



INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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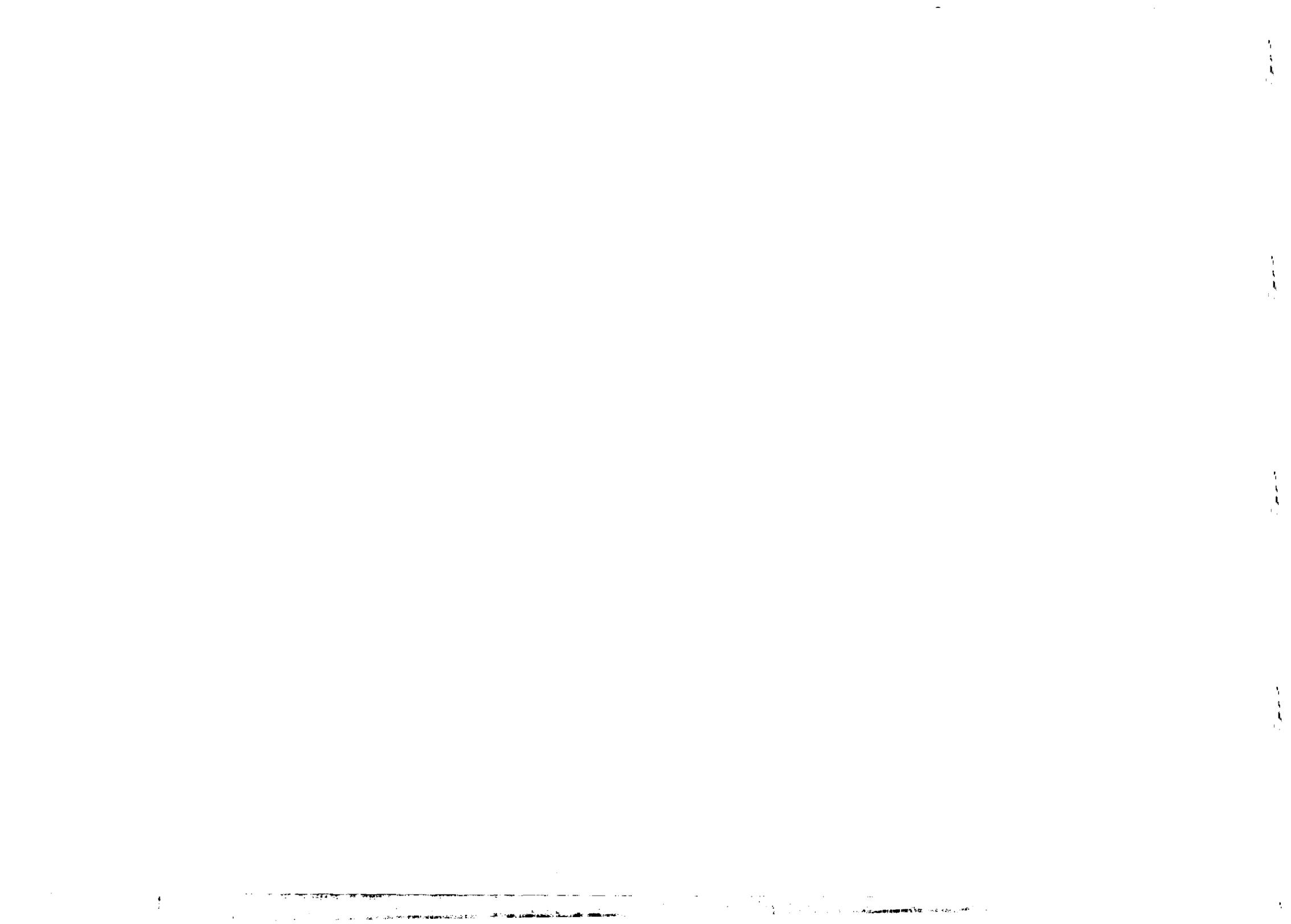


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OPERATOR ORDERING IN QUANTUM MECHANICS AND QUANTUM GRAVITY *

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ABSTRACT

A non-perturbative approach to the quantization of the canonical algebra of pure gravity is presented. The problem of factor ordering of operators in the constraints $\hat{\mathcal{H}}_\mu \psi = 0$ is resolved invoking hermiticity under the invariant inner product in hyperspace - the space of all three-dimensional metrics $g_{ij}(x)$ - and covariance under coordinate transformations. The resulting operators $\hat{\mathcal{H}}_\mu$ receive corrections of order \hbar and \hbar^2 only, and the algebra closes up to a conformal anomaly term. It is argued that, by a convenient choice of gauge, the anomalous term can be removed.

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1. INTRODUCTION

The attempts to quantize Einstein's theory of gravitation are more than fifty years old [1]. Nevertheless, the formulation of the theory was obscured by the existence of constraints among the dynamical variables. A consistent treatment of constrained systems was put forward by Dirac [2] and further developed by Teitelboim [3] and others. Following Dirac's original programme, the weak constraint equations $\mathcal{H}_\mu \approx 0$ ought to become conditions on the physical states of the corresponding quantum theory $\hat{\mathcal{H}}_\mu \psi = 0$. While the consistency of the classical constraints is ensured by the first class algebra obeyed by them

$$[\mathcal{H}_i, \mathcal{H}_j] = -[g^{ij} \mathcal{H}_i + g^{ij} \mathcal{H}_j] \delta_{,j}(x, \bar{x}) \quad (1.1a)$$

$$[\mathcal{H}_i, \mathcal{H}_j] = \mathcal{H}_j \delta_{,i}(x, \bar{x}) + \mathcal{H}_i \delta_{,j}(x, \bar{x}) \quad (1.1b)$$

$$[\mathcal{H}_i, \mathcal{H}_i] = \mathcal{H}_i \delta_{,i}(x, \bar{x}) \quad (1.1c)$$

(a tilde under a symbol is used to indicate that the argument of the corresponding function is \bar{x} ; otherwise it is assumed to be x), the realization of the corresponding quantum algebra is obstructed by ordering ambiguities in the operators $\hat{\mathcal{H}}_\mu$. Some authors [4] have come to the conclusion that there exists no hermitian factor ordering that gives a consistent (closed) algebra. Those investigations, however, have been restricted by the implicit assumption that hermiticity is to be defined in terms of the trivial inner product $\int \psi_1^* \psi_2 \overline{\int_x [d^6 g(x)]}$. Here we propose that the inner product should be $\int \psi_1^* \psi_2 \overline{\int_x [\sqrt{|G|} d^6 g]}$ instead, where G is the determinant of $G^{ijkl}(x)$ - the metric in hyperspace [5]. This seems to be a more natural choice in view of the fact that all Lagrangian theories are constructed in terms of generalized co-ordinates, and should therefore be covariant under general co-ordinate transformations. The co-ordinates in this case are the metric components $g_{ij}(x)$. This idea was previously exploited in the context of quantum cosmological models [6] and the present paper extends it to the general case, where no particular symmetry assumptions for the three space are made.

Recently, there has been growing interest in quantum cosmological models mainly in connection with the fate of the singularities of classical general relativity [7]. Statements based on the wave function(al) of the universe are, however, crucially dependent upon the choice of the quantum operator $\hat{\mathcal{H}}_1$ which defines it. It is, therefore, not of merely academic interest to resolve the ordering ambiguities for the quantum operators.

The paper is organized as follows. In Sec.II a resolution of the ordering ambiguity for operators of the form $\frac{1}{2}f(q) p^2$ in one dimension is presented and the extension to several degrees of freedom is discussed. In Sec.III we propose a hermitian ordering for $\hat{\mathcal{H}}_1$ which is naturally induced by the symmetry of hyperspace. In Sec.IV the remaining operators $\hat{\mathcal{H}}_i$ are given and the quantum algebra is presented. Sec.V contains some discussion on the results obtained.

II. QUANTUM MECHANICS

a) One degree of freedom

In writing the quantum-mechanical version of a classical theory it is necessary to invert the limiting process $\hbar \rightarrow 0$, but, as is well known, this problem does not possess a unique solution except in a few very simple cases - e.g. theories without derivative couplings in Cartesian co-ordinates. The problem is, in its simplest form, that there is more than one quantum operator $\hat{F}(\hat{q}, \hat{p})$ that in the limit $\hbar \rightarrow 0$ approaches a given classical function $F(q, p)$ [8]. (Here q, p are the classical co-ordinates and momenta and \hat{q}, \hat{p} are their quantal counterparts.)

Here we suggest a procedure that gives a unique prescription for the quantization of a wide class of theories which is a generalization of a prescription developed in the context of quantum cosmological models [6]. In this paper we shall only consider theories whose Hamiltonians are quadratic in momenta so that their quantum dynamics are given by second order (functional) differential equations.

In order to illustrate the idea, consider the Hamiltonian of a one-dimensional classical system of the form

$$H = H_0(p, q) + V(q) \quad (2.1)$$

where

$$H_0 = \frac{1}{2} f(q) p^2, \quad f(q) > 0$$

$$[q, p] = 1 \quad (2.2)$$

Clearly there are many possible orderings in the quantum theory which could give rise to (2.1) in the limit $\hbar \rightarrow 0$; to mention just a few, take

$$H_0^{(1)} = \frac{1}{2} f(q) p^2 \quad (2.3a)$$

$$H_0^{(2)} = \frac{1}{2} p^2 f(q) \quad (2.3b)$$

$$H_0^{(3)} = \frac{1}{2} p f(q) p \quad (2.3c)$$

$$H_0^{(4)} = \frac{1}{2} f^\alpha(q) p f^{1-2\alpha}(q) p f^\alpha(q), \quad (2.3d)$$

etc. In order to resolve this ambiguity, we first note that the Hamiltonian (2.1) is obtained from the Lagrangian [9]

$$L = \frac{1}{2} f^{-1}(q) \dot{q}^2 - V(q) \quad (2.4)$$

In the Lagrangian we can change the variable q by a new co-ordinate x defined by

$$x = x(q) = \int^q f^{-1/2}(q') dq', \quad \dot{x} = f^{-1/2} \dot{q} \quad (2.5)$$

and we observe that (2.4) now takes the form

$$L = \frac{1}{2} \dot{x}^2 - V(x) \quad (2.6)$$

The change of co-ordinates (2.5) is a point (canonical) transformation and therefore Lagrangian (2.6) describes the same system and contains the same information as (2.4). The Hamiltonian in the new variables is

$$H_0 = \frac{1}{2} p_x^2, \quad p_x = \dot{x} = f^{1/2} p \quad (2.7)$$

This familiar form can be quantized in the standard manner and has no ordering ambiguity. Since the Poisson bracket of x with p_x is one, we take in the Schrödinger representation

$$\hat{x} = x, \quad \hat{p}_x = -i \frac{d}{dx}, \quad (2.8)$$

and the quantum Hamiltonian is just

$$\hat{H}_0 = -\frac{1}{2} \frac{d^2}{dx^2}. \quad (2.9)$$

Now, either by a change of variables in (2.8) from x back to q , or by virtue of Eq.(2.7) we have

$$P_x = -i f^{1/2}(q) \frac{d}{dq} = f^{1/2}(q) \hat{p} \quad (2.10)$$

where

$$\hat{q} = q, \quad \hat{p} = -i \frac{d}{dq}.$$

Thus, the ordering assigned to \hat{H}_0 is naturally selected to be

$$\hat{H}_0 = \frac{1}{2} f^{1/2}(q) \hat{p} f^{1/2}(q) \hat{p}, \quad (2.11)$$

which is different from the more "plausible" ordering in (2.3). It should be stressed that the different choices (2.3), (2.11) give rise to radically different Schrödinger equations and it is therefore an important point to decide which one is the correct choice. In deriving (2.11) we have only assumed invariance of the system under co-ordinate transformations. This is correct classically, since the Lagrangian formalism is constructed using generalized co-ordinates, as well as quantum-mechanically, because (2.10) is a standard change of variables in a differential equation [10]. As a result, the canonical momentum transforms as a covariant vector and the Hamiltonian is the Laplace-Beltrami operator which is a scalar under co-ordinate transformations, as it should be.

There is still the question of hermiticity of \hat{H}_0 to be clarified. But the hermiticity of (2.9) is obviously guaranteed if we define the inner product in the x co-ordinates to be

$$\langle \psi_1 | \psi_2 \rangle = \int \psi_1^*(x) \psi_2(x) dx \quad (2.12)$$

and we require it to be invariant under co-ordinate transformations.

Then, in the q co-ordinates (2.11) is trivially hermitian under the inner product

$$\langle \psi_1 | \psi_2 \rangle = \int \psi_1^*(q) \psi_2(q) f^{-1/2}(q) dq, \quad (2.13)$$

where $f^{1/2}$ is the Jacobian of the transformation $x \rightarrow q$.

b) N degrees of freedom (point particle in curved space)

One can try to generalize the steps of the previous construction for several variables. The programme, however, is a non trivial one because it is impossible to diagonalize the metric everywhere in a generic higher dimensional manifold by a pure co-ordinate transformation.

Consider a mechanical system described by co-ordinates q^a ($a = 1, \dots, N$) and the corresponding momenta $p_a \equiv \frac{\partial L}{\partial \dot{q}^a}$ (where $\dot{q}^a = \frac{dq^a}{d\lambda}$, λ being some affine parameter). The generalization of (2.2) is

$$H_0 = \frac{1}{2} \gamma^{ab}(q) p_a p_b \quad (2.14)$$

with $[q^a, p_b] = \delta^a_b$. Here γ^{ab} is a non-degenerate arbitrary symmetric matrix function of the co-ordinates only. The expression (2.14) also corresponds to the Hamiltonian of a free point particle of unit mass on a manifold with metric γ_{ab} (the inverse of γ^{ab}), and can be derived from the Lagrangian

$$L(q(\lambda), \dot{q}(\lambda)) = \frac{1}{2} \gamma_{ab}(q) \dot{q}^a \dot{q}^b \quad (2.15)$$

so that

$$p_a = \frac{\partial L}{\partial \dot{q}^a} = \gamma_{ab}(q) \dot{q}^b \quad (2.16)$$

(here λ can be identified with the proper time or proper arc length $d\lambda^2 = \gamma_{ab} dq^a dq^b$). The signature of γ will be assumed to be:

$$\underbrace{(+, +, \dots, +)}_t, \underbrace{(-, -, \dots, -)}_s, \quad t + s = N \quad (2.17)$$

One can now try to proceed by analogy with the one-dimensional case and define new co-ordinates $s^A(q)$ such that

$$\gamma_{\alpha\beta} \dot{q}^\alpha \dot{q}^\beta = \eta_{ab} \dot{s}^a \dot{s}^b$$

$$\eta_{ab} = \text{diag}(\underbrace{+1, \dots, +1}_t, \underbrace{-1, \dots, -1}_s) \quad (2.18)$$

Obviously this cannot be done globally unless the manifold is flat. In the flat case - and only then - one can define the canonical momenta conjugate to s^a ,

$$p_a = \frac{\partial L}{\partial \dot{s}^a} = \eta_{ab} \dot{s}^b \quad (2.19)$$

and hence

$$\dot{s}^a = \eta^{ab} p_b$$

where η^{ab} is the inverse of η_{ab} . Then, in a straightforward way the quantum-mechanical counterpart of H_0 is found to be

$$\hat{H}_0 = -\frac{1}{2} \gamma^{\alpha\beta} D_\alpha D_\beta = -\frac{1}{2} \nabla^2, \quad (2.20)$$

where D_α is the covariant derivative on the manifold.

It should be stressed that the generalization of (2.20) to arbitrary spaces requires some extra assumptions. So far we have only required covariance of the Lagrangian formulation. This guideline is, however, insufficient to define uniquely a canonical ordering in a generic curved space. In fact, there are still many possible second order differential operators that reduce to (2.20) in flat space which are not the Laplacian.

One could invoke some principle like "naturalness", or "simplicity", etc. and define by fiat (2.20) as the correct form in an arbitrary manifold, but one should be aware that this does not follow from any principle of classical or quantum theory.

Taking the minimal substitution of ordinary derivatives by covariant derivatives in curved spaces, certainly eliminates the ordering problem: D_α and $\gamma^{\alpha\beta}$ commute. This does not mean, however, that $-iD_\alpha$ should be identified with the canonical momentum conjugate to q^μ : $[q^\mu, iD_\nu] \neq \delta^\mu_\nu$, whereas $[q^\mu, -i\partial_\nu] = \delta^\mu_\nu$.

One important case in which there are compelling reasons to choose the form (2.20) over other alternatives is that of maximally symmetric spaces of the form G/H . Then, besides the reparametrization - or co-ordinate transformation - invariance of the theory there exist the group of isometries of the space and the Laplacian can be written in the form [11]

$$\nabla^2 = \frac{1}{a^2} [c_2(G) - c_2(H)], \quad (2.21)$$

where $c_2(G)$ and $c_2(H)$ are the quadratic Casimir operators of the groups G and H , respectively, and a is some constant that sets the scale. Then the Laplacian choice is required if one wants to guarantee the invariance of the quantum theory under the isometry transformations of the manifold.

The choice of the Laplace-Beltrami operator amounts to selecting the ordering of p 's and q 's to be

$$\hat{H}_0 = -\frac{1}{2} \nabla^2 = \frac{1}{2} \gamma^{-1/2} \hat{p}_a \gamma^{1/2} \gamma^{\alpha\beta} \hat{p}_\beta, \quad \gamma = |\det[\gamma_{\alpha\beta}]| \quad (2.22)$$

where $\hat{p}_\alpha = -i \frac{\partial}{\partial q^\alpha}$. Naturally, the operator \hat{H}_0 is hermitian under the co-ordinate invariant inner product

$$\langle \psi_1 | \psi_2 \rangle = \int \psi_1^*(q) \psi_2(q) \sqrt{\gamma} d^N q. \quad (2.23)$$

It is trivial to check that in one dimension (2.22) and (2.23) reduce to (2.11) and (2.13), respectively. One might want to consider the most general linear combination of monomials constructed out of $\gamma^{\alpha\beta}$ and quadratic in p_α of the form

$$\hat{A} = \gamma^{\alpha\beta} \gamma^a \hat{p}_\alpha \gamma^b \hat{p}_\beta \gamma^c, \quad a + b + c = 0 \quad (2.24a)$$

$$\hat{B} = \gamma^t \hat{p}_\alpha \gamma^f \hat{p}_\beta \gamma^{\alpha\beta} \gamma^h \quad e + f + h = 0 \quad (2.24b)$$

$$\hat{C} = \gamma^k \hat{p}_\alpha \gamma^l \gamma^{\alpha\beta} \hat{p}_\beta \gamma^m \quad k + l + m = 0 \quad (2.24c)$$

$$\hat{D} = \gamma^p \gamma^{\alpha\mu} \hat{p}_\alpha \gamma^q \gamma_{\mu\nu} \hat{p}_\beta \gamma^r \gamma^{\nu\beta} \quad p + q + r = 0 \quad (2.24d)$$

$$\hat{E} = \gamma^t \gamma^{\alpha\mu} \hat{p}_\beta \gamma^u \gamma_{\mu\nu} \hat{p}_\alpha \gamma^v \gamma^{\beta\nu} \quad t + u + v = 0 \quad (2.24e)$$

...

etc., all of which reduce to (2.14) in the limit $\hbar \rightarrow 0$. One can observe that whatever linear combination of these expressions is chosen, the resulting operator has the form

$$\hat{H}_0 = -\frac{1}{2} \left[\gamma^{\mu\nu} \partial_\mu \partial_\nu + B^\mu \partial_\mu + c \right], \quad (2.25)$$

where B^μ is linear in first derivatives of $\gamma_{\mu\nu}$, while c is quadratic in first derivatives and linear in second derivatives of $\gamma_{\mu\nu}$. If one demands \hat{H}_0 to be a scalar it can be shown that $B^\mu = -\gamma^{\alpha\beta} \Gamma_{\alpha\beta}^\mu$ and c is a scalar, which cannot be anything else but the Ricci scalar (up to constants). Thus, the most general form admissible for \hat{H}_0 is

$$\hat{H}_0 = -\frac{1}{2} \nabla^2 + k R. \quad (2.26)$$

III. QUANTUM GRAVITY (infinitely many degrees of freedom)

The natural generalization of (2.14) to infinitely many degrees of freedom is obtained by introducing a set of continuous indices $x = (x^1, \dots, x^N)$. The co-ordinates are now field variables $q_A(x)$, and their canonical conjugate momenta $\pi^B(x)$ satisfy

$$[q_A(x), \pi^B(x')] = \delta_A^B \delta(x, x'). \quad (3.1)$$

We generalize (2.14) in the form

$$H_0 = \frac{1}{2} G_{AB} [q_c] (x, x') \pi^A(x) \pi^B(x'), \quad (3.2)$$

where a sum is understood over repeated indices including the continuous indices x, x' , and G_{AB} is in general a functional of the fields $q_A(x)$.

In gravity, the operator that plays the role of the Hamiltonian is the generator of normal deformations of the three space geometry, \mathcal{H}_\perp [3],[12]

$$\mathcal{H}_\perp = \frac{1}{2} G_{ijkl} \pi^{ij} \pi^{kl} - g^{1/2} R, \quad (3.3)$$

where

$$G_{ijkl} = g^{-1/2} (g_{ik} g_{jl} + g_{il} g_{jk} - g_{ij} g_{kl}), \quad g \equiv |\det g_{ij}| \quad (3.4)$$

Here $g_{ij}(x)$ stands for the metric of the 3-geometry and R is the Ricci scalar associated with it. Because $G_{ijkl}(x)$ is trivially diagonal in the continuous index x, x' (all the g_{ij} 's are taken at the same point), instead of (3.2), it is more convenient to consider the density

$$\mathcal{H}_0(x) = \frac{1}{2} G_{ijkl}(x) \pi^{ij}(x) \pi^{kl}(x), \quad (3.5)$$

where the sum runs over the discrete (latin) indices only.

It is clear that the operator ordering problem is particularly severe in this case. We would like to say in the spirit of our previous discussion that the quantum descendant of \mathcal{H}_0 is some operator $\hat{\mathcal{H}}_0$, which should be invariant under co-ordinate transformations $g_{ij} \rightarrow g'_{ij}[g]$ (These co-ordinate transformations have nothing to do with the diffeomorphisms on the three space surfaces. The latter should be thought of as changes in the space of indices $x \rightarrow x'$, that label the co-ordinates $g_{ij}(x)$ of hyperspace \mathcal{M} [13].) The changes $g_{ij} \rightarrow g'_{ij}[g]$ need not be local, namely the new co-ordinates $g'_{ij}(x)$ can be functionals of the old co-ordinates $\{g_{kl}(x')\}$. However, since the metric is diagonal in the continuous index x , we can restrict ourselves to only local co-ordinate transformations, $g_{ij}(x) \rightarrow g'_{ij}(x)$ so that the metric (3.4) remains diagonal. In other

words, since \mathcal{M} has the geometry of a direct product of a flat (infinite dimensional) space labelled by x , times a six-dimensional manifold M with metric $G_{AB}(g_c)$, ($A, B, C, = 1, \dots, 6$), we will only worry about the invariance of \mathcal{H}_0 under diffeomorphisms of M .

It has been shown by De Witt [12] that M is a manifold of hyperbolic signature $(-, +, +, +, +, +)$ formed by stacking up along the "time direction" five-dimensional manifolds (Ω_5) , having all the same intrinsic shape $SO(3)/SO(3)$, and differing only by a scale factor. Were we to restrict ourselves to one of these five-dimensional subspaces, we would be compelled to choose the Laplace-Beltrami operator for \mathcal{H}_0 . But, having at our disposal a family of Ω_5 's parametrized by the scale factor, we can consider the operator analogous to the more general form (2.26). Thus we take

$$\hat{\mathcal{H}}_0 = -\frac{1}{2} G_{ijkl} \frac{\mathcal{D}}{\mathcal{D}g_{ij}} \frac{\mathcal{D}}{\mathcal{D}g_{kl}} + k \mathcal{R}, \quad (3.6)$$

where $\mathcal{D}/\mathcal{D}g$ and \mathcal{R} are the covariant derivative and the Ricci scalar on \mathcal{M} , respectively. Using the results of Appx.A one finds

$$\hat{\mathcal{H}}_0 = \frac{1}{2} G_{ijkl} \hat{\pi}^{ijkl} - i \delta(0) g^{-1/2} \epsilon_{mn} \hat{\pi}^{mn} + k \delta(0)^2 g^{-1/2} - g^{1/2} R \quad (3.7)$$

Here $\hat{\pi}^{ij} = -i \frac{\delta}{\delta g_{ij}}$ is the operator conjugate to g_{ij} which acts on the space of functionals of g_{ij} , $\Psi[g]$. These functionals are supposed to be orthonormal under the invariant inner product

$$\langle \Psi_1 | \Psi_2 \rangle = \int \prod_x [\sqrt{G} d^6 g] \Psi_1^* \Psi_2, \quad (3.8)$$

where G is the absolute value of the determinant of G^{ijkl} with respect to the discrete indices only. In this functional Hilbert space, the operator $\hat{\mathcal{H}}_0$ is hermitian by construction.

IV. THE QUANTUM ALGEBRA OF THE CONSTRAINTS

The full dynamical content of Einstein's theory of gravity in the absence of matter can be expressed by the four classical constraint equations

$$\mathcal{H}_1 \approx 0$$

$$\mathcal{H}_i \approx 0 \quad (4.1)$$

where \mathcal{H}_1 is the generator of normal deformations of the three space given by (3.3) and \mathcal{H}_i are the generators of diffeomorphisms of the three geometries

$$\mathcal{H}_i = -2g_{ij} \pi^{kj}, k - 2g_{ij} \pi^{mn} \pi^{mn} \quad (4.2)$$

Consistency of the weak equations (4.1) is guaranteed by the fact that these constraints obey the classical (Poisson bracket) algebra

$$[\mathcal{H}_1, \mathcal{H}_1] = -[\mathcal{H}^i + \mathcal{H}^i] \delta_{,i}(x, \bar{x}) \quad (4.3a)$$

$$[\mathcal{H}_i, \mathcal{H}_j] = \mathcal{H}_j \delta_{,i}(x, \bar{x}) + \mathcal{H}_i \delta_{,j}(x, \bar{x}) \quad (4.3b)$$

$$[\mathcal{H}_i, \mathcal{H}_j] = \mathcal{H}_i \delta_{,j}(x, \bar{x}) \quad (4.3c)$$

Here $\mathcal{H}^i = g^{ij} \mathcal{H}_j$, with g^{ij} being the inverse of the "co-ordinate" g_{ij} , and $\delta(x, \bar{x})$ is a scalar density such that

$$\int f(x) \delta(x, \bar{x}) d^3x = f(\bar{x}) \quad (4.4)$$

In the quantum theory, Eqs.(4.1) are to be understood as conditions on the wave function(al)s which define the physical Hilbert space

$$\begin{aligned} \hat{\mathcal{H}}_1 \Psi[g] &= 0 \\ \hat{\mathcal{H}}_i \Psi[g] &= 0 \end{aligned} \quad (4.5)$$

In order to construct a consistent quantum theory of gravity along these lines one has to first define operators $\hat{\mathcal{H}}_1$ and $\hat{\mathcal{H}}_i$ and then test the consistency of these relations by constructing an algebra analogous to (4.3). The latter is, in general, a non-trivial requirement: the classical algebra can be spoiled by anomalies, or if the theory is non-renormalizable, by infinite series of quantum corrections to the classical form of the operators.

The procedure we adopt here is the following. We assume $\hat{\mathcal{K}}_1$ to be given by (3.6), and through the quantum analogue of (4.3a) we define $\hat{\mathcal{K}}^i$. In Appx.B it is shown that

$$[\hat{\mathcal{K}}_1, \hat{\mathcal{K}}_1] = -i [\hat{\mathcal{K}}^i + \hat{\mathcal{K}}^{\bar{i}}] \delta_{,i}(x, \bar{x}), \quad (4.6)$$

where

$$\hat{\mathcal{K}}^i = -2\hat{\pi}^{ij},_j - 2\Gamma_{mn}^i \hat{\pi}^{mn} - \frac{i}{2} \delta(0) g^{ij} \Gamma_{kj}^k. \quad (4.7)$$

The operator $\hat{\mathcal{K}}^i$ can be seen from Eq.(4.6) to be hermitian under the same inner product as $\hat{\mathcal{K}}_1$. Indeed one can write $\hat{\mathcal{K}}^i$ in the manifestly hermitian form

$$\hat{\mathcal{K}}^i = -2(G^{-1/4} \hat{\pi}^{ij} G^{1/4})_{,j} - \{ \Gamma_{mn}^i, G^{-1/4} \hat{\pi}^{mn} G^{1/4} \}, \quad (4.8)$$

where $\{A, B\}$ is the anticommutator of A and B. The hermiticity of $\hat{\mathcal{K}}^i$ can be easily seen in (4.8) since $G^{-1/4} \hat{\pi}^{ij} G^{1/4}$ is the analogue of the hermitian derivative operator $g^{-1/4} \partial_\mu g^{1/4}$ in ordinary curved space.

In order to define $\hat{\mathcal{K}}_i$ we multiply $\hat{\mathcal{K}}^j$ by g_{ij} from the left. This ensures that $\hat{\mathcal{K}}_i \psi = 0$, provided $\hat{\mathcal{K}}^i \psi = 0$. Thus we obtain

$$\hat{\mathcal{K}}_i = -2g_{ij} \hat{\pi}^{jk},_k - 2g_{ij} \Gamma_{mn}^j \hat{\pi}^{mn} - \frac{i}{2} \delta(0) \Gamma_{ki}^k \quad (4.9)$$

and the analogue of Eq.(4.3b) is found to be (see Appx.B for details)

$$[\hat{\mathcal{K}}_i, \hat{\mathcal{K}}_j] = i(\hat{\mathcal{K}}_j \delta_{,i}(x, \bar{x}) + \hat{\mathcal{K}}_i \delta_{,j}(x, \bar{x})). \quad (4.10)$$

Finally, the relation analogous to (4.3c) can be shown to be

$$[\hat{\mathcal{K}}_i, \hat{\mathcal{K}}_1] = i \hat{\mathcal{K}}_1 \delta_{,i}(x, \bar{x}) - \frac{\delta(0)}{4} \left[g^{1/2} (g_{mn} \hat{\pi}^{mn}) - i \left(\frac{\partial}{\partial t} - \frac{\partial}{\partial x} \right) \delta(0) \right] \delta(x, \bar{x}), \quad (4.11)$$

The discussion of the anomalous terms in (4.11) will be left for the following section.

The classical limit of the operators $\hat{\mathcal{K}}_1, \hat{\mathcal{K}}_i$ and their commutator algebra is recovered by dropping the terms that contain $\delta(0)$ and $\delta(0)^2$ since they arise from the commutators of $\hat{\pi}^{ij}$ and g_{kl} , which are of order \hbar .

V. DISCUSSION

As we have shown, it is possible, starting from first principles, to define a set of quantum operators $\hat{\mathcal{K}}_\mu$ that obey the correct classical algebra in the limit $\hbar \rightarrow 0$. The constraints $\hat{\mathcal{K}}_\mu \psi = 0$, however, cannot be consistently imposed on the states unless the anomalous terms appearing in (4.11) can be set to zero.

One way to avoid the problem is to restrict the class of allowed diffeomorphisms of three space to those generated by operators of the form

$$\hat{G}[f] = \int f^i(x) \hat{\mathcal{K}}_i(x) d^3x, \quad (5.1)$$

with $f^i_{,i} = 0$. In this case the anomalous terms in (4.11) drop out from the integrated out form of the commutator algebra. This has the disadvantage of replicating only the integrated out version of the classical algebra, thus obscuring the geometrical meaning of $\hat{\mathcal{K}}_\mu$.

An alternative approach [14] would be to impose an additional requirement of the form

$$\hat{A}\Psi \equiv \left(i g_{mn} \hat{\pi}^{mn} + \alpha \delta(0) \right) \Psi = 0, \quad (5.2)$$

and fix the value of $k = k(\alpha)$ so that the anomaly in (4.11) is just \hat{A} . This would be the quantum analogue of Dirac's maximal slicing gauge [3], $\pi \equiv \pi_{ij} = g_{ij} \pi^{ij} \approx 0$, where $\alpha \delta(0)$ in (5.2) can be viewed as a counter-term required by quantization. The geometrical meaning of $i g_{mn} \hat{\pi}^{mn}$ is that of a generator of conformal (scale) transformations: Consider the effect on $g_{ij}(x)$ produced by it, namely

$$\begin{aligned} g_{ij}(x) &\rightarrow \hat{\mathcal{C}}[\Omega] g_{ij}(x) \\ &= i \int \Omega(x') g_{mn}(x') \hat{\pi}^{mn}(x') d^3x' g_{ij}(x) \\ &= 3 \Omega(x) g_{ij}(x), \end{aligned} \quad (5.3)$$

which is indeed a conformal transformation. Thus, the appearance of these extra terms in the quantum algebra which were not present in its classical counterpart is reminiscent of the conformal anomalies found in the context of other quantum theories with massless fields [15].

The condition $\hat{A}\Psi = 0$ means that we have chosen the wave functional to be a constant along orbits in hyperspace which correspond to some particular rescalings of the metric g_{ij} . In order to make (5.2) consistent with the remaining constraints one has to evaluate their commutators. It is straightforward to check that

$$[\hat{A}, \hat{\mathcal{H}}_i] = 0 \quad (5.4)$$

for any value of α , and that

$$[\hat{A}, \hat{\mathcal{H}}_i] = -2i \left[\hat{A} + \left(\frac{3}{4} - \alpha \right) \right] \delta_{,i}(x, x) \quad (5.5)$$

Therefore \hat{A} and $\hat{\mathcal{H}}_i$ form a closed first class algebra if we take $\alpha = \frac{3}{4}$. This in turn fixes the value of k to be $-\frac{9}{32}$. The last commutator, $[\hat{A}, \hat{\mathcal{H}}_i]$, is not a linear combination of $\hat{\mathcal{H}}_\mu$ and \hat{A} , and therefore \hat{A} and $\hat{\mathcal{H}}_i$ are now second class operators: they express relations that link the

operators g_{ij} and $\hat{\pi}^{ij}$. This is also the case in the classical problem [16] and occurs because $\pi = 0$ corresponds to choosing a foliation of space-time into slices with vanishing extrinsic curvature and this slicing is obviously not invariant under the arbitrary normal deformations generated by $\hat{\mathcal{H}}_i$. We shall come back to these points in a forthcoming article where the gauge fixing conditions will be discussed in more detail.

In their final form, operators $\hat{\mathcal{H}}_\mu$ and \hat{A} exhibit corrections of order \hbar and \hbar^2 only, with respect to their classical counterparts C_μ and π . This suggests that in the action one would need at most two-loop counter terms. Furthermore, since some terms $O(\hbar)$ can be eliminated by setting $\hat{A} = 0$ this seems to support the perturbative claim that pure gravity is one-loop finite [17]. On the other hand, the fact that only $O(\hbar^2)$ corrections are needed in order to close the quantum algebra seems to indicate that a consistent (renormalizable) quantum theory of gravity might exist. Of course, all this is conditional on the consistent fixing of the gauge that we have not discussed here. Also our results should be revised when one considers matter fields coupled to gravity, a problem that we have so far avoided.

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In this appendix we give some useful relations concerning the geometry of the space of all matrices $g_{ij}(x)$, \mathcal{M} . Following De Witt, the metric on this space is taken to be the hypermetric

$$G_{ijkl}(g(x)) = g^{-\frac{1}{2}}(x) (g_{ik}(x)g_{jl}(x) + g_{il}(x)g_{jk}(x) - g_{ij}(x)g_{kl}(x)). \quad (A.1)$$

We assume the coordinates to be given by the entries of the 3-metric $g_{ij}(x)$. Thus, G_{ijkl} in Eq.(A.1) should transform as a contravariant second rank tensor in order that the contraction of it with π^{ij} , π^{kl} transforms as a scalar in \mathcal{M} . The inverse (covariant) metric is

$$G^{ijkl} = \frac{1}{4} g^{\frac{1}{2}} (g^{ik}g^{jl} + g^{il}g^{jk} - 2g^{ij}g^{kl}), \quad (A.2)$$

$$G_{ijkl} G^{klmn} = \delta_{ij}^{mn} \equiv \frac{1}{2} (\delta_i^m \delta_j^n + \delta_j^m \delta_i^n). \quad (A.3)$$

From now on, the x -dependence will be implicitly assumed except for ambiguous cases. Starting from definitions (A.1) and (A.2) one can find the Christoffel symbol

$$\left\{ \begin{matrix} ij \\ mn \end{matrix} \right\} \equiv \frac{1}{2} G_{mnpq} \left[\frac{\delta}{\delta g_{kl}} G^{ijpq} + \frac{\delta}{\delta g_{ij}} G^{klpq} - \frac{\delta}{\delta g_{pq}} G^{ijkl} \right], \quad (A.4)$$

to be

$$\left\{ \begin{matrix} ij \\ mn \end{matrix} \right\} = \frac{1}{4} \left[g^{kl} \delta_{mn}^{ij} + g^{ij} \delta_{mn}^{kl} - g^{ki} \delta_{mn}^{jl} - g^{il} \delta_{mn}^{jk} - g^{kj} \delta_{mn}^{il} - g^{il} \delta_{mn}^{ik} + g^{-\frac{1}{2}} G^{ijkl} g_{mn} \right] \delta(0). \quad (A.5)$$

Analogously, one defines the curvature tensor

$$R_{mn}^{ijklpq} \equiv \frac{\delta}{\delta g_{pq}} \left\{ \begin{matrix} ij \\ mn \end{matrix} \right\} - \frac{\delta}{\delta g_{kl}} \left\{ \begin{matrix} ij \\ mn \end{matrix} \right\} + \left\{ \begin{matrix} ij \\ rs \end{matrix} \right\} \left\{ \begin{matrix} pq \\ rs \end{matrix} \right\} - \left\{ \begin{matrix} ij \\ rs \end{matrix} \right\} \left\{ \begin{matrix} kl \\ mn \end{matrix} \right\}. \quad (A.6)$$

From this, the Ricci tensor R^{ijkl} and the scalar curvature R are found to be

$$R^{ijkl} = \frac{1}{16} g^{ij} g^{kl} \delta(0)^2 \quad (A.7)$$

and

$$R = -\frac{3}{16} g^{-\frac{1}{2}} \delta(0)^2 \quad (A.8)$$

respectively. Throughout this calculation use has been made of the definitions

$$\frac{\delta}{\delta g_{ij}(x)} g_{kl}(x') = \delta_{kl}^{ij} \delta(x, x') \quad (A.9)$$

$$\frac{\delta}{\delta g_{ij}(x)} g^{kl}(x') = -\frac{1}{2} (g^{ik} g^{jl} + g^{il} g^{jk}) \delta(x, x'). \quad (A.10)$$

Using the hyperspace analogue of the relation

$$\Gamma_{ki}^k = \frac{1}{2} \partial_i \ln g,$$

we can find the relationship between $G = \det G^{ijkl}$ and $g = |\det g_{ij}|$

$$G = -\frac{1}{256} g^{-1}, \quad (A.11)$$

where the factor $1/256$ has been fixed taking the flat space limit $g_{ij} = \delta_{ij}$.

In this appendix we outline the derivation of the quantum algebra for the constraints. The basic commutator between the canonical variables is

$$[\hat{\Pi}^{ij}(x), g_{kl}(x')] = -i \delta_{kl}^{ij} \delta(x, x') \quad (B.1)$$

in the units $\hbar = c = 1$. Using this relation and the definition of the Ricci scalar R ,

$$R = g^{nr} R_{nr} = g^{nr} g^{ms} (g_{ms, nr} - g_{nm, rs}) + g^{nr} g^{ml} g_{ost} (\Gamma_{nr}^s \Gamma_{ml}^t - \Gamma_{rm}^s \Gamma_{nl}^t),$$

one finds, after a little algebra,

$$[\hat{A}^{kl}, R] = 2i R^{kl} \delta(x, \bar{x}) - 2i \underline{g}^{-\frac{1}{2}} \underline{g}^{pqmn} \underline{\Gamma}_{mn}^r (2 \delta_{rp}^{kl} \delta_{,q}(x, \bar{x}) - \delta_{qp}^{kl} \delta_{,r}(x, \bar{x})) + 2i \underline{g}^{-\frac{1}{2}} \underline{g}^{klmn} \delta_{,mn}(x, \bar{x}). \quad (B.2)$$

where a tilde under a symbol denotes its evaluation at the point \bar{x} ; otherwise the function is understood to be evaluated at x . In order to calculate the commutator appearing in (4.6), we first observe that the only non-vanishing contributions are

$$[\hat{\mathcal{H}}_{\perp}, \hat{\mathcal{H}}_{\perp}] = -\frac{1}{2} [G_{ijkl} \hat{\Pi}^{ij} \hat{\Pi}^{kl}, g^{\frac{1}{2}} R] - \frac{1}{2} [g^{\frac{1}{2}} R, G_{ijkl} \hat{\Pi}^{ij} \hat{\Pi}^{kl}] + i \delta(x) \{ [g^{\frac{1}{2}} g_{ij} \hat{\Pi}^{ij}, g^{\frac{1}{2}} R] + [g^{\frac{1}{2}} R, g^{\frac{1}{2}} g_{ij} \hat{\Pi}^{ij}] \}. \quad (B.3)$$

The first two terms reduce to

$$i [2 \hat{\Pi}^{ij} g_{ij} + \{ \Gamma_{kl}^i, \hat{\Pi}^{kl} \} - \frac{3}{2} i \delta(x) \Gamma_{kl}^k g^{li}] - i [x \leftrightarrow \bar{x}], \quad (B.4)$$

where the last term is minus the first one with x and \bar{x} interchanged. The last two terms are

$$2 \delta(x) g^{ij} \Gamma_{kj}^k \delta_{,i}(x, \bar{x}) - [x \leftrightarrow \bar{x}]. \quad (B.5)$$

Combining (B.4) and (B.5) one obtains relation (4.6) with definition (4.7). In this derivation use has been made of the identities

$$\int \delta(x, \bar{x}) = \int \delta(x, \bar{x}) \quad (B.6a)$$

$$\int \delta_{,i}(x, \bar{x}) = \int \delta_{,i}(x, \bar{x}) + f_{,i} \delta(x, \bar{x}) \quad (B.6b)$$

$$\int \delta(x, \bar{x})_{,mn} - g \int \delta_{,mn}(x, \bar{x}) = \frac{1}{2} \{ (g_{\tilde{m}\tilde{n}} f_{,m} - g_{\tilde{m}\tilde{n}} f_{,n}) \delta(x, \bar{x})_{,\tilde{m}} + (g_{\tilde{m}\tilde{n}} f_{,m} - g_{\tilde{m}\tilde{n}} f_{,n}) \delta(x, \bar{x})_{,\tilde{m}} - (x \leftrightarrow \bar{x}) \}, \quad (B.6c)$$

where $\delta_{,i}(x, \bar{x}) \equiv \frac{\partial}{\partial x^i} \delta(x, \bar{x}) = -\delta(x, \bar{x})_{,i} = -\frac{\partial}{\partial \bar{x}^i} \delta(x, \bar{x})$. We have also adopted the traditional convention

$$\delta_{,i}(x, x) = \lim_{x' \rightarrow x} \delta_{,i}(x, x') = 0, \quad (B.7)$$

which implies, in particular, that

$$[\hat{\Pi}^{ij}, g_{kl}] = 0 = [\hat{\Pi}^{ij}, g_{mn,kl}]. \quad (B.8)$$

Relation (4.10) can now be easily deduced observing that in

$$\hat{\mathcal{H}}_{\perp} = -2 g_{ij} \hat{\Pi}^{jk} g_{,k} - 2 g_{ij} \Gamma_{mn}^j \hat{\Pi}^{mn} - \frac{1}{2} \delta(x) \Gamma_{kl}^k, \quad (B.9)$$

the first two terms have no factor ordering problem by virtue of (B.8). Then,

$$[\hat{\mathcal{H}}_i, \hat{\mathcal{H}}_j] = [\hat{C}_i, \hat{C}_j] - \frac{i}{2} \delta^{(0)} [\Gamma_{ki}^k, \hat{C}_j] - \frac{i}{2} \delta^{(0)} [\hat{C}_i, \Sigma_{kj}^k], \quad (\text{B.10})$$

where \hat{C}_i stands for the first two terms in (B.9), the $\hat{C}_i - \hat{C}_j$ commutator reproduces the "classical" result

$$[\hat{C}_i, \hat{C}_j] = i \hat{C}_j \delta_{,i}(x, \bar{x}) + i \hat{C}_i \delta_{,j}(x, \bar{x}). \quad (\text{B.11})$$

Furthermore, it can easily be verified that

$$[\Gamma_{ki}^k, \hat{C}_j] + [\hat{C}_i, \Sigma_{kj}^k] = i \Gamma_{kj}^k \delta_{,i}(x, \bar{x}) - i \Sigma_{ki}^k \delta_{,j}(x, \bar{x}). \quad (\text{B.12})$$

Adding (B.11) to (B.12) Eq.(4.10) follows.

The last commutator (Eq.(4.11)) is obtained as follows. The operator $\hat{\mathcal{H}}_1$ can be split into a "classical" part \hat{C}_0 and "quantum corrections" as

$$\hat{\mathcal{H}}_1 = \hat{C}_0 - i \delta^{(0)} g^{-\frac{1}{2}} g_{mn} \hat{\Pi}^{mn} + k \delta^{(0)^2} g^{-\frac{1}{2}}, \quad (\text{B.13})$$

where

$$\hat{C}_0 = \frac{1}{2} G_{ijkl} \hat{\Pi}^{ij} \hat{\Pi}^{kl} - g^{\frac{1}{2}} R. \quad (\text{B.14})$$

Then the commutator in (4.11) can be written as

$$\begin{aligned} [\hat{\mathcal{H}}_i, \hat{\mathcal{H}}_1] &= [\hat{C}_i, \hat{C}_0] - i \delta^{(0)} [\hat{C}_i, g^{-\frac{1}{2}} g_{mn} \hat{\Pi}^{mn}] - \frac{i}{2} \delta^{(0)} [\Gamma_{ki}^k, \hat{C}_0] \\ &\quad - \frac{1}{2} \delta^{(0)^2} [\Gamma_{ki}^k, g^{-\frac{1}{2}} g_{mn} \hat{\Pi}^{mn}] + k \delta^{(0)^2} [\hat{C}_i, g^{-\frac{1}{2}}]. \end{aligned} \quad (\text{B.15})$$

The first term on the right-hand side is

$$\begin{aligned} &\frac{1}{2} [\hat{C}_i, G_{pqrs}] \hat{\Pi}^{pq} \hat{\Pi}^{rs} + \frac{i}{2} G_{pqrs} ([\hat{C}_i, \hat{\Pi}^{pq}] \hat{\Pi}^{rs} \\ &\quad + \hat{\Pi}^{pq} [\hat{C}_i, \hat{\Pi}^{rs}]) - [\hat{C}_i, g^{\frac{1}{2}} R]. \end{aligned}$$

Since \hat{C}_i is linear in $\hat{\Pi}^{kl}$ and g_{mn} , all the $\hat{\Pi}$'s can be put to the far right in this expression without picking up any further commutators. Also, because \hat{C}_i has no factor ordering problem, the last commutator gives back i -times the classical value. Thus we conclude

$$[\hat{C}_i, \hat{C}_0] = i \hat{C}_0 \delta_{,i}(x, \bar{x}). \quad (\text{B.16})$$

The remaining terms in (B.15) can be found in a straightforward manner to be

$$\begin{aligned} &-\frac{\sqrt{3}}{4} \delta^{(0)} (g^{-\frac{1}{2}} g_{mn} \hat{\Pi}^{mn})_{,i} \delta(x, \bar{x}) - \frac{1}{4} \delta^{(0)} g^{-\frac{1}{2}} g_{mn} \hat{\Pi}^{mn} \delta_{,i}(x, \bar{x}) \\ &\quad + (\frac{3}{8} - k) i \delta^{(0)^2} g^{-\frac{1}{2}} \delta_{,i}(x, \bar{x}) - (\frac{3}{8} - 2k) i \delta^{(0)^2} g^{-\frac{1}{2}} \Gamma_{ki}^k \delta(x, \bar{x}). \end{aligned}$$

Then (B.15) becomes

$$\begin{aligned} [\hat{\mathcal{H}}_i, \hat{\mathcal{H}}_1] &= i \hat{\mathcal{H}}_1 \delta_{,i}(x, \bar{x}) - \frac{\sqrt{3}}{4} \delta^{(0)} (g^{-\frac{1}{2}} g_{mn} \hat{\Pi}^{mn} \delta(x, \bar{x}))_{,i} \\ &\quad + (\frac{3}{8} - 2k) i \delta^{(0)^2} (g^{-\frac{1}{2}} \delta(x, \bar{x}))_{,i} \end{aligned} \quad (\text{B.17})$$

which is the result claimed in (4.11).

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- Thus, unless one considers transformations which leave invariant the subspace defined by the polarization, it would be impossible to implement them as symmetries of the quantum theory. In this sense, general coordinate covariance is the maximal symmetry one could demand for a generic quantum theory, if one is to work in the configuration representation. (Particular systems may, of course, possess extra symmetries but these are not required by the canonical approach)
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