Title: Observables and Change in Totally Constrained Systems

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Abstract: We isolate an important physical distinction between gauge symmetries which exist at the level of histories and states, and those which exist at the level of histories and not states. This distinction is characterised explicitly using a generalized Hamilton-Jacobi formalism within which a non-standard prescription for the observables of classical totally constrained systems is developed. These ideas motivate a `relational quantization' procedure which is different from the standard `Dirac quanization'. In particular, relational quantization of totally constrained systems leads to a formalism with superpositions of energy eigenstates and an enlarged set of quantum observables. These `Kucha\v{r} observables' can change independently of each other, and thus are associated with measurable quantities in excess of the `perennials' of the standard Dirac approach.

Observables and Change in Totally Constrained Systems

Sean Gryb (Radboud) and Karim Thébault (LMU Munich)

Key Results

I. New framework for identifying and constructing observables and their evolution in totally constrained theories

II. Generalized Hamilton–Jacobi formalism containing 'Dirac observables' as a special case

III. Insight into partial and complete observables framework and (limited) support for Rovelli's (2002, 2007) interpretation of the partial observables as measurable.

IV. Schrödinger type formalism for quantum reparametrization invariant theories; featuring a dynamical wavefunctions, superpositions of energy eigenstates, and extra observables.

V. Alternative derivation of the dynamical minisuperspace model of Wald and Unurh (1989)

VI. New prescription for the canonical quantization of gravity that singles out the shape dynamics formalism as a classical starting point

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Motivation

On our view, one must distinguish between two notions of gauge invariance often taken as equivalent in the literature:

- The first notion arises when there exists an equivalence class of **states** in the state space of a theory that are identified as *physically indistinguishable*, leading to an under-determination problem in the evolution equations of the theory.
- A second notion of gauge invariance arises when there is an equivalence class of **histories** in the space of allowable histories of a theory. A symmetry at the level of histories is defined directly in terms of an invariance of the action.

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Motivation

- Although such an identification is justified in the case of a Type 1 symmetry, it is certainly *not* justified in the Type 2 case.
- Thus, in our view, the Dirac quantization algorithm is *only* justified for the Type 1 case.
- One then requires a *new* definition of observables and a *new* approach to quantization for gauge theories with Type 2 symmetries. This is precisely what the *relational quantization* approach presented here aims to provide

Plan of Talk

1. Generalized Hamilton-Jacobi Formalism
2. Relational Quantization
3. Gravity

– Consider the canonical action of a totally constrained Hamiltonian theory on a phase space Γ:

$$S = \int \left[p \cdot \dot{q} - \lambda^\alpha C_\alpha(q,p)\right] \mathrm{d}t\,. \tag{1}$$

– Our goal is to find a canonical transformation that parametrizes the flow of the (Abelianized) constraints C_α locally on Γ and restrict this flow to the constraint surface defined by $C_\alpha \approx 0$.

– Consider the modified action:

$$S_\mathrm{e} = \int \left[p \cdot \dot{q} + \dot{\phi}^\alpha \cdot \mathcal{E}_\alpha - \lambda^\alpha (\mathcal{E}_\alpha - C_\alpha(q,p))\right] \mathrm{d}t \tag{2}$$

defined on the *extended* phase space $\Gamma(q,p) \to \Gamma_\mathrm{e}(q,p;\phi^\alpha,\mathcal{E}_\alpha)$

– The new momenta $\mathcal{E}_\alpha$ are constants of motion. For the initial condition $\mathcal{E} = 0$, the extended theory defined by S_e is equivalent to the original theory defined by S.

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– We convert S to a type-2 generating functional $F(q, P; \phi^\alpha, \Phi_\alpha)$ by adding the boundary term $Q \wedge P$. The canonical transformation we are looking for can then be shown to satisfy the generalized Hamilton–Jacobi relations

$$\boxed{\frac{\partial F}{\partial \phi^\alpha} = C_\alpha\left(q, \frac{\partial F}{\partial q}\right)} \tag{4}$$

– Using a separation Ansatz for F

$$F(q, P; \phi^\alpha) = F(q, P; \phi^\alpha, \mathcal{E}_\alpha) = W(q, P) + \mathcal{E}_\alpha \phi^\alpha, \tag{5}$$

where we have identified the separations constants as the canonical coordinates $\mathcal{E}^\alpha$.

– We then obtain

$$\boxed{F(q, P, \phi^\alpha) = W(q, P) + \phi^\alpha C_\alpha\left(q, \frac{\partial W}{\partial q}\right)} \tag{6}$$

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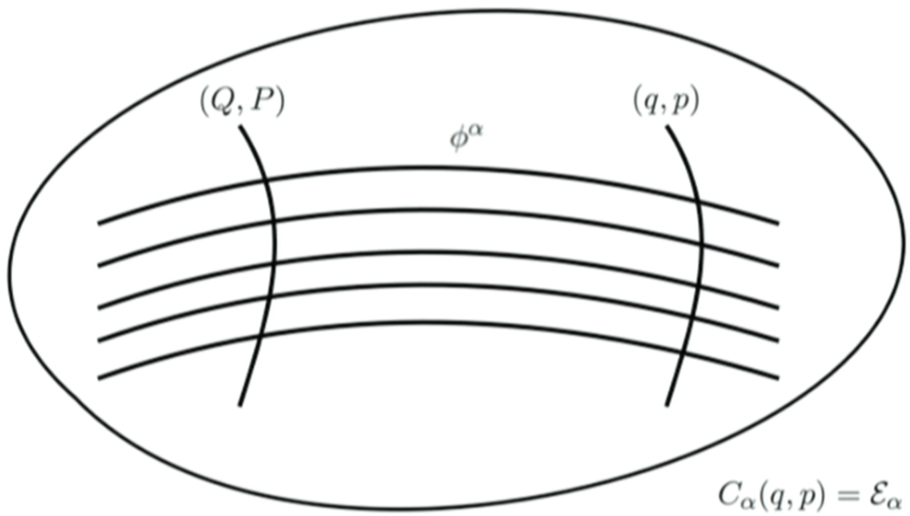
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– We aim to define a canonical transformation that parametrizes the flow of the constraints. This can be achieved by requiring that the new coordinates $(P, Q; \Phi^\alpha, E_\alpha)$ have zero flow under the transformed C_α, so that they are analogous to the 'initial data' of standard Hamilton–Jacobi theory.

– For the old coordinates (q, p), we additionally require that the momenta $\mathcal{E}_\alpha$ are constrained to be equal to the $C_\alpha(q, p)$.

– We can calculate a type-1 generating functional, $S(q, Q; \phi^\alpha, \Phi_\alpha)$, for a canonical transformation taking the lower case coordinates to upper case ones subject to our requirements:

$$\mathrm{d}S(q, Q; \phi^\alpha, \Phi_\alpha) = p \wedge \mathrm{d}q + C_\alpha(p, q) \wedge \mathrm{d}\phi^\alpha - P \wedge \mathrm{d}Q\,, \qquad (3)$$

where we set $\mathcal{E}_\alpha = C_\alpha(q, p)$ and $E_\alpha = 0$.

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– The Hamilton–Jacobi equation of motion are then

$$\boxed{Q = \frac{\partial F}{\partial P}\bigg|_{C_\alpha\left(q, \frac{\partial W}{\partial q}\right) = \mathcal{E}_\alpha}} \tag{7}$$

which should be read as an equation for q in terms of the 'initial data' (Q, P), the constants of motion, $\mathcal{E}_\alpha$, and the parameters ϕ^α. The interpretation of this equation depends crucially upon the type of symmetry at hand

– For Type 1 symmetries the ϕ^α parameterize unphysical flow. To compute observables we must impose $\mathcal{E}_\alpha = 0$ upon (7) and then eliminate the ϕ^α-dependance in the resulting expression. This can be done *either* by gauge fixing *or* constructing a family of complete observables. Gauge fixing is more natural.

– For Type 2 symmetries the ϕ^α parameterize physical change. To compute observables, impose $\mathcal{E}_\alpha = C_\alpha(q, p)$ upon (7). There is no necessity to eliminate the ϕ^α-dependance but we can do this by constructing a family of complete observables. Gauge fixing is unphysical.

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– We can illustrate these points explicitly using a finite dimensional model with total Hamiltonian:

$$H(\vec{q}_i, \vec{p}_i) = N\mathcal{H}(\vec{q}_i, \vec{p}_i) + \vec{\lambda} \cdot \vec{\mathcal{P}}(\vec{p}_i), \tag{8}$$

– Evolution of the particle positions, $\vec{q}_i$, and momenta, $\vec{p}_i$, is generated by the Hamiltonian constraint

$$\mathcal{H}(\vec{q}_i, \vec{p}_i) = \sum_i \frac{\vec{p}_i^{\,2}}{2m_i} - E \approx 0, \tag{9}$$

which is associated with a Type 2 reparamterization symmetry

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$$S_e = \int dt \left[\sum_i \dot{\vec{q}} \cdot \vec{p}_i + \dot{\vec{\sigma}} \cdot \vec{\Upsilon} - \dot{\tau}\mathcal{E} - N(\mathcal{E} - \mathcal{H}) - \vec{\lambda}\left(\vec{\Upsilon} - \vec{\mathcal{P}}\right) \right], \quad (11)$$

where the extended variables $(\tau, \vec{\sigma})$ are arbitrary labels parametrizing the time and centre of mass of the system respectively.

– The energy, $\mathcal{E}$, can be thought of as a redefinition of the zero of the total energy of the system $E \to E + \mathcal{E}$. The other conjugate momentum variable, $\vec{\Upsilon}$, is the total linear moment of the system

– The generating functional takes the form:

$$F(\vec{q}_i, \vec{P}_i; \vec{\sigma}, \tau) = \sum_i \vec{q}_i \cdot \vec{P}_i - \left(\sum_i \frac{\vec{P}_i^2}{2m_i} - E \right) \tau + \vec{\sigma} \cdot \sum_i \vec{P}_i . \quad (12)$$

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$$\boxed{\vec{q}_i = \left(\vec{Q}_i - \vec{\sigma}\right) + \frac{\vec{P}_i \tau}{m_i}} \tag{13}$$

where the $\vec{P}_i$'s must obey the constraints. This is just the usual integral of motion for the free particle plus an extra term which shifts the origin of each particle system by $\vec{\sigma}$,

– This model makes clear the importance of the Type 1 vs. Type 2 distinction: The $\vec{\sigma}$ parameterize unphysical changes, and the relevant conserved quantities (total linear momentum) are constrained to be zero. On the other hand, τ parameterizes dynamical physical change, and the relevant conserved quantity (energy) can be non-zero.

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– The Type 1 interpretation of the symmetry associated with σ implies a natural reduction in the original phase space degrees of freedom equivalent to a centre of mass gauge fixing:

$$\vec{\sigma} = \vec{Q}^{\mathrm{CM}} - \vec{q}^{\mathrm{CM}}, \tag{14}$$

– Reinserting this back into the integral of motion (13):

$$(\vec{q}_i - \vec{q}^{\mathrm{CM}}) = (\vec{Q}_i - \vec{Q}^{\mathrm{CM}}) + \frac{\vec{P}_i}{m_i}\tau, \tag{15}$$

$$q_i^{\mathrm{cm}} = \vec{Q}_i^{\mathrm{cm}} + \frac{\vec{P}_i}{m_i}\tau, \tag{16}$$

which are easily verified to fulfil the usual Dirac observables condition w.r.t the $\vec{\mathcal{P}} = 0$ constraint

– If we apply the same gauge fixing method to the Type 2 symmetries the 'integral of motion' would reduce to the trivial statement

$$\vec{q}_i^{\,\mathrm{cm}} = \vec{Q}_i^{\,\mathrm{cm}}. \tag{17}$$

The only way to obtain a notion of evolution for this system is to consider (16) as a genuine evolution equation for the system.

– We can identify the physically relevant observables of the system as those corresponding to the *entire* set of configuration space variables $\vec{q}_i^{\,\mathrm{cm}}$ after removing the centre of mass. These are are the Kuchař observables for this system since they commute with the 'Gauss' constraints $\mathcal{P}$ but not the Hamiltonian constraint $\mathcal{H}$.

– These Kuchař observables evolve according to (16), tracing out curves labelled by the arbitrary parameter τ, which is of course itself not an observable. Rather, τ is an independent parameter, and, as such, can be specified independently of quantities which are deemed measurable within the theory.

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– One might, however, wish to give a 'parameter free' expression for the relative variation of the observables. Consider our formalism in 1-dimension. We can choose the partial observables to be the centre of mass coordinates, Q_i^{cm}, meaning the q_i^{cm} defined via (16), play the role of the 'flow equations'.

– A natural choice of clock variables is the centre of mass coordinate of one of the particles, say particle 1. We can invert (16) for $i = 1$ to obtain

$$\tau = \frac{m_1}{P_1}\left(Q_1^{\mathrm{cm}} - q_1^{\mathrm{cm}}\right) . \tag{18}$$

– Using one of the initial value constraints we can express P_1 in terms of the remaining P_i's. Using this, we can deparametrize the evolution of the remaining q_a's (where $a = 2 \ldots n$) in terms of q_1^{cm}

$$q_a^{\mathrm{cm}}(Q_i^{\mathrm{cm}}, P_i, q_1^{\mathrm{cm}}) = Q_a^{\mathrm{cm}} - \frac{m_1}{m_a} P_a \frac{\left(Q_1^{\mathrm{cm}} - q_1^{\mathrm{cm}}\right)}{\left[2m_1\left(E + \mathcal{E} - \sum_a \frac{P_i^2}{m_i}\right)\right]^{1/2}} . \tag{19}$$

– For any $q_1^{\mathrm{cm}} = \kappa \in \mathbb{R}$ this expression defines a 'complete observable', which will also be a Dirac observable. One can use the complete and partial observables program to deparametrize the evolution purely in terms of observable quantities.

– This evolution is, however, fundamentally controlled by (16) and is *always* well-defined, even when a particular deparametrization breaks down. Thus, even if one wishes to use parameter-free 'complete observable' expressions, one is still required to retain the full the 'partial observables' representation given by (16).

– For the Type 2 Symmetries (although not for Type 1 symmetries) this supports Rovelli's (2002, 2007) idea that partial observables should be taken to correspond to measurable quantities.

- For any $q_1^{\mathrm{cm}} = \kappa \in \mathbb{R}$ this expression defines a ‘complete observable’, which will also be a Dirac observable. One can use the complete and partial observables program to deparametrize the evolution purely in terms of observable quantities.
- This evolution is, however, fundamentally controlled by (16) and is *always* well-defined, even when a particular deparametrization breaks down. Thus, even if one wishes to use parameter-free ‘complete observable’ expressions, one is still required to retain the full the ‘partial observables’ representation given by (16).
- For the Type 2 Symmetries (although not for Type 1 symmetries) this supports Rovelli’s (2002, 2007) idea that partial observables should be taken to correspond to measurable quantities.

Summary

- A Type 1 symmetry exists within a theory when there is a state symmetry with a corresponding history symmetry. The Type 1 labelling parameters and conserved charges do not have physical significance: the Hamilton–Jacobi characteristic functional should be independent of the parameters, and the conserved charges should be set to zero
- A Type 2 symmetry exists when there is history symmetry with no corresponding state symmetry. The labelling parameters and conserved charges do have physical significance: change of the Hamilton–Jacobi characteristic functional with respect to the parameters is dynamical, and the conserved charges are constants of motion
- Kuchař Observables, which commute with Type 1 constraints but not Type 2 constraints, parameterize the independently measurable degrees of freedom. This view supports the construction of complete observables for Type 2 constraints, so long as we take the Rovelli-type interpretation of the partial observables.

The requirements for a quantization technique that faithfully preserves the physical characteristics of a classical theory with Type 1 symmetries (labelled β) and Type 2 symmetries (labelled μ) are:

1. The classical Kuchař observables should be the basis for the algebra of quantum observables, which are defined as Hermitian operators on a physical Hilbert space.
2. We should define quantum wavefunctions as the elements of this physical Hilbert space that are invariant under change with respect to the Type 1 independent parameters, ϕ_β.
3. The wavefunctions should evolve according to an evolution equation that reduces in the semi-classical limit to the generazlied Hamilton–Jacobi evolution equation for the Type 2 parameters, ϕ_μ
4. The wavefunctions should be able to exist in superpositions of eigenstates of the constant of motion associated with the Type 2 symmetries, $\mathcal{E}_\mu$.

- For Type 1 symmetries (20) is implemented as a *kinematical* restrictions on the theory: physical states of the quantum theory, Ψ_{phys}, should be ϕ^{β}-independent.
- The physical Hilbert space should then be constructed in such a way that the inner product is invariant under the action of the relevant C_{β}'s. This coincides with the usual Dirac analysis and can be achieved by standard methods (e.g. group averaging)
- For Type 2 symmetries (20) is implemented as dynamical equations: they do not lead to any further kinematical restrictions upon the physical states, rather they give the change of such states with respect to the relevant (physical) ϕ^{μ}s.
- Observables are self-adjoint operators on the physical Hilbert space: they must commute with the Type 1 constraints, but not the Type 2 constraints. They are thus quantum Kuchař observables, with a generzlied Heisenberg evolution equation:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}\phi^{\mu}} \hat{\mathcal{O}} = [\hat{\mathcal{O}}, \hat{\mathcal{C}}^{\mu}] \qquad (21)$$

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The above considerations make clear the main difference between relationally quantized theories and Dirac quantized theories:

- In relational quantization, there is a larger set of observables because the relevant operators are not required to commute with the Type 2 constraints. These observables evolve according to the Heisenberg equations (21).
- This implies that we have a different quantum state than that obtained through Dirac quantization. Specifically, in relational quantization the state is allowed to be in a general superposition of eigenstates of the evolution operators $\hat{C}^\mu$
- While in the classical theory the introduction of the extended variables $(\phi^\mu, \mathcal{E}_\mu)$ did not change the physical predictions of the theory, the same is no longer true at the quantum level: relational quantization leads to physically different predictions for the behaviour of observables as compared with Dirac quantization.

- Our 'relational quantization' approach is based upon the assumption that, when they exist, state symmetries can be unambiguously identified at the level of phase space, this is the case for the spatial diffeomorphism symmetries associated with the momentum constraints
- However, it is explicitly not the case for general relativity: refoliation symmetry, connected to the Hamiltonian constraints H, is not represented in terms of sequences of physically indistinguishable states in phase space.
- This is despite the fact that the symmetry clearly leads to an under-determination problem in the evolution equations of the theory.
- Thus, without further articulation refoliation symmetries cannot be fitted into either the Type 1 or Type 2 categories.

– This might seem like a dire problem for relational quantization: however, on our view, the problem with refoliations is actually a barrier to *any* consistent canonical quantization approach.

– An ability to identify indistinguishable classical states is a *requirement* for a physically well motivated canonical quantization scheme based upon the notion of quantum state

– Without being able to identify which *classical* instantaneous states are physically equivalent, the problem of constructing a Hilbert space of distinct quantum states is not even well posed.

– That such an identification is not possible within the standard ADM formalism is a severe problem for any canonical quantization of gravity.

Quantization Requirements

This suggests the following quantization requirements for a reformulation of general relativity:

1. The (unconstrained) phase space is constructed from the ADM data, (g_{ab}, π^{ab}), on a spatial hypersurface
2. Instantaneous physical states are invariant under spatial diffeomorphisms i.e. the momentum constraint is preserved as a Type 1 symmetry generating constraint
3. All other constraints are required to be first class with respect to this constraint, and be unambiguously categorizable as either Type 1 or Type 2 generating
4. The physical degrees of freedom should match the original theory (i.e. two per spatial point) *and* be dynamical (i.e. propagated by a Hamiltonian function)

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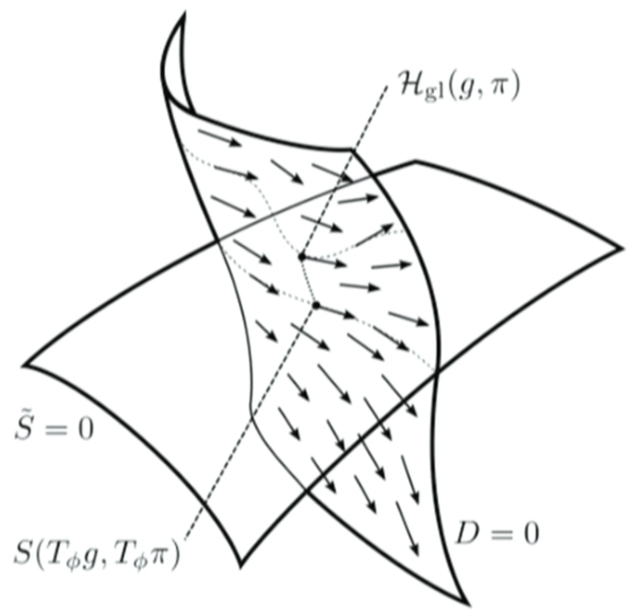
Shape Dynamics

The $\pi = 0$ condition singles out precisely the shape dynamics gauge fixing

Our quantization requirements thus point towards shape dynamics formalism as a classical starting point for quantum gravity



Key Results

I. New framework for identifying and constructing observables and their evolution in totally constrained theories

II. Generalized Hamilton–Jacobi formalism containing 'Dirac observables' as a special case

III. Insight into partial and complete observables framework and (limited) support for Rovelli's (2002, 2007) interpretation of the partial observables as measurable.

IV. Schrödinger type formalism for quantum reparametrization invariant theories; featuring a dynamical wavefunctions, superpositions of energy eigenstates, and extra observables.

V. Alternative derivation of the dynamical minisuperspace model of Unruh and Wald (1989)

VI. New prescription for the canonical quantization of gravity that singles out the shape dynamics formalism as a classical starting point