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Nonconventional functional calculus techniques in quantum field theories and in quantum gravity

Eyo Eyo Ita III

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Department of Applied Mathematics and Theoretical Physics
Centre for Mathematical Sciences, University of Cambridge, Wilberforce Road
Cambridge CB3 0WA, United Kingdom
eei20@cam.ac.uk

Abstract

In this exerpt we introduce the concept of the 'nonconventional' calculus, outlining a prescription for making sense of the ultraviolet singularities which occur in quantum field theories with a view to addressing quantm gravity. We first show how these singularities arise when interpreting the canonical commutation relations for a general quantum field theory and then discuss a new intepretation which deals with them without using regularization procedures. We then discuss the relative commutativity of functional with spacetime variation and its implications for addressing the issue of time in quantum gravity in contrast to nongravitational field theories. We end with a brief introduction into how these concepts may be applied to the quantization of gravity in Ashtekar variables coupled to matter fields.

1 Introduction

Consider a fibre bundle whose section consists of a functional $\Psi[\phi]$ defined on the functional space of fields $\phi = \phi(x)$ in four dimensional spacetime M. The functional Ψ might be defined with respect to a particular spacetime history of the fields ϕ, and we would like to assess the dependence of the functional Ψ on each of its variables. Let us define a fibre bundle whose base space B constitutes a direct product of a spacetime manifold $x \in M$ with a manifold comprising the functional space of quantum fields $\phi(x)$ living on spacetime. The notation is given by $B \sim (M \otimes \Gamma)$, where Γ constitutes the functional space. It seems reasonable to speculate that the dimension of this base space is $Dim(B) = \infty^4 \otimes \infty^N$, where N is the number of components, or individual degrees of freedom, of the quantum field ϕ. However, the question arises as to how one ensures that some portions of the base space have not been overcounted. This leads to the question of the trivializability of the base space with respect to spacetime, which ultimately leads to the question of the problem of time in quantum gravity as we will demonstrate in this work.

In the 3+1 decomposition of spacetime, one foliates spacetime M into a set of spatial 3-surfaces Σ labeled by time t via the decomposition $M = \Sigma \times R$. In the process one is in a certain sense singling out time from space from the starting point of a generally covariant description of nature. General covariance is a powerful principle upon which Einstein's general relativity is based, which requires that time and space be treated on the same footing with respect to the laws of nature. However, Einstein's theory as originally formulated is a classical theory. This leads one to pose the question as to whether classical theory of general relativity, a diffeomorphism invariant theory, can consistently be subjected to the laws and the axioms of quantum mechanics. The rules of quantum mechanics necessitate that one solve the Schrödinger equation, which by definition singles out the time direction from three space Σ. For many nongravitational theories this procedure has been successfully implemented, however in the case of general relativity one must ponder the following questions: (i) Does the principle of general covariance, a principle formulated within the classical realm of physics, apply to the quantum regime or does it break down, and to what extent if any does it break down? (ii) As a corollary to (i), was it Einstein's intent for this principle of covariance to be applied in this manner, given his expressed disapproval of quantum mechanics during the time he developed general relativity. (iii) If quantum mechanics and general covariance indeed are mutually inconsistent principles of nature, then how close can one get to reconciling general relativity with quantum mechanics? In other words,

what is the miniumum that one must absolutely relax, if anything at all?

It will become clear in the course of this work, from the above introduction, that the consistency of the quantization procedure for gravity is somehow related to the problem of time. The first question one must ascertain is the effect of the 3+1 decomposition of spacetime upon the fibre bundle structure upon which we define our quantum theory. One may think that the decomposition can be written as

$$E = \big(\Sigma \times R \otimes \Gamma, \Psi[\Sigma \times R \otimes \Gamma]\big), \tag{1}$$

where E constitutes the base space with fibre Ψ. Equation (1) assumes that the base space of the fibre bundle is trivializable with respect to spacetime. If this were to be the case, then one could conclude that general covariance has been preserved by the process of quantization[1] and that the dimension of the base space is given by $Dim(B) = \infty^4 \otimes \infty^N$. In this case, the field ϕ and spatial position $\boldsymbol{x}$ and time t can be considered truly independent variables. Note that if one restricts ϕ to a specific function of spacetime, then the dimension of the base space collapes to $Dim(B) = \infty^4$, since all field components N are uniquely determined once the spacetime position x is specified. The viability of a quantum theory of gravity by our interpretation then amounts to evaluation of which variables within spacetime can be considered as truly independent degrees of freedom with respect to the field ϕ. If it were to be the case that the time variable could not be distinguished from ϕ, then the dimension of the basespace would then collapse to $Dim(B) = \infty^3 \otimes \infty^N$. The relevant question to make this determination, as we will motivate and show in this work, is to determine which variables within the subspace M are such that variations within the subspace Γ commute with the former. It is this that determines the dimension of the base space B, and consequently the total space E of the fibre bundle.

Does functional variation commute with spatial variation or with time variation, with both or with neither? This is the question we will attempt to answer in this work, which we assert should shed some light on question (i) above. For question (iii) if one chooses not to make any consessions to either principle- in other words, maintain general covariance and quantization intact- then what consessions or restrictions elsewhere, if any, must be made. It is a conjecture of the present author that one becomes restricted in the class of allowed quantum states Ψ constituting the section of the fibre bundle, as we will show in subsequent works. As regards the question (iii) one can only speculate, given that Einstein in a certain sense motivated the study of quantum mechanics with his famous paper explaining the photoelectric effect, in which the concept of 'quanta' of light was invoked.

[1] This is the interpretation of the present author.

2 Ultraviolet field-theoretical singularities in quantum field theories

2.1 The canonical commutation relations

When one wants to quantize a classical theory via the Heisenberg prescription, one promotes the classical fields and their canonically conjugate momenta $\phi(x)$ and $\pi(x)$ to quantum operators $\hat{\phi}(x)$ and $\hat{\pi}(x)$ which act on a quantum state $\big|\Psi\big\rangle$. The equal-time commutation relations are defined such as to facilitate the manipulation of quantities involving functionals containing an infinite number of degrees of freedom. The equal-time commutation relations for a typical theory read

$$\big[\phi(\boldsymbol{x},t),\pi(\boldsymbol{y},t)\big] = i\hbar\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}) \tag{2}$$

Although the definition (2) makes it convenient to compute quantities in the functional formalism, the conventional thought is not to regard the Dirac-delta function seriously as a funtion but rather as a distribution designed to sift out a desired result. Stating (2) in words, the measurement of the field at the spacetime point $x = (\boldsymbol{x}, t)$ cannot affect the measurement at another spacetime point $y = (\boldsymbol{y}, t)$ if x and y are separated by a spacelike interval. The consequence if such a measurement at x did in fact affect a measurement at y is a violation of causality, an inviolable principle of quantum field theory consistent with Lorentz invariance, among other cherished principles of physics and intuition [1],[2].

An examination of the action for a massive Klein–Gordon scalar field in Minkowski spacetime,

$$L = \int_M d^4x\ \frac{1}{2}\big(\dot{\phi}(\boldsymbol{x},t)^2 - \partial_i\phi(\boldsymbol{x},t)^2 - \frac{1}{2}m^2\phi(\boldsymbol{x},t)^2\big) \tag{3}$$

in relation to the commutation relations (2) indicates a potential inconsistency. The time derivative term, which encodes evolution of the field orthogonal to the spatial hypersurface Σ_t on which the canonical commutation relations are defined, seems harmless enough. The mass squared term, which couples the field to itself at each point x as well seems to be self-consistent. It is the spatial derivative term where the apparent problem lies. Imagine discretizing three-space. As the field propagates from a position $\boldsymbol{x}_n$ to a point $\boldsymbol{x}_{n+1}$ there is a violation of causality, no matter how close $\boldsymbol{x}_n$ and $\boldsymbol{x}_{n+1}$ are together. One obvious way to mitigate this violation is to take the limit in which the points coincide, to allow propagation in infinitesimal steps from one spatial point to another. In this way, the causality violation is less severe, having being turned on and turned off in a continuous fashion.

The concept of particles and antiparticles in field theory resolves the paradox of causality since both propagate in opposite directions across the same spacelike interval when a measurement is made. This is an example of the introduction of an external structure, by Dirac, into a theory in order to solve a technical problem. Dirac's concept of particles and antiparticles is possible due to the ability to expand the solution to the classical equations of motion for a harmonic theory in terms of plane waves of positive and negative frequencies [2]. These plane waves correspond, in the quantized version of these harmonic theories, to noninteracting particles. In a usual treatment of anharmonic theories the anharmonic terms are treated as self-interactions which can usually be accomodated by perturbative expansion in a renormalizable theory. However in nonperturbative quantum gravity, the application of this particle-antiparticle concept breaks down due to perturbative nonrenormalizability in the metric representation. Also, due to the inherent nonlinearity of gravity, it is not possible to expand in plane wave solutions in the general case. Thus the concept of particles and antiparticles as a means for addressing causality violation in usual quantized field theories does not directly extend to quantized gravity without some additional provision to address the infinities that result.

In the extension of the canonical commutation relations to quantum gravity we must resist the temptation to alter them in order to avoid any unpleasantries of theoretical physics that the latter may portend. It is precisely the viability of these canonical commutation relations against Einstein's four-dimensional general relativity that we ultimately would like to examine. Any tampering with them is strictly forbidden in order for a reliable test of this viability to have been carried out. The process of regularization is in some cases tantamount to tampering, in that the result computed may leave behind traces of the regulator's presence even after removed. Such effects occur in various regularization prescriptions in loop quantum gravity [3],[4]. Therefore, we shall avoid regularization whenever possible in our approach, since the test for prescription independence for the set of all possible regulators is unfeasible.

2.2 Dirac delta functionals in quantum gravity

During the course of our quantization programme for Einstein's four-dimensional gravity we will occasionally need to evaluate the derivative of a delta function $\delta^{(3)}(\boldsymbol{x})$ at the spatial point $\boldsymbol{x}$. Recall that the definition of the one-dimensional delta function $\delta(x)$, as defined by the equal-time canonical commutation relations is conventionally such that

$$\int dx\ \delta(x) f(x) = f(0) \tag{4}$$

for all test functions $f(x)$. It will shed considerable light in our quantization programme to regard the delta function, as defined by the commutation relations, as a function or distribution in its own right independently of any test functions. The spatial derivative of this function or distribution can be given, just as one may intuitively define the derivative, by

$$\delta'(x) = \lim_{\epsilon\to 0}\frac{1}{2\epsilon}\big[\delta(x+\epsilon) - \delta(x-\epsilon)\big]. \tag{5}$$

We have taken the symmetric version of the derivative in (5). This appears suitable, since the delta function can be approximated by a sequence of even functions. Some familiar representations of the Dirac delta function are

$$\begin{aligned}
\delta_\epsilon(x) &= \lim_{\epsilon\to 0}\frac{1}{4\pi\epsilon}e^{-\frac{x^2}{\epsilon}} \\
\delta_\epsilon(x) &= \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{\epsilon^2+x^2} \\
\delta_\epsilon(x) &= \frac{1}{\pi}x^{-2}\sin^2(x/\epsilon)
\end{aligned} \tag{6}$$

Nonetheless, cast as a function the Dirac delta function should be independent of the representation. Equation (5) may appear to be not well-defined as a function in and of itself. However, when integrated against a test function $f(x)$ one finds

$$\begin{aligned}
\int dx f(x)\delta'(x) &= \lim_{\epsilon\to 0}\frac{1}{2\epsilon}\Big[\int dx f(x)\delta(x+\epsilon) - \int dx f(x)\delta(x-\epsilon)\Big] \\
&= \lim_{\epsilon\to 0}\frac{1}{2\epsilon}\big[f(-\epsilon) - f(\epsilon)\big] = -f'(0),
\end{aligned} \tag{7}$$

which is the required result. We have shown in (5) and (7) that the derivative of a delta function can be regarded formally, insofar as the delta function itself is formal, as a function producing the required effect by a well-defined mathematical operation. Note that we have not imposed any requirements on test functions such as fall-off conditions at infinity, since the Dirac delta function by definition already has compact support. Notice also in(7) how the Dirac delta function has sifted out the symmetric form of the derivative of f. It is natural, for field theoretical reasons which we will explain in more detail below, to apply the symmetric definition of the derivative when differentiating all functions. In the discretized version with spacing ϵ, one has

$$f'(x_n) = \lim_{\epsilon\to 0}\frac{1}{2\epsilon}\big[f(x_{n+1}) - f(x_{n-1})\big]. \tag{8}$$

2.3 Use of functional derivatives in field theory

We have defined the derivative of a delta function of x, but what about the spatial derivative of $\delta^{(3)}(0)$? Our interpretation will be such as to treat $\delta^{(3)}(0)$ as a (infinite) numerical constant, thus $\partial_j \delta^{(3)}(0) = 0$.[2] Such quantities will arise repeatedly in the analysis of the Hamiltonian constraint of quantum gravity in the Schrödinger representation, and are due to taking multiple functional derivatives evaluated at the same spatial point. This is a nonconventional interpretation, as strictly speaking one typically integrates delta functions against a test function $N(x)$ in order to try to make sense of such an expression as

$$\frac{\delta}{\delta\phi(x)}\frac{\partial\phi(y)}{\partial y} \equiv \frac{\partial}{\partial y}\delta^3(x-y). \tag{9}$$

One then writes, upon taking account of the fall-off conditions imposed upon $N(x)$,

$$\frac{\delta}{\delta\phi(x)}\int d^3y\ N(y)\frac{\partial\phi(y)}{\partial y} \equiv -\frac{\partial N(x)}{\partial x}. \tag{10}$$

However, when $x = y$ in (9), the the interpretation (10) in terms of distributions and test functions is not so clear. It seems more natural to conform to the functional definition as provided, making the identification

$$\frac{\delta}{\phi(x)}\Big[\frac{\partial}{\partial x^j}\phi(x)\Big] = \frac{\partial}{\partial x^j}\Big[\frac{\delta\phi(x)}{\delta\phi(x)}\Big] = \partial_j\delta^{(3)}(0) \equiv 0. \tag{11}$$

It may appear counterintuitive to interpret (17) the way it reads, namely that the field $\phi(x)$ and its spatial gradients $\partial\phi(x)$ at the same points can be regarded as independent variables.[3] Perhaps an analogy to motivate this notion is in order.

Consider the Lagrangian for a general system, being a functional of the fields and its derivatives

$$I = I(\phi, \partial\phi) = \int_M d^4x L[\phi(x), \partial\phi(x)]. \tag{12}$$

The Euler-Lagrange equations of motion follow from requiring the action to be stationary against independent variations of the fields. One varies the action with respect to the functional dependence of the Lagrangian upon the fields of the theory, which is the same at each point. In other words,

[2] This is a different interpretation to that presented in [5], in which it is argued that $\delta^{(3)}(0) = 0$, essentially as a consistency condition on the canonical quantization relations of metric gravity.

[3] Equation (17) carries the implicit assumption that spatial derivatiation and functional differentiation commute with one another.

any function of x for all x can be substituted in for $\phi(x)$ and the resulting action computed to give a number. Varying the action,

$$\delta I = \int_M d^4x \Big[\frac{\partial L}{\partial \phi(x)} \delta\phi(x) + \frac{\partial L}{\partial \phi_{,\mu}(x)} \delta\Big(\frac{\partial \phi(x)}{\partial x^\mu} \Big) \Big]. \tag{13}$$

We have maintained the position dependence of the fields in (12) explicit to signify that the fibre bundle structure consisting of the base space x with fibres $\phi(x)$ is in a certain sense trivializable. $\phi(x)$ can be regarded as a function independent of x at the point x when it is varied from one function to the next. The variable x then becomes a label.

Before one can proceed to the next step from (13), namely to integrate by parts to obtain the classical equations of motion, one must consider a detail often taken for granted in field theory. That is the question of commutativity of functional variation with partial differentiation. It is assumed that $\big[\delta, \partial\big] = 0$ which allows one to progress to the next step, in precise terms namely that functional variation in the functional space of fields at a fixed point commutes with spatial variation in the space of positions for a fixed function. Taking this into account one has

$$\begin{aligned} \delta I &= \int_M d^4x \Big[\frac{\partial L}{\partial \phi(x)} \delta\phi(x) + \frac{\partial}{\partial x^\mu} \Big(\frac{\partial L}{\partial \phi_{,\mu}(x)} \delta\phi(x) \Big) - \delta\phi(x) \Big(\frac{\partial}{\partial x^\mu} \frac{\partial L}{\partial \phi_{,\mu}} \Big) \Big] \\ &= \int_{\partial M} d^3x \; n^\mu \frac{\partial L}{\partial \phi_{,\mu}(x)} \delta\phi(x) + \int_M d^4x \; \delta\phi(x) \Big[\frac{\partial L}{\partial \phi(x)} - \partial_\mu \frac{\partial L}{\partial \phi_{,\mu}(x)} \Big] \end{aligned} \tag{14}$$

Only after these operations have been carried out[4] can one solve the classical equations of motion for $\phi(x)$, explicitly as a function of x subject to appropriate boundary conditions. In this case, one can find the gradients $\partial_\mu \phi(x)$ as well explicitly as a function of x. If the relation $Y = \phi(x)$ is locally inverted to find $x = \phi^{-1}(Y)$, then this can be substituted into the gradient to find

$$\phi'(x) = (\partial\phi)[x] = (\partial\phi)\big[\phi^{-1}(Y)\big]. \tag{15}$$

and the quantity $\partial\phi$ is explicitly a function of ϕ for a particular function $\phi(x)$ and they are no longer independent variables. However, there is no contradiction.

The operations carried out in order to obtain this relationship linking ϕ and $\partial\phi$ were successive restrictions upon the configuration space variables such that a unique classical solution could be obtained. There are two main differences in quantum field theory, and in particular in quantum gravity:
(i) In the quantum theory the evolution of the field is not deterministic as in the classical equations of motion. Any arbitrary function can be substituted

[4] With the appropriate bounday terms set to zero.

into the action, even funtions not satisfying the classical equations of motion, including functions which are not differentiable. The only restriction is that the function be continuous and have a well-defined value at each point of manifold of positions Σ. So in the space of functions, there is no apriori relation between ϕ and $\partial\phi$. In fact, the calculus of variations formalism has been extended to include functionals of higher derivatives, treating them each as independent variables. Hence from a starting action of the form $S = S[\phi, \phi_x, \phi_{xx}, \dots]$, where the subscript x denotes derivatives with respect to the variable x, one obtains

$$\frac{\delta S}{\delta\phi(x)} = \frac{\partial L}{\partial\phi} - \sum_n \frac{\partial^n}{\partial x^n}\Big(\frac{\partial L}{\partial\phi_{x\dots x}}\Big) = 0 \tag{16}$$

(ii) In quantum gravity, a constrained diffeomorphism invariant theory unlike the usual field theories, the processes of functional and spatial variation commute, however the processes of functional and time variation in general do not. This property provides a method to address the problem of time, which does not have a counterpart in ordinary field theory. These properties will be of great utility in our approach to the quantization of gravity.

3 Relative commutativity of functional variation and spacetime variation

3.1 Functional versus spatial variation

To make more precise the commutative relationship of spatial to functional differentiation, we will now see the utility of the symmetric definition of the derivative (8) when working with field theory and in particular, with quantum gravity. Let us compute the functional derivative of the spatial derivative of $\phi(x)$ at x. In order to visualize this procedure, which acts on infinite dimensional spaces, it is convenient to discretize space into intervals of length a. This can be justified by consideration, for example, of the predictions of loop quantum gravity which indicate that spacetime on a quantum level is discrete on the scale of the Planck length l_{Pl}, rather than continuous. So one has, applying the field theory relations to the discretized version of (17) at the point $\boldsymbol{x} \equiv \boldsymbol{x}_n$,

$$
\begin{aligned}
&\frac{\delta}{\phi(\boldsymbol{x},t)}\Big[\frac{\partial}{\partial x^j}\phi(\boldsymbol{x},t)\Big] \\
&= \frac{\delta}{\delta\phi(\boldsymbol{x}_n,t)}\lim_{a\to 0}\frac{1}{2a}\big[\phi(\boldsymbol{x}_{n+1},t)-\phi(\boldsymbol{x}_{n-1},t)\big] \\
&= \lim_{a\to 0}\frac{1}{2a}\Big[\frac{\delta\phi(\boldsymbol{x}_{n+1},t)}{\delta\phi(\boldsymbol{x}_n,t)}-\frac{\delta\phi(\boldsymbol{x}_{n-1},t)}{\delta\phi(\boldsymbol{x}_n,t)}\Big] \\
&= \lim_{a\to 0}\frac{1}{2a}\big[\delta(\boldsymbol{x}_{n+1}-\boldsymbol{x}_n)-\delta(\boldsymbol{x}_n-\boldsymbol{x}_{n-1})\big]. \qquad (17)
\end{aligned}
$$

Under the assumption that space is discrete, regardless of the spacing a, (17) vanishes. So one is free to make the spacing arbitrarily smaller than the Planck length scale $a << l_{Pl}$ and one would still have the same result. Therefore we will assume that functional and partial derivarives at the same point commute in the continuum limit, since the partial derivative of a function at a point depends upon the value of the function at adjacent separated points.

One may repeat the above exercise in the continuum limit, applying the definition of the functional derivative. Let us evaluate the functional and spatial derivatives of a function $F[\phi(x)]$ for both sequences. First, taking the spatial derivative of the functional derivative,

$$
\begin{aligned}
\frac{\partial}{\partial x}\Big[\frac{\delta F[\phi(x)]}{\phi(y)}\Big] &= \frac{\partial}{\partial x}\lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big(F[\phi(x)+\epsilon\delta(x-y)]-F[\phi(x)]\Big) \\
&= \frac{\partial}{\partial x}\lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big(F[\phi(x)]+\epsilon\delta(x-y)F'[\phi]+\cdots-F[\phi(x)]\Big). \qquad (18)
\end{aligned}
$$

All terms but the first order term in ϵ vanish, yielding

$$
\frac{\partial}{\partial x}\Big[\frac{\delta F[\phi(x)]}{\phi(y)}\Big] = \frac{\partial}{\partial x}\Big[\delta(x-y)F'[\phi]\Big] = \delta(x-y)F''[\phi]\frac{\partial\phi}{\partial x}+F'[\phi]\frac{\partial}{\partial x}\delta(x-y), \qquad (19)
$$

where we have applied the chain rule to the first term on the right hand side of (19). Prior to performing the differentiations in the opposite order one notes the chain rule

$$
\frac{\delta}{\delta\phi(y)}\Big[\frac{\partial F[\phi(x)]}{\partial x}\Big] = \frac{\delta}{\delta\phi(y)}\Big[F'[\phi]\frac{\partial\phi(x)}{\partial x}\Big] \qquad (20)
$$

as the rule for differentiating a function of a function with respect to its position dependence. Continuing with the expansion in (20), only the terms linear in ϵ prior to cancellation survive

$$\frac{\delta}{\delta\phi(y)}\Big[\frac{\partial F[\phi(x)]}{\partial x}\Big]$$
$$= \frac{1}{\epsilon}\lim_{\epsilon\to 0}\Big(F'\big[\phi(x)+\epsilon\delta(x-y)\big]\frac{\partial}{\partial x}\big(\phi(x)+\epsilon\delta(x-y)\big)+\cdots - F'[\phi(x)]\frac{\partial\phi(x)}{\partial x}\Big)$$
$$= F'[\phi]\frac{\partial}{\partial x}\delta(x-y)+F''[\phi]\delta(x-y)\frac{\partial\phi(x)}{\partial x}, \quad (21)$$

which is the same as (19). So we see that functional differentiation and spatial differentiation, even with respect to different points, do in fact commute.

One then asks the question as to whether functional and spatial integration commute as well. This follows from the algebraic properties of the integral. Consider the integral

$$\int_\Gamma \delta\phi \int_\Sigma F[\phi(x)]. \quad (22)$$

The notation in (22) signifies that we wish to integrate a function of position over the space of functions ϕ. This implies that the function $F = F(x)$, seen as a function of ϕ, is directly integrable into its antiderivative $G(x)$ such that $F(x) = \frac{dG(x)}{dx}$. Let us assume that the antiderivative G exists. One can see, by discretizing the spatial manifold Σ, that

$$\int_\Gamma \delta\phi \int_\Sigma d^3x F[\phi(x)] = \int_\Gamma \delta\phi \sum_n F[\phi(\boldsymbol{x}_n)]$$
$$= \sum_n \int_{G_1}^{G_2} \delta\phi(\boldsymbol{x}_n)F[\phi(\boldsymbol{x}_n)] = \sum_n \Big[G[\phi(\boldsymbol{x}_n]\Big]_{G_1(\boldsymbol{x}_n)}^{G_2(\boldsymbol{x}_n)}$$
$$= \int_\Sigma d^3x G_2(x) - \int_\Sigma d^3x G_1(x) \quad (23)$$

3.2 Functional versus time variation

We have shown in (17) that spatial derivatives commute with functional derivatives $[\partial_i, \delta] = 0$. But the question arises as to whether the same is true of time derivatives. First let us compute the result when the time derivative is evaluated last.

$$\frac{\partial}{\partial t}\Big[\frac{\delta\phi(\boldsymbol{y},t)}{\delta\phi(\boldsymbol{x},t)}\Big] = \frac{\partial}{\partial t}\Big(\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y})\Big) = 0. \quad (24)$$

For (24) we have made use of the equal-time commutation relations as well as the fact that spatial position $\boldsymbol{x}$ and time t are independent variables. Now let us perform the sequence in reverse.

$$\frac{\delta}{\phi(\boldsymbol{y},t)}\Big[\frac{\partial}{\partial t}\phi(\boldsymbol{x},t)\Big] \tag{25}$$

In the square brackets in (25) we must hold spatial position fixed and differentiate with respect to time. Discretizing the time interval,

$$\begin{aligned}\frac{\delta}{\phi(\boldsymbol{y},t)}\Big[\frac{\partial}{\partial t}\phi(\boldsymbol{x},t)\Big] &= \frac{\delta}{\delta\phi(\boldsymbol{y},t)}\lim_{\epsilon\to 0}\frac{1}{2\epsilon}\big[\phi(\boldsymbol{x},t_{n+1})-\phi(\boldsymbol{x},t_{n-1})\big]\\ &= \lim_{\epsilon\to 0}\frac{1}{2\epsilon}\Big[\frac{\delta\phi(\boldsymbol{x},t_{n+1})}{\delta\phi(\boldsymbol{y},t)}-\frac{\delta\phi(\boldsymbol{x},t_{n-1})}{\delta\phi(\boldsymbol{y},t)}\Big]\end{aligned} \tag{26}$$

Immediately in (26) arises the problem of how to interpret $\delta\phi(\boldsymbol{x},t_{n\pm 1})/\delta\phi(\boldsymbol{y},t_n)$. We cannot use (2), since the commutation relations are defined only at equal times. If we had a completely covariant description of nature in which space and time were on equal footing, then the commutation relations might read

$$\big[\phi(\boldsymbol{x},t),\pi(\boldsymbol{y},t')\big] = i\hbar\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y})\delta(t-t'). \tag{27}$$

But (27) restricted to equal times would read

$$\big[\phi(\boldsymbol{x},t),\pi(\boldsymbol{y},t)\big] = i\hbar\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y})\delta(0), \tag{28}$$

which is in contradiction with (2). So it would seem to imply that time and space are not necessarily exactly the same, at least on the quantum level.[5]

The most direct way to take into account the difference in times in (26) within the framework of quantum mechanics is to evolve the fields to equal times via the Heisenberg picture.

$$\phi(\boldsymbol{x},t) = e^{\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}(t')}\phi(\boldsymbol{x},t_0)e^{-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}(t')}. \tag{29}$$

Substituting into (26) for infinitesimal times,

$$\frac{\delta}{\phi(\boldsymbol{y},t)}\Big[\frac{\partial}{\partial t}\phi(\boldsymbol{x},t)\Big] = \frac{\delta}{\delta\phi(\boldsymbol{y},t)}\lim_{\epsilon\to 0}\frac{1}{2\epsilon}\big[e^{\frac{i\epsilon\hat{H}}{\hbar}}\phi(\boldsymbol{x},t)e^{-\frac{i\epsilon\hat{H}}{\hbar}}-e^{-\frac{i\epsilon\hat{H}}{\hbar}}\phi(\boldsymbol{x},t)e^{\frac{i\epsilon\hat{H}}{\hbar}}\big]. \tag{30}$$

[5] We do not make any inferences regarding the general covariance of Einstein's decription of space-time in this exerpt, but merely point out that one by definition singles out time as special by defining such things as equal time commutations, and also for other things such as the 3+1 ADM decomposition and for defining quantum gravitational wavefunctionals on spatial hypersurfaces.

Since functional variation with respect to the fields does not commute with the Hamiltonian, the most direct way to evaluate (30) is to expand the commutators. Hence,

$$e^{\frac{i\epsilon\hat{H}}{\hbar}}\phi(\boldsymbol{x},t)e^{-\frac{i\epsilon\hat{H}}{\hbar}} = \phi(\boldsymbol{x},t) + \frac{i}{\hbar}\epsilon\big[\hat{H},\phi(\boldsymbol{x},t)\big] + (\frac{i}{\hbar}\epsilon)^2\big[\hat{H},\big[\hat{H},\phi(\boldsymbol{x},t)\big]\big] + ... \quad (31)$$

Substituting into (30), the zeroth order term cancels out and we have

$$\frac{\delta}{\phi(\boldsymbol{y},t)}\Big[\frac{\partial}{\partial t}\phi(\boldsymbol{x},t)\Big] = \frac{2i}{\hbar}\frac{\delta}{\phi(\boldsymbol{y},t)}\lim_{\epsilon\to 0}\big[\hat{H},\phi(\boldsymbol{x},t)\big] + O(\epsilon) = \frac{2}{\hbar^2}\big[\hat{\pi}(\boldsymbol{y},t),\big[\hat{H},\phi(\boldsymbol{x},t)\big]\big] \quad (32)$$

where in (32) the $O(\epsilon)$ terms have vanished in the $\epsilon \to 0$ limit and we have made use of the equal-time commutation relations in the last line. In order to assess the relative commutativity of functional versus time variation, one must then ascertain under what conditions the right hand side of (32) vanishes. Clearly, for Hamiltonians for which there are no ordering ambiguities due to products of coordinates with momenta, the right hand side of (32) is zero. This encompasses all Hamiltonians that one is typically likely to encounter in usual nongravitational field theories on Minkowski spacetimes, such as can be decomposed into a kinetic term involving only momenta and potential terms involving only the fields.[6] For the Klein–Gordon scalar field in Minkowski spacetime with self-interaction potential $V(\phi)$, one has

$$\Big[\pi,\big[\frac{\pi^2}{2} + \frac{1}{2}\phi(\nabla^2 + m^2)\phi + V(\phi),\phi\big]\Big] = -i\hbar[\pi,\pi] = 0. \quad (33)$$

Equation (33) indicates that the results of (24) and (25) for this case are equal to each other, or that functional variation and time variation commute with each other, at least for the Klein–Gordon scalar field on Minkowski spacetime.

However, let us see what happens in the case of quantum gravity, a constrained diffeomorphism invariant, gauge invariant theory. For quantum gravity in Ashtekar variables, taking as an example the scenario of pure gravity alone with cosmological term the following commutation relations amongst the components of the Ashtekar potential A_i^a and its conjugate momentum, the densitized triad, $\widetilde{\sigma}_a^i$ are given by

$$\big[A_i^a(\boldsymbol{x},t),\frac{i}{G}\widetilde{\sigma}_b^j(\boldsymbol{y},t)\big] = i\delta_i^j\delta_b^a\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}). \quad (34)$$

The Hamiltonian density is then given, omitting any matter contributions for simplicity,

[6] This includes velocity-independent potentials.

$$H = \int_\Sigma d^3x \Big[\frac{\Lambda}{6}\epsilon_{ijk}\epsilon_{abc}\widetilde{\sigma}^i_a\widetilde{\sigma}^j_b\widetilde{\sigma}^k_c + \epsilon_{ijk}\epsilon^{abc}\widetilde{\sigma}^i_a\widetilde{\sigma}^j_b B^k_c\Big]. \tag{35}$$

In evaluating (32) one has, modulo Dirac delta functions,

$$\begin{aligned}
&\Big[\Big[\frac{\Lambda}{6}\epsilon_{ijk}\epsilon_{abc}\widetilde{\sigma}^i_a\widetilde{\sigma}^j_b\widetilde{\sigma}^k_c + \epsilon_{ijk}\epsilon^{abc}\widetilde{\sigma}^i_a\widetilde{\sigma}^j_b B^k_c, A^{d'}_{l'}\Big], \widetilde{\sigma}^n_f\Big] \\
&= \Big[\frac{\lambda}{2}\epsilon_{ijk}\epsilon^{abc}\widetilde{\sigma}^i_a\widetilde{\sigma}^j_b + 2\epsilon_{il'k}\epsilon^{ad'c}\widetilde{\sigma}^i_a B^k_c, \widetilde{\sigma}^n_f\Big] \\
&= 2\epsilon_{il'k}\epsilon^{ad'c}\widetilde{\sigma}^i_a\Big[\epsilon^{lkm}\partial_l A^c_m + \frac{1}{2}\epsilon^{klm}f^{cde}A^d_l A^e_m, \widetilde{\sigma}^n_f\Big] \\
&= \epsilon_{il'k}\epsilon^{ad'c}\epsilon^{kln}f^{cdf}\widetilde{\sigma}^i_a\big(A^d_l\delta^n_m\delta^e_f + A^e_m\delta^d_f\delta^n_l\big) = 2\epsilon_{il'k}\epsilon^{ad'c}\epsilon^{kln}f^{cdf}\widetilde{\sigma}^i_a A^d_l \neq 0
\end{aligned} \tag{36}$$

So we see that although functional variation commutes with spatial variation, it in general does not commute with time variation. The interpretation is that functional variation of fields for certain theories[7] includes time evolution of the fields. This effect sheds some light on the problem of time in quantum gravity, and a possible approach to its resolution.

3.3 Coincidence limit of delta functions

In the quantization of gravity in the Schrödinger representation we will need to take repeated functional derivatives. The functional derivative of a functional $H[\eta]$ is given, when the functional is the integral over all space

$$H[\eta] = \int_\Sigma d^3x\ G[\eta(x)] \tag{37}$$

for some function $G(x)$ is given by

$$\begin{aligned}
\frac{\delta}{\delta\eta(x)}H[\eta] &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big[\int_\Sigma d^3x' G\big[\eta(x') + \epsilon\delta^3(x)\big] - \int_\Sigma d^3x\ G[\eta(x)]\Big] \\
&= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big[\int_\Sigma d^3x' G\big[\eta(x')\big] + \epsilon\int_\Sigma d^3x' G(x)\delta^{(3)}(x-x') + ... - \int_\Sigma d^3x\ G[\eta(x)]\Big] \\
&= G[\eta(x)].
\end{aligned} \tag{38}$$

So we see that the functional derivative of the integral over three-space contains one degree of singularity less than the functional itself, having been reduced to the value at a point. The singularity is then cancelled out by the

[7] Particularly quantum gravity in Ashtekar variables, an effect we anticipate to be even more pronounced when coupled to matter fields

process of integration of the density. However, when the functional itself is explicitly a function of x, ultraviolet singularities result from the procedure. The functional derivative of a function $F[\eta(x)]$ evaluated at the same point x at equal times is given by

$$\frac{\delta}{\delta\eta(x)}F[\eta(x)] = \lim_{\epsilon\to 0}\frac{F[\eta(x)+\epsilon\delta^{(3)}(x)]-F[\eta(x)]}{\epsilon}$$
$$= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\big(F[\eta(x)]+\epsilon\delta^{(3)}(x)F'[\eta]+...-F[\eta(x)]\big) = F'[\eta]\delta^{(3)}(x) \qquad (39)$$

Our interpretation of this expression is that the functional relationship between $F[\eta(x)]$ and $\eta(x)$ at the point x has been exposed and the quantity $F'[\eta]$ is an exemplification of that relationship at the point x, a label which can be suppressed. The coefficient $\delta^{(3)}(x)$ ensures that this 'relationship' has compact support, valid only at the origin $x = 0$ but trivial (devoid of physical content) otherwise. We invoke the notation $F'[\eta]\delta^{(3)}(0)$ to highlight that the nontrivial physical content in this apparently ill-defined quantitity is transported to each point in space. To illustrate that it does in fact have physical content, let us take another functional derivative.

$$\frac{\delta}{\delta\eta(x)}\big(F'[\eta(x)]\delta^{(3)}(x)\big) = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big(F'[\eta(x)+\epsilon\delta^{(3)}(x)]\delta^{(3)}(x)-F'[\eta(x)]\delta^{(3)}(x)\Big)$$
$$= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big(F'[\eta(x)]+\epsilon\delta^{(3)}(x)F''[\eta]\big)\big(\delta^{(3)}(x)\big)+...-F'[\eta(x)]\delta^{(3)}(x)\Big)$$
$$= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big(F'[\eta]\delta^{3}(x)+\epsilon F''[\eta](\delta^{(3)}(x))^2+...-F'[\eta]\delta^{(3)}(x)\Big)$$
$$= F''[\eta](\delta^{(3)}(x))^2 \qquad (40)$$

Again, we interpret that due to the compact support of the $\delta^{(3)}(x)$ distribution, the operation contains nontrivial physical context only at the point $x = 0$ while the functional relationship $F[\eta]$ between F and η is maintained irrespective of the value of x. We illustrate this by the notation

$$F''[\eta](\delta^{(3)}(x))^2 \longrightarrow F''[\eta](\delta^{(3)}(0))^2. \qquad (41)$$

Since this operation could have been performed at any arbitrary point x yielding the same functional form and the origin of the coordinate system can be arbitrarily chosen, the functional relationship between $F[\eta]$ and η, which is independent of position, can be exploited to harness the encoded physics everywhere in Σ.[8] It is this property of which we make use in the analysis of the Hamiltonian constraint. Note due to the functional independence of

[8]The claim is that this subtlety can be exploited to treat the full theory of quantum gravity in a certain sense in direct analogy to minisuperspace. The functional relationship between $F[\eta]$ and η in the space of fields Γ is the same in each case, and the dependence

$\delta^{(3)}(x)$ upon $\eta(x)$, that functional derivatives can be taken to arbitrarily high order, producing arbitrarily singular products of delta functions.

Having defined the commutations relations and the process of functional differentiation, we will *not* perform regularization procedures in order to get rid of any infinities that result. This is because it is not guaranteed that we will always, or ever, be fortunate to obtain answers independent of the particular regularization prescription, for which there are be infinitely many to test. Granted, this in no way relieves us of the requirement to deliver finite results in quantum gravity, but we shall not make the use of regulators in order to do so. Regularization may have worked in ordinary field theory, which is more tractable and for which there are complementary regularization procedures for obtaining and double-checking the sensibility of results. However, for quantum gravity it is not so clear and the same luxuries are not available. In order to address quantize gravity we will avoid regularizations to the maximum extend feasible and attempt to extract the nontrivial physical content from the infinties themselves and from their coefficients. We have made our quantum mechanical bed by defining the canonical quantum relations, so we must lie in it.

4 Introduction: The Hamiltonian constraint and the semiclassical-quantum correspondence

We would like to solve the quantized version of the classical Hamiltonian constraint, given by

$$\frac{\Lambda}{6}\epsilon_{ijk}\epsilon^{abc}\widetilde{\sigma}^i_a\widetilde{\sigma}^j_b\widetilde{\sigma}^k_c + \epsilon_{ijk}\epsilon^{abc}\widetilde{\sigma}^i_a\widetilde{\sigma}^j_b B^k_c + G\Omega\big[A^a_i, \phi^\alpha, \pi_\alpha, \widetilde{\sigma}^i_a\big] = 0. \tag{42}$$

The Hamiltonian constraint arises from the classical equation of motion for the lapse density $\underline{N}$, given by

$$\frac{\delta I_{Ash}}{\delta \underline{N}(x)} = (H_{tot}) = 0 \ \forall x \ in \ M \tag{43}$$

which holds at all points in the spacetime manifold $M = \Sigma \times R$, where I_{Ash} is the action for general relativity in Ashtekar variables coupled to matter fields $\phi^\alpha(x)$. The diffeomorphism constraint arises from the classical equation of motion for the shift vector N^i

upon spatial position $\boldsymbol{x}$ in Σ has been 'factored' out. We exploit this subtlety in our quantization programme for the full theory of quantum gravity, since it is precisely in this theory that one must consider the effects of 'freezing' spatial position in order to implement the constraints. As we have shown, one cannot 'freeze' time as well.

$$\frac{\delta I_{Ash}}{\delta \underline{N}^i(x)} = (H_i)_{tot} = 0 \ \forall x \ in \ M, \tag{44}$$

and the Gauss' law constraint arises from the classical equation of motion for the $SU(2)_-$ rotation angle $\theta^a = A_0^a$

$$\frac{\delta I_{Ash}}{\delta \theta^a(x)} = (G_a)_{tot} = 0 \ \forall x \ in \ M. \tag{45}$$

First, the classical equation of motion for the densitized shift function (43), (42) must be quantized. This equation of motion must hold at all spacetime points (x,t) in the 4-manifold $M = \Sigma \times R$. However, in order to evaluate its quantized form one must make use of the canonical quantization relations for the dynamical variables. By the usual rules of quantum field theory one is restricted to the equal-time commutation relations [2], which restricts one to a particular spatial hypersurace Σ when promoting the classical fields into quantum operators acting on the state $\left|\Psi\right\rangle$ via the Dirac quantization procedure [7]. One has, upon promoting Poisson brackets to commutators,

$$\begin{aligned} \left[A_i^a(\boldsymbol{x},t), \frac{i}{G}\widetilde{\sigma}_b^j(y,t)\right]_{PB} &= \delta_i^j \delta_b^a \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}) \\ \longrightarrow \left[A_i^a(\boldsymbol{x},t), \frac{i}{G}\widetilde{\sigma}_b^j(\boldsymbol{y},t)\right] &= i\delta_i^j \delta_b^a \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}) \end{aligned} \tag{46}$$

for the gravitational variables and

$$\left[\phi^\alpha(\boldsymbol{x},t), \pi_\beta(\boldsymbol{y},t)\right]_{PB} = \delta_\beta^\alpha \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}) \longrightarrow \left[\phi^\alpha(\boldsymbol{x},t), \pi_\beta(\boldsymbol{y},t)\right] = i\delta_\beta^\alpha \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}) \tag{47}$$

for the matter variables. In order to solve the quantized Hamiltonian constraint one must put (46) and (47) into the Schrödinger representation. Since one is restricted by this field-theoretical quantization property to equal times, the quantized Hamiltonian constraint applies at all spatial points $\boldsymbol{x}$ in a given spatial hypersurface Σ_t corresponding to a given time t. This appears to be related to the problem of time in quantum gravity in that is no inherent mechanism to evolve the quantum state $\left|\Psi_{GKod}\right\rangle$ from the hypersurface Σ_t at time t to the hypersurface $\Sigma_{t+\delta t}$ at time $t+\delta t$. However, since the classical Hamiltonian constraint (42) must hold for all times t as a classical equation of motion, the problem of time is circumvented. It is circumvented because the classical constraint corresponding to each time t must be quantized and solved. This implies that the classical evolution in time corresponds to a quantum evolution in time,[9] since the functional form of the constraints is preserved on each spatial hypersurface Σ_t.

[9]This property is reminiscent of a new principle which we will make use of to construct quantum states of gravity namely, the principle of the semiclassical-quantum correspondence (SQC). Our assessment is that this principle implies the existence of special states in constrained field theories.

So one is free to transform the quantized Hamiltonian constraint into the Schrödinger representation by choosing a polarization in which the wave function is a functional of the configuration space variables via the replacements, for a given spatial hypersurface,

$$\hat{A}_i^a(\boldsymbol{x},t)\big|\Psi_{GKod}[A,\phi]\big\rangle = A_i^a(\boldsymbol{x},t)\big|\Psi_{GKod}[A,\phi]\big\rangle;$$
$$\hat{\tilde{\sigma}}_a^i(\boldsymbol{x},t)\big|\Psi_{GKod}[A,\phi]\big\rangle = \hbar G\frac{\delta}{\delta A_i^a(\boldsymbol{x},t)}\big|\Psi_{GKod}[A,\phi]\big\rangle; \tag{48}$$

for the gravitational dynamical variables, and

$$\hat{\phi}^\alpha(\boldsymbol{x},t)\big|\Psi_{GKod}[A,\phi]\big\rangle = \phi^\alpha\big|\Psi_{GKod}[A,\phi]\big\rangle;$$
$$\hat{\pi}_\alpha(\boldsymbol{x},t)\big|\Psi_{GKod}[A,\phi]\big\rangle = -i\hbar\frac{\delta}{\delta\phi^\alpha(\boldsymbol{x},t)}\big|\Psi_{GKod}[A,\phi]\big\rangle \tag{49}$$

for the gravity-coupled matter dynamical variables. We have chosen the name Ψ_{GKod} for our wavefunctions in order to signify the generalized Kodama states, the significance of which we will explain in greater detail in separate works. For now, consider the term $GKod$ as just a label. Then all that remains in the solution of the quantized Hamiltonian constraint $\hat{H}_{tot}\big|\Psi_{GKod}\big\rangle = 0$ in the Schrödinger representation is to make sense of the singular terms $\delta^{(3)}(0)$ which arise from quantum operator products evaluated at the same spatial point $\boldsymbol{x}$ at equal times. The quantized counterpart to (42), reads

$$0 = \hat{H}\big|\Psi_{Gkod}\big\rangle = \Bigg[\frac{\Lambda}{6}\hbar^3G^3\epsilon^{abc}\epsilon_{ijk}\frac{\delta}{\delta A_i^a(x)}\frac{\delta}{\delta A_j^b(x)}\frac{\delta}{\delta A_k^c(x)}$$
$$+\hbar^2G^2\epsilon^{abc}\epsilon_{ijk}B_a^i\frac{\delta}{\delta A_j^b(x)}\frac{\delta}{\delta A_k^c(x)} + G\hat{\Omega}\big[A_i^a(x)\phi(x),\frac{\delta}{\delta\phi(x)},\frac{\delta}{\delta A_i^a(x)}\big]\Bigg]\big|\Psi_{Gkod}\big\rangle$$
$$= \Big(\sum_n(\hbar G\delta^{(3)}(0))^n q_n\Big)\big|\Psi_{Gkod}\big\rangle \tag{50}$$

for some q_n. Equation (50) then requires that $q_n = 0$ for all n.

4.1 A bit of notation

We will need to make use of a few identities in dealing with the Ashtekar variables in quantum gravity. First, we note that three dimensions is special in that the SU(2) group has three generators with structure constants $f_{abc} \propto \epsilon_{abc}$ similar to the epsilon tensor ϵ_{ijk} for Cartesian space. This

allows us to regard the Ashtekar variables as 3 by 3 matrices. We will use interchangeably the symbols f_{abc} and ϵ_{abc} when refering to the SU(2) structure constants. The Ashtekar magnetic field B^i_a is given by $B^k_c = \epsilon^{klm}(\partial_l A^c_m + (1/2) f^{cde} A^d_l A^e_m)$. We have the following additional identities

$$\begin{aligned}
\frac{\delta B^k_c(\boldsymbol{x},t)}{\delta A^a_i(\boldsymbol{y},t)} &= \frac{\delta}{\delta A^b_j(\boldsymbol{y},t)}\Big[\epsilon^{klm} D_l A^c_m(\boldsymbol{x},t)\Big] \\
= \epsilon^{klm}\frac{\delta}{\delta A^a_i(\boldsymbol{y},t)}\Big[\frac{\partial}{\partial x^l} A^c_m(\boldsymbol{x},t) &+ \frac{1}{2} f^{cde} A^d_l(\boldsymbol{x},t) A^e_m(\boldsymbol{x},t)\Big] \\
&= \epsilon^{ikl}[\delta_{ac}\partial_l + f_{ace} A^e_l(\boldsymbol{x},t)\Big]\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}) \\
&\equiv \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}) D^{ik}_{ac}. \qquad (51)
\end{aligned}$$

Note that in evaluating functional derivatives we are restricted to performing operations on quantities evaluated at the same time t, e.g. on the same spatial 3-surface Σ_t in order to make use of the equal-time quantum commutation relations. For $\boldsymbol{x} = \boldsymbol{y}$ in (51), one must have $\delta^{(3)}(0) D^{ik}_{ac} = \epsilon^{ikl}\epsilon_{ace} A^e_l$, due to the commutativity of functional with partial differentiation. Moving on to the third functional derivative,

$$\begin{aligned}
\frac{\delta}{\delta A^a_i(\boldsymbol{x},t)}\frac{\delta}{\delta A^b_j(\boldsymbol{y},t)} B^k_c(\boldsymbol{z},t) &= \epsilon^{ijk} f_{abc}\delta^{(3)}(\boldsymbol{z}-\boldsymbol{x})\delta^{(3)}(\boldsymbol{z}-\boldsymbol{y}) \\
&\equiv \epsilon^{ijk}_{abc}\delta^{(3)}(\boldsymbol{z}-\boldsymbol{x})\delta^{(3)}(\boldsymbol{z}-\boldsymbol{y}). \qquad (52)
\end{aligned}$$

In the coincidence limit of (52) we have

$$\frac{\delta}{\delta A^a_i(\boldsymbol{x},t)}\frac{\delta}{\delta A^b_j(\boldsymbol{x},t)} B^k_c(\boldsymbol{x},t) = \epsilon^{ijk}_{abc}(\delta^{(3)}(0))^2. \qquad (53)$$

All functional derivatives higher than the second vanish, since ϵ^{ijk}_{abc} is a numerical constant. From now on we will suppress the position dependence of the variables when convenient and will insert the appropriate factors of $\delta^{(3)}(0)$ when necessary.

5 Ramifications of spacetime versus functional variation

5.1 Minisuperspace toy model

We will show how a quantum mechanical wavefunction $\Psi = \Psi[A(T), \phi(T)]$ as determined on the final hypersurface Σ_T at time T is independent of time derivatives of the fields living within M.

This can be more clearly seen by direct analogy to a simpler example in $0+1$ dimensional field theory. Define a functional $S = S(u, v)$ of two independent variables $u = u(t)$ and $v = v(t)$ which are each functions of a parameter t along a one-dimensional curve γ. The question is, under what conditions is the integral

$$S = \int_{t_0}^{T} dt\big(U\dot{u} + V\dot{v}\big) \tag{54}$$

independent of the velocities $\dot{u}$ and $\dot{v}$ as well as the histories of u and v along γ, where U and V are functionals of (u, v)? One obvious condition is that for which S in (54) is the integral of a total time derivative with U and V themselves being independent of the velocities. This is so due to the first-order nature of the integrand (54). Taking the time derivative of (54) yields

$$\frac{dS}{dt} = \dot{u}\Big(\frac{\partial S}{\partial u}\Big)\Big|_{v=const.} + \dot{v}\Big(\frac{\partial S}{\partial v}\Big)\Big|_{u=const.} = U(u,v)\dot{u} + V(u,v)\dot{v} \tag{55}$$

with the identifications $\partial S/\partial u = U$ at fixed v and $\partial S/\partial v = V$ at fixed u. Clearly U and V must be related by a condition of mixed partial derivatives in order to satisfy the conditions requested. Hence

$$\frac{\partial^2 S}{\partial u \partial v} = \frac{\partial^2 S}{\partial v \partial u} = \frac{\partial U}{\partial v} = \frac{\partial V}{\partial u}. \tag{56}$$

As long as (56) is satisfied, then S is the integral of a total time derivative and (54) can be deparametrized via $du = \dot{u}dt$, $dv = \dot{v}dt$ to yield

$$\begin{aligned} S = \int_{t_0}^{T} dt\big(U\dot{u} + V\dot{v}\big) &= \int_{u(t_0)}^{u(T)} U(u,v)du + \int_{v(t_0)}^{v(T)} V(u,v)dv \\ &= S[u(T), v(T)] - S[u(t_0), v(t_0)] \sim S(T) - S(t_0). \end{aligned} \tag{57}$$

The relevant features of this simple example are:(i) that the final form for S in (57) is obtained by integrating in the u direction for fixed v in the first term, and integration in the v direction for fixed u in the second term. Note that this integration is independent of the detailed time dependence or history of the functions $u(t), v(t)$ along γ and therefore the time dependence

can be arbitrarily chosen. (ii) The final result depends entirely on the values of the arguments u, v as defined at the endpoints of the one-dimensional curve γ, and also manifestly independent of any velocities $\dot{u}$ or $\dot{v}$. (iii) In light of the questions posed in the introduction, one may say that due to the time reparametrization invariance on the functional S, that time variation is indistinguishable from functional variations of the fields u and v. So while the dimension of the base space in this case may naively start at $Dim(u, v, t) = \infty^2 \otimes \infty$, the requirement that the fields u and v combine to produce a total derivative amounts to a collapse of the dimension to $Dim(u, v, t) = \infty^2$. Time has been 'absorbed' into the definition of the fields.

5.2 Application to the full theory

We are now ready to carry this simple minisuperspace analogy to the full theory by making the identifications $\gamma \to M$, $u \to A_i^a(\boldsymbol{x}, t)$, $v \to \phi(\boldsymbol{x}, t)$. Let us say that the quantum constraints of general relativity have been solved for the CDJ matrix elements Ψ_{ab} to the nine equations $C_{ab} = 0$ arising from the Dirac quantization procedure [8]. The next step then is to evaluate the starting action for the Ashtekar variables coupled to matter on the reduced phase space. The variable $\Psi_{ab} = \Psi_{ab}[A_i^a, \phi^\alpha]$ is known as the CDJ matrix, which can be considered as the transformation of the conjugate momentum $\widetilde{\sigma}_a^i$ into a new set of variables via the Ansatz

$$\widetilde{\sigma}_a^i(\boldsymbol{x}, t) = \Psi_{ae}(\boldsymbol{x}, t) B_e^i(\boldsymbol{x}, t) \tag{58}$$

The starting action in Ashtekar variables evaluated on the solution to the constraints is given by

$$iS = iS[A_i^a, \phi^\alpha] = \int_M \Big[(\hbar G)^{-1} \Psi_{ae} B_e^i \dot{A}_i^a + \frac{i}{\hbar} \pi \dot{\phi} \Big] \Big|_{C_{ab}(x)=0} \tag{59}$$

making use of the matter momentum eigenvalue π arising from the mixed partials condition. First we eliminate the time derivatives in (59). Note that S is a functional of two dynamical variables living on the spacetime manifold M. Write out the integral for the action

$$iS = \int_{t_0}^{T} dt \int_\Sigma d^3x \Big((\hbar G)^{-1} \Psi_{ae}(\boldsymbol{x}, t) B_e^i(\boldsymbol{x}, t) \dot{A}_i^a(\boldsymbol{x}, t) + \frac{i}{\hbar} \pi(\boldsymbol{x}, t) \dot{\phi}(\boldsymbol{x}, t) \Big) \tag{60}$$

and then interchange the order of spacetime integration in (60)[10]

$$iS = \int_\Sigma d^3x \int_{t_0}^T dt\Big((\hbar G)^{-1}\Psi_{ae}(\boldsymbol{x},t)B_e^i(x)\dot{A}_i^a(\boldsymbol{x},t) + \frac{i}{\hbar}\pi(\boldsymbol{x},t)\dot{\phi}(\boldsymbol{x},t)\Big) \quad (61)$$

Using the identities, suppressing the position dependence,

$$\begin{aligned} dA_i^a &= \frac{\partial A_i^a}{\partial t}dt + \frac{\partial A_i^a}{\partial x}dx + \frac{\partial A_i^a}{\partial y}dy + \frac{\partial A_i^a}{\partial z}dz; \\ d\phi &= \frac{\partial \phi}{\partial t}dt + \frac{\partial \phi}{\partial x}dx + \frac{\partial \phi}{\partial y}dy + \frac{\partial \phi}{\partial z}dz \end{aligned} \quad (62)$$

and the following identities involving differential forms

$$d^3x = dx \wedge dy \wedge dz; \quad dx \wedge dx = dy \wedge dy = dz \wedge dz = 0, \quad (63)$$

any contribution to (61) due to spatial gradients of $A_i^a(x)$ or of $\phi(x)$ automatically vanish. This is due to the fact that the top form in four-dimensional space M is the four form $dx \wedge dy \wedge dz \wedge dt$. See [10] for similar arguments by Rovelli in a covariant treatment of Hamiltonian mechanics using differential forms. The steps that follow can be seen as the projection of a covariant description onto a spacelike hypersurface, but should hold independently of whether the hypersurface is spacelike, timelike or null. Hence (61) can be simplified by noting that for four dimensional spacetime M,

$$\begin{aligned} dx \wedge dy \wedge dz \wedge dX_e^a\Psi_{ae} &= dx \wedge dy \wedge dz\Psi_{ae}\Big[\frac{\partial X_e^a}{\partial t}dt + \frac{\partial X_e^a}{\partial x}dx + \frac{\partial X_e^a}{\partial y}dy + \frac{\partial X_e^a}{\partial z}dz\Big] \\ &= dx \wedge dy \wedge dz \wedge dt\frac{\partial X_e^a}{\partial t}\Psi_{ae} = d^3x\ dt\dot{A}_i^a B_e^i\Psi_{ae} \end{aligned} \quad (64)$$

for the gravitational sector, and

$$\begin{aligned} dx \wedge dy \wedge dz\ \pi \wedge d\phi &= dx \wedge dy \wedge dz\pi\Big[\frac{\partial \phi}{\partial t}dt + \frac{\partial \phi}{\partial x}dx + \frac{\partial \phi}{\partial y}dy + \frac{\partial \phi}{\partial z}dz\Big] \\ &= dx \wedge dy \wedge dz \wedge dt\ \pi\frac{\partial \phi}{\partial t} = d^3xdt\ \pi\dot{\phi} \end{aligned} \quad (65)$$

for the matter sector. The left hand sides of (64) and (65) correspond to four-forms projected into two different four-dimensional spaces, different on

[10] We have assumed that space and time are independent variables in a second quantized theory, therefore any operations with respect to these variables, which take on the role of labels, must commute. We leave open for now the question as to whether time can be considered a dynamical variable as are the quantum fields.

the one hand since A_i^a and ϕ are two dynamically independent variables, the same space on the other hand since there is no other direction besides the time direction to project them into in a 3+1 dimensional spacetime M. This leads to the condition that

$$iS = \int_\Sigma d^3x \left((\hbar G)^{-1} \int_{A_i^a(\boldsymbol{x},t_0)}^{A_i^a(\boldsymbol{x},T)} \Psi_{ae}(\boldsymbol{x}) B_e^i(\boldsymbol{x}) dA_i^a(\boldsymbol{x}) + \frac{i}{\hbar} \int_{\phi(\boldsymbol{x},t_0)}^{\phi(\boldsymbol{x},T)} \pi(\boldsymbol{x}) d\phi(\boldsymbol{x}) \right) \quad (66)$$

Equation (66) can be written in the following notation, supressing the x dependence, to avoid cluttering the notation and to illustrate that the integration occurs in the functional space of fields for each fixed point $\boldsymbol{x}$ on the initial and final spatial hypersurfaces Σ_0 and Σ_T

$$iS = \int_\Sigma d^3x \left((\hbar G)^{-1} \int_{A_i^a(t_0)}^{A_i^a(T)} \Psi_{ae}[A,\phi] B_e^i \delta A_i^a + \frac{i}{\hbar} \int_{\phi(t_0)}^{\phi(T)} \pi[A,\phi] \delta\phi \right). \quad (67)$$

The assumption is that the processes of functional integration over the space of fields in (67) commutes with spatial integration over the manifold Σ_T and Σ_{t_0}. This can be seen more clearly by discretizing 3-dimensional space Σ as is often done in Feynman path integrals [11]. Suppressing the dependence on T and t_0,

$$iS = \sum_{\boldsymbol{x_n}} \left[(\hbar G)^{-1} \int_{A_i^a(t_0)}^{A_i^a(T)} \Psi_{ae}[A(\boldsymbol{x_n},t),\phi(\boldsymbol{x_n},t)] B_e^i(\boldsymbol{x_n},t) \delta A_i^a(\boldsymbol{x_n},t) \right.$$
$$\left. + \frac{i}{\hbar} \int_{\phi(t_0)}^{\phi(T)} \pi[A(\boldsymbol{x_n},t),\phi(\boldsymbol{x_n},t),\phi(\boldsymbol{x_n},t),\phi(\boldsymbol{x_n},t)] \delta\phi(\boldsymbol{x_n},t),\phi(\boldsymbol{x_n},t) \right]. \quad (68)$$

The interpretation of (68) and consequently of (67) is that for the first term, the integration occurs with respect to the A_i^a dependence of the term $\Psi_{ae}B_e^i$ for a given $\boldsymbol{x}_n$, holding the ϕ dependence of Ψ_{ae} fixed, and in the second term the integration occurs with respect to the ϕ dependence of π for a given $\boldsymbol{x}_n$, holding the A_i^a dependence of π fixed. That this is so can be seen from the analogue of the condition of mixed partial derivatives, shown in the toy model, as applied to the full theory

$$-i\hbar \frac{\delta A_i^a(x)}{\delta\phi(x)} = \hbar G \frac{\delta\phi(x)}{\delta A_i^a(x)} = 0 \ \forall x \quad (69)$$

from which it is clear that A_i^a and ϕ are truly dynamically independent variables irrespective of their individual time histories within M.

Once this functional integration (68) is carried out over the space of fields $\Gamma = (A_i^a, \phi)$, then 3-space can be 'undiscretized' by taking the limit in which the lattice spacing approaches zero, giving the field-theoretical analogue (67) whereupon the spatial integration d^3x is performed. The end result is that the action S depends upon the fields A_i^a and ϕ living on the initial and final hypersurfaces Σ_T and Σ_{t_0} exactly as in the $0+1$ example considered earlier. Equation (67) exhibits the same functional form as minisuperspace but is in fact still the full theory. Note that this argument holds in the case of the Chern–Simons action, since using (64) for $\Psi_{ae} = \delta_{ae}$ and writing in δ vice d notation for the field,

$$\int d^3x \int dt B_a^i \dot{A}_i^a = \int d^3x \int_\Gamma dA_i^a B_a^i$$
$$\sim \int d^3x \int_\Gamma B_e^i \delta A_i^a = \int_\Gamma \delta \int_\Sigma d^3x \Big(A \wedge dA + \frac{2}{3} A \wedge A \wedge A \Big) = I_{CS}[A]. \quad (70)$$

for the connection as a one-form [9].

6 Discussion

In quantum field theory, having imposed the canonical commutation relations (2) one often tries to avoid the consequences of the resulting singularities in order to make sense of the physical results. We argue that consistency requires that the same rules apply in all cases. One should impose the conditions whose coexistability one desires to test, namely that Einstein's four-dimensional general relativity coupled to arbitrary matter can be consistently reconciled with quantum mechanics and quantum field theory, and then examine the implications and possible manifestations of this in the classical limit. Our appraisal of such a reconciliation is that it can be made possible provided that one makes concessions in the form of a restriction of the space of allowable physical states of the theory. An irreconcilable result would imply a null space of such states.

We have also demonstrated a main difference between the usual field theories on Minkowski spacetime and the constrained theory of gravity in Ashtekar variables which relates to the problem of time. This follows from the noncommutativity of functional variation with time variation in the latter theory as opposed to the former, and stems from ordering ambiguities between products of configuration variables and their momenta. This noncommutativity implies that a time evolution by definition includes a variation of the fields in quantum gravity and that in this sense the quantum fields defining the theory can be utilized as a clock.

The usual objections against the utilization of physical degrees of freedom as a clock stem from nonmonotonicity of the fields and from a restriction to the semiclassical limit where the notion of time evolution is more meaningful. Our proposal is that the objections can be addressed by finding a special set of states for which the classical and the quantum regimes of the state are one and the same. This enables the association of a classical evolution in time by way of the classical equations of motion to a quantum evolution in time by way of their quantum counterparts. Secondly, the issue of lack of monotonicity would be resolved in spite of the arbitrary time dependence of a particular history between two spatial hypersurfaces Σ_0 and Σ_T, if such an evolution can be carried out by holographic effect. It then suffices to define the clock by the association of a time label to the state as defined on these hypersurfaces.

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