definition of a finite and dif-

feomorphism invariant physical-time-hamiltonian $\hat{H}$, and reduces the problem of computing its matrix elements to an algebraic problem in three-dimensional geometry and combinatorics. If the construction developed here is consistent, this geometrical action of the gravitational hamiltonian $\hat{H}$, which is just to add loops and rearrange rootings at the intersections of the knots states, should code the full content of the Einstein equations, in a diffeomorphism invariant form\(^3\).

We close with some comments. First, the techniques described here also provide a finite expression for the (full) hamiltonian constraint; in fact, we can define a finite operator that corresponds to $H(f) = \int_\Sigma f \sqrt{C}$ for any $f$. This makes it possible to define the hamiltonian constraint directly on the space of diffeomorphism invariant states. Using this operator, one should recover previous results \(^6\) \cite{15} on the kernel of the hamiltonian constraint. Second, as the $A^{-1}$ in (7) is cancelled against other factors, the limit taken in (6) does not define an area derivative. It would be of interest to investigate the space of loop functionals on which this limit is well defined; unlike the space of area differentiable states, this space includes the diffeomorphism invariant states. Third, we note that with the Einstein term left out, our construction provides a definition of the diffeomorphism invariant operator for the volume of the universe. Fourth, the Hamiltonian that we have defined here could be an important ingredient for determining the reality conditions, and hence the physical inner product \(^4\). Finally, we note that the finiteness of the Hamiltonian is not sufficient for the evolution operator to be finite. It is necessary to compute at least the second order term in the expansion in time of the evolution operator, to see whether the sums over virtual states converge \(^10\).

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\(^3\)as the harmonic oscillator equations of motion are coded in the number operator.
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