The Physical Hamiltonian in Nonperturbative Quantum Gravity

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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 [2,3], 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 based on the loop representation [4–7]. We use a scalar field as a clock as suggested in several recent papers [8], 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 [6,9] for diffeomorphism invariant theories. The main 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 [9] is implied by these conditions) finite. It follows that $\hat{H}$ is well defined on the space, $\mathcal{V}$, of the diffeomorphism invariant states of the gravitational field. As $\mathcal{V}$ is spanned by the basis given by the generalized knot classes [4] (diffeomorphism equivalence classes of finite sets of loops in Σ, 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]. We denote the physical regime in which this can be done (in which the scalar field grows monotonically everywhere on Σ) as the clock regime. The formalism developed here is meaningful only within this regime. If we denote its conjugate momentum by $\pi(x)$, the Hamiltonian constraint is

$$\mathcal{C}(x)=\frac{1}{2\mu}\pi^2+\frac{\mu}{2}\tilde{\tilde{q}}^{ab}\partial_a T\partial_b T+\mathcal{C}_{\rm grav}\,, \tag{1}$$

where μ is a constant. The gravitational contribution has the standard form $\mathcal{C}_{\rm grav}=\mathcal{C}_{\rm Einst}+\Lambda_q$ where $\mathcal{C}_{\rm Einst}=\epsilon_{ijk}\times\tilde{E}^{ai}\tilde{E}^{bj}F^k_{ab}$ and $q=\det(q_{ab})$. Here Λ is the cosmological constant, and all other symbols have the usual meaning in the Ashtekar formalism [10]. We then restrict the freedom of choosing the time coordinate by fixing the gauge $\partial_a T=0$. 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 $\mathcal{C}(x)$ turn out to be gauge fixed, except one, which is

$$\int_\Sigma \frac{\mathcal{C}}{\pi}=(2\mu)^{-1/2}\int_\Sigma \pi+\int_\Sigma\sqrt{-\mathcal{C}_{\rm grav}}=0\,. \tag{2}$$

In the quantum theory the diffeomorphism invariant states are then of the form $\Psi[\{\alpha\},T]$, where $\{\alpha\}$ indicates a generalized knot class and the real number T is the constant value of the time. These states satisfy a Schrödinger-type equation $i\hbar(d\Psi/dT)=\sqrt{2\mu}\hat{H}\Psi$ where $\hat{H}$ is the quantum operator corresponding to the observable

$$H=\int_\Sigma\sqrt{-\mathcal{C}_{\rm grav}}\,. \tag{3}$$

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. We write

$$\hat{H}=\lim_{L\to 0,A\to 0,\delta\to 0}\sum_I L^3\sqrt{-\hat{\mathcal{C}}^{L,\delta,A}_{{\rm Einst}\,I}-\Lambda\hat{q}^L_I}\,, \tag{4}$$

where we have divided the spatial manifold Σ 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 δ 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. Further, note that in the clock regime $-\mathcal{C}_{\rm grav}$ is strictly positive everywhere, so that the clock measures time to flow in the same direction everywhere. The Einstein term is

$$\hat{\mathcal{C}}^{L,\delta,A}_{\text{Einst}\,I}=\frac{1}{2L^3A}\int_{\text{cube}\,I}d^3x\int d^3y\int d^3z\,f^\delta(x,y)f^\delta(x,z)\sum_{\hat{a}\hat{b}}\{\hat{T}^{\hat{a}\hat{b}}[\gamma_{xyz}\circ\gamma^A_{x\hat{a}\hat{b}}](y,z)-\hat{T}^{\hat{a}\hat{b}}[\gamma_{xyz}\circ\gamma^{A}_{x\hat{a}\hat{b}}{}^{-1}](y,z)\}\,,\tag{5}$$

where $f^\delta(x,y)=(3/4\pi\delta^3)\Theta(\delta-|x-y|)$ regulates the distributional products (Θ is the step function). $\hat{T}^{ab}$ is defined in [4], γ_{xyz} is a zero area curve running from x to y to z and back, and $\gamma^A_{x\hat{a}\hat{b}}$ 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, δ, A, and L. It is straightforward to check that the classical expression corresponding to (4) and (5) reproduces (3) when the limits are taken.

Let us now study the action of (5) on a loop state $\Psi[\alpha]$. First, the limit is zero unless there is an intersection in the Ith cube. When there is an intersection, we will, for simplicity, restrict ourselves to the case in which the intersection is formed by a meeting of smooth curves. In these cases, let us label the n curves going through the intersection point, p, as $\alpha_i, i=1,\ldots,n$. Using the explicit forms of the operator $\hat{T}^{ab}$ [4], we have

$$\hat{\mathcal{C}}^{L,\delta,A}_{\text{Einst}\,I}\Psi[\alpha]=\frac{l^4_{\rm Pl}}{AL^3}\sum_{i<j\le n}X(I,i,j,\delta)\sin(\theta_{ij})\sum_r(-1)^r\{\Psi[(\alpha*_i*_j\gamma^A_{p\,\dot{\alpha}_i(p)\dot{\alpha}_j(p)})^r]-\Psi[(\alpha*_i*_j\gamma^A_{p\,\dot{\alpha}_i(p)\dot{\alpha}_j(p)}{}^{-1})^r]\},\tag{6}$$

where

$$X(I,i,j,\delta)=\int_{\text{cube}\,I}d^3x\int_{-\infty}^{\infty}ds\int_{-\infty}^{\infty}dt\,f^\delta(x,\alpha_i(s))f^\delta(x,\alpha_j(t))\,.\tag{7}$$

Here $l_{\rm Pl}$ is the Planck length, we have chosen a parametrization such that $|\dot{\alpha}^a_i(s)|=1$, and $*_i$ indicates the action of a "grasp" [4] on the line α_i. θ_{ij} is the angle between the ith and jth tangent vectors at the intersection point p and $\gamma^A_{p\,\dot{\alpha}_i(p)\dot{\alpha}_j(p)}$ 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

$$\sum_{\hat{a}>\hat{b}}v^{\hat{a}}w^{\hat{b}}\{\Psi[\alpha**\gamma^A_{x\hat{a}\hat{b}}]-\Psi[\alpha**\gamma^{A}_{x\hat{a}\hat{b}}{}^{-1}]\}=|\mathbf{v}||\mathbf{w}|\sin(\theta_{\mathbf{vw}})\{\Psi[\alpha**\gamma^A_{x\mathbf{vw}}]-\Psi[\alpha**\gamma^{A}_{x\mathbf{vw}}{}^{-1}]\},\tag{8}$$

which is true for every two vectors $\mathbf{v}$ and $\mathbf{w}$, with an angle $\theta_{\mathbf{vw}}$ 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 [11]. 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 (6) 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

$$\hat{\mathcal{C}}^{\delta}_{\text{Einst}\,I}\Psi[\alpha]=\frac{4\pi^2 l^4_{\rm Pl}}{\delta AL^3}\mathcal{O}^A_I\Psi[\alpha]+O(\delta^2/A)+O(\delta/L)\,,\tag{9}$$

where the operator $\mathcal{O}^A_I$ is zero unless there is an intersection in the box I, in which case it is given by

$$\mathcal{O}^A_I\Psi[\alpha]=\sum_{i<j\le n}\sum_r(-1)^r\{\Psi[(\alpha*_i*_j\gamma^A_{p\dot{\alpha}_i(p)\dot{\alpha}_j(p)})^r]-\Psi[(\alpha*_i*_j\gamma^A_{p\dot{\alpha}_i(p)\dot{\alpha}_j(p)}{}^{-1})^r]\}\,.\tag{10}$$

The action of the operator $\mathcal{O}$ 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 $\delta\rightarrow 0$, $A\rightarrow 0$, and $L\rightarrow 0$ can be taken, respecting the conditions assumed, namely, $\delta\ll L$ and $\delta^2\ll A$, so that the resulting operator in (4) is finite. We can accomplish this task if we pose $L=\kappa\delta$ and $A=\kappa^3\delta^2/Z$, with Z a free renormalization constant, and take first the limit $\delta\rightarrow 0$ at fixed κ, followed by the limit $\kappa\rightarrow\infty$. This limit exists and is finite because up to terms of order κ^{-1} the powers of δ and κ coming from the operator and from the volume L^3 outside the square root in the sum (4) 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. To zeroth order in κ^{-1} and δ, the action of $\mathcal{O}^A_I$ is diffeomorphism covariant, in the sense that $\mathcal{O}^A_I\Psi[\phi\circ\alpha]=\mathcal{O}^A_{\phi^{-1}\circ I}\Psi[\alpha]$, the reason being the following. For fixed α, and for small enough δ the action of the operator becomes independent of δ, because the added loop does not link any other component of α. More precisely, for each given α and κ, there is a δ_0 such that for all $\delta<\delta_0$ there is a diffeomorphism ϕ_δ such that $\mathcal{O}^{(\kappa^3\delta^2)}_I\Psi[\alpha]=\mathcal{O}^{(\kappa^3\delta_0^2)}_I\Psi[\phi_\delta\circ\alpha]=\mathcal{O}^{(\kappa^3\delta_0^2)}_I\Psi[\alpha]$ up to terms $O(\kappa^{-1})$, the last equality following from the diffeomorphism invariance of Ψ. It follows that on the diffeomorphism invariant states the limit exists trivially because close to $\delta=0$ we have that $\mathcal{O}^{(\kappa^3\delta^2)}_I\Psi[\alpha]$ is constant in δ

(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 α is (up to errors of order δ and κ^{-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 does not 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 α can be simply compensated by moving the box accordingly.

Next, the determinant of the three-metric is regulated as

$$\hat{q}_I^L = \frac{1}{10L^6}\sum_{\hat{a}\le\hat{b}\le\hat{c}}\int_{I\hat{a}} d^2S_a(\sigma_1)\int_{I\hat{b}} d^2S_b(\sigma_2)\int_{I\hat{c}} d^2S_c(\sigma_3)\hat{T}^{abc}(\sigma_1,\sigma_2,\sigma_3)\,, \tag{11}$$

where the integrals are over the faces of the cube, which we labeled as $I\hat{a}$, summing both front and back, and $d^2S_a=\epsilon_{abc}d^2S^{bc}$ is the area element of the $\hat{a}$th face of the Ith cube. 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 [6]) to the diffeomorphism covariant quantum action

$$\hat{q}_I^L\Psi[\alpha] = \frac{l_{\rm Pl}^6}{L^6}\sum_{\hat{a}\le\hat{b}\le\hat{c}}\sum_{i,j,k} I[I\hat{a},\alpha_i]I[I\hat{b},\alpha_j]I[I\hat{c},\alpha_k]\mathcal{W}\Psi[\alpha]+O(L)\,, \tag{12}$$

where $I[I\hat{a},\alpha_i]$ is the intersection number between $\hat{a}$th face of the Ith cube and the ith 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

$$L^6[\hat{\mathcal{C}}_{{\rm Einst}\,I}^{(\kappa\delta),\delta,(\kappa^3\delta^2)}+\Lambda\hat{q}_I^L]\Psi[\alpha]=\mathcal{M}_I\Psi[\alpha]+O(\kappa^{-1})+O(\delta)\,, \tag{13}$$

then we have found that when the Ith box contains an intersection

$$\mathcal{M}_I=\lim_{\delta\to 0}\left[4\pi^2 l_{\rm Pl}^4 Z\mathcal{O}_I^{\kappa^3\delta^2}+l_{\rm Pl}^6\Lambda\sum_{\hat{a}\le\hat{b}\le\hat{c}}\sum_{i,j,k}I[I\hat{a},\alpha_i]I[I\hat{b},\alpha_j]I[I\hat{c},\alpha_k]\mathcal{W}\right]+O(\kappa^{-1})\,. \tag{14}$$

To complete the definition of the operator $\hat{H}$ we have to take the square root and then take the limits. Since the only nonvanishing terms in the sum in (4) come when there is an intersection in the box, the sum reduces to a sum over the intersections of α. 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 δ and κ, $I(i)$ is the box in which there is the intersection i, plus terms that vanish as $\delta\to 0$ for all fixed κ. If we take the limit $\delta\to 0$ and then $\kappa\to\infty$, we obtain $\hat{H}\Psi[\alpha]=\sum_i[\mathcal{M}_i]^{1/2}\Psi[\alpha]$, where the sum is now over all the *intersections* i of α. The action indicated of $\hat{H}$ is now 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 we choose a basis for the diffeomorphism invariant bra states of the form $\langle m_1,\ldots,m_n;\mathcal{K}_P;a_1,\ldots,a_n|$. This refers to a graph with n intersections with $2m_i, i=1,\ldots,n$ 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 [12]), which are joined to the intersections; here $P=\sum_i 2m_i$. Knots with support on topologically equivalent graphs can still be inequivalent: We can vary the rooting through the intersections, and the linear dependences among the tangent vectors at intersection. These inequivalent knots span a subspace of the state space, which we denote as $\mathcal{S}[\mathcal{K}_P,m_1,\ldots,m_n]$. 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 labeled by a_i. [The diffeomorphism equivalence classes formed by loops with intersections (in which five or more lines join) are not denumerable but are labeled by continuous parameters.]

The operator $\mathcal{M}_i$ then has the form of an infinite dimensional matrix

$$\langle m_1,\ldots,m_n,\mathcal{K}_P,a_1,\ldots,a_i,\ldots,a_n|\mathcal{M}_i=\langle m_1,\ldots,\tilde{m}_i,\ldots,m_n,\tilde{\mathcal{K}}_P,a_1,\ldots,\tilde{a}_i,\ldots,a_n|[\mathcal{M}_i]_{a_i m_i\mathcal{K}_P}^{\tilde{a}_i\tilde{m}_i\tilde{\mathcal{K}}_P}\,. \tag{15}$$

The cosmological term is diagonal in the indices m_i and $\mathcal{K}_P$ because it only rearranges lines at the intersection. The Einstein term is nonvanishing only in the first upper diagonal in these indices; more precisely, it has the form $\delta_{\tilde{m}_i}^{m_i+1}\delta_{\tilde{\mathcal{K}}_P}^{\mathcal{K}_{P+2}}$, times a matrix in the a_i space. (Recall the action of $\mathcal{O}$ described above.) This structure gives $\mathcal{M}_i$ a relatively simple "block diagonal and upper diagonal" form

$$[\mathcal{M}_i]_{a_i m_i\mathcal{K}_P}^{\tilde{a}_i\tilde{m}_i\tilde{\mathcal{K}}_P}=\delta_{\tilde{m}_i}^{m_i}\delta_{\tilde{\mathcal{K}}_P}^{\mathcal{K}_P}[\mathcal{M}_i^q]_{a_i}^{\tilde{a}_i}+\delta_{\tilde{m}_i}^{m_i+1}\delta_{\tilde{\mathcal{K}}_P}^{\mathcal{K}_{P+2}^{\cup}}[\mathcal{M}_i^{\rm Einst}]_{a_i}^{\tilde{a}_i}\,, \tag{16}$$

where $\mathcal{K}_{P+2}^{\cup}$ is the $P+2$ tangle obtained from the P tangle $\mathcal{K}$ by adding a simple loop which links nothing else in $\mathcal{K}$. The explicit computation of the blocks $[\mathcal{M}_i^q]_{a_i}^{\tilde{a}_i}$ and $[\mathcal{M}_i^{\rm Einst}]_{a_i}^{\tilde{a}_i}$ is a slow but straightforward exercise in three-dimensional geometry and combinatorics, defined by the rearranging of rooting through the intersection produced by the grasps of the operators $\hat{T}^{ab}$ and $\hat{T}^{abc}$. The remaining problem is to compute the square root of the matrix

(16). A procedure to do this is under development, which exploits the block diagonal structure of the matrix.

In summary, the result we reported is the discovery of a regularization procedure that provides the definition of a finite and diffeomorphism invariant physical-time-Hamiltonian $\hat{H}$, and reduces the computation of its matrix elements to an algebraic problem in three-dimensional geometry and combinatorics. This geometrical action of the gravitational Hamiltonian $\hat{H}$, which is just to add loops and rearrange routing at the intersections of the knots states, should code the full content of the Einstein equations, in a diffeomorphism invariant form.

We close with some comments.

(i) The techniques described here also provide a finite expression for the (full) Hamiltonian constraint, since we can define the operator corresponding to $H(f)=\int_\Sigma f\sqrt{\mathcal{C}}$ 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 be able to recover previous results [4,13] on the kernel of the Hamiltonian constraint.

(ii) As the A^{-1} in (5) is canceled against other factors, the limit taken in (4) does not define a loop derivative. It would be of interest to investigate the space of loop functionals on which this limit is well defined; unlike the space of loop differentiable states, this space includes the diffeomorphism invariant states.

(iii) We do not expect the Hamiltonian to be self-adjoint and have only real eigenvalues: Outside the clock regime (defined above) the evolution with respect to the time defined by the scalar field becomes nonunitary. This simply signals that the system is exiting the clock regime (see [3,14] for more details). Thus, the formalism developed here can only be applied to a subspace of the quantum state space (corresponds to the classical clock regime) on which the Hamiltonian is well behaved. This is precisely those parts of the space of diffeomorphism invariant states spanned by the eigenstates of $\mathcal{M}_I$ whose eigenvalues have positive real part.

(iv) An extension to fermions of the present construction has been developed in Ref. [14].

(v) Our construction provides a definition of the diffeomorphism invariant operator for the volume of 3D space.

(vi) 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 [15].

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