

On Dirac's incomplete analysis of gauge transformations

Josep M. Pons *

Departament d'Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona Av. Diagonal 647, 08028 Barcelona Catalonia, Spain

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Abstract

Dirac's approach to gauge symmetries is discussed. We follow closely the steps that led him from his conjecture concerning the generators of gauge transformations *at a given time* —to be contrasted with the common view of gauge transformations as maps from solutions of the equations of motion into other solutions— to his decision to artificially modify the dynamics, substituting the extended Hamiltonian (including all first-class constraints) for the total Hamiltonian (including only the primary first-class constraints). We show in detail that Dirac's analysis was incomplete and, in completing it, we prove that the fulfilment of Dirac's conjecture —in the "non-pathological" cases— does not imply any need to modify the dynamics. We give a couple of simple but significant examples.

Keywords: gauge theories, gauge transformations, Dirac-Bergmann theory, constrained systems, Dirac conjecture.

^{*}pons@ecm.ub.es

1 Introduction

It has been more than fifty years since the formal development of the theory of constrained systems saw the light with the work of Dirac and Bergmann. By the end of the 1940's, these two physicists, independently, Peter Gabriel Bergmann with different collaborators (Bergmann 1949, Bergmann and Brunings 1949, Anderson and Bergmann 1951) and Paul Adrien Maurice Dirac (1950), working alone, began the systematic study of the canonical formalism for what we today call gauge theories (here including generally covariant theories), also known —in an almost¹ equivalent terminology— as constrained systems.

Since these early stages, Bergmann's purpose was nothing other than the quantization of gravity, whereas for Dirac the purpose was rather the generalization of Hamiltonian methods, in view also of quantization, but mostly for special relativistic theories, and the development of his ideas (1949) on the forms of relativistic dynamics. Eventually the application to general relativity made its way indirectly into Dirac's approach when he considered (1951) the quantization on curved surfaces (see also Dirac 1958, 1959, where general relativity was properly addressed).

The quantization of gravity is an elusive subject that still remains basically unresolved, because of both technical and conceptual obstacles. In addition to the fact that general relativity described gravity as a feature of the geometry of space-time, there was the problem that, since it was a gauge theory —in the form of diffeomorphism invariance—, its Hamiltonian formulation was unknown, because the standard procedure of translating the formulation from tangent space —with a Lagrangian as a starting point— to phase space met with some technical difficulties that had not yet been addressed. Solving these difficulties was part of the contribution by Bergmann and Dirac.

A Hamiltonian formulation was considered at that time a necessary step towards quantization: quantization had to proceed through the correspondence rules —which were worked out also by Dirac in the 1920's— that map the classical Poisson brackets of the canonical variables into commutators of operators. Curiously enough, as a matter of fact, it was at about the same time as Bergmann's and Dirac's first contributions to constrained systems, the end of the 1940's, that Richard Feynman (1948) developed the path integral approach to quantization, which renders the route through the canonical

¹This "almost" is to be explained below.

formalism basically unnecessary² and restores the Lagrangian function to its privileged role in defining a Quantum (Field) Theory.

The difficulties that gauge theories pose to their own canonical formulation were already present in Electromagnetism, but in that case were somewhat circumvented in a heuristic way by several methods of fixing the gauge freedom (e.g., Fermi 1932) and by "ad hoc" modifications of the Poisson brackets (e.g., Bjorken and Drell 1965) —thus discovering the Dirac ones, "avant la lettre". But a diffeomorphism invariant theory like general relativity (GR) was not so easy to tackle. Eventually, a general framework emerged, applicable to any particular case, that yielded general results on the canonical formulation of gauge theories. It was mostly Dirac who gave the final form to the standard formulation of what has been called thereafter Constrained Systems. His concise but largely influential Yeshiva "Lectures on Quantum Mechanics" (1964) became the little book from which generations of theoretical physicists learned the basics of Constrained Systems and were first acquainted with the key concepts of the formulation: constraints —primary, secondary, etc., in a terminology coined by Bergmann; first-class, second-class, in a different classification introduced by Dirac—, canonical Hamiltonian, total Hamiltonian, extended Hamiltonian, arbitrary functions, gauge transformations, Dirac bracket —substituting for the Poisson bracket—, etc. The classical canonical formulation of GR, the ADM formalism of Arnowitt, Deser and Misner (1962), was obtained also in the 1960s.

An introductory as well as conceptual overview of Constrained Systems and Dirac's approach to gauge symmetries can be found in Earman (2003). There has been a good deal of debate concerning generally covariant theories —like general relativity—, where the canonical Hamiltonian is a first class constraint (definitions given below) participating in the generation of gauge freedom. It has been suggested that because of this fact, these theories exhibit no physical dynamics in the canonical formalism, in the sense that the dynamics seems to be purely gauge. In fact it is not. This issue, which is related to the issue of observables for this kind of theories, is clarified in Pons and Salisbury (2005). Another approach as well as many references can be found in Lusanna and Pauri (2003).

Let us mention at this point that one can find in the literature other methods of

²Note however that the derivation of the path integral formalism from the canonical approach is the safest way to guarantee the unitarity of the S-matrix as well as the correct Feynman rules for some specific theories (Weinberg 1995).

obtaining a canonical formulation for theories originating from singular Lagrangians. For instance one can adopt the method of Faddeev and Jackiw (1988), which amounts to a classical reduction of all the gauge degrees of freedom. The equivalence of this method with that of Dirac and Bergmann was shown by Garcia and Pons (1997). Another method, which consists also in a classical reduction of the gauge degrees of freedom, considers a quotienting procedure (Sniatycki 1974, Abraham and Marsden 1978, Lee and Wald 1990) to obtain a physical phase space (endowed with a symplectic form) starting from the presymplectic form that is defined in the tangent bundle once the singular Lagrangian is given. It was shown by Pons, Salisbury and Shepley (1999) that this method is again equivalent to Dirac-Bergmann's.

The main objective of this paper is to discuss and give a critical assessment of Dirac's approach to gauge transformations, and his consequent proposal to modify the dynamics by the use of the extended Hamiltonian, instead of the one that is obtained from purely mathematical considerations, the total Hamiltonian. Dirac only considered gauge transformations *at a given time*, and this must be contrasted with the most common view of gauge transformations as *symmetries* that map *entire solutions* of the dynamics into new solutions, which was Bergmann's point of view. We will try to clarify some confusions originated from the use of these two different concepts of gauge transformation.

In Section 2 we start with a brief, though almost self-contained, introductory Section on Constrained Systems. In Section 3 we reproduce verbatim Dirac's own view (1964) on gauge transformations whereas in Section 4 we show the limitations of his approach and complete it. We make contact with Bergmann's view in Section 5. In Section 6 we comment upon the incompleteness of Dirac view and its possible explanations. In Section 7 it is shown that Dirac's modification of the dynamics has, after all, no damaging consequences. Finally we devote the last Section to some examples.

2 Dirac-Bergmann constrained systems in a nutshell

Although we are interested in gauge field theories, we will use mainly the language of mechanics —that is, of a finite number of degrees of freedom—, which is sufficient for our purposes. A quick switch to the field theory language can be achieved by using DeWitt's

(1963) condensed notation. Consider, as our starting point³ a time-independent firstorder Lagrangian $L(q, \dot{q})$ defined in configuration-velocity space TQ, that is, the tangent bundle of some configuration manifold Q that we assume to be of dimension n. Gauge theories rely on singular —as opposed to regular— Lagrangians, that is, Lagrangians whose Hessian matrix with respect to the velocities (where q stands, in a free index notation, for local coordinates in Q),

$$W_{ij} \equiv \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j},\tag{1}$$

is not invertible.

Two main consequences are drawn from this non-invertibility. First notice that the Euler-Lagrange equations of motion $[L]_i = 0$, with

$$[L]_i := \alpha_i - W_{ij} \ddot{q}^j \, ,$$

and

$$lpha_i := -rac{\partial^2 L}{\partial \dot{q}^i \partial q^j} \dot{q}^j + rac{\partial L}{\partial q^i},$$

cannot be written in a normal form, that is, isolating on one side the accelerations, $\ddot{q}^j = f^j(q, \dot{q})$. This makes the usual theorems about the existence and uniqueness of solutions of ordinary differential equations inapplicable. Consequently, there may be points in the tangent bundle where there are no solutions passing through the point, and others where there is more than one solution. This is in fact our first encounter with constraints and the phenomenon of gauge freedom. Much more on this will be said below.

The second consequence of the Hessian matrix being singular concerns the construction of the canonical formalism. The Legendre map from the tangent bundle TQ to the cotangent bundle —or phase space— T^*Q (we use the notation $\hat{p}(q, \dot{q}) := \frac{\partial L}{\partial \dot{q}}$),

$$\mathcal{F}L:TQ \longrightarrow T^*Q$$
 (2)

$$(q, \dot{q}) \longrightarrow (q, p = \hat{p})$$
 (3)

is no longer invertible because $\frac{\partial \hat{p}}{\partial \dot{q}} = \frac{\partial L}{\partial \dot{q} \partial \dot{q}}$ is the Hessian matrix. There appears then an issue about the projectability of structures from the tangent bundle to phase space: there will be functions defined on TQ that cannot be translated (projected) to functions on

 $^{^{3}}$ All functions are assumed to be continuous and differentiable as many times as the formalism requires.

phase space. This feature of the formalisms propagates in a corresponding way to the tensor structures, forms, vector fields, etc.

In order to better identify the problem and to obtain the conditions of projectability, we must be more specific. We will make a single assumption, which is that the rank of the Hessian matrix is constant everywhere. If this condition is not satisfied throughout the whole tangent bundle, we will restrict our considerations to a region of it, with the same dimensionality, where this condition holds. So we are assuming that the rank of the Legendre map $\mathcal{F}L$ is constant throughout TQ and equal to, say, 2n - k. The image of $\mathcal{F}L$ will be locally defined by the vanishing of k independent functions, $\phi_{\mu}(q, p), \mu = 1, 2, ..., k$. These functions are the primary constraints, and their pullback $\mathcal{F}L^*\phi_{\mu}$ to the tangent bundle is identically zero:

$$(\mathcal{F}L^*\phi_\mu)(q,\dot{q}) := \phi_\mu(q,\hat{p}) = 0, \quad \forall q,\dot{q}.$$
 (4)

The primary constraints form a generating set of the ideal of functions that vanish on the image of the Legendre map. With their help it is easy to obtain a basis of null vectors for the Hessian matrix. Indeed, applying $\frac{\partial}{\partial \dot{q}}$ to (4) we get

$$W_{ij} \left(\frac{\partial \phi_{\mu}}{\partial p_j} \right)_{|_{p=\hat{p}}} = 0, \quad \forall \, q, \dot{q} \, .$$

With this result in hand, let us consider some geometrical aspects of the Legendre map. We already know that its image in T^*Q is given by the primary constraints' surface. A foliation in TQ is also defined, with each element given as the inverse image of a point in the primary constraints' surface in T^*Q . One can easily prove that the vector fields tangent to the surfaces of the foliation are generated by

$$\Gamma_{\mu} = \left(\frac{\partial \phi_{\mu}}{\partial p_{j}}\right)_{|_{p=\hat{p}}} \frac{\partial}{\partial \dot{q}^{j}}.$$
(5)

The proof goes as follows. Consider two neighboring points in TQ belonging to the same sheet, (q, \dot{q}) and $(q, \dot{q} + \delta \dot{q})$ (the configuration coordinates q must be the same because they are preserved by the Legendre map). Then, using the definition of the Legendre map, we must have $\hat{p}(q, \dot{q}) = \hat{p}(q, \dot{q} + \delta \dot{q})$, which implies, expanding to first order,

$$\frac{\partial \hat{p}}{\partial \dot{q}}\delta \dot{q} = 0$$

which identifies $\delta \dot{q}$ as a null vector of the Hessian matrix (here expressed as $\frac{\partial \hat{p}}{\partial \dot{q}}$). Since we already know a basis for such null vectors, $\left(\frac{\partial \phi_{\mu}}{\partial p_{j}}\right)_{|p=\hat{p}}$, $\mu = 1, 2, ..., k$, it follows that the vector fields Γ_{μ} form a basis for the vector fields tangent to the foliation.

The knowledge of these vector fields is instrumental for addressing the issue of the projectability of structures. Consider a real-valued function $f^L: TQ \longrightarrow \mathbf{R}$. It will — locally— define a function $f^H: T^*Q \longrightarrow \mathbf{R}$ iff it is constant on the sheets of the foliation, that is, when

$$\Gamma_{\mu}f^{L} = 0, \quad \mu = 1, 2, ..., k.$$
 (6)

Equation (6) is the projectability condition we were looking for. We express it in the following way:

$$\Gamma_{\mu}f^{L} = 0, \quad \mu = 1, 2, ..., k \Leftrightarrow \text{there exists } f^{H} \text{such that } \mathcal{F}L^{*}f^{H} = f^{L}.$$

2.1 The canonical Hamiltonian

A basic ingredient of the canonical formalism is the Hamiltonian function. In the case of a regular theory (that is, with a non-singular Hessian matrix) it defines, by use of the Poisson bracket, the vector field that generates the time evolution —the dynamics— in phase space. The Hamiltonian is given in that case as the projection to phase space of the Lagrangian energy $E = \frac{\partial L}{\partial \dot{q}} - L$.

This procedure to define the Hamiltonian will still work in the singular case if the energy satisfies the conditions of projectability (6). Indeed we can readily check that $\Gamma_{\mu}E = 0$, so we have a canonical Hamiltonian H_c , defined as a function on phase space whose pullback is the Lagrangian energy, $\mathcal{F}L^*H_c = E$. It was Dirac that first realized in the general setting of constrained systems that a Hamiltonian always existed.

There is a slight difference, though, from the regular case, for now there is an ambiguity in the definition of H_c . In fact, since $\mathcal{F}L^*\phi_{\mu} = 0$, many candidates for canonical Hamiltonians are available, once we are given one. In fact, $H_c + v^{\mu}\phi_{\mu}$ —with $v^{\mu}(q, \dot{q}; t)$ arbitrary functions and with summation convention for μ — is as good as H_c as a canonical Hamiltonian. This "slight difference" is bound to have profound consequences: it is the door to gauge freedom.

2.2 Dynamics for constrained systems

The Hamiltonian —with arbitrary functions— $H_c + v^{\mu}\phi_{\mu}$ was called by Dirac the total Hamiltonian, although today it is usually referred to as the Dirac Hamiltonian H_D .

In the regular case, once the Hamiltonian is given, the equations of motion in phase space are deterministically formulated as

$$\dot{q} = \{q, H_c\}, \quad \dot{p} = \{p, H_c\}.$$
 (7)

So in the singular case we could try, taking into account the non-uniqueness of the canonical Hamiltonian,

$$\dot{q} = \{q, H_D\} = \{q, H_c\} + v^{\mu} \{q, \phi_{\mu}\},
\dot{p} = \{q, H_D\} = \{p, H_c\} + v^{\mu} \{p, \phi_{\mu}\},
0 = \phi_{\mu}(q, p).$$
(8)

Of course, as of now, this formulation (8) is just a reasonable guess. But it turns out that it is correct in a very precise sense, as already shown by Dirac (1950). To be a bit more precise, it was proven by Batlle, Gomis, Pons and Roman (1986) that the equations (8) are equivalent to the Euler-Lagrange equations $[L]_i = 0$. This is to say that if (q(t), p(t))is a trajectory in phase space satisfying (8), then q(t) is a solution of the Euler-Lagrange equations. And vice-versa, if q(t) is a solution of the Euler-Lagrange equations, then the definition $p(t) := \hat{p}(q(t), \frac{dq}{dt})$ makes (q(t), p(t)) a solution of (8). Note that although the arbitrary functions v^{μ} may depend on the time and the phase space variables, on a given solution (q(t), p(t)) they become just functions of the time variable. That is, assuming that the functions v^{μ} are simply arbitrary functions of time is sufficient in order to describe all solutions to the system (8).

So we have succeeded in obtaining a Hamiltonian formulation for a theory defined through a singular Lagrangian. It is worth noticing that the Hamiltonian equations of motion have two parts, a differential one, corresponding to the first two lines in (8), and an algebraic one, which is the third line —the primary constraints. Both types of equations are coupled in the sense that the constraints may impose severe restrictions on the solutions of the differential equations —or even may prevent them from existing. Dirac devised a clever way to disentangle the algebraic and differential components of (8), which we are going to summarise in the next two subsections. Let is emphasize, however, that the formulation of the dynamics is already complete in (8), and that the developments below are just convenient elements for dealing with equations of the type (8).

2.3 Dirac's classification of constraints

The Hamiltonian time evolution vector field, derived from the differential part in (8) is given by

$$\mathbf{X}_{\mathbf{H}} := \frac{\partial}{\partial t} + \{-, H_c\} + v^{\mu}\{-, \phi_{\mu}\},\tag{9}$$

where v^{μ} are arbitrary functions of time and we have introduced $\frac{\partial}{\partial t}$ to account for possible explicit dependences on time.

Let us now examine the marriage between the algebraic and differential parts in (8). First, we require the preservation in time of the primary constraints, that is, $\mathbf{X}_{\mathbf{H}}\phi_{\mu} = \mathbf{0}$ on any trajectory solution of (8). These are tangency conditions that may lead to new constraints and to the determination of some of the functions v^{μ} . Here enters Dirac's clever idea of splitting the primary constraints in two types: those that are first-class, ϕ_{μ_0} , and the rest, called second class, ϕ_{μ_1} . They are defined respectively by

$$\{\phi_{\mu_0}, \phi_{\mu}\} =_{pc} 0, \quad \text{and} \quad \det |\{\phi_{\mu_1}, \phi_{\nu_1}\}| \neq 0, \quad (10)$$

where $\{-, -\}$ is as before the Poisson Bracket and pc stands for a generic linear combination of the *primary* constraints. The subscript pc under the sign of equality (or inequality) means that such equality (or inequality) holds for all the points in phase space that lie on the primary constraints' surface. Let us mention the technical point that sometimes the inequality above does not hold for every point; this fact rises the issue that some constraints initially classified as second-class may eventually become first-class when new constraints appear in the formalism. We will not consider such a situation and will assume henceforth that the determinant in (10) will be different from zero everywhere on the surface of primary constraints.

Note that the concept of a function being first-class is not restricted to functions representing constraints. In fact, we say that a function f is first-class with respect to a given set of constraints if its Poisson bracket with these constraints vanishes in the constraints' surface.

2.4 Refining the dynamics

The requirement of the tangency of $\mathbf{X}_{\mathbf{H}}$ to the second class constraints fixes some arbitrariness in the Hamiltonian dynamics. The arbitrary functions v^{ν_1} —where ν_1 runs over the indices of the second class constraints⁴— become determined as canonical functions $v_c^{\nu_1}$ through

$$0 = \mathbf{X}_{\mathbf{H}} \phi_{\mu_1} = \{\phi_{\mu_1}, H_c\} + v_c^{\nu_1} \{\phi_{\mu_1}, \phi_{\nu_1}\}, \qquad (11)$$

which yields

$$v_c^{\mu_1} = -M^{\mu_1\nu_1} \{\phi_{\nu_1}, H_c\},$$

where $M^{\mu_1\nu_1}$ is the matrix inverse of the Poisson bracket matrix of the primary secondclass constraints, $\{\phi_{\mu_1}, \phi_{\nu_1}\}$.

Substituting $v_c^{\nu_1}$ for v^{ν_1} in (9) gives a more refined expression for the dynamics:

$$\mathbf{X}_{\mathbf{H}}^{1} := \frac{\partial}{\partial t} + \{-, H_{c}\}^{*} + v^{\mu_{0}}\{-, \phi_{\mu_{0}}\}, \qquad (12)$$

where a new structure, the Dirac bracket, has been introduced, at this level of the primary constraints, by the definition

$$\{A, B\}^* := \{A, B\} - \{A, \phi_{\mu_1}\} M^{\mu_1 \nu_1} \{\phi_{\nu_1}, B\},\$$

Next we must require the dynamics to preserve the primary first-class constraints ϕ_{μ_0} . The definition of the first class property in (10) makes irrelevant the choice between the initial form of the dynamics and the refined form. For with either choice this requirement ends up as the condition

$$\{\phi_{\nu_0}, H_c\} = 0,$$

on any solution of (8). If, for some ν_0 , the bracket $\{\phi_{\nu_0}, H_c\}$ already gives zero on the primary constraints' surface, nothing new needs to be done, but if $\phi_{\nu_0}^1 := \{\phi_{\nu_0}, H_c\}$ is different from zero on that surface, it means that we have found *new constraints* that further restrict the region where solutions to (8) may exist. These $\phi_{\nu_0}^1$ (for the appropriate ν_0 's) are called the *secondary* constraints (Anderson and Bergmann 1951).

Note that the evolutionary operator (12) can be alternatively expressed (taking into account the fulfillment of the primary constraints) as

$$\mathbf{X}_{\mathbf{H}}^{1} := \frac{\partial}{\partial t} + \{-, H_{c}^{*}\} + v^{\mu_{0}}\{-, \phi_{\mu_{0}}\}, \qquad (13)$$

⁴In the SHPMP version of this article, "second class constraints" is mistakenly written "secondary cosntraints".

with H_c^* itself a new canonical hamiltonian defined by

$$H_c^* := H_c - \{H_c, \phi_{\mu_1}\} M^{\mu_1 \nu_1} \phi_{\nu_1}, \tag{14}$$

thus making the use of the Dirac bracket unnecessary.

Summing up, an initial analysis of the internal consistency of the system (8) has led us to the equivalent system

$$\dot{q} = \{q, H_c^*\} + v^{\mu_0}\{q, \phi_{\mu_0}\},$$

$$\dot{p} = \{p, H_c^*\} + v^{\mu_0}\{p, \phi_{\mu_0}\},$$

$$0 = \phi_{\mu}(q, p)$$

$$0 = \phi_{\mu_0}^1(q, p),$$
(15)

which is a first step in our endeavour to decouple the differential and the algebraic sides in (8). In the language of the trade, we have undertaken the first step in the Dirac constraint algorithm.

Now the way is paved for the next steps to be taken. If new —i.e. secondary constraints have been introduced in the first step, we must ask again for the tangency of the new evolution operator, (12) or (13), to them. This requirement may bring some of the formerly primary first-class constraints into the second-class category (thus producing the determination of some of the remaining arbitrary functions) and, again, may give new —tertiary— constraints. We will not dwell on the details, easily reconstructed, but just mention that the application of the algorithm ends when we reach a final constraint surface to which the final form of the time evolution vector field is already tangent, so that no more constraints appear and no more arbitrary functions get determined by consistency requirements. This final evolution vector field will be written as

$$\mathbf{X}_{\mathbf{H}}^{\mathbf{F}} := \frac{\partial}{\partial t} + \{-, H'\} + v^{\mu'}\{-, \phi_{\mu'}\}, \qquad (16)$$

with H' the final, first-class, Hamiltonian⁵, and $\phi_{\mu'}$ the final primary first-class constraints.

So at this final stage a certain set of constraints, primary, secondary, tertiary, etc., will restrict the region of phase space where a solution can exist. Let us denote these generic constraints as ϕ_A , for some index A that will run through the whole set of primary,

⁵Note that H' is a specific choice of a canonical Hamiltonian.

secondary, tertiary, etc., constraints. So the final picture of the dynamics will be expressed with a system of equations equivalent to (8),

$$\dot{q} = \{q, H'\} + v^{\mu'}\{q, \phi_{\mu'}\},
\dot{p} = \{p, H'\} + v^{\mu'}\{p, \phi_{\mu'}\},
0 = \phi_A(q, p),$$
(17)

with $v^{\mu'}$ the arbitrary functions associated with the final primary first-class constraints $\phi_{\mu'}$.

Note the crucial difference between the initial equations (8) and the final ones (17). Since H' and $\phi_{\mu'}$ are first-class with respect to the whole set of constraints ϕ_A , we only need to choose the initial conditions —at, say, t = 0— (q(0), p(0)) in such a way that the constraints are satisfied. Then, for whatever arbitrary functions we may use for $v^{\mu'}$, the solution of the differential equations in the first two lines in (17) will always satisfy the constraints. The differential and the algebraic sides in (17) are now completely disentangled.

The presence of arbitrary functions in the final form of the dynamics (17) signals the existence of gauge freedom, which will be the subject of the next section. Note that there may exist constrained systems (that is, systems described by singular Lagrangians) that do not exhibit any gauge freedom, because all constraints eventually become second class. That is why the phrases of "gauge theories" and "constrained systems" are not entirely equivalent.

Finally, for further use, let us mention the notation invented by Dirac for the concepts of weak (\approx) and strong (\equiv) equalities, with respect to a set of constraints that we denote generically by ϕ . A function f is said to be *weakly equal* to zero,

$$f \approx 0$$
,

if it vanishes on the surface defined by the constraints, f = 0. A function f is said to be *strongly equal* to zero,

$$f\equiv 0\,,$$

if both f and its differential —that is, its partial derivatives $\frac{\partial f}{\partial q}$, $\frac{\partial f}{\partial p}$ — vanish on the surface defined by the constraints, $f \stackrel{=}{_{\phi=0}} 0$, $df \stackrel{=}{_{\phi=0}} 0$.

3 Gauge freedom: Dirac's view

As we said, when the final equations (17) exhibit arbitrary functions in the dynamics, the phenomenon of gauge freedom is present in our formulation, and there will exist gauge transformations connecting different solutions of (17) that share the same initial conditions. From the mathematical point of view, the dynamics is no longer deterministic.

Now we will reproduce in literal terms Dirac's analysis of gauge transformations. Let us say at the outset that, as the title of this paper indicates, we shall eventually find this analysis incomplete; but in this Section we will accurately reproduce Dirac's view in his own words. Our comments will be reserved for the next section. The source here will be exclusively the little book (1964), which was written when the theory of constrained systems was settled enough, and which probably represents Dirac's mature perspective on the subject.

Dirac, verbatim:

Let us try to get a physical understanding of the situation where we start with given initial variables and get a solution of the equations of motion containing arbitrary functions. The initial variables which we need are the q's and the p's. We don't need to be given initial values for the coefficients v. These initial conditions describe what physicists would call the *initial physical state* of the system. The physical state is determined only by the q's and the p's and not by the coefficients v.

Now the initial state must determine the state at later times. But the q's and the p's at later times are not uniquely determined by the initial state because we have the arbitrary functions v coming in. That means that the state does not uniquely determine a set of q's and p's, even though a set of q's and p's uniquely determines a state. There must be several choices of q's and p's which correspond to the same state. So we have the problem of looking for all the sets of q's and p's that correspond to one particular physical state.

All those values for the q's and p's at a certain time which can evolve from one initial state must correspond to the same physical state at that time. Let us take particular initial values for the q's and the p's at time t = 0, and consider what the q's and the p's are after a short time interval δt . For a general dynamical variable g, with initial value g_0 , its value at time δt is

$$g(\delta t) = g_0 + \delta t \, \dot{g}$$
(18)
= $g_0 + \delta t \{g, H_T\}$
= $g_0 + \delta t(\{g, H'\} + v^a \{g, \phi_a\}).$

The coefficients v are completely arbitrary and at our disposal. Suppose we take different values, v', for these coefficients. That would give a different $g(\delta t)$, the difference being

$$\Delta g(\delta t) = \delta t (v^{\prime a} - v^a) \{g, \phi_a\}.$$
⁽¹⁹⁾

We may write this as

$$\Delta g(\delta t) = \epsilon^a \{g, \, \phi_a\}\,,\tag{20}$$

where

$$\epsilon^a = \delta t (v'^a - v^a) \tag{21}$$

is a small arbitrary number, small because of the coefficient δt and arbitrary because the v's and v's are arbitrary. We can change all our Hamiltonian variables in accordance with the rule (20) and the new Hamiltonian variables will describe the same state. This change in the Hamiltonian variables consists in applying an infinitesimal contact transformation with a generating function $\epsilon^a \phi_a$. We come to the conclusion that the ϕ_a 's, which appeared in the theory in the first place as the primary first-class constraints, have this meaning: as generating functions of infinitesimal contact transformations, they lead to changes in the q's and the p's that do not affect the physical state. (Dirac 1964, p 20-21)

Dirac next shows in extreme detail that applying, after $\epsilon^a \phi_a$, a second contact transformation $\gamma^a \phi_a$, reversing the order and subtracting, and using the Jacobi identity for the Poisson brackets, one gets

$$\Delta g = \epsilon^a \gamma^b \{ g, \{ \phi_a, \phi_b \} \}, \qquad (22)$$

and then he infers that:

This Δg must also correspond to a change in the q's and the p's which does not involve any change in the physical state, because it is made up by processes which individually don't involve any change in the physical state. Thus we see that we can use

$$\{\phi_a, \phi_b\}\tag{23}$$

as a generating function of an infinitesimal contact transformation and it will still cause no change in the physical state.

Now the ϕ_a are first-class: their Poisson brackets are weakly zero, and therefore strongly equal to some linear function of the ϕ 's. This linear function of the ϕ 's must be first-class because of the theorem I proved a little while back, that the Poisson bracket of two first-class quantities is first-class. So we see that the transformations which we get this way, corresponding to no change in the physical state, are transformations for which the generating function is a first-class constraint. The only way these transformations are more general than the ones we had before is that the generating functions which we had before are restricted to be first-class primary constraints. Those that we get now could be first-class secondary constraints. The result of this calculation is to show that we might have a first-class secondary constraint as a generating function of an infinitesimal contact transformation which leads to a change in the q's and the p's without changing the state.

For the sake of completeness, there is a little bit of further work one ought to do which shows that a Poisson bracket $\{H', \phi_a\}$ of the first-class hamiltonian with a first-class ϕ is again a linear function of first-class constraints. This can also be shown to be a possible generator for infinitesimal contact transformation which do not change the state.

The final result is that those transformations of the dynamical variables which do not change physical states are infinitesimal contact transformations in which the generating function is a primary first-class constraint or possibly a secondary first-class constraint. A good many of the secondary first-class constraints turn up by the process (23) or as $\{H', \phi_a\}$. I think it may be that all the first-class secondary constraints should be included among the transformations which don't change the physical state, but I haven't been able to prove it. Also, I haven't found any example for which there exist first-class secondary constraints which do generate a change in the physical state. (Dirac 1964, p 22-23-24)

We were led to the idea that there are certain changes in the p's and the q's that do not correspond to a change of state, and which have as generators first-class secondary constraints. That suggests that one should generalize the equations of motion in order to allow as variations of a dynamical variable g with the time not only any variation given by

$$\dot{g} = \{g, H_T\},\$$

but also any variation which does not correspond to a change of state. So we should consider a more general equation of motion

$$\dot{g} = \{g, H_E\}$$

with an extended Hamiltonian H_E , consisting of the previous Hamiltonian H_T , plus all those generators that do not change the state, with arbitrary coefficients:

$$H_E = H_T + v^{\prime a'} \phi_{a'}.$$

Those generators $\phi_{a'}$, which are not included already in H_T , will be the firstclass secondary constraints. The presence of these further terms in the Hamiltonian will give further changes in g, but these further changes in g do not correspond to any change of state and so they should certainly be included, even though we did not arrive at these further changes of g by direct work from the Lagrangian." (Dirac 1964, p 25)

You notice that when we have passed over to the quantum theory, the distinction between primary constraints and secondary constraints ceases to be of any importance....Once we have gone over to the Hamiltonian formalism we can really forget about the distinction between primary constraints and secondary constraints. The distinction between first-class and second-class constraints is very important." (Dirac 1964, p 43)

4 Gauge freedom revisited: the incompleteness of Dirac's view

The limitation of Dirac's analysis is that he only examined the gauge transformations in an infinitesimal neighborhood of the initial conditions. This is shown by his using an infinitesimal parameter, that he took as δt , and an arbitrary function, which he took as the difference $v^a - v'^a$. Instead, we shall proceed to examine gauge transformations at any value of the parameter t, that is, gauge transformations for the entire trajectory. The infinitesimal parameter will no longer be δt , but a new δs that describes an infinitesimal motion that maps a trajectory into another in such a way that points are mapped into points corresponding to the same time. This new δs , times an arbitrary function f^a , will describe the difference $v'^a - v^a$, which now is taken to be infinitesimal. So the infinitesimal parameter and the arbitrary function appear together in

$$\epsilon^a := v'^a - v^a = \delta v^a = \delta s f^a$$

The two total Hamiltonians $H' + v^a \phi_a$ and $H' + v'^a \phi_a$, differ by an infinitesimal arbitrary function for any value of the time parameter t. This proposal goes beyond the scope of Dirac's work, which was circumscribed to an infinitesimal neighborhood of the canonical variables describing the trajectory at time t = 0.

We will see that when we complete the work by Dirac, the generators of gauge transformations (mapping solutions into solutions) will be characterized⁶ by nice mathematical expressions which, when restricted to the infinitesimal region examined by Dirac, that is, around the initial conditions, will reproduce his results.

Consider⁷ a dynamical trajectory generated by the total Hamiltonian $H_T = H' + v^a \phi_a$

 $^{^{6}}$ We present a slightly modified derivation from that in Gracia and Pons (1988), see also Banerjee, Rothe and Rothe (1999) for a parallel derivation.

⁷We keep using Dirac's notation: H' is a first-class canonical Hamiltonian and ϕ_a are the final primary

out of some initial conditions at t = 0. To emphasise the role of the arbitrary functions v^a , let us use the notation $g_v(t)$ for it. This trajectory satisfies the equations of motion

$$\dot{g}_v(t) = \{g, H'\}_{g_v(t)} + v^a \{g, \phi_a\}_{g_v(t)}$$

An infinitesimally close trajectory, sharing the same initial conditions and generated by $H' + v'^a \phi_a$, with $v' = v^a + \delta v^a$, will be denoted by $g_{v'}$. Let us define the variation $\Delta g = g_{v'} - g_v$, which is an equal-time variation, that is, $\Delta g(t) = g_{v'}(t) - g_v(t)$. Because of that, this variation commutes with the time derivative,

$$\left[\Delta, \, \frac{d}{dt}\right] = 0\,. \tag{24}$$

We shall make extensive use of this fact in the following.

First, notice that $\Delta g(t)$ can be conceived as the result of a chain of canonical transformations: bringing $g_v(t)$ down to $g_v(0) = g_{v'}(0)$ through the time evolution generated by $H' + v^a \phi_a$ (going backwards in time) and then up to $g_{v'}(t)$ using $H' + v'^a \phi_a$. Therefore $\Delta g(t)$ is an infinitesimal canonical transformation that can be written as

$$\Delta g(t) = \{g, G(t)\}_{q_t} \tag{25}$$

for some function $G(t)^8$ in phase space, that is, a function G(q, p; t). Note that a change of the coefficient functions v^a will also produce changes in G(t). Since the vector field $\{-, G(t)\}$ generates a map from solutions into solutions, it must preserve the constraints of the theory, therefore G(t) is first-class function.

Now let us use (24) to compute $\Delta \dot{g}$ in two different ways (we use $v'^a = v^a + \delta v^a$ and keep terms up to first order in δv^a).

First way

$$\begin{split} \Delta \dot{g} &= \dot{g}_{v'} - \dot{g}_{v} = \{g, H'\}_{g_{v+\delta v}} + (v^{a} + \delta v^{a})\{g, \phi_{a}\}_{g_{v+\delta v}} - \{g, H'\}_{g_{v}} - v^{a}\{g, \phi_{a}\}_{g_{v}} \\ &= \left(\{g, H'\}_{g_{v+\delta v}} - \{g, H'\}_{g_{v}}\right) + \left(v^{a}\{g, \phi_{a}\}_{g_{v+\delta v}} - v^{a}\{g, \phi_{a}\}_{g_{v}}\right) + \delta v^{a}\{g, \phi_{a}\}_{g_{v}} \\ &= \left(\frac{\partial\{g, H'\}}{\partial g}\right)_{g_{v}} \Delta g + v^{a} \left(\frac{\partial\{g, \phi_{a}\}}{\partial g}\right)_{g_{v}} \Delta g + \delta v^{a}\{g, \phi_{a}\}_{g_{v}} \end{split}$$

first-class constraints.

⁸Observe that G(t) is hiding an infinitesimal factor δs which for the sake of simplicity we do not make explicit.

$$= \left(\frac{\partial\{g, H'\}}{\partial g}\right)_{g_{v}}\{g, G\}_{g_{v}} + v^{a}\left(\frac{\partial\{g, \phi_{a}\}}{\partial g}\right)_{g_{v}}\{g, G\}_{g_{v}} + \delta v^{a}\{g, \phi_{a}\}_{g_{v}}$$

$$= \left(\{\{g, H'\}G\} + v^{a}\{\{g, \phi_{a}\}G\} + \delta v^{a}\{g, \phi_{a}\}\right)_{g_{v}}$$

$$= \left(\{\{g, H_{T}\}G\} + \delta v^{a}\{g, \phi_{a}\}\right)_{g_{v}}.$$

Second way

$$\Delta \dot{g} = \frac{d}{dt} \Delta g = \frac{d}{dt} \{g, G\}_{gv}$$
$$= \frac{\partial}{\partial t} \{g, G\}_{gv} + \{\{g, G\}, H_T\}_{gv}$$
$$= \left(\{g, \frac{\partial G}{\partial t}\} + \{\{g, G\}, H_T\}\right)_{gv}$$

Now, comparing these two expressions for $\Delta \dot{g}$ and using the Jacobi identities for the Poisson brackets leads to

$$\{g, \frac{\partial G}{\partial t} + \{G, H_T\} - \delta v^a \phi_a\}_{g_v} = 0.$$

At any time, the point $g_v(t)$ in phase space, for a generic dynamical trajectory g_v , can be any point on the surface of constraints. Thus, freed from a specific trajectory, the contents of the previous expression is just the weak equality

$$\{g, \frac{\partial G}{\partial t} + \{G, H_T\} - \delta v^a \phi_a\} \approx 0.$$

The variable g represents any canonical variable, therefore the last expression is equivalent to the strong equality

$$\frac{\partial G}{\partial t} + \{G, H_T\} - \delta v^a \phi_a \equiv f(t) \,,$$

for some function f that depends exclusively on the time parameter t. A trivial redefinition of G,

$$G(t) \to G(t) - \int^t d\tau f(\tau)$$

makes this function disappear without affecting (25). We obtain, with the redefined G,

$$\frac{\partial G}{\partial t} + \{G, H_T\} - \delta v^a \phi_a \equiv 0.$$
(26)

Recall that the δv^a 's are arbitrary infinitesimal functions, and the ϕ_a 's are the primary first-class constraints (**pfcc**). Then (26) can be alternatively written with no mention to the δv^a 's,

$$\frac{\partial G}{\partial t} + \{G, H_T\} \equiv \mathbf{pfcc} \,. \tag{27}$$

Finally, recalling that $H_T = H' + v^a \phi_a$ and that the functions v^a are arbitrary as well, we get the three conditions for G(t) to be a canonical generator of infinitesimal gauge transformations:

$$G(t)$$
 is a first class function, (28)

$$\frac{\partial G}{\partial t} + \{G, H'\} \equiv \mathbf{pfcc}, \qquad (29)$$

$$\{G, \phi_a\} \equiv \mathbf{pfcc} \,. \tag{30}$$

Note that putting **pc** (primary constraints) instead of **pfcc** in (29) and (30) would have been sufficient because the first class condition in these equations is already guaranteed by (28) taken together with the fact that H' and ϕ_a are first class.

Let us briefly comment on our result. We have found that, in addition to being firstclass, G is a constant of motion for the dynamics generated by H_T , for any values of the arbitrary functions v^a . This is just the meaning of (29) and (30). It is a constant of motion of a very specific type, as is seen directly in (27). One must notice that, in contrast with the case of regular theories, Dirac-Bergmann constrained systems have different types of constants of motion, according to the status of what appears in the right side of (27). For instance, if instead of the strong equality to a linear combination of primary first-class constraints, we had a strong or weak equality to *any* constraint, we still would have a constant of motion, but if (27) is not satisfied, it will not generate a gauge transformation.

But in fact our result goes beyond the consideration of gauge transformations. We have just found the conditions for G(t) in (25) to generate a symmetry, either rigid or gauge. Any object G satisfying the three conditions above is a canonical generator of a symmetry of the dynamics, that maps solutions into solutions. These symmetries may depend on arbitrary functions (more on this below) and then will be called gauge symmetries (or gauge transformations). If they do not depend on arbitrary functions they will be called rigid symmetries. What we have found in the three conditions (28), (29), (30) is the characterization of the generators of symmetries in phase space that are canonical transformations.

It is worth noticing that conditions (28), (29), (30) come very close to saying that G is a Noether conserved quantity, thus generating a Noether symmetry through (25). Indeed this would have been the case if our theory had been defined by a regular Lagrangian, and not by a singular one. But in gauge systems, Noether theory has some specific features. Let us just mention that the characterisation of a conserved quantity that generates a Noether symmetry projectable from tangent space to phase space⁹ is given in Batlle, Gomis, Gracia and Pons (1989) by the following conditions

$$\frac{\partial G}{\partial t} + \{G, H_c\} = \mathbf{pc}, \qquad (31)$$

$$\{G, \mathbf{pc}\} = \mathbf{pc} \,. \tag{32}$$

Note that the fulfillment of (31), (32) makes G first class. Equations (31), (32) are more restrictive than (28), (29), (30) in three ways. (a) The strong equality there is replaced here by an ordinary equality. (b) In (32) the Hamiltonian is the canonical one, H_c , which, unlike H', is not necessarily first-class. (c) In the Poisson bracket in (32) all primary constraints appear in the lhs, and not only those that are first-class.

5 Bergmann's version of gauge transformations

Probably inspired by the examples of electromagnetism, where the gauge transformation of the gauge potential is

$$\delta A_{\mu} = \{A_{\mu}, G\} = \partial_{\mu}\Lambda \,,$$

for an arbitrary function Λ , and general relativity, where the gauge transformations (diffeomorphisms) for the metric field read

$$\delta g_{\mu\nu} = \epsilon^{\rho} \partial_{\rho} g_{\mu\nu} + g_{\mu\rho} \partial_{\nu} \epsilon^{\rho} + g_{\rho\nu} \partial_{\mu} \epsilon^{\rho} \,,$$

(for some arbitrary functions ϵ^{ρ} , components of an arbitrary vector field), Anderson and Bergmann (1951) conceived a gauge transformation in a general field theory as (Φ_A representing any field or field component)

$$\delta \Phi_A = f_A \xi + f_A^{\mu} \partial_{\mu} \xi + f_A^{\mu\nu} \partial_{\mu\nu} \xi + \dots ,$$

where $\xi(x^{\mu})$ is an arbitrary function of the space-time coordinates and ∂_{μ} stands for the partial derivatives. In our formulation of canonical generators, and restricting ourselves

⁹In gauge theories, there may be Noether symmetries in the tangent bundle that are *not* projectable to phase space. This case has been discussed in Garcia and Pons (2000), see also Garcia and Pons (2001), Gracia and Pons (2001).

to the language of mechanics rather than that of field theory, this will correspond to an ansatz of the form (see also Castellani (1982))

$$G(t) = G_0\xi(t) + G_1\dot{\xi}(t) + G_2\ddot{\xi}(t) + \ldots = \sum_{i=0}^N G_i\xi^{(i)}(t), \qquad (33)$$

with ξ an arbitrary function of the time parameter and with G_i functions of the canonical variables, to be determined. We have assumed that a finite number of terms will suffice. Let us plug this ansatz into (29), (30) and take into account the arbitrariness of ξ . We get, from (30),

$$\{G_i, \phi_a\} \equiv \mathbf{pfcc}, \ i = 0, \dots, N.$$
(34)

and from (29),

$$\{G_0, H'\} \equiv \mathbf{pfcc}, \qquad (35)$$

$$G_{i-1} \equiv \{G_i, H'\} + \mathbf{pfcc}, \ i = 1, \dots, N.$$
 (36)

$$G_N \equiv \mathbf{pfcc}$$
. (37)

The intuitive idea behind these expressions is quite clear: the last one sets G_N to be a primary first-class constraint (up to pieces quadratic in the constraints). Next, using the iteration in (36), G_{N-1} is found to be a secondary first-class constraint (up to **pfcc** pieces), and so on, until we reach G_0 , which is required to satisfy (35), that puts a stop to the stabilisation algorithm.

In addition, every G_i must satisfy (34). It is by no means trivial to prove that there exist solutions for the ansatz (33). This existence was proved in Gomis, Henneaux and Pons (1990) under just the conditions a) that the rank of the Hessian matrix is constant, b) that the constraints that are initially second-class, remain always so under the stabilisation algorithm, and c) that no ineffective constraints¹⁰ appear in the theory.

So let us suppose that these conditions are met and that a gauge generator of the form (33) exists. This generator is made up of first-class constraints, so it automatically satisfies the first requirement (28), and therefore all three requirements (28), (29), (30) are fulfilled. In addition, since it is a combination of constraints, the value of G as a conserved quantity is zero¹¹.

¹⁰A constraint is said to be ineffective if its differential vanishes on the constraints' surface. See Pons, Salisbury and Shepley (2000), section 2, for further considerations.

¹¹This assertion needs a prompt qualification in field theory because of possible contributions from the

Now let us try to recover the results of Dirac. He considered a gauge transformation acting at time δt and which at time t = 0 did not produce any change because it preserved the initial conditions. Since

$$\delta g(t) = \{g, G(t)\} = \sum_{i=0}^{i=N} \{g, G_i\} \xi^{(i)}(t), \qquad (38)$$

we must impose $\xi^{(i)}(0) = 0$, $i = 0, \ldots, N$, in order to guarantee $\delta g(0) = 0$ for generic constraints G_i . Then, at an infinitesimal time δt , and to first order in δt ,

$$\xi^{(i)}(\delta t) = \xi^{(i)}(0) + \delta t \,\xi^{(i+1)}(0), \ i = 0, \dots, N \,, \tag{39}$$

thus implying, to this order,

$$\xi^{(i)}(\delta t) = 0, \ i = 0, \dots, N - 1; \ \xi^{(N)}(\delta t) = \delta t \,\xi^{(N+1)}(0) \,, \tag{40}$$

where the value of $\xi^{(N+1)}(0)$ is arbitrary. The choice $\xi^{(N+1)}(0) = v' - v$, where v' - v is $v'^a - v^a$ as in (21) but for a fixed *a*—corresponding to a single gauge transformation—, produces ($\epsilon = \delta t(v' - v)$, see (21))

$$\delta g(\delta t) = \epsilon \left\{ g, \, G_N \right\},\tag{41}$$

which is, recalling from (37) that G_N is a **pfcc**, Dirac's result (20). Here it has been obtained as a first order computation in δt , which was exactly Dirac's starting point.

Now we are ready to connect the concept of a gauge transformation as a map of solutions into solutions, which is Bergmann's view, with Dirac's concept of a gauge transformation at a given time, which can be understood as mapping a set of initial conditions into a gauge equivalent set. In view of equation (33), it is clear that the full generator of a gauge transformation, G(t), is equivalent to a set of different, independent generators of gauge transformations at a given time. It suffices to consider that, at any fixed time t_0 , the quantities $\xi^{(i)}(t_0)$ are just independent numerical quantities (remember that $\xi(t)$ was an arbitrary function), and therefore the functions G_i become independent generators of gauge transformations at a given time.

spatial boundary in the definition of a conserved charge from a conserved current, as happens in GR (Regge and Teitelboim 1974, York 1972, York 1986, Gibbons and Hawking 1977, Pons 2003).

6 Comments

Notice that if we expand to second order in δt the previous expressions, the role of the secondary first-class constraints emerges. This was probably the idea of Dirac in the paragraph reproduced above: "For the sake of completeness, there is a little bit or further work one ought to do which shows that a Poisson bracket $\{H', \phi_a\}$ of the first-class hamiltonian with a first-class ϕ is again a linear function of first-class constraints. This can also be shown to be a possible generator for infinitesimal contact transformation which do not change the state".

It is very curious, to say the least, that such a relevant argument, purely mathematical, does not appear more elaborated in Dirac's book, in contrast with his previous argument, also reproduced in section 3, where it is shown in detail that the Poisson bracket of two primary first-class constraints must be still a generator of gauge transformations at a given time. This argument, which is just mentioned with a concise *can also be shown*, is crucial to understanding the origin of the incompleteness of Dirac's analysis, because it could have been used to show that one does not need to modify the dynamics in order to ensure that all first-class constraints are allowed to generate gauge transformations at a given time. At this point Dirac seems to think of his argument as *physical* rather than *mathematical*, and so he is led to believe that the preservation, and pre-eminence, of the physical interpretation makes it necessary to artificially modify the dynamics.

Let us rephrase our main point. Dirac attempted to carefully distinguish the mathematical and the physical aspects of the formulation. On the other hand, he was convinced that a physically conceived gauge transformation at a given time, in order to be mathematically recognised as such, should have its generator explicitly appearing in the Hamiltonian, with its corresponding Lagrangian multiplier. Otherwise there would have been something wrong with the formalism. His thinking in this respect is clearly stated in the third paragraph reproduced in section 3. Then, in view of the fact that there could be secondary first-class constraints generating gauge transformations at a given time, and that they were not present in the total Hamiltonian, he proposed the extended Hamiltonian as the true generator of time evolution, to prevent the formalism from any contradiction. Thus, being afraid of an inconsistency between the mathematical formalism and its physical interpretation, Dirac proposed to modify the dynamics through the introduction of the Extended Hamiltonian. Considering in his view the subsidiary role of mathematics, and in full agreement with his approach to these disciplines (Kragh 1990), he put physical intuition first. Regretfully he did so in this case based on an incomplete analysis. Now, completion of his analysis shows that there is no tension whatsoever between the mathematical description and the physical content of gauge transformations, and that his proposal for the Extended Hamiltonian was totally unnecessary.

On the technical side we observe that, in constructing a gauge transformation, Dirac looked for an infinitesimal transformation containing an arbitrary function. The arbitrariness he found in the functions v (see (21)), whereas the infinitesimality he took from the time evolution, δt . This last step in his construction is responsible for the essential incompleteness of his analysis, because a gauge transformation *at a given time* should not have used the time as the governing parameter of the transformation.

A complementary argument was also developed by Dirac. Since there is always a mathematical jump in the process of quantization of a classical system, he conceived that although from the classical perspective, the classification of primary, secondary, etc. constraints was relevant, the quantization of the system made this nomenclature useless and for quantization the only useful concepts were those of first-class and second-class constraints. He made his point very clear in the last paragraph reproduced in Section Obviously a Hamiltonian including only the primary first-class constraints was at 3. odds with this new way of thinking, and the extended Hamiltonian was a remedy for it. It seems likely that these considerations helped Dirac in deciding to depart from what he thought was deducible from the pure mathematics of the system and to artificially introduce an ad hoc modification of the dynamics. In Dirac's view, therefore, the argument concerning the preservation of the physical interpretation of gauge transformations at a given time, against the purely mathematical interpretation (that, as we insist, he thought were mutually inconsistent), gets somewhat mixed with arguments concerning the process of quantization of a constrained classical system.

Dirac only dealt with gauge transformations at a given time, which can be taken as the time for the setting of the initial conditions. But the most common view of a gauge transformation is that of Bergmann: a symmetry that maps entire solutions (or solutions defined in a region of phase space) of the dynamics into new solutions. The misunderstandings created by the confusion between both concepts have been enormous. Indeed many authors take for granted from Dirac that first-class constraints generate gauge transformations without even making the distinction between Dirac's and Bergmann's concepts. As explained in the last paragraph of the preceding section, the difference between both concepts is neatly displayed when the complete analysis of the generators of gauge transformations is performed.

Let us finally say a few words on the so-called Dirac's conjecture. In fact, one should clearly distinguish between Dirac's formulation of a conjecture, namely, that *all firstclass constraints generate gauge transformations at a given time*, and what he thought —wrongly in our understanding— to be a compulsory consequence of the assumption of this conjecture: the necessity of modifying the dynamics. The conjecture can be proved (Gomis, Henneaux and Pons 1990) under the same assumptions that guarantee the existence of gauge transformations, already spelled out in Section 5. Examples of the failure of this conjecture for some "pathological" models, as well as other considerations on the formalism for these models, have been widely discussed in the literature (see for instance Allcock 1975, Cawley 1979, Frenkel 1980, Sugano and Kimura 1983, Costa, Girotti and Simoes 1985, Cabo and Louis-Martinez 1990, Lusanna 1991, Lusanna 1993, Wu 1994, Miskovic and Zanelli 2003, Rothe and Rothe 2004).

7 Saving the day: the definition of observables and the quantization in the operator formalism

If Dirac's approach to gauge transformations was so incomplete, and his proposal to modify the dynamics so gratuitous and unfounded, one may wonder to what extent has it affected the correct development and applications of the theory. The answer is: very little, and for various reasons.

First, because of the concept of observables, which will be the subject of the following paragraph. Second, because Dirac's method of quantisation in the operator formalism can be introduced either with the total Hamiltonian or with the extended Hamiltonian with equivalent results. A third reason is that important developments, for instance the most powerful theoretical tool for the quantization of constrained systems, the fieldantifield formalism (Batalin and Vilkovisky 1981, Batalin and Vilkovisky 1983a, Batalin and Vilkovisky 1983b, see Gomis, Paris and Samuel 1995 for a general review), did not incorporate these controversial features of Dirac's view¹². Indeed, the natural concept of gauge transformations —as Noether symmetries of the action— to be used in a pathintegral framework is that of mapping trajectories into trajectories (or field configurations into field configurations).

Let us give some details about the first two reasons.

In the classical setting, an observable is defined as a function that is gauge invariant. Consider a time dependent observable $\mathcal{O}(t)$ (the dependence with respect to the phase space variables exists, but is not made explicit) and consider for simplicity that there is only one gauge transformation in the formalism, whose gauge generator is of the form (33), that is

$$G(t) = \sum_{i=0}^{N} G_i \xi^{(i)}(t) ,$$

with G_i being first-class constraints. In fact they are *all* the first-class constraints of the theory if the conditions mentioned in Section 5 are met.

Thus, $\mathcal{O}(t)$ being an observable means that the equal-time Poisson bracket between $\mathcal{O}(t)$ and G(t) vanishes:

$$\{\mathcal{O}(t),\,G(t)\}=0$$

(strictly speaking, this vanishing of the Poisson bracket needs only to hold on the surface defined by the constraints). But, having in mind the expansion of G(t) above and the arbitrariness of the function $\xi(t)$, this is equivalent to the vanishing of the Poisson bracket of $\mathcal{O}(t)$ with respect to all the first-class constraints,

$$\{\mathcal{O}(t), G_i\} = 0, \forall i.$$

¹²In Henneaux and Teitelboim (1992) a mixed approach is taken. These authors first assume Dirac's analysis and consider the extended Hamiltonian formalism, on the grounds —see below— that quantization in the operator formalism only distinguishes between constraints of first or second class. But the authors are able to make contact with the standard gauge transformations —mapping solutions into solutions— by considering the combinations of the extended Hamiltonian gauge transformations —generated independently by the first class constraints— that are compatible with setting to zero in the extended Hamiltonian the Lagrange multipliers associated with the secondary first-class constraints. Clearly the total Hamiltonian formalism and its gauge transformations are recovered. The authors consider the generalization of taking the remaining Lagrange multipliers as new independent variables. This approach has been extended by Garcia and Pons (2001).

The immediate consequence is that the dynamical evolution of $\mathcal{O}(t)$ is deterministic and that in this respect it is irrelevant whatever we use the total Hamiltonian H_T or the extended Hamiltonian H_E . Indeed

$$\frac{d\mathcal{O}}{dt} = \frac{\partial\mathcal{O}}{\partial t} + \{\mathcal{O}, H_T\} = \frac{\partial\mathcal{O}}{\partial t} + \{\mathcal{O}, H_E\}$$

Since we can only attach physical significance to the gauge invariant functions, it is clear the Dirac's proposal of the extended Hamiltonian is harmless, as far as observables are concerned. This key result finally saves the day for Dirac's proposal.

A similar argument can be applied to Dirac's quantization in the operator formalism, where the physical states must be gauge invariant. Let us denote a generic Schrodinger physical state at time t by $|\psi(t)\rangle$. If the first-class constraints G_i can be expressed as linear quantum operators \tilde{G}_i , still remaining first class, where this is understood in terms of the commutator of operators instead of the Poisson bracket, and being stable under the quantum Hamiltonian, then the gauge invariance property of the physical states at a given time becomes

$$\tilde{G}_i|\psi(t)\rangle = 0, \forall i.$$
(42)

So we end up with the requirement that all first-class constraints must be enforced as operators on the quantum state at any time on an equal footing, regardless whether they were primary or not —which was Dirac's idea. Second-class constraints in Dirac formalism are used to eliminate pairs of canonical variables before the process of quantisation is undertaken.

Notice that equations (42) have naturally led us to identify the gauge invariance property of the states with the implementation of the first-class constraints as quantum operators acting on them and giving a vanishing eigenvalue. The difference with the classical picture is noticeable, because the classical trajectories satisfying the constraints are not gauge invariant and further elimination of gauge degrees of freedom is needed, for instance through a gauge fixing procedure. Thus the two issues of a) satisfying the constraints and b) being gauge invariant, which are different from the classical point of view, become identical in the operational quantum picture. This is the origin of the quantum *problem of time* (Isham 1992, Kuchar 1992) for generally covariant systems, for which the Hamiltonian is a first class constraint.

8 Examples

Finally, we illustrate our discussion with two examples.

8.1 The free relativistic particle with auxiliary variable

The relativistic massive free particle model with auxiliary variable is a good example for our purposes. It is described by the Lagrangian

$$L = \frac{1}{2e} \dot{x}^{\mu} \dot{x}^{\nu} \eta_{\mu\nu} - \frac{1}{2} em^2, \qquad (43)$$

where x^{μ} is the vector variable in Minkowski spacetime, with metric $(\eta_{\mu\nu}) = \text{diag}(-1, 1, 1, 1)$. The parameter m is the mass and the auxiliary variable e can be interpreted, in the standard language of canonical general relativity, as a lapse function, the world-line metric being defined by $g_{00} = -e^2$. Its own equation of motion determines $e = (-\dot{x}^{\mu}\dot{x}_{\mu})^{1/2}$, and substitution of this value into the Lagrangian¹³ leads to the free particle Lagrangian $L_f = -\frac{m}{2}(-\dot{x}^{\mu}\dot{x}_{\mu})^{1/2}$. Equation (43) is analogous to the Polyakov Lagrangian for the bosonic string, where the components of the world-sheet metric are auxiliary variables. Substitution of their dynamically determined values yields the Nambu-Goto Lagrangian, analogous to L_f .

The following Noether gauge transformation is well-known to describe the reparametrisation invariance for this Lagrangian $(\delta L = \frac{d}{dt}(\epsilon L))$:

$$\delta x^{\mu} = \epsilon \dot{x}_{\mu}, \ \delta e = \epsilon \dot{e} + \dot{\epsilon} e. \tag{44}$$

Here ϵ is an infinitesimal arbitrary function of the evolution parameter t. There is a primary constraint $\pi \approx 0$, where π is the variable conjugate to e. The only vector field in (5) is now $\Gamma = \partial/\partial \dot{e}$. The condition that a function f in configuration-velocity space be projectable to phase space is

$$\Gamma f = \frac{\partial f}{\partial \dot{e}} = 0.$$

The Noether transformation (44) is not projectable to phase space, since $\Gamma \delta e \neq 0$. Projectable transformations are of the form:

$$\epsilon(t, e) = \xi(t)/e. \tag{45}$$

¹³The legitimacy of this substitution is proved in a general framework in Garcia and Pons 1997.

The Noether variations then become:

$$\delta x^{\mu} = \xi \frac{\dot{x}^{\mu}}{e}, \ \delta e = \dot{\xi}.$$
(46)

The arbitrary function describing the Noether gauge transformation is now $\xi(t)$.

The canonical Hamiltonian is

$$H = \frac{1}{2}e(p^{\mu}p_{\mu} + m^2),$$

where p_{μ} is the variable canonically conjugate to x^{μ} . The evolution operator vector field $\{-, H\} + \lambda(t)\{-, \pi\}$ yields the secondary constraint $\frac{1}{2}(p^{\mu}p_{\mu} + m^2) \approx 0$. Both the primary and the secondary constraints are first class. The arbitrary function λ is a reflection of the gauge invariance of the model. The solutions of the equations of motion are:

$$\begin{aligned} x^{\mu}(t) &= x^{\mu}(0) + p^{\mu}(0) \left(e(0)t + \int_{0}^{t} d\tau \int_{0}^{\tau} d\tau' \,\lambda(\tau') \right), \\ e(t) &= e(0) + \int_{0}^{t} d\tau \,\lambda(\tau), \\ p^{\mu}(t) &= p^{\mu}(0), \\ \pi(t) &= \pi(0), \end{aligned}$$

with the initial conditions satisfying the constraints.

The canonical generator of gauge transformations, satisfying (28), (29) and (30), is

$$G = \xi(t)\frac{1}{2}(p^{\mu}p_{\mu} + m^2) + \dot{\xi}(t)\pi.$$
(47)

Gauge transformations relate trajectories obtained through different choices of $\lambda(t)$. Consider an infinitesimal change $\lambda \to \lambda + \delta \lambda$. Then the change in the trajectories (keeping the initial conditions intact) is:

$$\delta x^{\mu}(t) = p^{\mu}(0) \left(\int_{0}^{t} d\tau \int_{0}^{\tau} d\tau' \,\delta\lambda(\tau') \right),$$
$$\delta e(t) = \int_{0}^{t} d\tau \,\delta\lambda(\tau),$$
$$\delta p^{\mu}(t) = 0, \ \delta\pi(t) = 0,$$

which is nothing but a particular case of the projectable gauge transformations displayed above with

$$\xi(t) = \int_0^t d\tau \int_0^\tau d\tau' \,\delta\lambda(\tau').$$

Notice that the structure of the gauge generator (47) is that of (33). It is only this particular combination of primary and secondary first-class constraints that generates gauge transformations mapping solutions to solutions.

8.2 Maxwell theory

The case of pure electromagnetism is described with the Lagrangian

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

where $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$ and A_{μ} is the Maxwell gauge field. We take again the metric in Minkowski spacetime as $(\eta_{\mu\nu}) = \text{diag}(-1, 1, 1, 1)$. The canonical Hamiltonian is

$$H_c = \int d\mathbf{x} \left[\frac{1}{2} (\vec{\pi}^2 + \vec{B}^2) + \vec{\pi} \cdot \nabla A_0 \right] \,,$$

where the electric field $\vec{\pi}$ stands for the spatial components of π^{μ} , the variables canonically conjugate to A_{μ} . The Lagrangian definition of π^{μ} is $\hat{\pi}^{\mu} = -F^{0\mu}$ and so π^{0} is a primary constraint, $\pi^{0} \approx 0$. The magnetic field is defined as $B_{i} = \frac{1}{2} \epsilon_{ijk} F^{jk}$. Stability of the constraint π^{0} under the Hamiltonian dynamics leads to the secondary constraint $\dot{\pi}^{0} =$ $\{\pi^{0}, H_{c}\} = \nabla \cdot \vec{\pi} \approx 0$. Both constraints are first-class and no more constraints arise.

Now, similarly to the previous example, the gauge generator takes the form

$$G[t] = \int d^3x \left[-\dot{\Lambda}(\mathbf{x},t) \,\pi^0(\mathbf{x},t) + \Lambda(\mathbf{x},t) \,\nabla \cdot \vec{\pi}(\mathbf{x},t) \right]$$

with $\Lambda(\mathbf{x}, t)$ an arbitrary scalar function of the space-time coordinates. The gauge transformation of the gauge field is then

$$\delta A_{\mu} = \{A_{\mu}, G\} = -\partial_{\mu}\Lambda,$$

which is the usual Noether U(1) symmetry for the Lagrangian \mathcal{L}_M . Let us observe again that a primary and a secondary constraint are necessary to build the gauge generator. Notice also that the particular combination of both constraints, together with the role of the function Λ and its time derivative, eventually ensures that the gauge field A_{μ} transforms covariantly.

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