# Quantum spin dynamics (QSD): VI. Quantum Poincaré algebra and a quantum positivity of energy theorem for canonical quantum gravity

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**Abstract.** We quantize the generators of the little subgroup of the asymptotic Poincaré group of Lorentzian four-dimensional canonical quantum gravity in the continuum.

In particular, the resulting ADM energy operator is densely defined on an appropriate Hilbert space, symmetric and essentially self-adjoint.

Moreover, we prove a quantum analogue of the classical positivity of the energy theorem due to Schoen and Yau. The proof uses a certain technical restriction on the space of states at spatial infinity which is suggested to us given the asymptotically flat structure available. The theorem demonstrates that several of the speculations regarding the stability of the theory, spelled out recently by Smolin, are false once a quantum version of the pre-assumptions underlying the classical positivity of the energy theorem is imposed in the quantum theory as well.

The quantum symmetry algebra corresponding to the generators of the little group faithfully represents the classical algebra.

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#### 1. Introduction

Following the canonical approach to a quantum theory of gravity, a (Dirac) observable is by definition a self-adjoint operator on the full Hilbert space (not only on the Hilbert space induced from the full Hilbert space by restricting to the space of solutions of the quantum constraints) which weakly commutes with the constraint operators. Equivalently, an observable leaves the physical Hilbert space of solutions to the quantum constraints invariant and is self-adjoint with respect to the physical inner product.

At this point no Dirac observables are known for pure general relativity (the situation improves when adding matter), neither for classical nor for quantum gravity. An exception is given by the asymptotically flat case where it is well known that the Poincaré generators at spatial infinity form a closed Dirac classical observable algebra.

In the present paper we address the question of how to quantize these generators. We work with the real version of the originally complex connection formulation of Lorentzian general relativity [1] which was first considered in [2] (a real-valued connection formulation for Euclidean gravity was earlier considered in [3]). The associated real connection representation has been made into a solid foundation for quantum theory in the series

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of papers [4–10]. This rigorous mathematical framework which is based on the earlier pioneering work on loop variables, for instance [11, 12] for gauge theories and gravity, respectively (the latter of which was designed for the complex variables and thus was lacking an appropriate inner product), equips us with the tools necessary to ask the question of whether the various operators constructed are densely defined, symmetric, self-adjoint, diffeomorphism invariant and so forth.

But even though this kinematical framework is available, it is still quite surprising that something like an ADM energy operator can actually be constructed. The reason for this is that in the representation under consideration the ADM energy function turns out to be a rather non-polynomial function of the canonical momenta and thus it is far from clear how to define it. It turns out that the same technique that enabled one to define the Wheeler–DeWitt operator for 3 + 1 Lorentzian gravity [13–15], the Wheeler–DeWitt operator for 2 + 1 Euclidean gravity [16], length operators [17] and matter Hamiltonians when coupled to gravity [18] can be employed to define Poincaré quantum operators.

The present paper is organized as follows. In section 2 we review the necessary mathematical background from [4–10, 19]. In section 3 we regularize the ADM energy operator. There are at least two natural orderings, one in which the operator becomes densely defined on the full physical Hilbert space as defined in [19] and one in which it is not. Nevertheless, the latter operator should be the physically relevant one because when restricting the Hilbert space to a subspace which is suggested to us given the asymptotically flat structure available, then this operator turns out to be positive-semidefinite by inspection and essentially self-adjoint on the physical Hilbert space. This result reveals that several of the speculations spelled out in [20] and which were based on several unproved assumptions were premature: after taking the quantum dynamics of the theory and the quantum asymptotic and regularity conditions on the Hilbert space appropriately into account, the quantum positivity of energy theorem is *not* violated.

It should be said from the outset, however, that the 'quantum positivity of energy theorem' that we provide rests, besides on a quite particular regularization procedure of the ADM energy operator which exploits the fall-off behaviour of the fields at spatial infinity quite crucially, on one additional technical assumption (the *tangle assumption*, see below) whose physical significance is unclear. Although it can be motivated also given the structure available at spatial infinity, it should be stressed that without this assumption the positivity theorem would not hold.

In section 4 we naturally extend the unitary representation of the diffeomorphism group to include asymptotic translations and rotations and compute the symmetry algebra between time translations and the spatial Euclidean group, that is, we verify the algebra of the little group of the Poincaré group. We find no anomaly. As is well known, the little group suffices to induce the unitary irreducible representations of the Poincaré group. In this paper we do not, however, address the more difficult problem of how to define a boost quantum operator.

#### 2. Preliminaries

We begin with a compact review of the relevant notions from [10, 19]. The interested reader is urged to consult these papers and references therein.

We assume that spacetime is of the form  $M = \mathbb{R} \times \Sigma$  where  $\Sigma$  has an asymptotically flat topology, that is, there is a compact set  $B \subset \Sigma$  such that  $\Sigma - B$  is homeomorphic with  $\mathbb{R}^3$  with a compact ball cut out. We also assume that  $\partial \Sigma$  is homeomorphic with the 2-sphere. The case of more than one component of  $\partial \Sigma$  (e.g. several asymptotic ends or horizons, etc) can be treated in a similar way.

Denote by  $a,b,c,\ldots$  spatial tensor indices and by  $i,j,k,\ldots$  su(2) indices. The gravitational phase space is described by a canonical pair  $\left(A_a^i,E_i^a/\kappa\right)$  where  $A_a^i$  is an SU(2) connection on the hypersurface  $\Sigma$ ,  $E_i^a$  is an ad(SU(2)) transforming vector density and  $\kappa$  is the gravitational coupling constant. This means that the symplectic structure is given by  $\left\{A_a^i(x),E_j^b(y)\right\}=\kappa\delta(x,y)\delta_a^b\delta_j^i$ . The relation with the co-triad  $e_a^i$ , the extrinsic curvature  $K_{ab}$  and the 3-metric  $q_{ab}=e_a^ie_b^i$  is  $E_i^a=\frac{1}{2}\epsilon^{abc}\epsilon_{ijk}e_b^je_c^k$  and  $A_a^i=\Gamma_a^i+\mathrm{sgn}\left(\det\left((e_c^j)\right)\right)K_{ab}e_j^b$  where  $\epsilon^{abc}$  is the metric-independent, completely skew tensor density of weight one,  $\Gamma_a^i$  is the spin connection of  $e_a^i$  and  $e_a^i$  is the inverse of the matrix  $e_a^i$ .

By  $\gamma$  we will denote in the following a closed, piecewise analytic graph embedded into a d-dimensional smooth manifold  $\Sigma$  (the case of interest in general relativity is d=3). The set of its edges will be denoted by  $E(\gamma)$  and the set of its vertices  $V(\gamma)$ . By suitably subdividing edges into two halves we can assume that all of them are outgoing from a vertex (the remaining endpoint of the so divided edges is not a vertex of the graph because it is a point of analyticity). Let A be a G connection for a compact gauge group G (the case of interest in general relativity is G=SU(2)). We will denote by  $h_e(A)$  the holonomy of A along the edge e. Let  $\pi_j$  be the (once and for all fixed representative of the equivalence class of the set of) jth irreducible representations of G (in general relativity j is just a spin quantum number) and label each edge e of  $\gamma$  with a label  $j_e$ . Let v be an n-valent vertex of  $\gamma$  and let  $e_1, \ldots, e_n$  be the edges incident at v. Consider the decomposition of the tensor product  $\bigotimes_{k=1}^n \pi_{j_{e_k}}$  into irreducibles and denote by  $\pi_{c_v}(1)$  the linearly independent projectors onto the irreducible representations  $c_v$  that appear.

Definition 2.1. An extended spin-network state is defined by

$$T_{\nu,\vec{l},\vec{c}}(A) := \operatorname{tr}(\bigotimes_{v \in V(\gamma)} [\pi_{c_v}(1) \cdot \bigotimes_{e \in E(\gamma), v \in e} \pi_{j_e}(h_e(A))]) \tag{2.1}$$

where  $\vec{j} = \{j_e\}_{e \in E(\gamma)}$ ,  $\vec{c} = \{c_v\}_{v \in V(\gamma)}$ . In what follows we will use a compound label  $I \equiv (\gamma(I), \vec{j}(I), \vec{c}(I))$ . An ordinary spin-network state is an extended one with all vertex projectors corresponding to singlets.

Thus, a spin-network state is a particular function of smooth connections restricted to a graph with definite transformation properties under gauge transformations at the vertices. Their importance is that they form an orthonormal basis for a Hilbert space  $\mathcal{H} \equiv \mathcal{H}_{aux}$ , called the auxiliary Hilbert space. Orthonormality means that

$$\langle T_{\gamma,\vec{j},\vec{c}}, T_{\gamma',\vec{j}',\vec{c}'} \rangle \equiv \langle T_{\gamma,\vec{j},\vec{c}}, T_{\gamma',\vec{j}',\vec{c}'} \rangle_{aux} = \delta_{\gamma\gamma'} \delta_{\vec{j},\vec{j}'} \delta_{\vec{c},\vec{c}'}. \tag{2.2}$$

Another way to describe  $\mathcal{H}$  is by displaying it as a space of square-integrable functions  $L_2(\overline{\mathcal{A}/\mathcal{G}}, d\mu_0)$ . Here  $\overline{\mathcal{A}/\mathcal{G}}$  is a space of distributional connections modulo gauge transformations, typically non-smooth and  $\mu_0$  is a rigorously defined,  $\sigma$ -additive, diffeomorphism-invariant probability measure on  $\overline{\mathcal{A}/\mathcal{G}}$ . The space  $\overline{\mathcal{A}/\mathcal{G}}$  is the maximal extension of the space  $\mathcal{A}/\mathcal{G}$  of smooth connections such that (the Gel'fand transform of) spin-network functions are still continuous. The inner product can be extended, with the same orthonormality relations, to any smooth (rather than analytic) graph with a finite number of edges and to non-gauge-invariant functions. It is only the latter description of  $\mathcal{H}$  which enables one to verify that the inner product  $\langle \cdot, \cdot \rangle$  is the unique one that incorporates the correct reality conditions that A, E are in fact real valued. The inner product (2.2) was postulated earlier (see remarks in [31]) for the *complex* connection formulation. But it was not until the construction of the Ashtekar–Lewandowski measure  $\mu_0$  that one could show that this inner product is actually the correct one for the real connection formulation only.

We will denote by  $\Phi$  the finite linear combinations of spin-network functions and call it the space of cylindrical functions. A function  $f_{\gamma}$  is said to be cylindrical with respect to a graph  $\gamma$  whenever it is a linear combination of spin-network functions on that graph such that  $\pi_{j_e}$  is not the trivial representation for no  $e \in E(\gamma)$ . The space  $\Phi$  can be equipped with one of the standard nuclear topologies induced from  $G^n$  because on each graph  $\gamma$  every cylindrical function  $f_{\gamma}$  becomes a function  $f_n$  on  $G^n$  where n is the number of edges e of  $\gamma$  through the simple relation  $f_{\gamma}(A) = f_n(h_{e_1}(A), \ldots, h_{e_n}(A))$ . This turns it into a topological vector space. By  $\Phi'$  we mean the topological dual of  $\Phi$ , that is, the bounded linear functionals on  $\Phi$ . General theorems on nuclear spaces show that the inclusion  $\Phi \subset \mathcal{H} \subset \Phi'$  (Gel'fand triple) holds.

So far we have dealt with solutions to the Gauss constraint only, that is, we have explicitly solved it by dealing with gauge-invariant functions only. We now turn to the solutions to the diffeomorphism constraint (we follow [19]).

Roughly speaking one constructs a certain subspace  $\Phi_{Diff}$  of  $\Phi'$  by 'averaging spinnetwork states over the diffeomorphism group' by following the subsequent recipe: take a spin-network state  $T_I$  and consider its orbit  $\{T_I\}$  under the diffeomorphism group. Here we mean orbit under asymptotically identity diffeomorphisms only! Then construct the distribution

$$[T_I] := \sum_{T \in \{T_I\}} T \tag{2.3}$$

which can be shown explicitly to be an element of  $\Phi'$ . Any other vector is averaged by first decomposing it into spin-network states and then averaging those spin-network states separately. Certain technical difficulties having to do with superselection rules and graph symmetries [10] were removed in [19].

An inner product on the space of the thus constructed states is given by

$$\langle [f], [g] \rangle_{Diff} := [f](g) \tag{2.4}$$

where the brackets stand for the averaging process and the right-hand side means evaluation of a distribution on a test function. The completion of  $\Phi_{Diff}$  with respect to  $\langle \cdot, \cdot \rangle_{Diff}$  is denoted by  $\mathcal{H}_{Diff}$ .

Finally, the Hamiltonian constraint is solved as follows [15]: one can explicitly write down an algorithm of how to construct the most general solution. It turns out that one can construct 'basic' solutions  $s_{\mu} \in \Phi'$  which are mutually orthonormal with respect to  $\langle \cdot, \cdot \rangle_{Diff}$  (in a generalized sense) and diffeomorphism invariant. The span of these solutions is equipped with the natural orthonormal basis  $s_{\mu}$  (in the generalized sense). One now defines a 'projector'

$$\hat{\eta}f := [[f]] := \sum_{\mu} s_{\mu} \langle s_{\mu}, [f] \rangle_{Diff}$$

$$(2.5)$$

for each  $f \in \Phi$  and so obtains a subspace  $\Phi_{Ham} \subset \Phi'$ . The physical inner product [19] is defined by

$$\langle [[f]], [[g]] \rangle_{phys} := [[f]]([g]).$$
 (2.6)

Finally, the physical Hilbert space is just the completion of  $\Phi_{Ham}$  with respect to  $\langle \cdot, \cdot \rangle_{Ham}$ .

# 3. Regularization of the ADM Hamiltonian

There are many ways to write the ADM Hamiltonian which are all classically weakly identical. We are going to choose a form which is a pure surface integral and which

depends only on  $E_i^a$  because in this case the associated operator will be almost diagonal in a spin-network basis so that we can claim that spin-network states really do provide a nonlinear Fock representation for quantum general relativity as announced in [13, 14].

The appropriate form of the classical symmetry generators was derived in [21, 22]. Although that paper was written for the *complex* Ashtekar variables, all results can be taken over by carefully removing factors of i at various places. We find for the surface part of the Hamiltonian (expression (4.31) in [21], we use that  $N = N/\sqrt{\det(q)}$ ,  $N = (D_a N)/\sqrt{\det(q)}$  where N is the scalar lapse function)

$$E(N) = -\frac{2}{\kappa} \int_{\partial \Sigma} dS_a \frac{N}{\sqrt{\det(q)}} E_i^a \partial_b E_i^b.$$
 (3.1)

It is easy, instructive and for the sign of the ADM energy crucial to see that (3.1) really equals the classical expression  $+(1/\kappa)\int_{\partial\Sigma}\mathrm{d}S_a\,(q_{ab,b}-q_{bb,a})$  due to ADM: using that  $E^a_i=\frac{1}{2}\epsilon^{abc}\epsilon_{ijk}e^j_ae^k_b$  we have the chain of identities

$$-\frac{2}{\sqrt{\det(q)}}E_{i}^{a}\partial_{b}E_{i}^{b} = -\operatorname{sgn}(\det(e))e_{i}^{a}\epsilon^{bcd}\epsilon_{ijk}\left[e_{c}^{j}e_{d}^{k}\right]_{,b}$$

$$= -2\operatorname{sgn}(\det(e))e_{i}^{a}\epsilon^{bcd}\epsilon_{ijk}e_{c}^{j}e_{d,b}^{k}$$

$$= -2\operatorname{sgn}(\det(e))q^{af}\epsilon^{bcd}\epsilon_{ijk}e_{f}^{i}e_{c}^{j}e_{d,b}^{k}$$

$$= -4q^{ac}\delta_{[c}^{b}\delta_{e]}^{d}\sqrt{\det(q)}e_{i}^{e}e_{d,b}^{i}$$

$$= 4\sqrt{\det(q)}q^{ac}q^{ed}e_{d}^{i}e_{[c,e]}^{i} = 2\sqrt{\det(q)}q^{ac}q^{bd}e_{d}^{i}\left[e_{c,b}^{i} - e_{b,c}^{i}\right]$$

$$= \sqrt{\det(q)}q^{ac}q^{bd}\left[2e_{(d}^{i}e_{c),b}^{i} + 2e_{[d}^{i}e_{c],b}^{i} - 2e_{(d}^{i}e_{b),c}^{i} - 2e_{[d}^{i}e_{b],c}^{i}\right]$$

$$= \sqrt{\det(q)}q^{ac}q^{bd}\left[(q_{cd,b} - q_{bd,c}) + 2e_{[d}^{i}e_{c],b}^{i}\right]. \tag{3.2}$$

Now we expand  $e_a^i(x) = \delta_a^i + f_a^i(x/r)/r + o(1/r^2)$  where  $r^2 = \delta_{ab}x^ax^b$  defines the asymptotic Cartesian frame. The function  $f_a^i(x/r)$  only depends on the angular coordinates of the asymptotic sphere and is related to the analogous expansion  $q_{ab}(x) = \delta_{ab} + f_{ab}(x/r)/r + o(1/r^2)$  by  $f_{ab}\delta_i^b = f_a^i$ . Consider now the remainder in the last line of (3.2). Its  $o(1/r^2)$  part vanishes because  $f_{[ab]} = 0$  and this concludes the proof.

In the following we focus on the energy functional  $E_{ADM} = E(N = 1)$ . We will quantize it in two different ways corresponding to two quite different factor orderings. Each of the orderings has certain advantages and certain disadvantages which we will point out.

# 3.1. Ordering I: no state space restriction

In this subsection we will derive a form of the operator which is densely defined on the whole Hilbert space  $\mathcal{H}$  (and extends to the spaces  $\mathcal{H}_{Diff}$ ,  $\mathcal{H}_{phys}$  defined above) without imposing any further restriction that corresponds to asymptotic flatness.

Using again that  $E_i^a = \frac{1}{2} \epsilon_{ijk} \epsilon^{abc} e_b^j e_c^k$  we can write it as

$$E_{ADM} = \lim_{S \to \partial \Sigma} E_{ADM}(S) \qquad \text{where} \quad E_{ADM}(S) = -\frac{2}{\kappa} \int_{S} \frac{1}{\sqrt{\det(q)}} \epsilon^{ijk} e^{j} \wedge e^{k} \partial_{b} E_{i}^{b} \quad (3.3)$$

and S is a closed 2-surface which is topologically a sphere. The idea is to point-split expression (3.3) and to use that

$$\left[\operatorname{sgn}(\det(e))e_a^i\right](x) = \frac{1}{2\kappa} \left\{ A_a^i(x), V(x, \epsilon) \right\}$$

where  $V(x, \epsilon) = \int_{\Sigma} d^3y \, \chi_{\epsilon}(x, y) \sqrt{\det(q)}(y)$  and  $\chi_{\epsilon}$  is the (smoothed out) characteristic function of a box of coordinate volume  $\epsilon^3$ . Since

$$\lim_{\epsilon \to 0} \frac{\chi_{\epsilon}(x, y)}{\epsilon^{3}} = \delta(x, y) \qquad \text{so that} \quad \lim_{\epsilon \to 0} \frac{V(x, \epsilon)}{\epsilon^{3}} = \sqrt{\det(q)}(x)$$

we have

$$E_{ADM}(S) = \lim_{\epsilon \to 0} -\frac{2}{\kappa} \int_{S} \frac{1}{\epsilon^{3} \sqrt{\det(q)}(x)} e^{ijk} e^{j}(x) \wedge e^{k}(x) \int_{\Sigma} d^{3}y \, \chi_{\epsilon}(x, y) (\partial_{b} E_{i}^{b})(y)$$

$$= \lim_{\epsilon \to 0} -\frac{2}{\kappa} \int_{S} \frac{\epsilon^{ijk}}{V(x, \epsilon)} e^{j}(x) \wedge e^{k}(x) \int_{\Sigma} d^{3}y \, \chi_{\epsilon}(x, y) (\partial_{b} E_{i}^{b})(y)$$

$$= \lim_{\epsilon \to 0} -\frac{1}{2\kappa^{3}} \int_{S} \frac{\epsilon^{ijk}}{V(x, \epsilon)} \left\{ A^{j}(x), V(x, \epsilon) \right\} \wedge \left\{ A^{k}(x), V(x, \epsilon) \right\}$$

$$\times \int_{\Sigma} d^{3}y \, \chi_{\epsilon}(x, y) (\partial_{b} E_{i}^{b})(y)$$

$$= \lim_{\epsilon \to 0} -\frac{2}{\kappa^{3}} \int_{S} \epsilon^{ijk} \left\{ A^{j}(x), \sqrt{V(x, \epsilon)} \right\} \wedge \left\{ A^{k}(x), \sqrt{V(x, \epsilon)} \right\}$$

$$\times \int_{\Sigma} d^{3}y \, \chi_{\epsilon}(x, y) (\partial_{b} E_{i}^{b})(y)$$

$$= \lim_{\epsilon \to 0} \frac{4}{\kappa^{3}} \int \operatorname{tr} \left( \left\{ A(x), \sqrt{V(x, \epsilon)} \right\} \wedge \left\{ A(x), \sqrt{V(x, \epsilon)} \right\} \right)$$

$$\times \int_{\Sigma} d^{3}y \, \chi_{\epsilon}(x, y) (\partial_{b} E^{b})(y)$$

$$= -\lim_{\epsilon \to 0} \frac{4}{\kappa^{3}} \int_{S} \operatorname{tr} \left( \left\{ A(x), \sqrt{V(x, \epsilon)} \right\} \wedge \left\{ A(x), \sqrt{V(x, \epsilon)} \right\} \right)$$

$$\times \int_{\Sigma} d^{3}y \, \left[ \partial_{y^{b}} \chi_{\epsilon}(x, y) \right] E^{b}(y)$$

$$= \lim_{\epsilon \to 0} E^{\epsilon}_{ADM}(S)$$
(3.4)

where in the second to last step we have taken a trace with respect to generators  $\tau_i$  of su(2) obeying  $[\tau_i, \tau_j] = \epsilon_{ijk}\tau_k$  and in the last step we have performed an integration by parts (the boundary term at  $\partial \Sigma$  does not contribute for finite S and  $\epsilon$  sufficiently small). Thus, we absorbed the  $1/\sqrt{\det(q)}$  into a square root within a Poisson bracket and simultaneously the singular  $1/\epsilon^3$  into a volume functional. Classically we could have dropped the  $1/\sqrt{\det(q)}$  (although the integrand would then no longer be a density of weight one and is strictly speaking not the boundary integral of a variation of the Hamiltonian constraint) due to the classical boundary conditions which tell us that  $\det(q)$  tends to 1.

We now quantize  $E_{ADM}^{\epsilon}(S)$ . This consists of two parts: in the first we focus on the volume integral in (3.4) and replace  $E_i^a$  by  $\hat{E}_i^a = -i\hbar\kappa\delta/\delta A_a^i$ . In the second step we triangulate S exactly as the hypersurface of 2+1 gravity in [16], replace the volume functional by the volume operator and Poisson brackets by commutators times  $1/i\hbar$ .

So let  $f_{\gamma}$  be a function cylindrical with respect to a graph  $\gamma$ . Since we are only interested in the limit  $S \to \partial \Sigma$  we may assume that

- (i)  $\gamma$  lies entirely within the closed ball whose boundary is S, but
- (ii)  $\gamma$  may intersect S at an endpoint of one of its edges and may even have edges that lie entirely inside S.

Furthermore, we can label the edges of  $\gamma$  in such a way that an edge either intersects S transversally (with an orientation outgoing from the intersection point with S) or lies entirely within S.

Coming to the first step we have for the y integral involved in  $E_{ADM}^{\epsilon}(S)$ :

$$\int_{\Sigma} d^{3}y \left[\partial_{a}\chi_{\epsilon}(x,y)\right] \hat{E}_{i}^{a}(y) f_{\gamma} = -i\hbar\kappa \sum_{e \in E(\gamma)} \int_{\Sigma} d^{3}y \left[\partial_{a}\chi_{\epsilon}(x,y)\right] 
\times \int_{0}^{1} dt \, \dot{e}^{a}(t) \, \delta(y,e(t)) \, X_{e}^{i}(t) \, f_{\gamma} 
= -i\hbar\kappa \sum_{e \in E(\gamma)} \int_{0}^{1} dt \, \dot{e}^{a}(t) \left[\partial_{y^{a}}\chi_{\epsilon}(x,y)_{y=e(t)}\right] X_{e}^{i}(t) \, f_{\gamma} 
= -i\hbar\kappa \sum_{e \in E(\gamma)} \int_{0}^{1} dt \left[\frac{d}{dt}\chi_{\epsilon}(x,e(t))\right] X_{e}^{i}(t) \, f_{\gamma} 
= -i\hbar\kappa \sum_{e \in E(\gamma)} \lim_{n \to \infty} \sum_{k=1}^{n} \left[\chi_{\epsilon}(x,e(t_{k})) - \chi_{\epsilon}(x,e(t_{k-1}))\right] X_{e}^{i}(t_{k-1}) \, f_{\gamma} \tag{3.5}$$

where  $E(\gamma)$  is the set of edges of  $\gamma$ ,  $X_e^i(t) := [h_e(0, t) \tau_i h_e(t, 1)]_{AB} \partial/\partial [h_e(0, 1)]_{AB}$  and  $0 = t_0 < t_1 < \cdots < t_n = 1$  is an arbitrary partition of the interval [0, 1].

It is important for what follows that for each t, e, i  $X_e^i(t) f_{\gamma}$  is still a function cylindrical with respect to  $\gamma$ .

We now come to the second step. This involves, first of all, a triangulation of the *two-dimensional* surface S in adaption to the graph  $\gamma$ . Besides the prescription explained in detail in [16] which deals with the triangulation of S in the neighbourhood of a vertex formed by edges of  $\gamma$  that lie entirely within S we just need to deal with the case that a vertex v of  $\gamma$  also has edges incident at it which lie entirely inside the open ball with boundary S except for the one point v. In the case where there are at least two edges  $e_1, e_2$  of  $\gamma$  incident at v such that  $e_1, e_2 \subset S$  we can still take over the triangulation from [16]. However, if there is only *one or no* such edge (indeed, since we do not allow for gauge transformations at spatial infinity we can allow for open edges that lie entirely within or end at S without ruining gauge invariance) we need an additional prescription: in the case where there is only one edge  $e \subset S$  incident at v, choose an arbitrary edge e' not intersecting  $\gamma$  except at v such that the tangents of the edges e, e', e'' are positively oriented at v where e'' is any of the edges of  $\gamma$  incident at v but transversal to S.

In the case where there is no edge  $e \subset S$  incident at v, choose two arbitrary edges e, e' not intersecting  $\gamma$  except at v such that the tangents of the edges s, e', e'' are positively oriented at v where e'' is any of the edges of  $\gamma$  incident at v but transversal to S. These arbitrary edges will disappear from the stage again at the end of the calculation.

Given this set-up, at each vertex v of  $\gamma$  that lies inside S we have now at least two edges  $e_1, e_2$  incident at it that are inside S and we can define the triangles  $\Delta$  associated with pairs of edges incident at v and inside S exactly as in [16]. As in [16] we then have two segments  $s_1(\Delta), s_2(\Delta)$  for each triangle  $\Delta$  which are actually segments of edges of  $\gamma$  incident at v and that lie inside S. Now observe that

$$\epsilon^{ij} h_{s_i(\Delta)} \left\{ h_{s_i(\Delta)}^{-1}, V(v, \epsilon) \right\} h_{s_j(\Delta)} \left\{ h_{s_j(\Delta)}^{-1}, V(v, \epsilon) \right\} \\
= \delta^2 \epsilon^{ij} \dot{s}_i^a(0) \dot{s}_j^b(0) \left\{ A_a(v), \sqrt{V(v, \epsilon)} \right\} \left\{ A_b(v), \sqrt{V(v, \epsilon)} \right\} + o(\delta^2) \\
= 2 \operatorname{vol}(\Delta) \epsilon^{ab} \left\{ A_a(v), \sqrt{V(v, \epsilon)} \right\} \left\{ A_b(v), \sqrt{V(v, \epsilon)} \right\} \tag{3.6}$$

where  $\delta$  is a small parameter corresponding to the parameter length of the  $s_i(\Delta)$  and  $\epsilon^{ab}$  the metric independent totally skew tensor density of weight one on S. Altogether we therefore conclude that the surface integral  $\int_S \left\{ A(x), \sqrt{V(x, \epsilon)} \right\} \wedge \left\{ A(x), \sqrt{V(x, \epsilon)} \right\}$  involved in  $E_{ADM}(S)$  can be quantized by

$$-\frac{1}{2\hbar^2} \sum_{v \in V(\gamma)} \frac{4}{E(v)} \sum_{v(\Delta)=v} \epsilon^{ij} h_{s_i(\Delta)} \left[ h_{s_i(\Delta)}^{-1}, \sqrt{\hat{V}(v, \epsilon)} \right] h_{s_j(\Delta)} \left[ h_{s_j(\Delta)}^{-1}, \sqrt{\hat{V}(v, \epsilon)} \right] f_{\gamma}. \tag{3.7}$$

We do not wish to give a full derivation of (3.7) for which the reader should consult [16], however, a few remarks are in order which intuitively explain (3.7):

- (i) First of all as has already been mentioned, we do not work with a fixed triangulation but with a whole finite family of triangulations that depend on the graph  $\gamma$  of the state that we act on. More precisely, a particular member of the family of triangulations is defined such that for each vertex v of  $\gamma$  which lies in S we (i) pick one pair  $e_1, e_2$  of edges of  $\gamma$  incident at it which are such that  $e_2$  is next to  $e_1$  to its right while the tangents of  $e_1, e_2$  enclose an angle less than or equal to  $\pi$  (with respect to  $\delta_{ab}$ ); (ii) take proper subsegments  $s_i(\Delta) \subset e_i$  incident at v; (iii) construct two more segments  $s_{\bar{i}}(t) = 2v s_i(t)$ ; (iv) construct four obvious triangles from  $s_i, s_{\bar{i}}$  which saturate v and (v) choose a triangulation which embeds those four triangles for each v as basic ones and is otherwise arbitrary only subject to the restriction that none of the remaining  $\Delta$  has its basepoint on  $\gamma$ .
- (ii) Next, each of the four triangles  $\Delta_{12}$ ,  $\Delta_{2\bar{1}}$ ,  $\Delta_{\bar{1}\bar{2}}$ ,  $\Delta_{\bar{2}1}$  contributes classically the same to the surface integral  $\int_{\mathcal{S}} = \sum_{\Delta} \int_{\Delta}$  as the triangle  $\Delta_{12}$  so that we can classically replace these four terms by  $4\int_{\Delta_{12}}$ . This explains the factor of 4 in (3.7).
- (iii) Now, since we do not want to distinguish one particular pair of edges as compared to any other, we average over the choice of pairs which explains the factor of 1/E(v) where E(v) = n(v) or E(v) = n(v) 1 is the possible number of pairs depending on whether the angles less than or equal to  $\pi$  add up to  $2\pi$  (with respect to  $\delta_{ab}$ ) or not and n(v) is the valence of v.
- (iv) Finally, the fact that we sum over vertices of  $\gamma$  only comes from the presence of the volume operator which has non-trivial action at vertices only. Therefore the contribution of all other triangles which define the triangulation drop out (all triangles such that there is no edge of  $\gamma$  transversal to S at its basepoint since the three-dimensional volume operator annihilates co-planar vertices).

It should be mentioned that any of the so-defined 'averaged family of triangulations of S adapted to  $\gamma$ ' has as classical continuum limit the original integral  $\int_{\Sigma}$ !

Putting (3.5) and (3.7) together we obtain as the final result

$$\hat{E}_{ADM}^{\epsilon,n}(S) f_{\gamma} = \frac{4}{\kappa^{3}} \left( -\frac{1}{2\hbar^{2}} \right) (-i\hbar\kappa) \sum_{v \in V(\gamma)} \frac{4}{E(v)} 
\times \sum_{v(\Delta)=v} \epsilon^{ij} \operatorname{tr} \left( h_{s_{i}(\Delta)} \left[ h_{s_{i}(\Delta)}^{-1}, \sqrt{\hat{V}(v, \epsilon)} \right] h_{s_{j}(\Delta)} \left[ h_{s_{j}(\Delta)}^{-1}, \sqrt{\hat{V}(v, \epsilon)} \right] \right) 
\times \sum_{e \in E(\gamma)} \sum_{k=1}^{n} \left[ \chi_{\epsilon}(v, e(t_{k})) - \chi_{\epsilon}(v, e(t_{k-1})) \right] X_{e}^{i}(t_{k-1}) f_{\gamma}.$$
(3.8)

Now we perform the limit  $n \to \infty$  and  $\epsilon \to 0$  in reverse order†: keeping n fixed, for small enough  $\epsilon$  only the term with k=1 in the sum survives provided that e(0)=v. Therefore also the sum over k and with it the n dependence drops out. Also the operator  $\hat{V}(v,\epsilon)$  actually has a limit as  $\epsilon \to 0$  which we call  $\hat{V}_v$  and which is defined by  $\lim_{\epsilon \to 0} \hat{V}(v,\epsilon) f_\gamma =: (\hat{V}_v)_\gamma f_\gamma$  for all  $\gamma$ . That the limit exists relies on the fact that either  $\gamma$  has v as a vertex or it does not. In the latter case the limit just vanishes, in the former case for sufficiently small  $\epsilon$  the  $\epsilon$  box around v does not include any other vertex of  $\gamma$  other than v and so there is only one contribution  $(\hat{V}_v)_\gamma f_\gamma$  which is constant as  $\epsilon \to 0$ . The family of operators  $(\hat{V}_v)_\gamma$  is consistently defined because  $\hat{V}$  is. For a more explicit formula in terms of analytic germs of edges see [16].

Now, the limit  $n \to \infty$  is trivial and the resulting operator derived for arbitrary but finite S can be extended to  $\partial \Sigma$ . The result is

$$\hat{E}_{ADM} f_{\gamma} = \frac{2i}{\hbar \kappa^{2}} \sum_{v \in V(\gamma)} \frac{4}{E(v)} \sum_{v(\Delta) = v} \epsilon^{ij} \operatorname{tr} \left( h_{s_{i}(\Delta)} \left[ h_{s_{i}(\Delta)}^{-1}, \sqrt{\hat{V}(v, \epsilon)} \right] h_{s_{j}(\Delta)} \right) \times \left[ h_{s_{j}(\Delta)}^{-1}, \sqrt{\hat{V}(v, \epsilon)} \right] \sum_{e \in E(\gamma), e(0) = v} X_{e}^{i} f_{\gamma} \tag{3.9}$$

where  $X_e^i(0) = X_e^i = X^i(h_e)$  and  $X^i(g)$  is the right invariant vector field at  $g \in SU(2)$ .

The virtue of (3.9) is that it displays the ADM energy operator as a densely defined operator on all of the Hilbert space. Also, the dependence on the 'arbitrarily short edges'  $s_i(\Delta)$  drops out at the end of the calculation because of gauge invariance as explained in [17]. The disadvantage is that the operator (3.9) is not a manifestly positive semi-definite operator. This is, however, not surprising because even the classical ADM energy is not a positive semi-definite functional on the full phase space of general relativity. It is only when evaluating it on (i) asymptotically flat, (ii) solutions of the Einstein equations which (iii) satisfy an energy condition for allowed matter and (iv) allow for a regular initial data set, that the positive energy theorem has been proved [23, 24] and, in fact, one can easily produce negative ADM energy when one of these conditions is violated. As we did not impose any (quantum analogue of) such restrictions we cannot expect to find a manifestly non-negative operator.

In the next subsection we will derive another quantization of the ADM energy which is only densely defined on a subspace of the Hilbert space, however, the definition of that subspace is a quite natural quantum translation of the classical condition that there be an asymptotically flat regular initial data set. The virtue will be that the ADM operator acquires non-negative discrete spectrum on that subspace of the Hilbert space thus proving a 'quantum positivity of the energy theorem'.

## 3.2. Ordering II: restrictions on the state space

In order to make sense of the operator to be defined in this section we need to give some definition of 'asymptotically flat state'. The following definition is a first attempt

 $\dagger$  One can also make  $\epsilon$  y dependent in (3.4) in a state-dependent way which then leads to a dependence  $\epsilon = \mathrm{o}(1/n)$ . If one then takes  $n \to \infty$  one gets classically back to the original expression for the ADM energy. If one takes n large but finite then one arrives at the same result as below on the quantum level without an interchange of limits being necessary. Therefore the calculations that follow are justified. The state dependence of the regularization drops out in the final expression because before actually taking the limit  $n \to \infty$  the operator will be n-independent. The family of operators thus obtained for each state is consistently defined as we will see. See [16, 18] for a more detailed explanation.

towards a precise notion of 'quantum asymptotic flatness' to be considerably refined in future publications.

Definition 3.1. An asymptotically flat state  $\Psi$  on the Hilbert space  $\mathcal{H}$  is a distribution in  $\Phi'$  satisfying the following conditions:

- (i)  $\Psi$  is a normalized solution  $\hat{\eta}\xi$  to all quantum constraints  $\hat{U}(\varphi) 1 = 0$ ,  $\hat{H}(N) = 0$  (the diffeomorphism and Hamiltonian constraint) of general relativity where  $\varphi$ , N are arbitrary 3-diffeomorphisms and lapse functions subject to the condition that they be pure gauge, that is,  $\varphi(x) \to \operatorname{id}$  and  $N(x) \to 0$  as  $x \to \partial \Sigma$  and where  $\hat{\eta}$  is the operator [19] that maps elements of  $\Phi$  to solutions to all constraints.
- (ii)  $\Psi = \hat{\eta} \xi$  is asymptotically flat. That is, consider any compact region R, surface S and loop  $\alpha$  (which is embedded in the graph underlying the definition of  $\xi$ ) of  $\Sigma \partial \Sigma$  and which are large as compared to Planck volume, area and length, respectively, as measured by the Euclidean metric  $q_{ab}^{(0)} := \delta_{ab}$ . Then, as  $R, S, \alpha$  tend to  $\partial \Sigma$ , the quantities  $\Psi([\hat{V}(R) V_0(R)]\xi), \Psi([\hat{A}(S) A_0(S)]\xi), \Psi([\operatorname{tr}(h_{\alpha}) 2]\xi)$ , respectively, are of order  $\ell_p^3, \ell_p^2, \ell_p/L(c)$ , respectively, where  $V_0(R), A_0(S), L_0(\alpha)$  are the volume, area and length of  $R, S, \alpha$  as measured by  $q_{ab}^{(0)}$ .
- (iii)  $\Psi$  transforms according to an unitary, irreducible representation of the Poincaré group at spatial infinity.
- (iv)  $\Psi$  satisfies the dominant energy condition: let  $\hat{H}'_{matter}(N)$  be the dual of the matter part of the Hamiltonian constraint (not the Hamiltonian!) and  $\hat{V}'_{matter}(\vec{N})$  be the dual of the matter part of the diffeomorphism constraint.

The 4-vector  $N^{\mu} = (N, \vec{N})$  is said to be a future-directed timelike vector in a state  $\Psi$  if (a) N > 0 and (b) there exists  $\epsilon > 0$  such that  $-t^2N^2(x) + \Psi[\hat{L}(c(\vec{N}, x, t))^2\xi] < 0$  for each  $0 < t < \epsilon$  where  $\hat{L}(c)$  is the length operator [17] and  $c(\vec{N}, x, t)$  is the segment of the integral curve of  $\vec{N}$  beginning in x and ending after a parameter distance t.

 $\Psi$  is said to satisfy the dominant energy condition provided that for every 4-vector  $N^{\mu}$  which is future-directed and timelike for  $\Psi$  then there is an  $\epsilon > 0$  such that the 4-vector  $\hat{P}^{\mu}(x,t) := (\hat{H}'_{matter}(N_{x,t}) + \hat{V}'_{matter}(\vec{N}_{x,t}), 0)$  is either zero or future-directed and timelike for every  $x \in \Sigma$  and  $0 < t < \epsilon$  in the state  $\Psi$  where  $N_{x,t}(y) = \chi_t(x,y) N(y)$  and likewise for  $\vec{N}_{x,t}(y)$  ( $\chi_t(x,y)$ ) is the characteristic function of a box of coordinate volume  $t^3$  and centre x). In other words,  $\Psi([\hat{H}_{matter}(N_{x,t}) + \hat{V}_{matter}(\vec{N}_{x,t})]\xi) > 0$  for each  $x, 0 < t < \epsilon$ . Here we have adopted the convention that the signature of the Lorentz metric be -, +, +, +.

The subspace of  $\xi$  in  $\mathcal{H}$  satisfying these conditions will be called  $\mathcal{H}_{af}$  where 'af' stands for asymptotically flat.

Condition (i) makes sure that  $\Psi$  is a solution of the 'quantum Einstein equations'. Condition (ii) is a possible way of defining asymptotic flatness  $q_{ab} \to \delta_{ab}, K_{ab} \to 0$  (although not very carefully, no fall-off and parity conditions were imposed [21, 22] and certainly this condition needs to be refined in future publications. For instance, one might imagine that the error of  $\Psi(\hat{V}(R)\xi)/V_0(R)-1$  is even smaller than  $\ell_p^3/V_0(R)$  in the sense that it could depend on some negative power of the value of the radius r (with respect to  $\delta_{ab}$ ) at the centre of R). Condition (iii) makes contact with physics and allows us to identify certain states with elementary particles. In particular, in the present context of pure gravity we should be able to isolate the graviton (spin-2, massless) states. Notice that in order to allow for non-trivial representations of the little subgroup of the Lorentz group we must specify the appropriate diffeomorphism group in the group averaging process in order to arrive at the diffeomorphism-invariant states [10] which means, roughly speaking, that we

include only those diffeomorphisms in the averaging process that approach identity at  $\partial \Sigma$ . Finally, condition (iv) is the most imprecise one and attempts at defining a possible quantum analogue for the dominant energy condition: recall that the classical energy–momentum tensor  $T_{\mu\nu}$  is said to satisfy the dominant energy condition if for every future-directed timelike vector field  $v^{\mu}$ , the vector field  $T^{\mu}_{\nu}v^{\nu}$  is zero or future-directed and timelike. Now if  $t^{\mu} = Nn^{\mu} + N^{\mu}$  is the future-directed timelike foliation vector field underlying the split  $M = \mathbb{R} \times \Sigma$  and  $n^{\mu}$  the normal vector field of  $\Sigma$  then we may pick a frame such that  $n^{\mu}T_{\mu\nu}t^{\nu} = NH_{matt} + N^{a}(V_{matt})_{a}$  is the only non-vanishing component of the vector  $T_{\mu\nu}t^{\nu}$  and so we need to ask that it be non-negative, in particular, for  $\vec{N} = 0$ , we ask that the matter Hamiltonian densities be non-negative. This condition is, of course, incomplete since it is frame dependent and needs to be improved in the future. Notice that  $(t^{2}g_{\mu\nu}t^{\mu}t^{\nu})(x) = -t^{2}N^{2}(x) + t^{2}(q_{ab}N^{a}N^{b})(x) \approx -N^{2}(x)t^{2} + L(c(\vec{N},x,t))^{2}$  which motivates our definition of future directedness of  $t^{\mu}$ . We conclude with the remark that condition (iv) is certainly satisfied in the vacuum case that we are interested in here.

One might think that a state satisfying all those conditions is rather hard to construct. Let us pause for a moment to argue that it is rather simple.

Consider for simplicity a  $\Sigma$  with topology of  $\mathbb{R}^3$  and distribute a countable number of vertices  $v_n$  randomly into  $\Sigma$  with an average next-neighbour distance of a Planck length as measured by  $q_{ab}^{(0)}$ . Make  $v_n$  the only vertex of a graph  $\gamma_n$  which is 4-valent and non-coplanar (for instance,  $\gamma_n = \alpha_n \cap \beta_n$  where  $\alpha_n$ ,  $\beta_n$  are two kinks with vertex  $v_n$ ). The graphs  $\gamma_n$  are supposed to be contained in a box  $B_n$  of  $q^{(0)}$  volume  $k\ell_p^3$  for some positive number kand the  $B_n$  are mutually non-intersecting. Consider normalized vectors  $f_n$  which are finite linear combination of spin-network states defined on  $\gamma_n$  and which are eigenstates of the volume operator  $\hat{V}(R)$  for any region R, all with the same eigenvalue  $\lambda_n \ell_p^3 = \lambda \ell_p^3 > 0$ if  $v_n \in R$ . Thus we have  $\hat{V}(B_m)f_n = \lambda \ell_p^3 \delta_{m,n} f_n$ . Consider the infinite product state  $\xi := \prod_{n=1}^{\infty} f_n$  which is a regular (non-cylindrical) spin-network state on the infinite graph  $\gamma = \bigcup_n \gamma_n$  and which is in fact normalized,  $\|\xi\| = 1$  thanks to the disjointness of the graphs  $\gamma_n$  because of which  $\|\xi\| = \prod_n \|f_n\|$  due to the properties of the Ashtekar-Lewandowski measure. We now choose  $k := \lambda$  and find that for any macroscopic R, that is, any Rthat contains many of the boxes  $B_n$ , it holds that  $\hat{V}(R)\xi = V_0(R)[1 + o(\ell_p^3/V_0(R))]\xi$ . Now, since no state which is cylindrical with respect to any of the graphs  $\gamma_n$  can be in the image of the Hamiltonian constraint [13–15] it follows from its definition [19] that the  $\hat{\eta}$ operator reduces to group averaging with respect to the diffeomorphism group because of which the group-averaged diffeomorphism-invariant state  $\Psi = [\xi] = \hat{\eta}\xi$  is normalized as well with respect to the physical inner product [19]  $\|\Psi\|_{phys}^2 = \Psi(\xi) = \|\xi\|^2 = 1$ . Thus indeed  $\Psi([\hat{V}(R) - V_0(R)]\xi) = o(\ell_p^3/V_0(R))$  is satisfied. It is clear that the construction can be repeated for the surface operator as well because most of the intersections of the macroscopic surface S with the  $\gamma_n$  will not be in vertices of the  $\gamma_n$  so that  $\hat{V}(R)$ ,  $\hat{A}(S)$  can be simultaneously diagonalized up to errors of order of  $\ell_n^2/A_0(S)$ . Thus, almost every  $f_n$ can be chosen as a simultaneous eigenvector of  $\hat{V}(R)$ ,  $\hat{V}(S)$ . Finally, any macroscopic, for simplicity non-self-intersecting (any loop is a product of these), loop  $\alpha$  on our particular  $\gamma$ is of the product form  $\alpha = \circ^n \alpha_n^{k_n}$ ,  $\alpha_n \subset \gamma_n$ ,  $k_n \in \{0, 1\}$  where  $k_n = 0$  except for finitely many. The SU(2) Mandelstam algebra is too complicated as to exhibit an explicit solution for SU(2) so let us argue with an U(1) substitute that the condition stated in definition 3.1 is reasonable. For U(1) we have  $h_{\alpha} = \prod_{k_n=1} h_{\alpha_n}$ . Now, if we choose for simplicity  $\alpha_n = \gamma_n$  then  $f_n = \sum_{k=-N}^N a_k h_{\alpha_n}^k$  where  $\chi_k(g) = g^k$  is the character of the irreducible representation of U(1) with weight k. Since  $T = \chi_k \chi_l = \chi_{k+l}$  the condition stated in the definition amounts to asking that (for U(1))  $1 = \prod_{k_n=1}^{N} \sum_{k_n=1}^{N} \sum_{k_n=1}^{N} \sum_{k_n=1}^{N} \bar{a}_k a_{k+1}$ 

up to some corrections. Indeed, if we could choose all  $a_k$  to be equal  $(=1/\sqrt{2N+1})$  then the error would be  $1-\prod_{k_n=1}[1-1/(2N+1)]$  which is small provided that  $\sum_{k_n=1}1=\mathrm{o}(L(\alpha)/\ell_p)\ll N$ . For instance, we may choose  $N=[L/\ell_p]^2$  where L is the bound on the length of a macroscopic loop that we wish to consider. This will suffice to motivate definition 3.1. Obviously one has to refine it but this seems impossible without the notion of coherent states and will be left for future publications [25].

We will now show that on an asymptotically flat state the ADM energy operator as defined below is non-negative. We will not show that vanishing energy corresponds to Minkowski space. Our definition of asymptotically flat states as of yet is not restrictive or precise enough for that. As we will see, in order for the ADM operator to be densely defined we need the following stronger condition:

(ii)' A state  $\Psi = \hat{\eta}\xi$  is said to be asymptotically flat provided (ii) of definition 3.1 holds and, in addition:

Let  $\gamma$  be the (infinite) graph on which  $\xi$  depends, p a point in  $\partial \Sigma \cap V(\gamma)$  and  $B_t$ ,  $t \in [0, 1]$  any homotopy of regions in  $\Sigma$  such that  $p \in B_t$  for each t and  $B_0 = \{p\}$ . Then we require that for each such p there exists  $\epsilon > 0$  such that  $\xi$  is, for each  $0 < t < \epsilon$ , a finite linear combination of eigenstates with non-vanishing and t-independent eigenvalues of the volume operator  $\hat{V}(B_t)$ .

It is not clear that condition (ii) implies (ii)' and if that should not be the case then we must add the requirement (ii)' stated as an additional restriction on  $\mathcal{H}_{af}$ ! Notice, however, that (ii)' is not unreasonable in the asymptotically flat context.

It will turn out in the course of the derivation that the positivity of energy theorem then holds if we impose one additional condition on the thus already restricted space of states.

We write expression (3.4) this time in the form (setting  $S = \partial \Sigma$  right from the beginning)

$$E_{ADM} = \lim_{\epsilon \to 0} -\frac{2}{\kappa} \int_{\partial \Sigma} dS_a \, E_i^a(x) \frac{1}{\epsilon^3 \sqrt{\det(q)}(x)} \int_{\Sigma} d^3 y \, \chi_{\epsilon}(x, y) \, \left(\partial_b E_i^b\right)(y)$$

$$= \lim_{\epsilon \to 0} -\frac{2}{\kappa} \int_{\partial \Sigma} dS_a \, E_i^a(x) \frac{1}{V(x, \epsilon)} \int_{\Sigma} d^3 y \, \chi_{\epsilon}(x, y) \, \left(\partial_b E_i^b\right)(y)$$

$$= \lim_{\epsilon \to 0} -\frac{2}{\kappa} \int_{\partial \Sigma} dS_a(x) \, E_i^a(x) \frac{1}{V(x, \epsilon)} \int_{\Sigma} d^3 y \, \chi_{\epsilon}(x, y) \left[G_i(y) - \epsilon_{ijk} A_b^j(y) E_k^b(y)\right]$$

$$=: \lim_{\epsilon \to 0} E_{ADM}^{\epsilon}$$
(3.10)

where  $G_i = \partial_a E_i^a + \left[A_a, E^a\right]_i$  is the Gauss law constraint. Recall that  $G_i = 0$  only needs to hold in the interior of  $\Sigma$  because the Lagrange multiplier  $\Lambda^i$  of the Gauss constraint falls off like  $1/r^2$  so that at  $\partial \Sigma$  every function of  $E_i^a$ ,  $A_a^i$  is gauge invariant. More precisely we have the following: it is of interest by itself to derive the quantum Gauss law operator on a function of *smooth* connections cylindrical with respect to a graph  $\gamma$ :

$$\begin{split} \int_{\Sigma} \mathrm{d}^3x \, \Lambda^i(x) \, \hat{G}_i(x) f_{\gamma} &= -\mathrm{i} \hbar \kappa \sum_{e \in E(\gamma)} \int \mathrm{d}^3x \, \Lambda^i(x) \\ &\times \int_0^1 \mathrm{d}t \, \dot{e}^a(t) \Big( \big[ \partial_{x^a} \delta_{ik} + \epsilon_{ijk} A^j_a(x) \big] \delta(x, e(t)) \Big) \Big( X^k_e(t) f_{\gamma} \Big) \\ &= -\mathrm{i} \hbar \kappa \sum_{e \in E(\gamma)} \int \mathrm{d}^3x \, \Lambda^i(x) \\ &\int_0^1 \mathrm{d}t \Big( \Big[ -\frac{\mathrm{d}}{\mathrm{d}t} \delta_{ik} + \epsilon_{ijk} \dot{e}^a(t) A^j_a(x) \Big] \delta(x, e(t)) \Big) \Big( X^k_e(t) f_{\gamma} \Big) \end{split}$$

$$\begin{split} &= -\mathrm{i}\hbar\kappa \left\{ \sum_{e \in E(\gamma)} \int \mathrm{d}^3x \; \Lambda^i(x) \bigg[ -\delta(x,e(1)) X_e^i(1) + \delta(x,e(0)) X_e^i(0) \\ &+ \int_0^1 \mathrm{d}t \; \delta(x,e(t)) \Big( \dot{X}_e^i(t) + \epsilon_{ijk} \, \dot{e}^a(t) \; A_a^j(x) \; X_e^k(t) \Big) \bigg] f_\gamma \right\} \\ &= -\mathrm{i}\hbar\kappa \left\{ \sum_{e \in E(\gamma)} \bigg[ -\Lambda^i(e(1)) \; X_e^i(1) + \Lambda^i(e(0)) \; X_e^i(0) \\ &+ \int_0^1 \mathrm{d}t \; \Lambda^i(e(t)) \Big( \dot{X}_e^i(t) + \epsilon_{ijk} \, \dot{e}^a(t) \; A_a^j(e(t)) \; X_e^k(t) \Big) \bigg] f_\gamma \right\}. \end{split} \tag{3.11}$$

Here we have made use of  $\partial_x \delta(x, y) = -\partial_y \delta(x, y)$  in the third step which holds on spaces of test functions of rapid decrease. But since for smooth connections  $h_e(t, t + \delta t)^{\pm 1} = 1 \pm \dot{e}^a(t) \, \delta t \, A_a(e(t)) + o(\delta t^2)$  we have

$$X_{e}^{i}(t+\delta t) - X_{e}^{i}(t) = \operatorname{tr}(h_{e}(0, t+\delta t)\tau_{i} h_{e}(t+\delta t, 1) \partial_{h_{e}(0,1)}) - X^{i}(t)$$

$$= \operatorname{tr}(h_{e}(0, t) h_{e}(t, t+\delta t) \tau_{i} h_{e}^{-1}(t, t+\delta t) h_{e}(t, 1) \partial_{h_{e}(0,1)}) - X^{i}(t)$$

$$= \delta t \dot{e}^{a}(t) \operatorname{tr}(h_{e}(0, t)[A_{a}(e(t)), \tau_{i}]h_{e}(t, 1) \partial_{h_{e}(0,1)}) + o(\delta t^{2})$$

$$= -\epsilon_{ijk} \delta t \dot{e}^{a}(t) A_{a}^{j}(e(t)) \operatorname{tr}(h_{e}(0, t) \tau_{k} h_{e}(t, 1) \partial_{h_{e}(0,1)}) + o(\delta t^{2})$$

$$= -\epsilon_{ijk} \delta t \dot{e}^{a}(t) A_{a}^{j}(e(t)) X_{e}^{k}(t) + o(\delta t^{2}). \tag{3.12}$$

This shows that the t integral in (3.11) vanishes identically for smooth connections. Now  $X_e^i(0) = X^i(h_e) =: X_e^i$  where  $X^i(g)$  is the right invariant vector field at  $g \in SU(2)$  and  $X_e^i(1) = -X^i(h_e^{-1})$ . Thus, when splitting each edge into two halves  $e = e_1 \circ e_2^{-1}$  where both  $e_1, e_2$  are outgoing at the vertex different from their intersection point then  $e(1) = e_2(0)$  and the right invariance of X now implies  $X(h_e) = X(h_{e_1}), -X(h_e^{-1}) = X(h_{e_2})$ . Summarizing we find that the quantum Gauss constraint is given by

$$\hat{G}(\Lambda)f_{\gamma} = -i\hbar\kappa \sum_{e \in E(\gamma)} \Lambda^{i}(e(0)) X_{e}^{i} f_{\gamma} = -i\hbar\kappa \sum_{v \in V(\gamma)} \Lambda^{i}(v) X_{v}^{i} f_{\gamma}$$
(3.13)

where  $-iX_v = -i\sum_{e(0)=v} X_e$  is the total 'internal' angular momentum operator. Notice that (3.13) can be extended from smooth to distributional connections and that no assumption on asymptotic behaviour or smoothness of  $\Lambda$  had to be made. The quantum Gauss constraint is obviously a self-adjoint operator on  $\mathcal{H}$  and anomaly free: it is trivial to check that  $[\hat{G}(\Lambda), \hat{G}(\Lambda')] = \hat{G}([\Lambda, \Lambda'])$  precisely mirroring the classical constraint algebra. Moreover, the quantum Gauss law constraint is identically satisfied as  $\gamma$  tends to  $\partial \Sigma$  because  $\Lambda_{|\partial \Sigma} = 0$ , that is, there are no internal charges in general relativity [1]. This allows quantum states of distributional connections to be non-gauge invariant at spatial infinity, a fact that we are going to exploit in the following.

Now let the state  $\xi \in \mathcal{H}_{af}$  be considered as a function  $f_{\gamma}$  cylindrical with respect to a graph  $\gamma$  which is a finite subgraph of the graph on which  $\xi$  depends and which intersects  $\partial \Sigma$ . Because  $\xi \in \mathcal{H}_{af}$  we know that  $f_{\gamma}$  is a finite linear combination of eigenstates of the volume operator  $\hat{V}(R)$  with non-zero eigenvalue for sufficiently small regions R and such that  $R \cap V(\gamma)|_{\partial \Sigma} \neq \emptyset$ . Consider first the volume integral in (3.10). Setting  $\Lambda(y) = \chi_{\epsilon}(x, y)$  there is an obvious quantization for the term proportional to  $G_i$  in view of (3.13). However,

for the remainder we have, again on functions of smooth connections only to begin with

$$\begin{split} \epsilon_{ijk} \int_{\Sigma} \mathrm{d}^{3}y \, \chi_{\epsilon}(x, y) \, A_{a}^{j}(y) \, \hat{E}_{k}^{a}(y) \, f_{\gamma} \\ &= -\mathrm{i}\hbar \kappa \epsilon_{ijk} \sum_{e \in E(\gamma)} \int_{\Sigma} \mathrm{d}^{3}y \, \chi_{\epsilon}(x, y) \, A_{a}^{j}(y) \int_{0}^{1} \mathrm{d}t \, \dot{e}^{a}(t) \, \delta(y, e(t)) \, X_{e}^{k}(t) \, f_{\gamma} \\ &= -\mathrm{i}\hbar \kappa \epsilon_{ijk} \sum_{e \in E(\gamma)} \int_{0}^{1} \mathrm{d}t \, \dot{e}^{a}(t) \, A_{a}^{j}(e(t)) \, \chi_{\epsilon}(x, e(t)) \, X_{e}^{k}(t) \, f_{\gamma} \\ &= 2\mathrm{i}\hbar \kappa \sum_{e \in E(\gamma)} \lim_{n \to \infty} \sum_{k=1}^{n} \chi_{\epsilon}(x, e(t_{k-1})) \, \mathrm{tr}(\tau_{i}[h_{e}(t_{k-1}, t_{k}) - 1]) X_{e}^{i}(t_{k-1}) \, f_{\gamma}. \end{split} \tag{3.14}$$

Now recall that  $x \in \partial \Sigma$  and that  $\gamma \subset B(\partial \Sigma)$ . Pick a particular edge e in (3.14). Then for sufficiently small  $\epsilon$  the corresponding term either vanishes or e(0) = x and the term becomes  $\operatorname{tr}(\tau_i[h_e(0,t(\epsilon))-1])X_e^if_\gamma + \operatorname{o}(\epsilon^2)$  where  $t(\epsilon)$  is the largest value of t such that  $\chi_\epsilon(x,e(t))=1$ . Now for a classical, smooth connection which approaches infinity as  $1/r^2$  the term  $h_e(0,t(\epsilon))-1$  is at most of order  $\epsilon/r$  (the 'length' of  $e(\epsilon)$  is at most of order r) and so vanishes even at finite  $\epsilon$  because  $x\to\partial\Sigma$ . Therefore expression (3.14) vanishes and the volume integral contribution of  $\hat E_{ADM}$  becomes

$$\int_{\Sigma} d^3 y \, \chi_{\epsilon}(x, y) \, \partial_a \hat{E}_i^a(y) \, f_{\gamma} = -i\hbar \kappa \sum_{v \in V(\gamma)} \chi_{\epsilon}(x, v) \, X_v^i f_{\gamma}$$
(3.15)

which one can extend to non-smooth connections.

We turn to the surface integral of (3.10) and write  $f_{\gamma,v} = X_v^i f_{\gamma}$ . We have, ordering the  $1/\hat{V}(x,\epsilon)$  to the left

$$\int_{\partial \Sigma} \chi_{\epsilon}(x, v) \, dS_{a} \frac{1}{\hat{V}(x, \epsilon)} \hat{E}_{i}^{a} f_{\gamma, v} = -i\hbar \kappa \sum_{e \in E(\gamma)} \int_{0}^{1} dt \, \dot{e}^{a}(t) 
\times \int_{\partial \Sigma} dS_{a}(x) \, \delta(x, e(t)) \frac{\chi_{\epsilon}(x, v)}{\hat{V}(x, \epsilon)} X_{e}^{i}(t) f_{\gamma, v} 
= -i\hbar \kappa \sum_{e \in E(\gamma), e(0) \in \partial \Sigma} \operatorname{sgn}(\partial \Sigma, e) \frac{\chi_{\epsilon}(e(0), v)}{\hat{V}(e(0), \epsilon)} X_{e}^{i} f_{\gamma, v} 
= i\hbar \kappa \sum_{e \in E(\gamma), e(0) \in \partial \Sigma, e \notin \partial \Sigma} \frac{\chi_{\epsilon}(e(0), v)}{\hat{V}(e(0), \epsilon)} X_{e}^{i} f_{\gamma, v}$$
(3.16)

where  $\operatorname{sgn}(S, e)$  is the sign of the intersection of e with the surface S (which is outward oriented) at e(0) which is thus -1 because all edges e are outgoing from a vertex e(0) and, because of  $\gamma \subset B(\partial \Sigma)$ , they are thus running away from  $\partial \Sigma$  (there is no contribution from edges that run inside  $\partial \Sigma$  because  $\operatorname{sgn}(\partial \Sigma, e)_{|e(t)} = 0$  for all t as was shown in [26]). Thus, only edges which run transversally into  $\partial \Sigma$  contribute to the sum in (3.16).

We can take now the limit  $\epsilon \to 0$ . Notice that for small enough  $\epsilon$  we have  $\chi_{\epsilon}(e(0),v)=1$  as  $\epsilon \to 0$  provided that e(0)=v is a vertex of  $\gamma$ . Moreover, for small enough  $\epsilon$ , v is the only vertex of  $\gamma$  in the  $\epsilon$  box around v. Thus, we may replace  $\hat{V}(v,\epsilon)$  by  $\hat{V}_v$  interpreting the operator  $1/\hat{V}_v$  by its spectral resolution. Now the only critical point is whether the two operators  $X_e^i$ ,  $X_v^i$  that are to the right of  $1/\hat{V}_v$  will leave the crucial property of  $f_\gamma$  intact, namely, that  $f_\gamma = \sum_{i=1}^N f_i$  with  $\hat{V}_v f_i = \lambda_i f_i$ ,  $\lambda_i \neq 0$ . But this is easily seen to be the case provided we impose the following additional restriction on  $\mathcal{H}_{af}$ :

Tangle property. An asymptotically flat state is a linear combination of diffeomorphism group-averaged elements of the kinematical Hilbert space  $\mathcal{H}_{af}$  each of which depends on an (infinite) graph  $\gamma$  all of whose intersections with  $\partial \Sigma$  are transversal, that is, there are no edges of  $\gamma$  which lie inside  $\partial \Sigma$ . Thus, any path along  $\gamma$  between two distinct points of  $\gamma \cap \partial \Sigma$  is a generalized tangle [27], that is, a piecewise analytic path intersecting  $\partial \Sigma$  transversally and points of non-analyticity are vertices of  $\gamma$ , equivalently, intersections of tangles. The subspace of  $\mathcal{H}_{af}$  having the tangle property will be called  $\mathcal{H}_{tangle}$ .

The tangle property is a rather natural assumption about states  $\xi$  because curves of non-zero parameter length running in  $\partial \Sigma$  themselves between vertices automatically have infinite length with respect to  $\delta_{ab}$ . This is not the case for curves between vertices which just approach  $\partial \Sigma$  but otherwise lie in the interior.

Under this additional assumption, we have in the limit  $\epsilon \to 0$ , putting (3.13), (3.16) and the remaining pre-factor of  $-2/\kappa$  from (3.10) together

$$\hat{E}_{ADM}(S)f_{\gamma} = -2\hbar^{2}\kappa \sum_{v \in \partial \Sigma \cup V(\gamma)} \frac{1}{\hat{V}_{v}} X_{v}^{i} X_{v}^{i} f_{\gamma}. \tag{3.17}$$

But recognizing  $-\mathrm{i} X_v = \hat{J}_v$  as the total angular momentum of  $f_\gamma$  at v we finally find

$$\hat{E}_{ADM} f_{\gamma} = 2\hbar^2 \kappa \sum_{v \in \partial \Sigma \cup V(\gamma)} \frac{1}{\hat{V}_v} \hat{J}_v^i \hat{J}_v^i f_{\gamma}. \tag{3.18}$$

Expression (3.18) defines a self-consistent family of operators  $\{\hat{E}_{ADM,\gamma}\}$  of operators which can be extended to infinite graphs and thus to  $\mathcal{H}_{tangle}$  provided that the number of punctures of  $\gamma$  with  $\partial \Sigma$  is finite. This defines the domain of  $\hat{E}_{ADM}$ .

A number of remarks are in order.

- The operator  $\hat{J}_v^i$  is the infinitesimal generator of gauge transformations at v and therefore commutes with  $\hat{V}_v$  because the volume operator is gauge invariant proving that (3.18) is densely defined on the restricted state space. If we would not require the tangle property then while the volume integral in (3.10) gives essentially  $X_v$ , the surface integral does not, rather it gives  $X_v' = X_v \sum_{e(0)=v,e\subset\partial\Sigma} X_v$  which does not commute with  $\hat{V}_v$  and so may map  $f_\gamma$  into a linear combination of states some of which may acquire zero volume and so (3.18) would blow up. Thus, the tangle property is *sufficient* for  $\hat{E}_{ADM}$  to be a densely defined operator. Although we do not have a proof, it is almost granted that  $X_v' f_\gamma$  will contain zero-volume eigenstates in its expansion and so the tangle property would also be *necessary*!
- As a striking bonus of the tangle property we easily see that (3.18) indeed defines a positive-semidefinite self-adjoint operator on the Hilbert space  $\mathcal{H}_{tangle}$ : first of all, since the volume operator and the  $X_v^i$  are defined in terms of the operators  $X_e^i$  it follows that the family of operators (3.18) is consistently defined because the  $X_e^i$  are. Next, since  $[X_v^i, \hat{V}_v] = 0$  we see that we may order (3.18) symmetrically involving only terms of the form  $\hat{J}_v^i(1/\hat{V}_v)\hat{J}_v^i$  and so (3.18) defines a symmetric operator because it leaves the graph  $\gamma$  invariant [5–7]. Finally, the Laplacian  $-\Delta_v := J_v^i J_v^i$  has non-negative discrete spectrum  $j_v(j_v+1)$  where  $j_v$  is the spin of the contractor of the generalized (non-gauge-invariant) spin-network states into which  $f_\gamma$  can be decomposed. Moreover, since  $-\Delta_v$  and  $\hat{V}_v$  commute, they can be simultaneously diagonalized. Thus, if  $\lambda_v$  is the eigenvalue of the volume operator then the simultaneous eigenstate  $f_\gamma$  is an eigenstate of the ADM energy with eigenvalue  $\sum_v j_v(j_v+1)/\lambda_v$ . This provides an explicit diagonalization of  $\hat{E}_{ADM}$  on  $\mathcal{H}_{tangle}$  and demonstrates that it is a self-adjoint operator on  $\mathcal{H}_{tangle}$ . Now,

since states in  $\mathcal{H}_{tangle}$  are not diffeomorphism averaged at spatial infinity the part of the graph which is responsible for the spectrum of the ADM energy is untouched by the diffeomorphism-group averaging. Next, the map  $\hat{\eta}$  that makes a diffeomorphism-invariant state a solution of the Hamiltonian constraint is a generalized projector at each vertex of the graph separately [13–15, 19]. Therefore, it is the identity map at those vertices of  $\gamma$  that lie in  $\partial \Sigma$  because for a gauge transformation  $N \to \partial \Sigma$  the action of the constraint at those vertices is trivially zero. Thus the part of the state responsible for the spectrum and the adjointness relations of  $\hat{E}_{ADM}$  is unchanged by the map  $\hat{\eta}$  and is thus preserved when we go to the physical Hilbert space  $\mathcal{H}_{phys} = \hat{\eta} \mathcal{H}_{tangle}$ . Moreover, the spectrum is entirely discrete and non-negative, thus we have proved a quantum positivity energy theorem!

• Astonishingly, the proof of this theorem turned out to be surprisingly simple: the proof of the classical positivity theorem is much more complicated and uses the boundary conditions and the Einstein equations at various stages. Why did we not need (a quantum analogue of) these assumptions? The answer is that we actually did use them: we used them in the definition of an asymptotically flat state, in particular, that the volume of the state be non-vanishing and that it be a solution of the quantum Einstein equations. Since the energy functional is really given by  $E(N) = H(N) + E_{ADM}(N)$  where the Hamiltonian constraint only vanishes on a solution, likewise the ADM energy operator  $\hat{E}_{ADM}$  only represents energy if we apply it to a solution  $\Psi$  of  $\hat{H}'(N)\Psi=0$ . Here we have written the dual  $\hat{H}'(N)$  on  $\Phi'$  of  $\hat{H}(N)$  because, as stated above, solutions  $\Psi$  actually lie in  $\Phi'$  [10, 15]. Finally, we used a regularization of the operator consisting (i) of the restriction of the space of states to functions of classical connections (this means here that they are smooth and decay at infinity as  $1/r^2$ ) and then (ii) in the extension of the expression for the operator obtained to all of  $\bar{A}$ . In the derivation of the operator we made crucial use of the fact that a classical connection decays at infinity.

Now a subtle issue is the following: by definition a solution  $\Psi$  satisfies  $H'(N)\Psi=0$  for any N which vanishes at  $\partial \Sigma$ . But how about lapse functions N that approach a constant value at  $\partial \Sigma$ ? It is now not a consequence of the formalism any longer that  $\hat{H}'(N)\Psi=0$  should hold, very much like in the case of the Gauss constraint. The only guideline of what to do is the classical theory and there it is indeed true that on classical solutions  $(A_0, E_0)$  to the Einstein equations E(N) just equals  $E_{ADM}(N)_{A=A_0, E=E_0}$  so that we will require that  $\hat{H}'(N)\Psi=0$  even for asymptotically constant lapse.

Now, by definition the operator  $\hat{\eta}$  acts like the identity operator at  $\partial \Sigma$ . Therefore we conclude that any physical state has the property that it is annihilated by  $\hat{H}'(N)$  even for N= constant and, moreover, it is a linear combination of eigenstates with non-zero eigenvalue of the volume operator  $\hat{V}_v$  for each vertex of the graph  $\gamma$  on which  $\xi$  depends (with  $\hat{\eta}\xi=\Psi$ ) such that  $v\in\partial \Sigma$ . One might suspect that the number of states that satisfy this condition is rather tiny but the opposite is the case: the volume operator has the particular property that it does not change the graph or the labelling of that graph with spin quantum numbers. Now there exist an infinite number of states which are annihilated by  $\hat{H}'(N)$  just because the graph or its labellings are of a particular type (see [15] where such states were labelled by 'spin-webs', more precisely, 'sources' of spin-webs) and so one can construct eigenstates of the volume operator of such states while they are still annihilated by  $\hat{H}'(N)$ . As an aside, this might shed some light on the issue of how to interpret those special solutions of the Hamiltonian constraint.

These remarks are sufficient to show that then  $\hat{E}'_{ADM}(N) = \hat{E}_{ADM}(N)$ .

The fact that the ADM energy operator is essentially diagonal on spin-network states
can be interpreted as saying that the spin-network representation is the nonlinear Fock

representation of quantum general relativity. Namely, if we compare the spin that the edges of a spin-network carry with the occupation number of momentum modes of, say, the free Maxwell field then we may interpret this spin essentially as the occupation number of a gravitational mode which is not labelled by a momentum but by an edge.

Notice that each vertex of  $\gamma$  which lies in  $\partial \Sigma$  must be at least 3-valent (not 4-valent because the function does not need to be gauge invariant at infinity) in order that it can have non-vanishing volume. Also notice that the gravitational energy is quantized in quanta of the Planck mass: the eigenvalues of the volume operator are multiples of  $\ell_p^3$  so the eigenvalues of energy, according to (3.18) are multiples of  $\hbar^2 \kappa / \ell_p^3 = \sqrt{\hbar/\kappa} = m_p$ . Notice, however, that the spectrum does *not* just consist of integers times  $m_p$ : in fact, we can arrange, by appropriate choice of the spins of the edges that meet at spatial infinity in a vertex, that the volume operator assigns arbitrarily high volume to that vertex, while we can choose the total (non-vanishing) spin of that vertex to be as low as we wish, for instance,  $\frac{1}{2}$ . This follows from simple Clebsh–Gordan theory. Thus, while the spectrum is discrete, the value 0 is certainly an accumulation point. This is important because we expect that in a low-energy approximation the theory correctly describes scattering of low-frequency gravitons. The fact that the spectrum contains such quanta is a first hint (although no proof) that the theory might have the expected low-energy (large-distance) limit.

On the other hand, the spectrum is certainly unbounded from above because we may have an arbitrary number of vertices at spatial infinity. Even the 'spectrum per vertex', is unbounded: we can choose the spins of vertices meeting at a vertex of given valence n to add up to highest weight  $J = j_1 + \cdots + j_n$  and we can choose them to be equal  $j_i = j$ . The volume eigenvalue then is bounded from above by  $k(n)j^{3/2}$  where k(n) is some constant depending on the valence of n while the total spin squared is bounded from below by  $n^2j^2$  so that for any fixed n the asymptotic behaviour is  $\propto j^{1/2}$ .

- For a classical connection every function at  $\partial \Sigma$  is gauge invariant because it decays like  $1/r^2$  which results in a holonomy of order  $\exp(i/r) \to 1$ , i.e. a trivial holonomy. In quantum theory this is lifted by the distributional nature of a connection, smooth connections are assigned zero volume by the Ashtekar–Lewandowski measure in the space of distributional connections and are unimportant.
- Gauge-invariant states at  $\partial \Sigma$  correspond to vanishing energy eigenvalue. Thus, energy seems to sit at non-gauge-invariant vertices. We may interpret this observation as follows: the gravitational energy in a state labelled by an (infinite) graph  $\gamma$  is concentrated at the vertices of  $\gamma$ , and energy flows from vertex to vertex along the edges of  $\gamma$  in quantized packages labelled by the spin of those edges. Non-zero energy at a vertex corresponds to lack of gauge invariance at this vertex meaning that the spins that flow out or into a vertex do not add up to zero. Now in the interior of  $\Sigma$  the quantum Gauss constraint requires that all spins add up to zero. We interpret this as the connection dynamics version of the geometrodynamics result that there is no energy location in general relativity in the interior of  $\Sigma$ , gravitational energy can be gauged away locally, it is pure gauge. However, while it can be pushed around at one's will, one cannot entirely delete it, one can push it all the way to spatial infinity where it eventually shows up in the form of a non-zero net spin flow at the vertices of  $\gamma$  at  $\partial \Sigma$ .
- The fact that (representations of) the SU(2) gauge group of general relativity should play an essential role in the energy is very unexpected from a geometrodynamics point of view where one never even talks about the SU(2) gauge freedom. Even the classical ADM expression  $\int_{\partial \Sigma} dS_a \, (q_{ab,b} q_{bb,a})$  is manifestly gauge invariant, so how did the

SU(2) gauge group enter the stage†? The answer is the following: notice that while the classical ADM expression is manifestly gauge invariant, it is not at all covariant; the derivatives that appear in  $\int_{\partial \Sigma} dS_a (q_{ab,b} - q_{bb,a})$  are not covariant derivatives (in fact, if they were covariant derivatives then the energy would vanish identically). This does not need to concern us because at  $\partial \Sigma$  the diffeomorphisms that underlie the diffeomorphism constraint must die off. Now as we showed in (3.2), when writing  $\int_{\partial \Sigma} dS_a (q_{ab,b} - q_{bb,a})$  in terms of  $E_i^a$  this lack of 3-diffeomorphism covariance, by means of the boundary conditions, gets translated into non-gauge invariance, while installing covariance because in (3.2) a correction term drops out due to the boundary conditions which explains why one and the same function can be written in a manifestly gauge invariant or diffeomorphism covariant way but not both. Indeed, the expression  $-2\int_{\partial\Sigma} dS_a E_i^a \partial_b E_i^b / \sqrt{\det(q)}$  is manifestly 3-diffeomorphism covariant but it fails to be gauge invariant. This is not unexpected: after all the triad formulation reduces the local diffeomorphism gauge freedom to local rotation freedom. In conclusion, the fact that states with non-zero energy are not gauge invariant is in fact very natural, the more so as gauge transformations at spatial infinity are not allowed as follows from the classical theory [1] so that any manifestly gauge-invariant function is in fact gauge invariant.

- Another function for which SU(2) gauge transformations and diffeomorphisms get mixed up is the classical vector constraint  $V_a = \text{tr}(F_{ab}E^b)$ . Strictly speaking this constraint function does not generate diffeomorphisms but only on gauge-invariant functions.
- Notice that although  $-2 \int_{\partial \Sigma} dS_a \, E_i^a \, \partial_b E_i^b / \sqrt{\det(q)}$  is not gauge invariant the quantum expression (3.18) in fact is. The reason why that is possible lies in the structure of quantum theory: in the classical theory we only have functions on phase space. In quantum theory those functions get translated into operators on a Hilbert space, but values of those functions really correspond to expectation values. Thus non-gauge-invariant functions correspond to expectation values of either a gauge-invariant operator in a non-gauge-invariant state or vice versa. The quantization (3.18) picks the latter possibility.
- In principle, we have now solved the 'problem of time': since we have a true Hamiltonian we can introduce the *Schrödinger time parameter t* and our state vectors  $\Psi \in \Phi'$ , being distributions which are invariant under asymptotically identity diffeomorphisms, are supposed to satisfy the *non-stationary Schrödinger equation*

$$\hat{E}_{ADM}(N=1)\Psi = -i\hbar \partial_t \Psi. \tag{3.19}$$

Notice that, as we showed above, the ADM energy operator is its own dual so that (3.19) makes sense.

• In the next section the operator (3.18) will be shown to commute with all quantum constraints of general relativity and it is therefore a *strong quantum Dirac observable* for quantum gravity in the strict sense of the word. This is not unexpected because it is built purely from momentum operators.

<sup>†</sup> This question actually arises already in connection with the spectrum of the geometrical operators volume, area and length [17, 28–32], however, since irreducible representations also carry gauge-invariant information the fact that these operators have a spectrum which is determined by spin-quantum numbers of *gauge-invariant states* is maybe not that surprising. What *is* surprising for the energy operator is that it is the spins of non-gauge-invariant states which determine the spectrum.

## 4. The Poincaré algebra

We now wish to define the rest of the quantum generators of the little group of the asymptotic Poincaré group and check whether their algebra is anomalous or not<sup>†</sup>. This is enough to construct particle states since the irreducible unitary representations of the little group induce a unique unitary irreducible representation of the full Poincaré group. So far we have not constructed an operator corresponding to a boost generator which is more difficult to obtain than the ADM energy operator.

First of all we must clarify on which space to represent the Poincaré group (respectively its generators). To that end it is helpful to remember how the classical Poincaré generators are realized as a subalgebra of the Poisson algebra [21, 22].

Let H(N), V(N) be the Hamiltonian and diffeomorphism constraint functional, respectively. Both functionals are integrals over  $\Sigma$  of local densities and both converge and are functionally differentiable only if the lapse and shift functions N,  $\vec{N}$  vanish at  $\partial \Sigma$ . In order to be able to describe the Poincaré group corresponding to the asymptotically constant or even diverging functions ( $x^a$  is a Cartesian frame at spatial infinity)  $N = a + \chi_a x^a$ ,  $N^a = a^a + \epsilon^{abc} \phi_b x^c$  where  $(a, a^a)$  is a 4-translation,  $\phi^a$  are rotation angles and  $\chi^a$  are boost parameters, one proceeds as follows: let S be a bounded 2-surface that is topologically a sphere and let B(S) be the (intersection of  $\Sigma$  with the) closed ball such that  $\partial B(S) = S$ . For each S one defines  $E(N,S) := H(N,S) + E_{ADM}(N,S) + B(N,S)$ ,  $P(N,S) := V(\vec{N},S) + P_{ADM}(N,S)$  where the parameter S means that volume integrals are restricted to B(S) only (a classical regularization of the divergent integrals) and the 'counter-terms'  $E_{ADM}(N,S)$ ,  $E_{ADM}(N,S)$ ,  $E_{ADM}(N,S)$  are the surface integrals defined in [21] and correspond to ADM energy, boost and momentum. One can show that  $\lim_{S\to\partial\Sigma} E(N,S)$ ,  $\lim_{S\to\partial\Sigma} P(\vec{N},S)$  exist. Moreover, for each finite  $E_{ADM}(N,S)$  are functionally differentiable so that it is meaningful to compute the Poisson brackets

$$\begin{aligned}
\{E(M, S), E(M, S)\} &= P(q^{ab}(MN_{,b} - M_{,b}N), S) \\
\{E(M, S), P(\vec{N}, S)\} &= E(\mathcal{L}_{\vec{N}}M, S) \\
\{P(\vec{M}, S), P(\vec{N}, S)\} &= P(\mathcal{L}_{\vec{M}}\vec{N}, S).
\end{aligned} \tag{4.1}$$

The crucial point is that one computes the Poisson brackets (i) at finite S and (ii) on the full phase space and then takes the limit  $S \to \partial \Sigma$  or restricts to the constraint surface of the phase space (where  $H(N,S) = V(\vec{N},S) = 0$ ). Notice that the numerical value of, say, E(N,S) equals H(N,S) for a gauge transformation for which  $N \to 0$  as  $S \to \partial \Sigma$ . On the other hand, on the constraint surface for a symmetry for which  $N \to 0$  as  $S \to \partial \Sigma$  it equals a time translation or a boost, respectively. A similar remark holds for  $P(\vec{N},S)$ . One therefore interprets (4.1) as follows: if M,N are both pure gauge then the constraint algebra closes. If M is a symmetry and N pure gauge then energy (or boost generator) are gauge invariant. If M,N are both symmetry then time translations commute with each other, time translations and boosts give a spatial translation and a boost with a boost gives a rotation, in other words the symmetry algebra closes.

† By little group of the Poincaré group we mean the group generated by the 4-translations and the little subgroup of the connected component of the Lorentz group. The latter, as is well known, is the stabilizator subgroup of the Lorentz group associated with a standard 4-vector  $\bar{s}$ . In the massive case  $\bar{s}^2 > 0$  the standard vector is associated with the spin of the particle in the rest frame and the covering group of the stabilizator group is given by SU(2). In the massless case the standard vector is associated with the helicity of the particle (spin in the momentum direction) and the covering group of the stabilizator group is given by U(1), physically important representations being 2-valued. Thus, the rotations at spatial infinity determine the unitary irreducible representation of the particle state in question.

In quantum theory we will therefore proceed as follows. Recall [13–15, 19] that the Hamiltonian constraint  $\hat{H}(N)$  (for asymptotically vanishing N) is only well defined on the subspace of  $\Phi'$  corresponding to distributions on  $\Phi$  which are invariant under diffeomorphisms that approach identity at  $\partial \Sigma$ . Thus we can expect the symmetry algebra to hold only on such distributions as well. In fact, we will just choose  $\Psi$  to be a solution to all constraints.

Next, in view of the fact that even the classical symmetry algebra only holds provided one first computes Poisson brackets at finite S and then takes the limit, we will check the quantum algebra first by evaluating  $\Psi$  on  $\hat{E}(N_S)$   $f_S$  for functions  $f_S \in \Phi$  which are cylindrical with respect to a graph which lies in the interior of B(S) (it may intersect S in such a way that the volume operator does not vanish at the intersection point for none of the eigenvectors into which  $f_S$  may be decomposed) and lapse functions  $N_S$  which grow at infinity like symmetries but which are supported in  $B(S) \cup S$  including S, and then to take the limit  $S \to \partial \Sigma$  (the support fills all of  $\Sigma$  as  $S \to \partial \Sigma$  in this process).

We come to the definition of  $\hat{E}(N)$  and  $\hat{P}(\vec{N})$ . First we treat the spatial Euclidean group. The unitary representation of the diffeomorphism group defined by  $\hat{U}(\varphi)f_{\gamma} = f_{\varphi(\gamma)}$  which was for matters of solving the diffeomorphism constraint so far only defined for diffeomorphisms that approach the identity asymptotically, can easily be extended to 3-diffeomorphisms which correspond to asymptotic spatial translations or rotations. Instead of defining the generator  $\hat{P}(\vec{N})$  though (which does not exist on  $\mathcal{H}[10]$ ) we content ourselves with the exponentiated version  $\hat{U}(\varphi(\vec{N}))$  where  $\varphi(\vec{N})$  is the diffeomorphism generated by the six-parameter shift vector field  $N^a = a^a + \epsilon_{abc}\phi^b x^c$  for some Cartesian frame  $x^a$  possibly corrected by an asymptotically vanishing vector field corresponding to a gauge transformation. It is trivial to check that

$$\hat{U}(\varphi(\vec{N}))\,\hat{U}(\varphi(\vec{N}'))\,\hat{U}(\varphi(\vec{N}))^{-1}\,\hat{U}(\varphi(\vec{N}'))^{-1} = \hat{U}(\varphi(\mathcal{L}_{\vec{N}}\vec{N}')) \tag{4.2}$$

where  $\mathcal{L}$  denotes the Lie derivative so that there are no anomalies coming from the spatial Euclidean group. This expression was derived by applying it to any function  $f_S$  cylindrical with respect to a graph with support in B(S).

We now turn to the time translations. As already mentioned we will not consider boosts in this paper so that  $\chi_a \equiv 0$  in the four parameter family of lapse functions  $N = a + \chi_a x^a$  (modulo a correction which vanishes at  $\partial \Sigma$ ). Define the operator on  $\mathcal{H}$ 

$$\hat{E}(N) := \hat{H}(N) + \hat{E}_{ADM}(N) \tag{4.3}$$

where  $\hat{H}(N)$  is the Lorentzian Hamiltonian constraint. Notice that  $\hat{E}(N)$  just as the Hamiltonian constraint in [13–15, 19] carries a certain prescription dependence which is removed by evaluating its dual on  $\Phi_{Diff}$ . We will not repeat these details here and refrain from indicating this prescription dependence in (4.3), however, the prescription dependence has consequences for the commutator algebra that we will discuss below in great detail.

Let us verify the commutators between the time translations among themselves and between time translations and spatial translations and rotations. We have

$$\Psi([\hat{E}(M), \hat{E}(N)]f_{\gamma}) = \Psi([\hat{H}(M), \hat{H}(N)]f_{\gamma}) + \Psi([\hat{E}_{ADM}(M), \hat{E}_{ADM}(N)]f_{\gamma}) 
+ \Psi(\{[\hat{E}_{ADM}(M), \hat{H}(N)] + [\hat{H}(M), \hat{E}_{ADM}(N)]\}f_{\gamma}).$$
(4.4)

The first term vanishes for the same reason as in [13–15, 19] although one needs one additional argument: the Hamiltonian constraint does not act at vertices that it creates. Therefore, it can be written as a double sum over vertices v, v' of  $\gamma$  alone and each of these terms is of the form

$$(M(v) N(v') - M(v') N(v)) \Psi([\hat{H}_{v',\gamma(v)} \hat{H}_{v,\gamma} - \hat{H}_{v,\gamma(v')} \hat{H}_{v',\gamma}] f_{\gamma})$$

where the notation means that  $\hat{H}_{v,\gamma}$  is a family of consistently defined operators each of which acting on cylindrical functions which depend on the graph  $\gamma$  and  $\gamma(v)$  is a graph on which  $\hat{H}_{v,\gamma} f_{\gamma}$  depends. This expression is clearly non-vanishing only if  $v \neq v'$  but then it can be shown that the operators  $\hat{H}_{v,\dots}$  and  $\hat{H}_{v',\dots}$  actually commute. Now this still does not show that the term above vanishes, however, it can be shown that  $\hat{H}_{v',\gamma(v)}\hat{H}_{v,\gamma}f_{\gamma}$ and  $\hat{H}_{v,\gamma(v')}\hat{H}_{v',\gamma}f_{\gamma}$  are related by a diffeomorphism [14]. Now in [14] that was enough to show that the commutator vanishes because we were dealing there only with vertices which do not intersect S as otherwise both lapse functions vanish identically for a pure gauge transformation. Thus the diffeomorphism that relates the two terms above could be chosen to have a support inside B(S) and  $\Psi$  is invariant under such diffeomorphisms. In the present context that does not need to be true. However, the crucial point is now that by the tangle property all edges of  $\gamma$  that intersect S must intersect S transversally. Therefore the arcs that the Hamiltonian constraint attaches to  $\nu$  and whose position is the only thing by which the two above vectors differ lie inside B(S) and do not intersect S. Therefore, again the two vectors are related by a diffeomorphism which has support inside B(S), that is, they are related by a gauge transformation and therefore the commutator vanishes.

We turn to the second term in (4.4). Now we obtain a double sum over vertices of  $\gamma$  which lie in S and each term is of the form

$$(M(v) N(v') - M(v') N(v)) \Psi([\hat{E}_{v',ADM}, \hat{E}_{v,ADM}] f_{\gamma})$$

which is significantly simpler than before because  $\hat{E}_{v,ADM}$  does not alter the graph. Notice that the commutator makes sense because  $\hat{E}_{ADM,v}$  leaves the span of non-zero volume eigenvectors invariant. Now for  $v \neq v'$  the commutator vanishes trivially, this time without employing diffeomorphism invariance of  $\Psi$ .

Finally the last term in (4.4) is a double sum over vertices v, v' of  $\gamma$ , where v must lie in S, of the form

$$(M(v) N(v') - M(v') N(v)) \Psi([\hat{H}_{v',\gamma}, \hat{E}_{v,ADM}] f_{\gamma}). \tag{4.5}$$

The fact that  $\hat{E}_{ADM}$  does not alter the graph was used to write (4.5) as a commutator without employing diffeomorphism invariance of  $\Psi$ . Now it may happen that, although  $f_{\gamma}$  is in the domain of  $\hat{E}_{v,ADM}$ , that  $\hat{H}_{v,\gamma}f_{\gamma}$  is not any longer in the domain and so (4.5), for v=v', is in danger of being a meaningless product of something that blows up times zero while that cannot happen for  $v \neq v'$ . However, since  $\Psi$  is a solution we conclude first of all that (4.5) equals

$$-(M(v) N(v') - M(v') N(v))[\hat{E}_{v,ADM}\Psi](\hat{H}_{v',\gamma}f_{\gamma})$$
(4.6)

and since  $\Psi$  is also in the domain of  $\hat{E}_{ADM}$  both  $\hat{E}_{v,ADM}\Psi$  and  $\hat{H}_{v',\gamma}f_{\gamma}$  are well defined elements of  $\Phi'$  and  $\Phi$ , respectively, we conclude that in case v=v' equation (4.5) does indeed vanish. On the other hand, the same argument as before shows that the commutator trivially vanishes for  $v\neq v'$ .

Let us now check the commutator between time translations and spatial translations and rotations  $\varphi$ . We have

$$\Psi([\hat{U}(\varphi)^{-1} \hat{E}(N) \hat{U}(\varphi) - \hat{E}(N)] f_{\gamma}) 
= \sum_{v \in V(\gamma)} [N(\varphi(v)) \Psi(\hat{U}(\varphi^{-1}) \hat{H}_{\varphi(v),\varphi(\gamma)} f_{\varphi(\gamma)}) - N(v) \Psi(\hat{H}_{v,\gamma} f_{\gamma})] 
+ \sum_{v \in V(\gamma) \cap S} [N(\varphi(v)) \Psi(\hat{U}(\varphi^{-1}) \hat{E}_{ADM,\varphi(v)} f_{\varphi(\gamma)}) - N(v) \Psi(\hat{H}_{ADM,v} f_{\gamma})].$$
(4.7)

Since  $\hat{E}_{ADM}$  does not change the graph on which a function depends we have identically  $\hat{U}(\varphi^{-1})\hat{E}_{ADM,\varphi(v)}f_{\varphi(v)} = \hat{E}_{ADM,v}f_{\gamma}$ .

Now, as explained in more detail in [14], the operator  $\hat{H}(N)$  depends on a certain prescription of how to attach loops to graphs. Since in the interior of B(S) there is no background metric available, this prescription can only be topological in nature and therefore graphs differing by a diffeomorphism  $\varphi$  are assigned graphs by  $\hat{H}(N)$  which are diffeomorphic by a diffeomorphism  $\varphi'$  which may not coincide with  $\varphi$ . That is, in the interior of B(S),  $\hat{H}(N)$  is only covariant up to a diffeomorphism. On the other hand, since one has the fixed background metric  $\delta_{ab}$  at S one can make  $\hat{H}(N)$  precisely covariant at S, that is, the prescription satisfies  $\varphi_{|S} = \varphi'_{|S}$ . Therefore, with this sense of covariance of  $\hat{H}(N)$  it is true that  $\hat{U}(\varphi^{-1})$   $\hat{H}_{\varphi(v),\varphi(\gamma)}f_{\varphi(\gamma)}$  and  $\hat{H}_{v,\gamma}f_{\gamma}$  differ at most by a diffeomorphism with support in the interior of B(S).

In conclusion we obtain

$$\Psi([\hat{E}(N), \hat{U}(\varphi)]f_{\nu}) = \Psi(\hat{E}(\varphi^{\star}N - N) f_{\nu})$$

which is what we were looking for.

We conclude that the little algebra of the Poincaré algebra is faithfully implemented.

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