What Are Observables in Hamiltonian Theories? Testing Definitions with Empirical Equivalence

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Abstract

Change seems missing in Hamiltonian General Relativity's observables. The typical definition takes observables to have 0 Poisson bracket with each first-class constraint. Another definition aims to recover Lagrangian-equivalence: observables have 0 Poisson bracket with the gauge generator G, a $tuned\ sum$ of first-class constraints.

Empirically equivalent theories have equivalent observables. That platitude provides a test of definitions using de Broglie's massive electromagnetism. The non-gauge "Proca" formulation has no first-class constraints, so everything is observable. The gauge "Stueckelberg" formulation has first-class constraints, so observables vary with the definition. Which satisfies the platitude? The team definition does; the individual definition does not.

Subsequent work using the gravitational analog has shown that observables have not a 0 Poisson bracket, but a Lie derivative for the Poisson bracket with the gauge generator G. The same should hold for General Relativity, so observables change locally and correspond to 4-dimensional tensor calculus.

Key words: gauge freedom, constrained Hamiltonian dynamics, theoretical equivalence, problem of time

1 Artificial Gauge Freedom

It is well known that many important physical theories have considerable descriptive redundancy. The gauge theories for the four fundamental forces— Maxwell's electromagnetism, the Yang-Mills theories for the weak and strong nuclear forces, and GTR—display this descriptive redundancy. gauge freedom arguably has a deep philosophical significance of some kind, gauge freedom poses something of a challenge technically. In some contexts, especially Maxwell's electromagnetism or its quantum successor, it can be useful to make a conventional choice of a specific gauge, make calculations in a convenient fashion, and then show that the results did not depend on that specific gauge choice (Weinberg 1995, p. 345). Unfortunately this simple procedure tends to fail for Yang-Mills theories due to the Gribov ambiguity (Sundermeyer 1982; Kaku 1993; Guay 2008); this failure can be relevant when nonperturbative effects matter. A more elegant, but more abstract and technically difficult procedure, is to work with a space of physically distinct configurations by taking gauge equivalence classes; the resulting reduced phase space (in a Hamiltonian formalism) or other reduction to the "true degrees of freedom" might be difficult to find or use explicitly, however. These sorts of procedures take gauge freedom to be an obstacle to overcome. Thus Freund, Maheshwari and Schonberg (FMS) discussed how the absence of gauge freedom in their massive variant of GTR made it easier to quantize than GTR (Freund, Maheshwari, and Schonberg 1969). One can take the second-class constraints as identities for eliminating unnecessary field variables (Sundermeyer 1982; Weinberg 1995).

The pragmatic challenges in dealing with Dirac brackets and the progress in handling gauge theories have led to a change of viewpoint. More recently the view has appeared that gauge freedom is an asset and not so much a liability. Thus technologies have been developed to take theories with constraints but no gauge freedom (such as Proca massive electromagnetisms) and install gauge freedom artificially by adding extra fields and extra symmetries ensuring that the extra fields make no empirical difference. One might call such techniques forms of de-Ockhamization; de-Ockhamization turns out to be more useful scientifically than philosophers might have expected (Quine

1975; Glymour 1977). The ad hoc Stueckelberg trick developed gradually in the middle of the 20th century (Ruegg and Ruiz-Altaba 2004), and a paper from the 1970s left the name "Wess-Zumino fields" for certain purposes (Wess and Zumino 1971; Neto 2006), but the subject of installing artificial gauge freedom reached a more mature form in the 1980s. What is most important for present purposes is not an algorithm for installing gauge freedom, but the result of doing so in massive electromagnetism. Then we will have two (empirically equivalent) formulations of a theory, one with gauge freedom, one without, or perhaps two empirically equivalent theories. Either classification will serve my purposes.

2 Proca and Stueckelberg Formulations

The most compact and perspicuous way to begin a technical discussion of a classical field theory is to exhibit its Lagrangian density, a function of some fields and their derivatives, such that the space-time integral of the Lagrangian density \mathcal{L} , the "action" S of the theory, satisfies the principle of least (or perhaps merely stationary) action. The source-free Maxwell field equations (in manifestly Lorentz-covariant form) follow from a Lagrangian density of the form

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu},\tag{1}$$

where the indices are moved using the Lorentz metric diag(-1, 1, 1, 1) and $F_{\mu\nu} =_{def} \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$ is the electromagnetic field strength. For Maxwell's theory, the vector potential A_{μ} admits the gauge transformation

$$A_{\mu} \to A_{\mu} + \partial_{\mu} \phi$$

for an arbitrary function ϕ ; this transformation makes no observable difference. This Lagrangian density is manifestly gauge invariant, because it is built from the gauge-invariant field strength only. For the massive Proca electromagnetisms, the Lagrangian density is

$$\mathcal{L}_p = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{m^2}{2} A_\mu A^\mu. \tag{2}$$

Evidently the A^2 term breaks the gauge symmetry in the massive case. Whereas Maxwell's theory has 2 degrees of freedom at each spatial point (written as $2\infty^3$ degrees of freedom), Proca's theories have $3\infty^3$ degrees of freedom. The extra degree of freedom (at each point), however, is weakly coupled for small photon masses and so is not readily noticed experimentally. The treatment of the two using the Dirac-Bergmann constrained dynamics formalism is straightforward and, in the Proca case, already known (Sundermeyer 1982; Gitman and Tyutin 1990). The approximate empirical equivalence between Maxwell's theory and Proca's theories for small enough photon masses is preserved under quantization: massive quantum electrodynamics (QED) approximates the standard massless QED arbitrarily well (Belinfante 1949; Glauber 1953; Bass and Schrödinger 1955; Stueckelberg 1957; Boulware and Gilbert 1962; Boulware 1970; Goldhaber and Nieto 1971; Slavnov and Faddeev 1971; Boulware and Deser 1972; Slavnov 1972; Shizuya 1975; Ruegg and Ruiz-Altaba 2004; Goldhaber and Nieto 2010; Pavel and Pervushin 1999). In thermal contexts, where one might expect the third degree of freedom to be relevant, it decouples in the massless limit, so that the time to reach equilibrium is inversely related to the photon mass. As the mass goes to zero, a system takes forever to reach equilibrium; hence equilibrium thermodynamic quantities based on three field degrees of freedom are physically irrelevant and unobservable (Bass and Schrödinger 1955; Goldhaber and Nieto 1971). It follows that in a world with electromagnetism as the only force, it would be impossible for finite beings to rule out all of the massive electromagnetic theories empirically, and thus impossible to determine empirically whether gauge freedom was a fundamental feature of the electromagnetic laws. Thus one has permanent underdetermination between massless and massive electromagnetism with only approximate empirical equivalence (Pitts 2011).

Given the starring role playing by Maxwell's electromagnetism, Yang-

¹The reader will observe the importance of distinguishing $2\infty^3$ from $3\infty^3$, notwith-standing rules for Cantorian transfinite arithmetic (Moore 1990). The lesson seems to be that physical theories involve continuity properties of sets from which cardinality abstracts. Evidently cardinality does not exhaust the useful notions of "same size" or counting for infinite collections.

Mills theory, and Einstein's gravity in contemporary physics, and consequently the non-negligible importance of their massive cousins (whether those theories are physically viable or not), it seems reasonable to seek a procedure for converting non-gauge formulations into gauge formulations that is as convenient as possible for massive electromagnetism, massive Yang-Mills theory, and massive GTR. In the electromagnetic and gravitational cases, it turns out that the gauge formulations were found in an ad hoc way without the need for such elaborate conversion algorithms as have appeared in recent decades. In the electromagnetic case, the answer is Stueckelberg's trick, which adds the gradient of a new scalar field to the vector field A_{μ} in the mass term; adding such a term in the kinetic term $-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$ would make no difference because such a term, like a gauge transformation, has no effect on $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$. In massive quantum electrodynamics, unitary is proven using what is in effect the Proca formulation, whereas renormalizability is proven by exploiting the Stueckelberg formulation having the true degrees of freedom manifest, but proves renormalizability (getting rid of infinities) using the Stueckelberg formulation with gauge freedom (Peskin and Schroeder 1995, pp. 738, 739) (Weinberg 1996, chapter 21) (Kaku 1993, chapter 10). This commonplace in quantum field theory inspires a somewhat analogous move in a classical Hamiltonian context: the Proca and Stueckelberg formulations are so closely related (at least empirically equivalent, if not formulations of the same theory) that their observables must be equivalent as well.

2.1 Non-Gauge Formulation: Proca

For the massive Proca electromagnetism, the Lagrangian density is (Sundermeyer 1982, pp. 183-186)

$$\mathcal{L}_{p} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{m^{2}}{2} A_{\mu} A^{\mu}.$$

Here as elsewhere I used the -+++ signature, letting Greek indices run from 0 to 3 and Latin indices from 1 to 3. The primary constraint (at each point) is

$$\pi^0 = \frac{\partial \mathcal{L}_p}{\partial A_{0,0}} = 0.$$

Performing the Legendre transformation to get the canonical Hamiltonian density (not a redundant term in the constrained dynamics literature (Sundermeyer 1982)) gives

$$\mathcal{H}_{pc} = \pi^{\alpha} A_{\alpha,0} - \mathcal{L}_p = \frac{1}{2} (\pi^a)^2 + \pi^a A_{0,a} + \frac{1}{4} F_{ij} F_{ij} + \frac{m^2}{2} (A_i)^2 - \frac{m^2}{2} (A_0)^2.$$

Using the canonical Hamiltonian $\int d^3x \mathcal{H}_{pc}$ (or the primary Hamiltonian—it does not matter) to find the time evolution of π^0 and to enforce its continued vanishing gives

$$\{\pi^{0}(y), \int d^{3}x \mathcal{H}_{pc}(x)\} = \pi^{a},_{a}(y) + m^{2}A_{0}(y) \approx 0.$$

Thus the secondary constraint is $\pi^a_{,a} + m^2 A_0$ everywhere. Demanding that the secondary constraint be preserved by the time evolution requires the use of the primary Hamiltonian $H_{pp} = H_{pc} + \int d^3x v(x) \pi^0(x)$, where v is a new Lagrange multiplier. Preserving the secondary constraint (with the help of an arbitrary test function to smear the Dirac delta functions from the fields' Poisson brackets as needed) gives

$$\{\pi^{a},_{a}(y) + m^{2}A_{0}(y), H_{pp}\} = -m^{2}A_{i,i} + m^{2}v \approx 0,$$

fixing v and leaving no arbitrariness in the evolution of the system. The Poisson brackets of the constraints among themselves are

$$\{\pi^{0}(x), \pi^{0}(y)\} = 0,$$

$$\{\pi^{0}(x), \pi^{a},_{a} + m^{2}A_{0}(y)\} = -m^{2}\delta(x, y),$$

and

$$\{\pi^a, a+m^2A_0(x), \pi^i, i+m^2A_0(y)\} = 0.$$

The vanishing Poisson brackets here vanish without the use of the constraints themselves. The matrix of Poisson brackets of constraints has non-vanishing determinant, so the theory is indeed second-class as advertised. Because there are no first-class constraints, all quantities in the theory have 0 Poisson bracket with all first-class constraints (of which there are none) and with the gauge generator (which also doesn't exist or perhaps is just 0). Consequently, everything is observable—at any rate everything that isn't 0 as π^0 is.

2.2 Gauge Formulation: Stueckelberg

How does the constrained dynamics treatment of the Stueckelberg gauge formulation of massive electromagnetism differ? The Lagrangian density is²

$$\mathcal{L}_s = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{m^2}{2}(A_\mu + \partial_\mu\phi)(A^\mu + \partial^\mu\phi).$$

Amusingly, it does not matter if the Stueckelberg scalar ϕ is varied or not. The reason is that the gauge transformation formula for the Stueckelberg field ϕ is algebraic in the gauge parameters. If ϕ is not varied, then its erstwhile equation of motion will still follow from the Euler-Lagrange equation for A_{μ} , either using the generalized Bianchi identity or by simply taking the divergence. But not varying that field would sit oddly with the spirit of the theory, so let us vary it.

Turning to the Hamiltonian formalism, the primary constraint is

$$\pi^0 = \frac{\partial \mathcal{L}_s}{\partial A_{0,0}} = 0,$$

as before; the momenta for A_i are also unchanged. The new momentum for the new field ϕ is

$$P = \frac{\partial \mathcal{L}_s}{\partial \phi_{,0}} = m^2 A_0 + m^2 \phi_{,0} \,,$$

so the vanishing of the new momentum (part of the BFT boundary condition) and the vanishing of the new field's time derivative (part of the new boundary condition proposed here) are in general incompatible. Performing the Legendre transformation to get the canonical Hamiltonian density gives

$$\mathcal{H}_{sc} = \frac{1}{2} (\pi^a)^2 + \pi^a A_{0,a} + \frac{1}{4} F_{ij} F_{ij} + \frac{m^2}{2} (A_i)^2 + \frac{P^2}{2m^2} - A_0 P + m^2 A_i \phi_{,i} + \frac{m^2}{2} (\phi_{,i})^2.$$

Preserving the primary constraint yields the secondary constraint

$$\pi^a$$
, $_a + P \approx 0$.

Preserving the secondary constraint gives neither a fixed Lagrange multiplier v nor a tertiary constraint. The primary constraint, being unchanged,

²It is sometimes useful to absorb one power of the photon mass m into the Stueckelberg field ϕ , but I have not done so here.

still Poisson-commutes with itself. The new secondary constraint also Poisson-commutes with itself. Most importantly, $\{\pi^0(x), \pi^a, +P(y)\} = 0$, $\{\pi^0(x), \pi^0(y)\} = 0$, and $\{\pi^a, +P(x), \pi^b, +P(y)\} = 0$, so the Stueckelberg formulation is first-class, as advertised. This is the same Poisson bracket algebra as in the Maxwell theory. One advantage of the Stueckelberg formulation of massive electromagnetism over the Proca formulation is the ease of taking the massless limit (Zinoviev 2007); the gauge freedom remains, while the extra degree of freedom decouples as $m \to 0$.

3 Testing Definitions of Observables

These familiar points within high-energy physics now let us do something of considerable philosophical importance for canonical) quantum gravity, namely, test definitions of "observables" in constrained Hamiltonian dynamics. Observables are supposed to comprise the real gauge-invariant physical content of a theory. Remarkably, it has long appeared (going back to (Bergmann and Goldberg 1955; Anderson 1962)) that the observables in General Relativity do not change over time or vary with place (Torre 1993). These claims are derived from the usual definition of observables as quantities with 0 Poisson bracket with all first-class constraints (Bergmann 1961; Dirac 1964; Henneaux and Teitelboim 1992). That definition, in turn, is largely due to the widespread idea that each first-class constraint generates a gauge transformation, a change of description that leaves the world (or at least the history of the world) unchanged. The implausibility of such results has led to criticisms of this definition that were not accompanied by systematic alternatives (Kuchař 1992; Smolin 2001).

A different view was present in some of the earliest works on constrained Hamiltonian dynamics (Rosenfeld 1930; Anderson and Bergmann 1951), according to which a tuned sum of first-class constraints generated a gauge transformation, which was expected to be equivalent to the familiar Lagrangian transformations. Such as view has reappeared since c. 1980 (Mukunda 1980; Castellani 1982; Sugano, Saito, and Kimura 1986; ?; Sugano, Kagraoka, and Kimura 1992; Pons, Salisbury, and Shepley 1997; Shepley, Pons, and Salisbury 2000; Pons and Salisbury 2005). That tuned sum

has been called the "gauge generator" G, which by construction maps solutions of Hamilton's equations to other solutions of Hamilton's equations. Surely observables need not be preserved by transformations that are not gauge transformations (such as separate first-class transformations in most theories, according to this view). Instead one defines observables as quantities with 0 Poisson bracket with the gauge generator G. This is a looser requirement, so observables are less scarce.

Which definition is correct? No one can doubt that the manifestly Lagrangian-equivalent view is permissible. But is it required, or just an option within a larger realm of good options? According to the separate first-class constraints view (presently the majority), the richer class of transformations generated by first-class constraints constitute a distinctive Hamiltonian sort of gauge freedom, but the view is supposed to be equivalent to the Lagrangian for "observables" (Henneaux and Teitelboim 1992). But the entities that are called "observables" depend on whether the individual first-class constraint view or the team view is held. Clearly it is crucial to let the mathematics, not stipulation, answer such questions. But can the mathematics be made to speak clearly?

In fact the mathematics can be made to speak decisively, as long as we agree that empirically equivalent theories have equivalent observables. That requirement sounds almost too obvious to bother saying, but it does need saying. If observables need not be equivalent for empirically equivalent theories, then the word "observables" has become a technical term detached from the intention of their main inventor, Peter Bergmann (Bergmann 1962, p. 250). Then it is unclear why one cares about observables. To ensure that observables are interesting and have some connection to their inventor's intention, let us assume that empirically equivalent theories have equivalent observables.

Because the Proca formulation has no first-class constraints, everything in the theory (at least everything that isn't 0) is observable, including the 4-vector potential A_{μ} and the non-zero canonical momenta π^a . (It doesn't matter whether one calls π^0 observable because it is just 0.) The two definitions agree on this point, because theories with no second-class constraints trivially satisfy the condition that observables have 0 Poisson bracket with

(i) each first-class constraint (the right criterion on the individual view) and with (ii) the gauge generator G (the right criterion on the team view).

The less trivial question is what the observables are for the Stueckelberg formulation. Possibly the gauge generator has not been presented for Stueckelberg massive electromagnetism previously. But it should be similar to that of Maxwell's theory and should be tuned sum of the first-class constraints. These constraints were found above to be π^0 and $\pi^a_{,a} + P \approx 0$.

One can take an arbitrary sum of first-class constraints and restrict it so that it leaves the action invariant (perhaps up to a boundary term). The result will be the gauge generator G (Pitts 2014b; Pitts 2014a); the requirement is equivalent to the requirement of preserving Hamilton's equations (Castellani 1982). The calculation, though somewhat longer than the Maxwell case, is straightforward. The Poisson bracket of the (smeared) primary constraint with the canonical Lagrangian $\int d^3x (\pi^a \dot{A}_i + P\dot{\phi} - \mathcal{H}_{sc})$ is just proportional to the secondary constraint (not identically 0 or a total divergence). The Poisson bracket of the (smeared) secondary constraint with the canonical Lagrangian is also proportional to the secondary constraint. Adding the two terms and demanding cancellation relates the arbitrary smearing functions, so that one is the negative time derivative of the other. This is all analogous to the Maxwell case, just with some extra terms (Pitts 2014b). Thus the gauge generator is

$$G = \int d^3x (-\dot{\epsilon}(t,x)\pi^0 + \epsilon[\pi^i,_i + P]).$$

It is very easy to see what the gauge generator G does to all the canonical momenta: it leaves them alone, because their canonically conjugate coordinates are absent from it. Thus all the (nonzero) momenta are observables on either definition—both π^i and P. Finding what G does to the canonical coordinates takes one line each:

$$\{G, A_0(y)\} = \dot{\epsilon},$$

$$\{G, A_j(y)\} = \epsilon_{,j}(y),$$

$$\{G, \phi(y)\} = -\epsilon(y).$$

Each of these results comes from a single nonzero Poisson bracket.

It is obvious by inspection that in the Stueckelberg formulation the quantity $A_{\mu} + \partial_{\mu}\phi$ plays just the role that A_{μ} plays in the Proca formulation. A_{μ} is observable in the Proca formulation, because everything is. Thus one strongly suspects that $A_{\mu} + \partial_{\mu}\phi$ should be an observable in the Stueckelberg formulation also. One could also say that gauge-fixing $\phi = 0$ turns the Stueckelberg formulation into the Proca formulation; in a Hamilton context one would impose $\frac{\partial \mathcal{H}_{sc}}{\partial P} = 0$ as well, thus making $\dot{\phi}$ vanish. But let us calculate, not suspect, and see what happens.

The nontrivial fundamental Poisson brackets are

$$\{A_{\mu}(x), \pi^{\nu}(y)\} = \delta^{\nu}_{\mu}\delta(x, y),$$

 $\{\phi(x), P(y)\} = \delta(x, y);$

the rest vanish. The smeared primary constraint by itself, acting on $A_{\mu} + \partial_{\mu} \phi$, immediately gives

$$\{ \int d^3x \xi(t, x) p^0(x), A_{\mu}(y) + \partial_{\mu} \phi(y) \} = -\xi(y) \delta_{\mu}^0,$$

which is not 0. The smeared secondary gives

$$\{ \int d^3x \epsilon(t,x) [\pi^k,_k(x) + P(x)], A_\mu(y) + \partial_\mu \phi(y) = -\dot{\epsilon} \delta^0_\mu$$

after a little cancellation and the use of the Anderson-Bergmann velocity Poisson bracket (Anderson and Bergmann 1951) $\{\dot{q}, F\} = \frac{\partial}{\partial t} \{q, F\}$ as needed.

For the separate first-class constraints definition of observables, it follows that $A_{\mu} + \partial_{\mu}\phi$ is not an observable; either one of these non-zero brackets makes that point. But for the team view with the gauge generator, one adds these two expressions and sets $\xi = -\dot{\epsilon}$. Then they cancel, so $A_{\mu} + \partial_{\mu}\phi$ is observable according to the Pons-Salisbury-Sundermeyer definition using the gauge generator G. These verdicts disagree, so one of these definitions must be wrong, but which? Recalling that empirically equivalent theories must have equivalent observables, it follows that the Stueckelberg and Proca observables must be equivalent. That holds for the gauge generator definition of observables, but fails for the separate first-class constraints view. Thus the separate first-class constraints view has been falsified by calculation, using

the platitude that observables for empirically equivalent formulations are equivalent.

What one be observed in massive electromagnetism in practice hasn't been terribly worrisome, but the resolution is important because it shows that at least one aspect of the usual paradox-generating definition of observables, that the constraints generate gauge transformations individually, is mistaken. Consequently General Relativity and all other gauge theories inherit the same lesson.³ Thus observables in General Relativity must also be sought using the gauge generator G, not using separate first-class constraints. The condition is weaker, so there might be more observables. It is, of course, possible that external symmetries behave differently from internal symmetries (Kuchař 1992; Barbour and Foster 2008; Pitts 2014a). Thus one should entertain the possibility that an adequate definition for General Relativity looks different, not regarding the team vs individual question, but on the issue of 0 Poisson bracket (invariance) vs some weaker condition yielding mere covariance. Such matters can also be tested by calculation with suitable examples.

4 Appendix

Subsequent work using the gravitational analog has shown that observables have not a 0 Poisson bracket, but a Lie derivative for the Poisson bracket with the gauge generator G. The same should hold for General Relativity, so observables change locally and correspond to 4-dimensional tensor calculus. Thus requiring equivalent observables for empirically equivalent formulations helps to address the problem of time. This work is described elsewhere (Pitts 2016).

³Special cases of certain theory formulations in which each first-class constraint does generate a gauge transformation, because there are no secondary first-class constraints and hence no teammates available, should not detain us. The standard formulations of Maxwell, Yang-Mills, and General Relativity are certainly not in that category.

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