

# **The Classical and Quantum Mechanics of Systems with Constraints**

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May 23, 2002

## **Abstract**

In this paper, we discuss the classical and quantum mechanics of finite dimensional mechanical systems subject to constraints. We review Dirac's classical formalism of dealing with such problems and motivate the definition of objects such as singular and non-singular action principles, first- and second-class constraints, and the Dirac bracket. We show how systems with first-class constraints can be considered to be systems with gauge freedom. A consistent quantization scheme using Dirac brackets is described for classical systems with only second class constraints. Two different quantization schemes for systems with first-class constraints are presented: Dirac and canonical quantization. Systems invariant under reparameterizations of the time coordinate are considered and we show that they are gauge systems with first-class constraints. We conclude by studying an example of a reparameterization invariant system: a test particle in general relativity.

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# 1 Introduction

In this paper, we will discuss the classical and quantum mechanics of finite dimensional systems whose orbits are subject to constraints. Before going any further, we should explain what we mean by “constraints”. We will make the definition precise below, but basically a constrained system is one in which there exists a relationship between the system’s degrees of freedom that holds for all times. This kind of definition may remind the reader of systems with constants of the motion, but that is not what we are talking about here. Constants of the motion arise as a result of equations of motion. Constraints are defined to be restrictions on the dynamics before the equations of motion are even solved. For example, consider a ball moving in the gravitational field of the earth. Provided that any non-gravitational forces acting on the ball are perpendicular to the trajectory, the sum of the ball’s kinetic and gravitational energies will not change in time. This is a consequence of Newton’s equations of motion; i.e., we would learn of this fact after solving the equations. But what if the ball were suspended from a pivot by a string? Obviously, the distance between the ball and the pivot ought to be the same for all times. This condition exists quite independently of the equations of motion. When we go to solve for the ball’s trajectory we need to input information concerning the fact that the distance between the ball and the pivot does not change, which allows us to conclude that the ball can only move in directions orthogonal to the string and hence solve for the tension. Restrictions on the motion that exist prior to the solution of the equations of motion are called constraints.

An other example of this type of thing is the general theory of relativity in vacuum. We may want to write down equations of motion for how the spatial geometry of the universe changes with time. But because the spatial geometry is really the geometry of a 3-dimensional hypersurface in a 4-dimensional manifold, we know that it must satisfy the Gauss-Codazzi equations for all times. So before we have even considered what the equations of motion for relativity are, we have a set of constraints that must be satisfied for any reasonable time evolution. Whereas in the case before the constraints arose from the physical demand that a string have a constant length, here the constraints arise from the mathematical structure of the theory; i.e., the formalism of differential geometry.

Constraints can also arise in sometimes surprising ways. Suppose we are confronted with an action principle describing some interesting theory. To derive the equations of motion in the usual way, we need to find the conjugate momenta and the Hamiltonian so that Hamilton’s equations can be used to evolve dynamical variables. But in this process, we may find relationships between these same variables that must hold for all time. For example, in electromagnetism the time derivative of the  $A_0$  component of the vector potential appears nowhere in the action  $F^{\mu\nu}F_{\mu\nu}$ . Therefore, the momentum conjugate to  $A_0$  is always zero, which is a constraint. We did not have to demand that this momentum be zero for any physical or math-

emational reason, this constraint just showed up as a result of the way in which we define conjugate momenta. In a similar manner, unforeseen constraints may manifest themselves in theories derived from general action principles.

From this short list of examples, it should be clear that systems with constraints appear in a wide variety of contexts and physical situations. The fact that general relativity fits into this class is especially intriguing, since a comprehensive theory of quantum gravity is the subject of much current research. This makes it especially important to have a good grasp of the general behaviour of physical systems with constraints. In this paper, we propose to illuminate the general properties of these systems by starting from the beginning; i.e., from action principles. We will limit ourselves to finite dimensional systems, but much of what we say can be generalized to field theory. We will discuss the classical mechanics of constrained systems in some detail in Section 2, paying special attention to the problem of finding the correct equations of motion in the context of the Hamiltonian formalism. In Section 3, we discuss how to derive the analogous quantum mechanical systems and try to point out the ambiguities that plague such procedures. In Section 4, we special to a particular class of Lagrangians with implicit constraints and work through an example that illustrates the ideas in the previous sections. We also meet systems with Hamiltonians that vanish, which introduces the much talked about “problem of time”. Finally, in Section 5 we will summarize what we have learnt.

## 2 Classical systems with constraints

It is natural when discussing the mathematical formulation of interesting physical situations to restrict oneself to systems governed by an action principle. Virtually all theories of interest can be derived from action principles; including, but not limited to, Newtonian dynamics, electromagnetism, general relativity, string theory, etc. . . . So we do not lose much by concentrating on systems governed by action principles, since just about everything we might be interested in falls under that umbrella. In this section, we aim to give a brief accounting of the classical mechanics of physical systems governed by an action principle and whose motion is restricted in some way. As mentioned in the introduction, these constraints may be imposed on the systems in question by physical considerations, like the way in which a “freely falling” pendulum is constrained to move in a circular arc. Or the constraints may arise as a consequence of some symmetry of the theory, like a gauge freedom. These two situations are the subjects of Section 2.1 and Section 2.2 respectively. We will see how certain types of constraints generate gauge transformations in Section 2.4. Our treatment will be based upon the discussions found in references [1, 2, 3].

## 2.1 Systems with explicit constraints

In this section, we will review the Lagrangian and Hamiltonian treatment of classical physical systems subject to explicit constraints that are added-in “by hand”. Consider a system governed by the action principle:

$$S[q, \dot{q}] = \int dt L(q, \dot{q}). \quad (1)$$

Here,  $t$  is an integration parameter and  $L$ , which is known as the Lagrangian, is a function of the system’s *coordinates*  $q = q(t) = \{q^\alpha(t)\}_{\alpha=1}^n$  and *velocity*  $\dot{q} = \dot{q}(t) = \{\dot{q}^\alpha(t)\}_{\alpha=1}^n$ . The coordinates and velocity of the system are viewed as functions of the parameter  $t$  and an overdot indicates  $d/dt$ . Often,  $t$  is taken to be the time variable, but we will see that such an interpretation is problematic in relativistic systems. However, in this section we will use the term “time” and “parameter” interchangeably. As represented above, our system has a finite number  $2n$  of degrees of freedom given by  $\{q, \dot{q}\}$ . If taken literally, this means that we have excluded field theories from the discussion because they have  $n \rightarrow \infty$ . We note that most of what we do below can be generalized to infinite-dimensional systems, although we will not do it here.

Equations of motion for our system are of course given by demanding that the action be stationary with respect to variations of  $q$  and  $\dot{q}$ . Let us calculate the variation of  $S$ :

$$\begin{aligned} \delta S &= \int dt \left( \frac{\partial L}{\partial q^\alpha} \delta q^\alpha + \frac{\partial L}{\partial \dot{q}^\alpha} \delta \dot{q}^\alpha \right) \\ &= \int dt \left( \frac{\partial L}{\partial q^\alpha} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^\alpha} \right) \delta q^\alpha. \end{aligned} \quad (2)$$

In going from the first to the second line we used  $\delta \dot{q}^\alpha = d(\delta q^\alpha)/dt$ , integrated by parts, and discarded the boundary term. We can justify the latter by demanding that the variation of the trajectory  $\delta q^\alpha$  vanish at the edges of the  $t$  integration interval, which is a standard assumption.<sup>1</sup> Setting  $\delta S = 0$  for arbitrary  $\delta q^\alpha$  leads to the Euler-Lagrange equations

$$0 = \frac{\partial L}{\partial q^\alpha} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^\alpha}. \quad (3)$$

When written out explicitly for a given system, the Euler-Lagrange equations reduce to a set of ordinary differential equations (ODEs) involving  $\{q, \dot{q}, \ddot{q}\}$ . The solution of these ODEs then gives the time evolution of the system’s coordinates and velocity.

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<sup>1</sup>This procedure is fine for Lagrangians that depend only on coordinates and velocities, but must be modified when  $L$  depends on the accelerations  $\ddot{q}$ . An example of such a system is general relativity, where the action involves the second time derivative of the metric. In such cases, integration by parts leads to boundary terms proportional to  $\delta \ddot{q}$ , which does not necessarily vanish at the edges of the integration interval.

Now, let us discuss how the notion of constraints comes into this Lagrangian picture of motion. Occasionally, we may want to impose restrictions on the motion of our system. For example, for a particle moving on the surface of the earth, we should demand that the distance between the particle and the center of the earth be a constant. More generally, we may want to demand that the evolution of  $q$  and  $\dot{q}$  obey  $m$  relations of the form

$$0 = \phi_a(q, \dot{q}), \quad a = 1 \dots m. \quad (4)$$

The way to incorporate these demands into the variational formalism is to modify our Lagrangian:

$$L(q, \dot{q}) \rightarrow L^{(1)}(q, \dot{q}, \lambda) = L(q, \dot{q}) - \lambda^a \phi_a(q, \dot{q}). \quad (5)$$

Here, the  $m$  arbitrary quantities  $\lambda = \{\lambda^a\}_{a=1}^m$  are called Lagrange multipliers. This modification results in a new action principle for our system

$$0 = \delta \int dt L^{(1)}(q, \dot{q}, \lambda). \quad (6)$$

We now make a key paradigm shift: instead of adopting  $q = \{q^\alpha\}$  as the coordinates of our system, let us instead take  $Q = q \cup \lambda = \{Q^A\}_{A=1}^{n+m}$ . Essentially, we have promoted the system from  $n$  to  $n + m$  coordinate degrees of freedom. The new Lagrangian  $L^{(1)}$  is independent of  $\dot{\lambda}^a$ , so

$$\frac{\partial L^{(1)}}{\partial \dot{\lambda}^a} = 0 \quad \Rightarrow \quad \phi_a = 0, \quad (7)$$

using the Euler-Lagrange equations. So, we have succeeded in incorporating the constraints on our system into the equations of motion by adding a term  $-\lambda^a \phi_a$  to our original Lagrangian.

We now want to pass over from the Lagrangian to Hamiltonian formalism. The first thing we need to do is define the momentum conjugate to the  $q$  coordinates:

$$p_\alpha \equiv \frac{\partial L^{(1)}}{\partial \dot{q}^\alpha}. \quad (8)$$

Note that we could try to define a momentum conjugate to  $\lambda$ , but we always get

$$\pi_a \equiv \frac{\partial L^{(1)}}{\partial \dot{\lambda}^a} = 0. \quad (9)$$

This is important, the momentum conjugate to Lagrange multipliers is zero. Equation (8) gives the momentum  $p = \{p_\alpha\}$  as a function of  $Q$  and  $\dot{q}$ . For what follows, we would like to work with momenta instead of velocities. To do so, we will need to be able to invert equation (8) and express  $\dot{q}$  in terms of  $Q$  and  $p$ . This is only

possible if the Jacobian of the transformation from  $\dot{q}$  to  $p$  is non-zero. Viewing (8) as a coordinate transformation, we need

$$\det \left( \frac{\partial^2 L^{(1)}}{\partial \dot{q}^\alpha \partial \dot{q}^\beta} \right) \neq 0. \quad (10)$$

The condition may be expressed in a different way by introducing the so-called mass matrix, which is defined as:

$$M_{AB} = \frac{\partial^2 L^{(1)}}{\partial \dot{Q}^A \partial \dot{Q}^B}. \quad (11)$$

Then, equation (10) is equivalent to demanding that the minor of the mass matrix associated with the  $\dot{q}$  velocities  $M_{\alpha\beta} = \delta_\alpha^A \delta_\beta^B M_{AB}$  is non-singular. Let us assume that this is the case for the Lagrangian in question, and that we will have no problem in finding  $\dot{q} = \dot{q}(Q, p)$ . Velocities which can be expressed as functions of  $Q$  and  $p$  are called *primarily expressible*. Note that the complete mass matrix for the constrained Lagrangian is indeed singular because the rows and columns associated with  $\dot{\lambda}$  are identically zero. It is clear that the Lagrange multiplier velocities cannot be expressed in terms of  $\{Q, p\}$  since  $\dot{\lambda}$  does not appear explicitly in either (8) or (9). Such velocities are known as *primarily inexpressible*.

To introduce the Hamiltonian, we consider the variation of a certain quantity

$$\begin{aligned} \delta(p_\alpha \dot{q}^\alpha - L) &= \delta(p_\alpha \dot{q}^\alpha - L^{(1)} - \lambda^a \phi_a) \\ &= \dot{q}^\alpha \delta p_\alpha + p_\alpha \delta \dot{q}^\alpha - \left( \frac{\partial L^{(1)}}{\partial q^\alpha} \delta q^\alpha + \frac{\partial L^{(1)}}{\partial \dot{q}^\alpha} \delta \dot{q}^\alpha + \frac{\partial L^{(1)}}{\partial \lambda^a} \delta \lambda^a \right) \\ &\quad - \phi_a \delta \lambda^a - \lambda^a \delta \phi_a \\ &= \left( \dot{q}^\alpha - \lambda^a \frac{\partial \phi_a}{\partial p_\alpha} \right) \delta p_\alpha - \left( \dot{p}^\alpha + \lambda^a \frac{\partial \phi_a}{\partial q^\alpha} \right) \delta q^\alpha. \end{aligned} \quad (12)$$

In going from the second to third line, we applied the Euler-Lagrange equations and used

$$\frac{\partial L^{(1)}}{\partial \lambda^a} = -\phi_a. \quad (13)$$

This demonstrates that the quantity  $p_\alpha \dot{q}^\alpha - L$  is a function of  $\{q, p\}$  and not  $\{\dot{q}, \lambda\}$ . Let us denote this function by

$$H(q, p) = p_\alpha \dot{q}^\alpha - L. \quad (14)$$

Furthermore, the variations of  $q$  and  $p$  can be taken to be arbitrary<sup>2</sup>, so (12) implies that

$$\dot{q}^\alpha = + \frac{\partial H}{\partial p_\alpha} + \lambda^a \frac{\partial \phi_a}{\partial p_\alpha}, \quad (15a)$$

$$\dot{p}_\alpha = - \frac{\partial H}{\partial q^\alpha} - \lambda^a \frac{\partial \phi_a}{\partial q^\alpha}. \quad (15b)$$

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<sup>2</sup>This is justified in Appendix A.



Following the usual custom, we attempt to write these in terms of the Poisson bracket. The Poisson bracket between two functions of  $q$  and  $p$  is defined as

$$\{F, G\} = \frac{\partial F}{\partial q^\alpha} \frac{\partial G}{\partial p_\alpha} - \frac{\partial G}{\partial q^\alpha} \frac{\partial F}{\partial p_\alpha}. \quad (16)$$

We list a number of useful properties of the Poisson bracket that we will make use of below:

1.  $\{F, G\} = -\{G, F\}$
2.  $\{F + H, G\} = \{F, G\} + \{H, G\}$
3.  $\{FH, G\} = F\{H, G\} + \{F, G\}H$
4.  $0 = \{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\}$

Now, consider the time derivative of any function  $g$  of the  $q$ 's and  $p$ 's, but not the  $\lambda$ 's:

$$\begin{aligned} \dot{g} &= \frac{\partial g}{\partial q^\alpha} \dot{q}^\alpha + \frac{\partial g}{\partial p_\alpha} \dot{p}_\alpha \\ &= \{g, H\} + \lambda^a \{g, \phi_a\} \\ &= \{g, H + \lambda^a \phi_a\} - \phi_a \{g, \lambda^a\}. \end{aligned} \quad (17)$$

In going from the first to second line, we have made use of equations (15). The last term in this expression is proportional to the constraints, and hence should vanish when they are enforced. Therefore, we have that

$$\dot{g} \sim \{g, H + \lambda^a \phi_a\}. \quad (18)$$

The use of the  $\sim$  sign instead of the  $=$  sign is due to Dirac [1] and has a special meaning: two quantities related by a  $\sim$  sign are only equal after all constraints have been enforced. We say that two such quantities are weakly equal to one another. It is important to stress that the Poisson brackets in any expression must be worked out before any constraints are set to zero; if not, incorrect results will be obtained.

With equation (18) we have essentially come to the end of the material we wanted to cover in this section. This formula gives a simple algorithm for generating the time evolution of any function of  $\{q, p\}$ , including  $q$  and  $p$  themselves. However, this cannot be the complete story because the Lagrange multipliers  $\lambda$  are still undetermined. And we also have no guarantee that the constraints themselves are conserved; i.e., does  $\dot{\phi}_a \sim 0$ ? We defer these questions to Section 2.3, because we should first discuss constraints that appear from action principles without any of our meddling.

## 2.2 Systems with implicit constraints

Let us now change our viewpoint somewhat. In the previous section, we were presented with a Lagrangian action principle to which we added a series of constraints. Now, we want to consider the case when our Lagrangian has contained within it implicit constraints that do not need to be added by hand. For example, Lagrangians of this type may arise when one applies generalized coordinate transformations  $Q \rightarrow \tilde{Q}(Q)$  to the extended  $L^{(1)}$  Lagrangian of the previous section. Or, there may be fundamental symmetries of the underlying theory that give rise to constraints (more on this later). For now, we will not speculate on why any given Lagrangian encapsulates constraints, we rather concentrate on how these constraints may manifest themselves.

Suppose that we are presented with an action principle

$$0 = \delta \int dt L(Q, \dot{Q}), \quad (19)$$

which gives rise to, as before, the Euler-Lagrange equations

$$0 = \frac{\partial L}{\partial Q^A} - \frac{d}{dt} \frac{\partial L}{\partial \dot{Q}^A}. \quad (20)$$

Here, early uppercase Latin indices run over the coordinates and velocities. Again, we define the conjugate momentum in the following manner

$$P_A \equiv \frac{\partial L}{\partial \dot{Q}^A}. \quad (21)$$

A quick calculation confirms that for this system

$$\begin{aligned} \delta(P_A \dot{Q}^A - L) &= P_A \delta \dot{Q}^A + \dot{Q}^A \delta P_A - \left( \frac{\partial L}{\partial Q^A} \delta Q^A + \frac{\partial L}{\partial \dot{Q}^A} \delta \dot{Q}^A \right) \\ &= \dot{Q}^A \delta P_A - \dot{P}_A \delta Q^A. \end{aligned} \quad (22)$$

Hence, the function  $P_A \dot{Q}^A - L$  depends on coordinates and momenta but not velocities. Similar to what we did before, we label the function

$$H(Q, P) = P_A \dot{Q}^A - L(Q, \dot{Q}). \quad (23)$$

Looking at the functional dependence on either side, it is clear we have somewhat of a mismatch. To rectify this, we should try to find  $\dot{Q} = \dot{Q}(Q, P)$ . Then, we would have an explicit expression for  $H(Q, P)$ .

Now, we have already discussed this problem in the previous section, where we pointed out that a formula like the definition of  $p_A$  can be viewed as a transformation of variables from  $P$  to  $\dot{Q}$  via the substitution  $P = P(Q, \dot{Q})$ . We want to do the

reverse here, which is only possible if the transform is invertible. Again the condition for inversion is the non-vanishing of the Jacobian of the transformation

$$0 \neq \det \frac{\partial P_A}{\partial \dot{Q}^B} = \det \frac{\partial^2 L}{\partial \dot{Q}^A \partial \dot{Q}^B} = \det M_{AB}. \quad (24)$$

Lagrangian theories which have mass matrices with non-zero determinant are called non-singular. When we have non-singular theories, we can successfully find an explicit expression for  $H(Q, P)$  and proceed with the Hamiltonian-programme that we are all familiar with.

But what if the mass matrix has  $\det M_{AB} = 0$ ? Lagrangian theories of this type are called singular and have properties which require more careful treatment. We saw in the last section that when we apply constraints to a theory, we end up with a singular (extended) Lagrangian. We will now demonstrate that the reverse is true, singular Lagrangians give rise to constraints in the Hamiltonian theory. It is clear that for singular theories it is impossible to express all of the velocities as function of the coordinates and momenta. But it may be possible to express some of velocities in that way. So we should divide the original sets of coordinates, velocities and momenta into two groups:

$$Q = q \cup \lambda, \quad (25a)$$

$$\dot{Q} = \dot{q} \cup \dot{\lambda}, \quad (25b)$$

$$P = p \cup \pi. \quad (25c)$$

In strong analogy to the discussion of the last section,  $\dot{q}$  is the set of primarily expressible velocities and  $\dot{\lambda}$  is the set of primarily inexpressible velocities. As before, we will have the Greek indices range over the  $(q, \dot{q}, p)$  sets and the early lowercase Latin indices range over the  $(\lambda, \dot{\lambda}, \pi)$  sets. Because  $\dot{q}$  is primarily expressible, we should be able to find  $\dot{q} = \dot{q}(Q, P)$  explicitly. So, we can write  $H(Q, P)$  as

$$H(Q, P) = p_\alpha \dot{q}^\alpha(Q, P) + \pi_a \dot{\lambda}^a - \bar{L}(Q, P, \dot{\lambda}), \quad (26)$$

where

$$\bar{L}(Q, P, \dot{\lambda}) = L(Q, \dot{q}(Q, P), \dot{\lambda}). \quad (27)$$

It is extremely important to keep in mind that in these equations,  $\dot{\lambda}$  cannot be viewed as functions of  $Q$  and  $P$  because they are primarily inexpressible. Now, let us differentiate (26) with respect to  $\dot{\lambda}^b$ , treating  $\pi_a$  as an independent variable:

$$0 = \pi_b - \frac{\partial \bar{L}}{\partial \dot{\lambda}^b}, \quad (28)$$

and again with respect to  $\dot{\lambda}^c$ :

$$0 = \frac{\partial^2 \bar{L}}{\partial \dot{\lambda}^b \partial \dot{\lambda}^c}. \quad (29)$$

The second equation implies that  $\partial\bar{L}/\partial\dot{\lambda}^b$  is independent of  $\dot{\lambda}$ . Defining

$$f_a(Q, P) = \frac{\partial\bar{L}}{\partial\dot{\lambda}^a}, \quad (30)$$

we get

$$0 = \phi_a^{(1)}(Q, P) = \pi_a - f_a(Q, P). \quad (31)$$

These equations imply relations between the coordinates and momenta that hold for all times; i.e. they are equations of constraint. The number of such constraint equations is equal to the number of primarily inexpressible velocities. Because these constraints  $\phi^{(1)} = \{\phi_a^{(1)}\}$  have essentially arisen as a result of the existence of primarily inexpressible velocities, we call them *primary constraints*. We can also justify this name because they ought to appear directly from the momentum definition (21). That is, after algebraically eliminating all explicit references to  $\dot{Q}$  in the system of equations (21), any non-trivial relations between  $Q$  and  $P$  remaining must match (31). This is the sense in which Dirac [1] introduces the notion of primary constraints. We have therefore shown that singular Lagrangian theories are necessarily subjected to some number of primary constraints relating the coordinates and momenta for all times.<sup>3</sup>

Note that we can prove that theories with singular Lagrangians involve primary constraints in an infinitesimal manner. Consider conjugate momentum evaluated at a particular value of the coordinates and the velocities  $Q_0$  and  $\dot{Q}_0$ . We can express the momentum at  $Q_0$  and  $\dot{Q}_0 + \delta\dot{Q}$  in the following way

$$P_A(Q_0, \dot{Q}_0 + \delta\dot{Q}) = P_A(Q_0, \dot{Q}_0) + M_{AB}(Q_0, \dot{Q}_0) \delta\dot{Q}^B. \quad (32)$$

Now, if  $M$  is singular at  $(Q_0, \dot{Q}_0)$ , then it must have a zero eigenvector  $\xi$  such that  $\xi^A(Q_0, \dot{Q}_0)M_{AB}(Q_0, \dot{Q}_0) = 0$ . This implies that

$$\xi^A(Q_0, \dot{Q}_0)P_A(Q_0, \dot{Q}_0 + \delta\dot{Q}) = \xi^A(Q_0, \dot{Q}_0)P_A(Q_0, \dot{Q}_0). \quad (33)$$

In other words, there exists a linear combination of the momenta that is independent of the velocities in some neighbourhood of every point where the  $M$  matrix is singular. That is,

$$\xi^A(Q_0, \dot{Q}_0)P_A(Q, \dot{Q}) = \text{function of } Q \text{ and } P \text{ only in ball}(Q_0, \dot{Q}_0). \quad (34)$$

This is an equation of constraint, albeit an infinitesimal one. This proof reaffirms that singular Lagrangians give rise to primary constraints. Note that the converse is also true, if we can find a linear combination of momenta that has a vanishing derivative with respect to  $\dot{Q}$  at  $\dot{Q} = \dot{Q}_0$ , then the mass matrix must be singular at that point. If we can find a linear combination of momenta that is completely

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<sup>3</sup>Note that we have not proved the reverse, which would be an interesting exercise that we do not consider here.

independent of the velocities altogether (i.e., a primary constraint), then the mass matrix must be singular for all  $Q$  and  $\dot{Q}$ .

We digress for a moment and compare how primary constraints manifest themselves in singular Lagrangian theories as opposed to the explicit way they were invoked in Section 2.1. Previously, we saw that Lagrange multipliers had conjugate momenta which were equal to zero for all times. In the new jargon, the equations  $\pi = 0$  are primary constraints. In our current work, we have momenta conjugate to coordinates with primarily inexpressible velocities being functionally related to  $Q$  and  $P$ . It is not hard to see how the former situation can be changed into the latter; generalized coordinate transformations that mix coordinates  $q$  with the Lagrange multipliers  $\lambda$  will not preserve  $\pi = 0$ . So we see that the previous section's work can be absorbed into the more general discussion presented here.

So we now have some primary constraints that we think ought to be true for all time, but what shall we do with them? Well, notice that the fact that each constraint is conserved implies

$$0 = \delta\phi_a^{(1)} = \frac{\partial\phi_a^{(1)}}{\partial Q^A} \delta Q^A + \frac{\partial\phi_a^{(1)}}{\partial P_A} \delta P_A. \quad (35)$$

Since the righthand side of this is formally equal to zero, we should be able to add it to any equation involving  $\delta Q$  and  $\delta P$ . In fact, we can add any linear combination of the variations  $u^a \phi_a^{(1)}$  to an expression involving  $\delta Q$  and  $\delta P$  without doing violence to its meaning. Here,  $u^a$  are undetermined coefficients. Let us do precisely this to (22), while at the same time substituting in equation (23). We get

$$0 = \left( \dot{Q}^A - \frac{\partial H}{\partial P_A} - u^a \frac{\partial\phi_a^{(1)}}{\partial P_A} \right) \delta P_A - \left( \dot{P}_A + \frac{\partial H}{\partial Q^A} + u^a \frac{\partial\phi_a^{(1)}}{\partial Q^A} \right) \delta Q^A. \quad (36)$$

Since  $Q$  and  $P$  are supposed to be independent of one another, this then implies that

$$\dot{Q}^A = + \frac{\partial H}{\partial P_A} + u^a \frac{\partial\phi_a^{(1)}}{\partial P_A}, \quad (37a)$$

$$\dot{P}_A = - \frac{\partial H}{\partial Q^A} - u^a \frac{\partial\phi_a^{(1)}}{\partial Q^A}. \quad (37b)$$

This is the exact same structure that we encountered in the last section, except for the fact that  $\lambda$  has been relabeled as  $u$ , we have appended the (1) superscript to the constraints, and that  $(Q, P)$  appear instead of  $(q, p)$ . Because there are essentially no new features here, we can immediately import our previous result

$$\dot{g} \sim \{g, H + u^a \phi_a^{(1)}\}, \quad (38)$$

where  $g$  is any function of the  $Q$ 's and  $P$ 's (also know as a function of the phase space variables) and there has been a slight modification of the Poisson bracket to

fit the new notation:

$$\{F, G\} = \frac{\partial F}{\partial Q^A} \frac{\partial G}{\partial P_A} - \frac{\partial G}{\partial Q^A} \frac{\partial F}{\partial P_A}. \quad (39)$$

So we have arrived at the same point that we ended Section 2.1 with: we have found an evolution equation for arbitrary functions of coordinates and momenta. This evolution equation is in terms of a function  $H$  derived from the original Lagrangian and a linear combination of primary constraints with undetermined coefficients. Some questions should currently be bothering us:

1. Why did we bother to add  $u^a \delta \phi_a^{(1)}$  to the variational equation (22) in the first place? Could we have just left it out?
2. Is there anything in our theory that ensures that the constraints are conserved? That is, does  $\phi_a^{(1)} = 0$  really hold for all time?
3. In deriving (37), we assumed that  $\delta Q$  and  $\delta P$  were independent. Can this be justified considering that equation (35) implies that they are related?

It turns out that the answers to these questions are intertwined. We will see in the next section that the freedom introduced into our system by the inclusion of the undetermined coefficients  $u^a$  is precisely what is necessary to ensure that the constraints are preserved. There is also a more subtle reason that we need the  $u$ 's, which is discussed in the Appendix. In that section, we show why the variations in (36) can be taken to be independent and give an interpretation of  $u^a$  in terms of the geometry of phase space. For now, we take (38) for granted and proceed to see what must be done to ensure a consistent time evolution of our system.

### 2.3 Consistency conditions

Obviously, to have a consistent time evolution of our system, we need to ensure that any constraints are preserved. In this section, we see what conditions we must place on our system to guarantee that the time derivatives of any constraints is zero. In the course of our discussion, we will discover that there are essentially two types of constraints and that each type has different implications for the dynamics governed by our original action principle. We will adopt the notation of Section 2.2, although what we say can be applied to systems with explicit constraints like the ones studied in Section 2.1.

Equation (38) governs the time evolution of quantities that depend on  $Q$  and  $P$  in the Hamiltonian formalism. Since the primary constraints themselves are functions of  $Q$  and  $P$ , their time derivatives must be given by

$$\dot{\phi}_b^{(1)} \sim \{\phi_b^{(1)}, H\} + u^a \{\phi_b^{(1)}, \phi_a^{(1)}\}. \quad (40)$$

But of course, we need that  $\dot{\phi}_b^{(1)} \sim 0$  because the time derivative of constraints should vanish. This then gives us a system of equations that must be satisfied for consistency:

$$0 \sim \{\phi_b^{(1)}, H\} + u^a \{\phi_b^{(1)}, \phi_a^{(1)}\}. \quad (41)$$

We have one such equation for each primary constraint. Now, the equations may have various forms that imply various things. For example, it may transpire that the Poisson bracket  $\{\phi_b^{(1)}, \phi_a^{(1)}\}$  vanishes for all  $a$ . Or, it may be strongly equal to some linear combination of constraints and hence be weakly equal to zero. In either event, this would imply that

$$0 \sim \{\phi_b^{(1)}, H\}. \quad (42)$$

If the quantity appearing on the righthand side does not vanish when the primary constraints are imposed, then this says that some function of the  $Q$ 's and  $P$ 's is equal to zero and we have discovered another equation of constraint. This is not the only way in which we can get more constraints. Suppose for example the matrix  $\{\phi_b^{(1)}, \phi_a^{(1)}\}$  has a zero eigenvector  $\xi^b = \xi^b(Q, P)$ . Then, if we contract each side of (41) with  $\xi^b$  we get

$$0 \sim \xi^b \{\phi_b^{(1)}, H\}. \quad (43)$$

Again, if this does not vanish when we put  $\phi_a^{(1)} = 0$ , then we have a new constraint. Of course, we may get no new constraints from (41), in which case we do not need to perform the algorithm we are about to describe in the next paragraph.

All the new constraints obtained from equation (41) are called *second-stage secondary constraints*. We denote them by  $\phi^{(2)} = \{\phi_i^{(2)}\}$  where mid lowercase Latin indices run over the number of secondary constraints. Just as we did with the primary constraints, we should be able to add any linear combination of the variations of  $\phi_i^{(2)}$  to equation (22).<sup>4</sup> Repeating all the work leading up to equations (38), we now have

$$\dot{g} \sim \{g, H + u^I \phi_I\}. \quad (44)$$

Here,  $\phi = \phi^{(1)} \cup \phi^{(2)} = \{\phi_I\}$ , where late uppercase Latin indices run over all the constraints. We now need to enforce that the new set of constraints has zero time derivative, which then leads to

$$0 \sim \{\phi_I, H\} + u^J \{\phi_I, \phi_J\}. \quad (45)$$

Now, some of *these* equations may lead to new constraints — which are independent of the previous constraints — in the same way that (41) led to the second-stage secondary constraints. This new set of constraints is called the *third-stage secondary constraints*. We should add these to the set  $\phi^{(2)}$ , add their variations to (22), and repeat the whole procedure again. In this manner, we can generate *fourth-stage*

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<sup>4</sup>And indeed, as demonstrated in Appendix A, we must add those variations to obtain Hamilton's equations.

secondary constraints, fifth-stage secondary constraints, etc. . . . This ride will end when equation (45) generates no non-trivial equations independent of  $u^J$ . At the end of it all, we will have

$$\dot{g} \sim \{g, H_T\}. \quad (46)$$

Here,  $H_T$  is called the *total Hamiltonian* and is given by

$$H_T \equiv H + u^I \phi_I. \quad (47)$$

The index  $I$  runs over all the constraints in the theory.

So far, we have only used equations like (45) to generate new constraints independent from the old ones. But by definition, when we have finally obtained the complete set of constraints and the total Hamiltonian, equation (45) cannot generate more time independent relations between the  $Q$ 's and the  $P$ 's. At this stage, the demand that the constraints have zero time derivative can be considered to be a condition on the  $u^I$  quantities, which have heretofore been considered undetermined. Demanding that  $\dot{\phi} \sim 0$  is now seen to be equivalent to

$$0 \sim \{\phi_I, H\} + u^J \Delta_{IJ}, \quad (48)$$

where the matrix  $\Delta$  is defined to be

$$\Delta_{IJ} \equiv \{\phi_I, \phi_J\}. \quad (49)$$

Notice that our definition of  $\Delta$  involves a strong equality, but that it must be evaluated weakly in equation (48). Equation (48) is a linear system of the form

$$0 \sim \Delta \mathbf{u} + \mathbf{b}, \quad \mathbf{u} = u^J, \quad \mathbf{b} = \{\phi_I, H\}, \quad (50)$$

for the undetermined vector  $\mathbf{u}$  where the  $\Delta$  matrix and  $\mathbf{b}$  vector are functions of  $Q$  and  $P$ . The form of the solution of this linear system depends on the value of the determinant of  $\Delta$ .

**Case 1:**  $\det \Delta \approx 0$ . Notice that this condition implies that  $\det \Delta \neq 0$  strongly, because a quantity that vanishes strongly cannot be nonzero weakly. In this case we can construct an explicit inverse to  $\Delta$ :

$$\Delta^{-1} \equiv \Delta^{IJ}, \quad \delta_J^I = \Delta^{IK} \Delta_{KJ}, \quad \Delta^{-1} \Delta = \mathbf{I}, \quad (51)$$

and  $\mathbf{u}$  can be found as an explicit weak function of  $Q$  and  $P$

$$u^I \sim -\Delta^{IJ} \{\phi_J, H\}. \quad (52)$$

Having discovered this, we can write the equation of evolution for an arbitrary function as

$$\dot{g} \sim \{g, H\} - \{g, \phi_I\} \Delta^{IJ} \{\phi_J, H\}. \quad (53)$$



We can write this briefly by introducing the *Dirac bracket* between two functions of phase space variables:

$$\{F, G\}_D = \{F, G\} - \{F, \phi_I\} \Delta^{IJ} \{\phi_J, G\}. \quad (54)$$

The Dirac bracket will satisfy the same basic properties as the Poisson bracket, but because the proofs are tedious we will not do them here. The interested reader may consult reference [4]. Then, we have the simple time evolution equation in terms of Dirac brackets

$$\dot{g} \sim \{g, H\}_D. \quad (55)$$

Notice that because  $\Delta^{-1}$  is the strong inverse of  $\Delta$ , the following equation holds strongly:

$$\begin{aligned} \{\phi_K, g\}_D &= \{\phi_K, g\} - \{\phi_K, \phi_I\} \Delta^{IJ} \{\phi_J, H\} \\ &= \{\phi_K, g\} - \Delta^{JI} \Delta_{IK} \{\phi_J, g\} \\ &= 0, \end{aligned} \quad (56)$$

where  $g$  is any function of the phase space variables. In going from the first to third line we have used that  $\Delta$  and  $\Delta^{-1}$  are anti-symmetric matrices. In particular, this shows that the time derivative of the constraints is strongly equal to zero. We will return to this point when we quantize theories with  $\det \Delta \approx 0$ .

**Case 2:**  $\det \Delta \approx 0$ . In this case the  $\Delta$  matrix is singular. Let us define the following integer quantities:

$$D \sim \dim \Delta, \quad R \sim \text{rank } \Delta, \quad N \sim \text{nullity } \Delta, \quad D = R + N. \quad (57)$$

Since,  $N$  is the dimension of the nullspace of  $\Delta$ , we expect there to be  $N$  linearly independent  $D$ -dimensional vectors such that

$$\xi_r^I = \xi_r^I(Q, P), \quad 0 \sim \xi_r^I \Delta_{IJ}. \quad (58)$$

Here, late lowercase Latin indices run over the nullspace of  $\Delta$ . Then, the solution of our system of equations  $0 \sim \Delta \mathbf{u} + \mathbf{b}$  is

$$u^I = U^I + w^r \xi_r^I, \quad (59)$$

where  $U^I = U^I(Q, P)$  is the non-trivial solution of

$$U^J \Delta_{IJ} \sim -\{\phi_I, H\}, \quad (60)$$

and the  $w^r$  are *totally arbitrary quantities*. The evolution equation now takes the form of

$$\dot{g} \sim \{g, H^{(1)} + w^r \psi_r\}, \quad (61)$$

where

$$H^{(1)} = H + U^I \phi_I, \quad (62)$$

and

$$\psi_r = \xi_r^I \phi_I. \quad (63)$$

There are several things to note about these definition. First, notice that  $H^{(1)}$  and  $\psi_r$  are explicit functions of phase space variables. There is nothing arbitrary or unknown about them. Second, observe that the construction of  $H^{(1)}$  implies that it commutes with all the constraints weakly:

$$\begin{aligned} \{\phi_I, H^{(1)}\} &= \{\phi_I, H\} + \{\phi_I, U^J \phi_J\} \\ &\sim \{\phi_I, H\} + U^J \Delta_{IJ} \\ &\sim \{\phi_I, H\} - \{\phi_I, H\} \\ &= 0. \end{aligned} \quad (64)$$

Third, observe that the same is true for  $\psi_r$ :

$$\begin{aligned} \{\phi_I, \psi_r\} &= \{\phi_I, \xi_r^J \phi_J\} \\ &\sim \xi_r^J \Delta_{IJ} \\ &\sim 0. \end{aligned} \quad (65)$$

We call quantities that weakly commute with all of the constraints *first-class*.<sup>5</sup> Therefore, we call  $H^{(1)}$  the *first-class Hamiltonian*. Since it is obvious that  $\psi_r \sim 0$ , we can call them *first-class constraints*. We have hence succeeded in writing the total Hamiltonian as a sum of the first-class Hamiltonian and first-class constraints. This means that

$$\dot{\Phi}_I \sim \{\Phi_I, H^{(1)}\} + w^r \{\Phi_I, \psi_r\} \sim 0. \quad (66)$$

That is, we now have a consistent time evolution that preserves the constraints. But the price that we have paid is the introduction of completely arbitrary quantities  $w^r$  into the Hamiltonian. What is the meaning of their presence? We will discuss that question in detail in Section 2.4.

However, before we get there we should tie up some loose ends. We have discovered a set of  $N$  quantities  $\psi_r$  that we have called first-class constraints. Should there not exist *second-class constraints*, which do not commute with the complete set  $\phi$ ? The answer is yes, and it is intuitively obvious that there ought to be  $R$  such quantities. To see why this is, we, note that any linear combination of constraints is also a constraint. So, we can transform our original set of constraints into a new set using an some matrix  $\Gamma$ :

$$\tilde{\phi}_J = \Gamma_J^I \phi_I. \quad (67)$$

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<sup>5</sup>Anticipating the quantum theory, we will often call the Poisson bracket a commutator and say that  $A$  commutes with  $B$  if their Poisson bracket is zero.

Under this transformation, the  $\Delta$  matrix will transform as

$$\begin{aligned}\tilde{\Delta}_{MN} &= \{\tilde{\phi}_M, \tilde{\phi}_N\} \\ &= \{\Gamma_M^I \phi_I, \Gamma_N^J \phi_J\} \\ &\sim \Gamma_M^I \Gamma_N^J \Delta_{IJ}.\end{aligned}\tag{68}$$

This says that one can obtain  $\tilde{\Delta}$  from  $\Delta$  by performing a series of linear operations on the rows of  $\Delta$  and then the same operations on the columns of the result. From linear algebra, we know there must be a choice of  $\Gamma$  such that  $\tilde{\Delta}$  is in a row-echelon form. Because  $\tilde{\Delta}$  is related to  $\Delta$  by row and column operations, they must have the same rank and nullity. Therefore, we should be able to find a  $\Gamma$  such that

$$\tilde{\Delta} \sim \begin{pmatrix} \Lambda & \\ & 0 \end{pmatrix},\tag{69}$$

where  $\Lambda$  is an  $R \times R$  antisymmetric matrix that satisfies

$$\det \Lambda \approx 0 \quad \Rightarrow \quad \det \Lambda \neq 0.\tag{70}$$

Let make such a choice for  $\Gamma$ . When written in this form, the a linearly independent set of null eigenvectors of  $\tilde{\Delta}$  are trivially easy to find:  $\xi_r^I = \delta_{r+R}^I$ , where  $r = 1, \dots, R$ . Hence, the primary constraints are simply

$$\psi_r = \xi_r^I \tilde{\phi}_I = \tilde{\phi}_{r+R};\tag{71}$$

i.e., the last  $R$  members of the  $\tilde{\phi}$  set. Let us give a special label to the first  $R$  members of  $\tilde{\phi}$ :

$$\chi_{r'} = \delta_{r'}^I \tilde{\phi}_I, \quad r' = 1, \dots, R.\tag{72}$$

With the definition of  $\chi = \{\chi_{r'}\}$ , we can give an explicit strong definition of  $\Lambda$

$$\Lambda_{r's'} = \{\chi_{r'}, \chi_{s'}\}.\tag{73}$$

Now, since we have  $\det \Lambda \approx 0$  then we cannot have all the entries in any row or column  $\Lambda$  vanishing weakly. This implies that each of member of  $\chi$  set of constraints must not weakly commute with at least one other member. Therefore, each element of  $\chi$  is a second-class constraint. Hence, we have seen that the original set of  $\tilde{\phi}$  constraints can be split up into a set of  $N$  first-class constraints and  $R$  second-class constraints. Furthermore, we can find an explicit expression for  $\tilde{\mathbf{u}}$  in terms of  $\Lambda^{-1}$ . We simply need to operate the matrix

$$\tilde{\Delta}^* = \begin{pmatrix} \Lambda^{-1} & \\ & 0 \end{pmatrix},\tag{74}$$

on the left of the equation of conservation of constraints (48) written in terms of the  $\tilde{\phi}$  set and in matrix form

$$0 \sim \tilde{\Delta} \tilde{\mathbf{u}} + \tilde{\mathbf{b}}\tag{75}$$

to get

$$\tilde{\mathbf{u}} = \begin{pmatrix} -\Lambda^{-1}\{\chi, H\} \\ w \end{pmatrix}. \quad (76)$$

In the lower sector of  $\tilde{\mathbf{u}}$ , we again see the set of  $N$  arbitrary quantities  $w^r$ . This solution gives the following expression for the first-class Hamiltonian

$$H^{(1)} = H - \chi_{r'} \Lambda^{r's'} \{\chi_{s'}, H\}, \quad (77)$$

and the following time evolution equation:

$$\dot{g} = \{g, H\} - \{g, \chi_{r'}\} \Lambda^{r's'} \{\chi_{s'}, H\} + w^r \{g, \psi_r\}. \quad (78)$$

Here,  $\Lambda^{r's'}$  are the entries in  $\Lambda^{-1}$ , *viz.*

$$\delta_{s'}^{r'} = \Lambda^{r't'} \Lambda_{t's'}. \quad (79)$$

This structure is reminiscent of the Dirac bracket formalism introduced in the case where  $\det \Delta \approx 0$ , but with the different definition of  $\{, \}_D$ :

$$\{F, G\}_D = \{F, G\} - \{F, \chi_{r'}\} \Lambda^{r's'} \{\chi_{s'}, G\}. \quad (80)$$

Keeping in mind that  $\{\chi, \psi\} \sim 0$ , this then gives

$$\dot{g} \sim \{g, H + w^r \psi_r\}_D. \quad (81)$$

Like in the case of  $\det \Lambda \approx 0$ , we see that the Dirac bracket of the second-class constraints with any phase space function vanishes strongly:

$$0 = \{g, \chi_{r'}\}. \quad (82)$$

This has everything to do with the fact that the definitions of  $\Lambda$  and  $\Lambda^{-1}$  are strong equalities. We should point out that taking the extra steps of transforming the constraints so that  $\Delta$  has the simple form (69) is not strictly necessary at the classical level, but will be extremely helpful when trying to quantize the theory.

We have now essentially completed the problem of describing the classical Hamiltonian formalism of system with constraints. Our final results are encapsulated by equation (55) for theories with only second-class constraints and equation (81) for theories with both first- and second-class constraints. But we will need to do a little more work to interpret the latter result because of the uncertain time evolution it generates.

## 2.4 First class constraints as generators of gauge transformations

In this section, we will be concerned with the time evolution equation that we derived for phase space functions in systems with first class constraints. We showed in Section 2.3 that the formula for the time derivative of such functions contains  $N$  arbitrary quantities  $w^r$ , where  $N$  is the number of first-class constraints. We can take these to be arbitrary functions of  $Q$  and  $P$ , or we can equivalently think of them as arbitrary function of time. Whatever we do, the fact that  $\dot{g}$  depends on  $w^r$  means that the trajectory  $g(t)$  is *not uniquely determined* in the Hamiltonian formalism. This could be viewed as a problem.

But wait, such situations are not entirely unfamiliar to us physicists. Is it not true that in electromagnetic theory we can describe the same physical systems with functionally distinct vector potentials? In that theory, one can solve Maxwell's equations at a given time for two different potentials  $A$  and  $A'$  and then evolve them into the future. As long as they remain related to one another by the gradient of a scalar field for all times, they describe the same physical theory.

It seems likely that the same this is going on in the current problem. The quantities  $g$  can evolve in different ways depending on our choice of  $w^r$ , but the real physical situation should not care about such a choice. This motivates us to make somewhat bold leap: *if the time evolution of  $g$  and  $g'$  differs only by the choice of  $w^r$ , then  $g$  and  $g'$  ought to be regarded as physically equivalent*. In analogy with electromagnetism, we can restate this by saying that  $g$  and  $g'$  are related to one another by a *gauge transformation*. Therefore, theories with first-class constraints must necessarily be viewed as gauge theories if they are to make any physical sense.

But what is the form of the gauge transformation? That is, we know that for electromagnetism the vector potential transforms as  $A \rightarrow A + \partial\varphi$  under a change of gauge. How do the quantities in our theory transform? To answer this, consider some phase space function  $g(Q, P)$  with value  $g_0$  at some time  $t = t_0$ . Let us evolve this quantity a time  $\delta t$  into the future using equation (61) and a specific choice of  $w^r = a^r$ :

$$\begin{aligned} g(t_0 + \delta t) &= g_0 + \dot{g} \delta t \\ &\sim g_0 + \{g, H^{(1)}\} \delta t + a^r \{g, \psi_r\} \delta t. \end{aligned} \quad (83)$$

Now, lets do the same thing with a different choice  $w^r = b^r$ :

$$g'(t_0 + \delta t) \sim g_0 + \{g, H^{(1)}\} \delta t + b^r \{g, \psi_r\} \delta t. \quad (84)$$

Now we take the difference of these two equations

$$\delta g \equiv g(t_0 + \delta t) - g'(t_0 + \delta t) \sim \varepsilon^r \{g, \psi_r\}, \quad (85)$$

where  $\varepsilon^r = (a^r - b^r) \delta t$  is an arbitrary small quantity. But by definition,  $g$  and  $g'$  are gauge equivalent since their time evolution differs by the choice of  $w^r$ . Therefore,

we have derived how a given phase space function transforms under an infinitesimal gauge transformation characterized by  $\varepsilon^r$ :

$$\delta g_\varepsilon \sim \{g, \varepsilon^r \psi_r\}. \quad (86)$$

This establishes an important point: *the generators of gauge transformations are the first-class constraints*. Now, we all know that when we are dealing with gauge theories, the only quantities that have physical relevance are those which are gauge invariant. Such objects are called *physical observables* and must satisfy

$$0 = \delta g_{\text{phys}} \sim \{g_{\text{phys}}, \psi_r\}. \quad (87)$$

It is obvious from this that all first-class quantities in the theory are observables, in particular the first class Hamiltonian  $H^{(1)}$  and set of first-class constraints  $\psi$  are physical quantities. Also, any second class constraints must also be physical, since  $\psi$  commutes with all the elements of  $\phi$ . The gauge invariance of  $\phi$  is particularly helpful; it would not be sensible to have constraints preserved in some gauges, but not others.

First class quantities clearly play an important role in gauge theories, so we should say a little bit more about them here. We know that the Poisson bracket of any first class quantity  $F$  with any of the constraints is weakly equal to zero. It is therefore strongly equal to some phase space function that vanishes when the constraints are enforced. This function may be expanded in a Taylor series in the constraints that has no terms independent of  $\phi$  and whose coefficients may be functions of phase space variables. We can then factor this series to be of the form  $f_I^J \phi_J$ , where the  $f_I^J$  coefficients are in general functions of the constraints and phase space variables. The net result is that we always have the strong equality:

$$\{F, \phi_I\} = f_I^J \phi_J, \quad (88)$$

where  $F$  is any first class quantity. We can use this to establish that the commutator of the two first class quantities  $F$  and  $G$  is itself first class:

$$\begin{aligned} \{\{F, G\}, \phi_I\} &= \{\{F, \phi_I\}, G\} - \{\{G, \phi_I\}, F\} \\ &= \{f_I^J \phi_J, G\} - \{g_I^J \phi_J, F\} \\ &\sim f_I^J \{\phi_J, G\} - g_I^J \{\phi_J, F\} \\ &\sim 0, \end{aligned} \quad (89)$$

where we used the Jacobi identity in the first line. This also implies that the Poisson bracket of two observables is also an observable. Now, what about the Poisson bracket of two first class constraints? We know that such an object must correspond to a linear combination of constraints because it vanishes weakly and that it must be first class. The only possibility is that it is a linear combination of first-class constraints. Hence, we have the strong equality

$$\{\psi_r, \psi_s\} = f_{rs}^p \psi_p, \quad (90)$$

where  $f_{rs}^p$  are phase space functions known as structure constants. Therefore, the set of first class constraints form a closed algebra, which is what we would also expect from the interpretation of  $\psi$  as the generator of the gauge group of the theory in question.<sup>6</sup>

The last thing we should mention before we leave this section is that one is sometimes presented with a theory where the first-class Hamiltonian can be expressed as a linear combination of first-class constraints:

$$H^{(1)} = h^r \psi_r. \quad (91)$$

For example, the first-class Hamiltonian of Chern-Simons theory, vacuum general relativity and the free particle in curved space can all be expressed in this way. In such cases, the total Hamiltonian vanished on solutions which preserve the constraints, which will have interesting implications for the quantum theory. But at the classical level, we can see that such a first class Hamiltonian implies

$$g(t_0 + \delta t) - g(t_0) \sim (h^r + w^r) \delta t \{g, \psi_r\} \quad (92)$$

for the time evolution of  $g$ . But the quantity on the right is merely an infinitesimal arbitrary gauge transformation since  $w^r$  are freely specifiable. Therefore, in such theories all phase space functions evolve by gauge transformations. Furthermore, all physical observables do not evolve at all. Such theories are completely static in a real physical sense, which agrees with our intuition concerning dynamics governed by a vanishing Hamiltonian. This is the celebrated “problem of time” in certain Hamiltonian systems, most notably general relativity. We will discuss aspects of this problem in subsequent sections.

### 3 Quantizing systems with constraints

We now have a rather comprehensive picture of the classical Hamiltonian formulation of systems with constraints. But we have always had quantum mechanics in the back of our minds because we believe that Nature prefers it over the classical picture. So, it is time to consider how to quantize our system. We have actually done the majority of the required mechanical work in Section 2, but that does not mean that the quantization algorithm is trivial. We will soon see that it is rife with ambiguities and *ad hoc* procedures that some may find somewhat discouraging. Most of the confusion concerns theories with first-class constraints, which are dealt with in Section 3.2, as opposed to theories with second-class constraints only, which are the subject of Section 3.1. We will try to point out these pitfalls along the way.

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<sup>6</sup>Since the Dirac bracket for theories with first-class constraints has the same computational properties as the Poisson bracket, we have that the first class constraints form an algebra under the Dirac bracket as well. Of course, the structure constants with respect to each bracket will be different. We will use this in the quantum theory.

### 3.1 Systems with only second-class constraints

In this section, we follow references [1, 2, 3]. As mentioned above, the problem of quantizing theories with second-class constraints is less ambiguous than quantizing theories with first-class constraints, so we will work with the latter first. But before we do even that, we should talk a little about how we quantize an unconstrained system.

The canonical quantization programme for such systems is to promote the phase space variables  $Q$  and  $P$  to operators  $\hat{Q}$  and  $\hat{P}$  that act on elements of a Hilbert space, which we denote by  $|\Psi\rangle$ . It is convenient to collapse  $Q$  and  $P$  into a single set

$$X = Q \cup P = \{X^a\}_{a=1}^{2d}, \quad (93)$$

where  $2d$  is the phase space dimension.<sup>7</sup> The commutator between phase space variables is taken to be their Poisson bracket evaluated at  $X = \hat{X}$ :

$$[\hat{X}^a, \hat{X}^b] = i\hbar\{X^a, X^b\}_{X=\hat{X}}. \quad (94)$$

Ideally, one would like to extend this kind of identification to include arbitrary functions of phase space variables, but we immediately run into troubles. To illustrate this, let's consider a simple one-dimensional system with phase space variables  $x$  and  $p$  such that  $\{x, p\} = 1$ . Then, we have the Poisson bracket

$$\{x^2, p^2\} = 4xp. \quad (95)$$

Now, when we quantize, we get

$$[\hat{x}^2, \hat{p}^2] = i\hbar 2(\hat{x}\hat{p} + \hat{p}\hat{x}). \quad (96)$$

Therefore, we will only have  $[x^2, p^2] = i\hbar\{x^2, p^2\}_{X=\hat{X}}$  if we order  $x$  and  $p$  in a certain way in the classical expression. This is an example of the ordering ambiguity that exists whenever we try to convert classical equations into operator expressions. Unfortunately, it is just something we have to live with when we use quantum mechanics. But note that we do have that

$$[\hat{x}^2, \hat{p}^2] = i\hbar\{x^2, p^2\}_{X=\hat{X}} + O(\hbar^2), \quad (97)$$

regardless of what ordering we choose for in the classical Poisson bracket. Because the Poisson bracket and commutator share the same algebraic properties, it is possible to demonstrate that this holds for arbitrary phase space functions

$$[F(\hat{X}), G(\hat{X})] = i\hbar\{F(X), G(X)\}_{X=\hat{X}} + O(\hbar^2). \quad (98)$$

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<sup>7</sup>We apologize for having early lowercase Latin indices take on a different role than they had in Sections 2.1 and 2.2, where they ran over Lagrange multipliers and primarily inexpressible velocities. We are simply running out of options.



Therefore, in the classical limit  $\hbar \rightarrow 0$  operator ordering issues become less important.

We will adopt the Schrödinger picture of quantum mechanics, where the physical state of our system will be represented by a time-dependent vector  $|\Psi(t)\rangle$  in the Hilbert space. The time evolution of the state is then given by

$$i\hbar \frac{d}{dt} |\Psi\rangle = \hat{H} |\Psi\rangle, \quad (99)$$

where  $\hat{H} = H(\hat{X})$  and  $H(X)$  is the classical Hamiltonian. The expectation value of a phase space function is constructed in the familiar way:

$$\langle g \rangle = \langle \Psi | \hat{g} | \Psi \rangle, \quad (100)$$

where  $\hat{g} = g(\hat{X})$  and  $\langle \Psi |$  is the dual of  $|\Psi\rangle$ . Note that we still have ordering issues in writing down an operator for  $\hat{g}$ . Taken with the evolution equation, this implies that for any phase space operator

$$\frac{d}{dt} \langle g \rangle = \frac{1}{i\hbar} \langle \Psi | [\hat{g}, \hat{H}] | \Psi \rangle = \langle \{g, H\} \rangle + O(\hbar). \quad (101)$$

In the classical limit we recover something very much like the classical evolution equation  $\dot{g} = \{g, H\}$  for an unconstrained system. With this example of Bohr's correspondence principle, we have completed our extremely brief review of how to quantize an unconstrained system.

But what if we have second-class constraints  $\phi$ ? We certainly want the classical limit to have

$$\langle f(\phi) \rangle = 0 \quad (102)$$

for any function that satisfies  $f(0) = 0$ . The only way to guarantee this for all times and all functions  $f$  is to have

$$\hat{\phi}_I |\Psi\rangle = 0. \quad (103)$$

This appears to be a restriction placed on our state space, but we will soon show that this really is not the case. Notice that it implies that

$$0 = [\phi_I, \phi_J] |\Psi\rangle. \quad (104)$$

This should hold independently of the value of  $\hbar$  and for all  $|\Psi\rangle$ , so we then need

$$\{\phi_I, \phi_J\} = 0 \quad (105)$$

at the classical level. Now, we have a problem. Because we are dealing with second-class constraints, it is impossible to have  $\{\phi_I, \phi_J\} = 0$  for all  $I$  and  $J$  because that would imply  $\det \Delta = 0$ . We do not even have that  $\{\phi_I, \phi_J\}$  vanishes weakly, so we cannot express it as strong linear combination of constraints. So, it is impossible to

enforce  $\langle f(\phi) \rangle = 0$  and it seems our straightforward attempt to quantize a theory with constraints has failed.

But how can we modify our approach to get a workable theory? Well, recall that we do have classically that

$$\{\phi_I, \phi_J\}_D = 0, \quad (106)$$

which is a strong equality. This formula suggests a way out of this mess. What if we quantize using Dirac brackets instead of Poisson brackets? Then, we will have

$$[\hat{X}^a, \hat{X}^b] = i\hbar\{X^a, X^b\}_{D, X=\hat{X}}. \quad (107)$$

and

$$[F(\hat{X}), G(\hat{X})] = i\hbar\{F(X), G(X)\}_{D, X=\hat{X}} + O(\hbar^2). \quad (108)$$

This quantization scheme has a nice feature:

$$[\hat{\phi}_I, g(\hat{X})] = O(\hbar^2), \quad (109)$$

since the Dirac bracket of a second-class constraint with any phase space function is strongly zero. Therefore, if we neglect terms of order  $\hbar^2$  (or conversely, we ignore operator ordering issues) the second-class constraint operators commute with everything in the theory, including the Hamiltonian. Now any operator that commutes with every conceivable function of  $\hat{Q}$  and  $\hat{P}$  cannot itself be a function of the the phase space operators. The only possibility is that the  $\hat{\phi}$  operators are  $c$ -numbers; that is, their action on states is scalar multiplication:

$$\hat{\phi}_I|\Psi\rangle = \lambda_I|\Psi\rangle, \quad (110)$$

where the  $\lambda_I$  are simple numbers. Then, to satisfy the constraints, we merely need to assume that  $\lambda_I = 0$ . Therefore, the condition that  $\hat{\phi}|\Psi\rangle = 0$  is not a constraint on our phase space, it is rather an operator identity

$$\hat{\phi} = 0 \quad (111)$$

when we quantize with Dirac brackets; i.e. *constraints can be freely set to zero in any operator*. Of course, we can only do this when we have already established the fundamental commutator (107). That formula along with (111) is the basis of our quantization scheme for systems with second-class constraints.

### 3.2 Systems with first-class constraints

So now we come to the case of systems with first-class constraints, i.e. systems with gauge degrees of freedom. There are two distinct ways of dealing with such systems, both of which we will describe. The first method is due to Dirac, and essentially involves restricting the Hilbert space in the quantum theory to ensure that constraints are obeyed. We call this ‘‘Dirac quantization of first-class systems’’.

The second method involves fixing the gauge of the theory classically by the addition of more constraints and then quantizing. Our term for this “canonical quantization of first-class systems”. The friction between the two methods can be boiled down to the following question:

Should we first quantize then constrain, or constrain then quantize?

We will not give you an answer here, we will merely outline both lines of attack.

### 3.2.1 Dirac quantization

In this section, our treatment is based on references [1, 3]. The working of Section 3.1 tells us that we should not waste too much time try to quantize a system with both first- and second-class constraints by converting Poisson brackets into commutators. We should instead work with Dirac brackets *ab initio*, and hence save ourselves some work. To do this, we will need to perform linear operations on our constraints  $\phi$  until we have  $\phi = \chi \cup \psi$ , where  $\chi$  is the set of second-class constraints and  $\psi$  is the set of first class constraints. When we have done so, we can define a Dirac bracket akin to equation (80) such that

$$\{\chi, g\}_D = 0, \quad \{\psi_r, \psi_s\}_D = f_{rs}^p \psi_c. \quad (112)$$

Quantization in the Dirac scheme proceeds pretty much as before with the introduction of the fundamental commutator (107). Again, the fact that the second-class constraints commute with everything means that we may set their operators equal to zero and not worry about them any more. But we cannot do this for the first class constraints. Therefore, unlike the previous section, the requirement

$$\hat{\psi}|\Psi\rangle = 0 \quad (113)$$

is a real restriction on our Hilbert space. State vectors which satisfy this property are called *physical* and the portion of our original Hilbert space spanned by them is call the *physical state space*. Dirac’s quantization procedure for systems with first-class constraints is hence relatively simple: first quantize using Dirac brackets and then restrict the Hilbert space by demanding that constraint operators annihilate physical states. Of course, many things are easier said than done.

There are several consistency issues we should address. First, since at a classical level we expect the Dirac bracket of a first-class quantity with the constraints to be strongly equal to some linear combination of first-class constraints, we ought to have the following commutators:

$$[\hat{\psi}_r, \hat{\psi}_s] = i\hbar \hat{f}_{rs}^p \hat{\psi}_p + O(\hbar^2), \quad (114)$$

and

$$[\hat{\psi}_r, H^{(1)}] = i\hbar \hat{g}_r^s \hat{\psi}_s + O(\hbar^2). \quad (115)$$

We have assumed an operator ordering that allows us to have the constraints appear to the right of the coefficients  $\hat{f}_{r_s}^p$  and  $\hat{g}_s^r$ , which themselves are functions of  $\hat{X}$ . Again only retaining terms linear in  $\hbar$ , these imply that

$$[\hat{\psi}_r, \hat{\psi}_s]|\Psi\rangle = 0 \quad (116)$$

and that

$$\hat{H}_T \hat{\psi}_a |\Psi\rangle = \hat{\psi}_a \hat{H}_T |\Psi\rangle \quad (117)$$

for physical states  $|\Psi\rangle$ . The first equation is the quantum consistency condition we met in the last section. We see that it will be satisfied for states in the physical Hilbert space. The second equation guarantees that as we evolve a physical state in time, it will remain a physical state. Note that we have made a modification of the Schrödinger equation for theories with first-class constraints:

$$i\hbar \frac{d}{dt} |\Psi\rangle = \hat{H}_T |\Psi\rangle; \quad (118)$$

i.e., we are using  $\hat{H}_T$  to evolve states as opposed to  $\hat{H}$  in order to match the classical theory. But when we act on physical states, there is no difference between the two Hamiltonians:

$$\hat{H}_T |\Psi\rangle = \hat{H} |\Psi\rangle, \quad (119)$$

provided we choose the operator ordering

$$\hat{H}_T = \hat{H} + \hat{w}^r \hat{\psi}_r. \quad (120)$$

(Recall that we have set  $\hat{\chi} = 0$ .)

What about operators  $\hat{O}$  corresponding to observables? On a quantum level, we would like to be able to only work with operators that map physical states into physical states. That is, we want

$$|\Phi\rangle = \hat{O}|\Psi\rangle \text{ and } \hat{\phi}_r |\Psi\rangle = 0 \quad \Rightarrow \quad \hat{\phi}_r |\Phi\rangle = 0. \quad (121)$$

If this were not the case,  $\hat{O}$  would have no eigenbasis in the physical state space and we could not even define its expectation value. This condition is equivalent to demanding

$$[\hat{\psi}_r, \hat{O}] = i\hbar \hat{o}_r^s \hat{\psi}_s + O(\hbar^2), \quad (122)$$

where we have again chosen a convenient operator ordering. At the classical level, this implies that the classical quantities equivalent to quantum observables are first-class, modulo the usual operator ordering problems. But we saw in Section 2.4 that first-class quantities are gauge-invariant in the Hamiltonian formalism. Therefore, quantum observables in Dirac's quantization scheme correspond to classical gauge invariant quantities. It seems as if our reduction of the original Hilbert space has somehow removed the gauge degrees of freedom from our system, provided that we

only work with operators whose domain is the physical Hilbert subspace. Indeed, when such a choice is made, the arbitrary operators  $\hat{w}^r$  in the operator for the total Hamiltonian play no role and the time evolution of  $|\Psi\rangle$  is determined conclusively. Also, recall that classically, the first-class constraints generated gauge transformations, but in our construction they annihilate physical states. So in some sense, physical states are gauge invariant quantities, which is a pleasing physical interpretation.

This completes our discussion of the Dirac quantization programme in general terms. While the procedure is simply stated, it is not so easily implemented. One thing that we have been doing here is to consistently ignore the operator ordering issues by retaining only terms to lowest order in  $\hbar$ , which is not really satisfactory. Ideally, when confronted with a first-class Hamiltonian system, one would like to find an operator representation where equations (114), (115) and (122) hold exactly; i.e. with only terms linear in  $\hbar$  appearing on the right. There is no guarantee that such a thing is possible, especially when we try to satisfy the last condition for every classical gauge-invariant quantity. This is a highly non-trivial problem in loop quantum gravity, and is the subject of much current research.

### 3.2.2 Converting to second-class constraints by gauge fixing

Because finding the physical state space and quantum observables in the Dirac programme is not always easy, it may be to our advantage to try something else. All our problems seem to stem from the gauge freedom in the classical theory. So, a plausible way out is to fix the gauge classically, and then quantize the system. This not a terribly radical suggestion. The usual way one quantizes the electromagnetic field in introductory field theory involves writing down the Lagrangian in a non-gauge invariant manner. In this section, we will not attempt gauge fixing in the Lagrangian, we instead work with the Hamiltonian structure described in Section 2.3. Our discussion relies on the treatment found in reference [2].

How do we remove the gauge freedom from the system? A clumsy method would be to simply make some choice for the undetermined functions  $w^r$  in the total Hamiltonian. But when we go to quantize such a system, we would still have a non-trivial algebra for the first-class constraints and would still have to enforce quantum conditions like  $[\hat{\psi}_r, \hat{\psi}_s]|\Psi\rangle$  by restricting the state space. A better way would be to try to remove the gauge freedom by further constraining the system. In this vein, let us add *more* constraints to our system by hand. Clearly, the number of supplementary constraints needed is the same as the number of first-class constraints on the system. Let the set of the extra constraints be  $\eta = \{\eta_r\}_{r=1}^N$ . By adding these constraints, we hope to have the system transform from a first-class to second-class situation. To see what requirement this places on  $\eta$ , consider the case where we have written the original constraints in the form  $\phi = \chi \cup \psi$ . Then, the total set of constraints is  $\bar{\phi} = \phi \cup \eta = \{\phi_I\}_{I=1}^{D+N}$ . For the whole system to be second class we need that the new  $\Delta$  matrix be weakly invertible; i.e.,  $\det \Delta \approx 0$ . The structure of

$\Delta$  matrix is as follows:

$$\Delta \sim \begin{pmatrix} \Lambda & 0 & \Pi \\ 0 & 0 & \Gamma \\ -\Pi^T & -\Gamma^T & \Theta \end{pmatrix}, \quad (123)$$

where  $\Gamma$  and  $\Theta$  are  $N \times N$  matrices

$$\Gamma_{rs} = \{\psi_r, \eta_s\}, \quad \Theta_{rs} = \{\eta_r, \eta_s\}, \quad (124)$$

and  $\Pi$  is the  $R \times N$  matrix

$$\Pi_{r's} = \{\chi_{r'}, \eta_s\}. \quad (125)$$

For  $\Delta$  to be invertible, we must have

$$\det \Gamma \approx 0 \quad \Rightarrow \quad \det \Gamma \neq 0. \quad (126)$$

This is one condition that we must place on our gauge fixing conditions.

The other condition that must be satisfied is that the consistency relations

$$0 = \dot{\bar{\phi}}_I \sim \{\bar{\phi}_I, H\} + u^J \Delta_{IJ} \quad (127)$$

not lead to any more constraints in the manner in which the primary constraints led to secondary constraints in Section 2.3. That is, our gauge choice must be consistent with the equations of motion without introducing any more restrictions on the system. If more constraints are needed to ensure that  $\dot{\bar{\phi}}_I = 0$ , then we have over-constrained our system and its orbit will not in general be an orbit of original gauge theory.

If we can find  $\eta$  subject to these two conditions, we have succeeded in transforming our first-class system into a second-class one. The only thing left to establish is that if we pick a different gauge  $\eta'$ , the difference between the time evolution of our system under  $\eta$  and  $\eta'$  can be described by a gauge transformation. The proof of this is somewhat involved and needs more mathematical structure than we have presented here. We will therefore direct the interested reader to reference [2, Section 2.6] for more details.

Having transformed our classical gauge system into a system with only second-class constraints, we can proceed to find an expression for the Dirac bracket as before. Quantization proceeds smoothly from this, with the commutators given by Dirac brackets and the complete set of constraints  $\bar{\phi}$  realized as operator identities. But now the question is whether or not this quantization procedure is equivalent to the one presented in the previous section. Could we have lost something in the quantum description by gauge fixing too early? As far as we know, there is no general proof that Dirac quantization is equivalent to canonical quantization for first-class systems. So, yet again we are faced with a choice that represents another ambiguity in the quantization procedure. In the next section, we will discuss an important type of Lagrangian theory that will necessitate such a choice.

## 4 Reparameterization invariant theories

In this section, we would like to discuss a special class of theories that are invariant under transformations of the time parameter  $t \rightarrow \tau = f(t)$ . We are interested in these models because we expect any general relativistic description of physics to incorporate this type of symmetry. That is, Einstein has told us that real world phenomena is independent of the way in which our clocks keep time. So, when we construct theories of the real world, our answers should not depend on the timing mechanism used to describe them. Realizations of this philosophy are called reparameterization invariant theories. We will first discuss a fairly general class of such Lagrangians in Section 4.1 and then specialize to a simple example in 4.2.

### 4.1 A particular class of theories

In this section, we follow reference [1]. Mathematically, reparameterization invariant theories must satisfy

$$\int dt L\left(Q, \frac{dQ}{dt}\right) = \int d\tau L\left(Q, \frac{dQ}{d\tau}\right) = \int dt \frac{d\tau}{dt} L\left(Q, \frac{dt}{d\tau} \frac{dQ}{dt}\right). \quad (128)$$

This will be satisfied if the Lagrangian has the property

$$L(Q^A, \lambda \dot{Q}^B) = \lambda L(Q, \dot{Q}^B), \quad (129)$$

where  $\lambda$  is some arbitrary quantity. In mathematical jargon, this says that  $L$  is a first-order homogeneous function of  $\dot{Q}$ . Note that this is not the most general form  $L$  can have for a reparameterization theory. We would, for example, have a reparameterization invariant theory if the quantities on the left and right differed by a total time derivative. But for the purposes of this section, we will work under the assumption that (129) holds. If we differentiate this equation with respect to  $\lambda$  and set  $\lambda = 1$ , we get the following formula

$$\dot{Q}^A \frac{\partial L}{\partial \dot{Q}^A} = L, \quad (130)$$

which is also known as Euler's theorem. If we write this in terms of momenta, we find

$$0 = P_A \dot{Q}^A - L. \quad (131)$$

That is, the  $H$  function associated with Lagrangians of the form (129) vanishes identically. So what governs the evolution of such systems? If we differentiate (130) with respect to  $\dot{Q}^B$ , we obtain

$$\dot{Q}^A \frac{\partial^2 L}{\partial \dot{Q}^A \partial \dot{Q}^B} = 0. \quad (132)$$

This means the mass matrix associated with our Lagrangian has a zero eigenvector and is hence non-invertible. So we are dealing with a singular Lagrangian theory, and we discovered in Section 2.2 that such theories necessarily involve constraints. So, the total Hamiltonian for this theory must be a linear combination of constraints:

$$H_T = u^I \phi_I \sim 0. \quad (133)$$

Now, the conservation equation for the constraints is

$$0 \sim u^I \Delta_{IJ}, \quad (134)$$

which means that  $\Delta$  is necessarily singular. Therefore, we must have at least one first-class constraint and we are dealing with a gauge theory. This is not surprising, the transformation  $t \rightarrow \tau = f(t)$  is a gauge freedom in our system by assumption. Furthermore, if we only have first-class constraints then all phase space functions will evolve by gauge transformations as discussed in Section 2.4. Hence our system at a given time will be gauge equivalent to the system at any other time.

When we go to quantize such theories, we will need to choose between Dirac and canonical quantization. If we go with the former, we are confronted with the fact that we have no Schrödinger equation because the total Hamiltonian must necessarily annihilate physical states. This rather bizarre circumstance is another manifestation of the problem of time, in the quantum world we have lost all notion of evolution and changing systems. We might expect the same problem in the canonical scheme, but it turns out that we can engineer things to end up with a non-trivial Hamiltonian at the end of it all. The key is in imposing supplementary constraints  $\eta$  that depend on the time variable, hence fixing it uniquely. This procedure is best illustrated by an example, which is what we will present in the next section.

## 4.2 An example: quantization of the relativistic particle

In this section, we illustrate properties of reparameterization invariant systems by studying the general relativistic motion of a particle in a curved spacetime. We also hope that this example will serve to demonstrate a lot of the other things we have talked about in this paper. In Section 4.2.1, we introduce the problem and derive the only constraint on our system. We also demonstrate that this constraint is first class and generates time translations. We then turn to the rather trivial Dirac quantization of this system in Section 4.2.2 and obtain the Klein-Gordon equation. In Section 4.2.3, we specialize to static spacetimes and discuss how we can fix the gauge of our theory in the Hamiltonian by imposing a supplementary constraint. Finally, in Section 4.2.4 we show how the same thing can be done at the Lagrangian level for stationary spacetimes.



### 4.2.1 Classical description

The work done in this section is loosely based on reference [3]. We can write down the action principle for a particle moving in an arbitrary spacetime as

$$0 = \delta \int d\tau m \sqrt{g_{\alpha\beta} \dot{x}^\alpha \dot{x}^\beta}, \quad (135)$$

where  $\alpha, \beta$ , etc.  $\dots = 0, 1, 2, 3$ . The Lagrangian clearly satisfies

$$L(x^\alpha, \lambda \dot{x}^\beta) = \lambda L(x^\alpha, \dot{x}^\beta), \quad (136)$$

so we are dealing with a reparameterization theory of the type discussed in the previous section. The momenta are given by

$$p_\alpha = m \frac{g_{\alpha\beta} \dot{x}^\beta}{\sqrt{g_{\alpha\beta} \dot{x}^\alpha \dot{x}^\beta}}. \quad (137)$$

Notice that when defined in this way,  $p_\alpha$  is explicitly a one-form in the direction of  $\dot{x}_\alpha$ , but with length  $m$ . In other words, the momentum carries no information about the length of the velocity vector, only its orientation. Therefore, it will be impossible to express the all of the velocities as functions of the coordinates and momenta. So we have a system with inexpressible velocities and is therefore singular and should have at least one primary constraint. This is indeed that case, since it is easy to see that

$$p_\alpha \dot{x}^\alpha = L, \quad \psi = g^{\alpha\beta} p_\alpha p_\beta - m^2 = 0. \quad (138)$$

The first equation says that the function  $H = p_\alpha \dot{x}^\alpha - L = 0$ , and the second is a relation between the momenta and the coordinates that we expect to hold for all  $\tau$ ; i.e. it is a constraint. We do not have any other constraints coming from the definition of the momenta. Because  $H$  vanishes and we only have one constraint, the consistency conditions

$$\dot{\psi} \sim \{\psi, H\} + u\{\psi, \psi\} = 0 \quad (139)$$

are trivially satisfied. They do not lead to new constraints and they do not specify what the coefficient  $u$  must be. Therefore, the only constraint in our theory is  $\psi$  and it is first-class constraint.

What are the gauge transformations generated by this constraint? We have the Poisson brackets

$$\{x^\alpha, \psi\} = 2p^\alpha, \quad \{p_\alpha, \psi\} = -p_\mu p_\nu \partial_\alpha g^{\mu\nu}. \quad (140)$$

Let's look at the one on the left first. It implies that under an infinitesimal gauge transformation generated by  $\varepsilon\psi$ , we have

$$\delta x^\alpha = \left( \frac{2\varepsilon m^2}{L} \right) \dot{x}^\alpha, \quad (141)$$

where  $\varepsilon$  is a small number. So, the gauge group governed by  $\psi$  has the effect of moving the particle from its current position at time  $t$  to its position at time  $t + 2\varepsilon m^2/L$ . The action of the gauge group on  $p_\alpha$  is a little more complicated. To see what is going on, consider

$$\begin{aligned}
\Gamma_{\alpha\beta}^\gamma p_\gamma p^\beta &= \frac{1}{2} p_\gamma p^\beta g^{\gamma\delta} (\partial_\beta g_{\alpha\delta} + \partial_\alpha g_{\beta\delta} - \partial_\delta g_{\alpha\beta}) \\
&= \frac{1}{2} p^\lambda p^\nu \partial_\alpha g_{\lambda\nu} \\
&= \frac{1}{2} p_\mu p^\nu g^{\lambda\mu} \partial_\alpha g_{\lambda\nu} \\
&= -\frac{1}{2} p_\mu p_\nu \partial_\alpha g^{\mu\nu} \\
&= \frac{1}{2} \{p_\alpha, \psi\}.
\end{aligned} \tag{142}$$

In going from the third to the fourth line, we have used  $0 = \partial_\alpha \delta_\nu^\mu = \partial_\alpha (g^{\mu\lambda} g_{\lambda\nu})$ . This gives

$$\delta p_\alpha = \left( \frac{2\varepsilon m^2}{L} \right) \Gamma_{\alpha\beta}^\gamma p_\gamma \dot{x}^\beta. \tag{143}$$

Now, we know that the solution to the equations of motion for this particle must yield the geodesic equation in an arbitrary parameterization:

$$\frac{D\dot{x}^\alpha}{d\tau} = \left( \frac{d}{d\tau} \ln L \right) \dot{x}^\alpha \quad \Rightarrow \quad \frac{Dp_\alpha}{d\tau} = 0, \tag{144}$$

where  $D/d\tau = \dot{x}^\mu \nabla_\mu$  and  $\nabla_\mu$  is the covariant derivative. The righthand equation then gives

$$\frac{dp_\alpha}{dt} = \Gamma_{\alpha\beta}^\gamma p_\gamma \dot{x}^\beta. \tag{145}$$

Therefore, just as for  $x^\alpha$ , the action of the gauge group on the momentum is to shift it from its current value at time  $t$  to its value at time  $t + 2\varepsilon m^2/L$ . It now seems clear that the gauge transformations generated by  $\varepsilon\psi$  are simply time-translations. We have not found anything new here; the reparameterization invariance of our system already implied that infinitesimal time translations ought to be a gauge symmetry. But we have confirmed that these time translations are generated by a first class constraint.

What are the gauge invariant quantities in this theory? Obviously, they are anything independent of the parameter time  $\tau$ . This means that things like the position of the particle at a particular parameter time  $\tau = \tau_0$  is not a physical observable! This makes sense if we think about it; the question ‘‘where is the particle when  $\tau = 1$  second?’’ is meaningless in a reparameterization invariant theory.  $\tau = 1$  second could correspond to any point on the particle’s worldline, depending on the choice of parameterization. Good physical observables are things like constants of the motion. That is, if  $g$  is gauge invariant

$$0 = \{g, \psi\}, \tag{146}$$

we must have

$$\dot{g} \sim \{g, H_T\} \sim u\{g, \psi\} = 0; \quad (147)$$

i.e.,  $g$  is a conserved quantity. A good example of this is the case when the metric has a Killing vector  $\xi$ . Then, we expect that  $\xi^\alpha p_\alpha$  will be a constant of the motion. To confirm that this quantity is gauge invariant, consider

$$\begin{aligned} \{\xi^\alpha p_\alpha, \psi\} &= \xi^\alpha \{p_\alpha, \psi\} + \{\xi^\alpha, \psi\} p_\alpha \\ &= 2\xi^\alpha \Gamma_{\alpha\beta}^\gamma p_\gamma p^\beta + 2p_\alpha p^\beta \partial_\beta \xi^\alpha \\ &= 2p_\alpha p^\beta (\partial_\beta \xi^\alpha + \Gamma_{\gamma\beta}^\alpha \xi^\gamma) \\ &= p^\alpha p^\beta (\nabla_\alpha \xi_\beta + \nabla_\beta \xi_\alpha) \\ &= 0. \end{aligned} \quad (148)$$

In going from the first to second line, we used equation (142). In going from the fourth to fifth line, we used the fact that  $\xi$  is a Killing vector. This establishes that  $\xi^\alpha p_\alpha$  is a physical observable of the theory.

This completes our classical description. We have seen a concrete realization of a reparameterization invariant theory with a Hamiltonian that vanishes on solutions. The theory has one first-class constraint that generates time translations and the physical gauge-invariant quantities are constants of the motion. We study the quantum mechanics of this system in the next two sections.

#### 4.2.2 Dirac quantization

Let us now pursue the quantization of our system. First we tackle the Dirac programme. We must first choose a representation of our Hilbert space. A standard selection is the space of functions of the coordinates  $x$ . Let a vector in the space be denoted by  $\Psi(x)$ . Now, we need representations of the operators  $\hat{x}$  and  $\hat{p}$  that satisfy the commutation relation

$$[\hat{x}^\alpha, \hat{p}_\beta] = i\hbar \{x^\alpha, p_\beta\}_{X=\hat{X}} = i\hbar \delta_\beta^\alpha. \quad (149)$$

Keeping the notion of general covariance in mind, we choose

$$\hat{x}^\alpha \Psi(x) = x^\alpha \Psi(x), \quad \hat{p}_\alpha \Psi(x) = -i\hbar \nabla_\alpha \Psi(x). \quad (150)$$

We have represented the momentum operator with a covariant derivative instead of a partial derivative to make the theory invariant under coordinate changes. This choice also ensures the the useful commutators

$$[\hat{g}_{\alpha\beta}, \hat{p}_\gamma] = [\hat{g}^{\alpha\beta}, \hat{p}_\gamma] = 0. \quad (151)$$

The restriction of our state space is achieved by demanding  $\hat{\psi}\Psi = 0$ , which translates into

$$(\hbar^2 \nabla^\alpha \nabla_\alpha + m^2) \Psi(x) = 0; \quad (152)$$

i.e. the massive Klein-Gordon equation. Notice that our choice of momentum operator means that we have no operator ordering issues in writing down this equation.

It is important to point out the the Klein-Gordon equation appears here as a constraint, not an evolution equation in parameter time  $\tau$ . Indeed, we have no such Schrödinger equation because the action of the Hamiltonian  $\hat{H}_T = \hat{u}\hat{\psi}$  on physical states is annihilation. So this is an example of a quantization procedure that results in quantum states that do not change in parameter time  $\tau$ . This makes sense if we remember that the classical gauge invariant quantities in our theory were independent of  $\tau$ . Since these objects become observables in the quantum theory, we must have that  $\Psi$  is independent  $\tau$ . If it were not, the expectation value of observable quantities would themselves depend on  $\tau$  and would hence break the gauge symmetry of the classical theory. This would destroy the classical limit, and therefore cannot be allowed.

Now, we should confirm that our choice of operators results in a consistent theory. We have trivially that the only constraint commutes with itself and that the constraints commute with the Hamiltonian, which is identically zero when acting on physical state vectors. This takes care of two of our consistency conditions (114) and (115). But we should also confirm that  $\hat{\psi}$  commutes with physical observables. Now, we cannot do this for *all* the classically gauge invariant quantities in the theory because we do not have closed form expressions for them in terms of phase space variables. But we can demonstrate the commutative property for the  $\hat{\xi}^\alpha \hat{p}_\alpha$  operator, which corresponds to a classical constant of the motion if  $\xi$  is a Killing vector. Consider

$$\begin{aligned}
i\hbar^{-3}[\hat{\xi}^\alpha \hat{p}_\alpha, \hat{\psi}]\Psi(x) &= \nabla^\beta \nabla_\beta (\xi^\alpha \nabla_\alpha \Psi) - \xi^\alpha \nabla_\alpha (\nabla^\beta \nabla_\beta \Psi) \\
&= (\nabla^\beta \nabla_\beta \xi^\alpha)(\nabla_\alpha \Psi) + \xi^\alpha g^{\beta\gamma} (\nabla_\gamma \nabla_\beta \nabla_\alpha - \nabla_\alpha \nabla_\gamma \nabla_\beta) \Psi \\
&= -R^\alpha{}_\beta \xi^\beta \nabla_\alpha \Psi + \xi^\alpha g^{\beta\gamma} (\nabla_\gamma \nabla_\alpha - \nabla_\alpha \nabla_\gamma) \nabla_\beta \Psi \\
&= -R^\alpha{}_\beta \xi^\beta \nabla_\alpha \Psi + \xi^\alpha g^{\beta\gamma} R_{\beta\lambda\gamma\alpha} \nabla^\lambda \Psi \\
&= 0.
\end{aligned} \tag{153}$$

In going from the second to the third line, we used that  $\square \xi^\alpha = -R^\alpha{}_\beta \xi^\beta$  because  $\xi$  is a Killing vector.<sup>8</sup> We also used that  $\nabla_\alpha \nabla_\beta \Psi = \nabla_\beta \nabla_\alpha \Psi$  because we assume that we are in a torsion-free space. In going from the third to fourth line, we used the defining property of the Riemann tensor:

$$(\nabla_\alpha \nabla_\beta - \nabla_\beta \nabla_\alpha) A_\mu = R_{\mu\nu\alpha\beta} A^\nu \tag{154}$$

for any vector  $A$ . Hence,  $\hat{\xi}^\alpha \hat{p}_\alpha$  commutes with  $\hat{\phi}$ . So the action of the quantum operator corresponding to the gauge-invariant quantity  $\xi^\alpha p_\alpha$  will not take a physical state vector  $\Psi$  out of the physical state space. We mention finally that there is no ambiguity in the ordering of the  $\hat{\xi}^\alpha \hat{p}_\alpha$  operator, since

$$[\hat{\xi}^\alpha, \hat{p}_\alpha]\Psi = -i\hbar[\xi^\alpha \nabla_\alpha \Psi - \nabla_\alpha (\xi^\alpha \Psi)] = i\hbar \Psi g^{\alpha\beta} \nabla_\alpha \xi_\beta = 0. \tag{155}$$

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<sup>8</sup>Curvature tensors have their usual definitions.

The last equality follows from  $\xi$  being a Killing vector.

So, it seems that we have successfully implemented the Dirac quantization programme for this system. Some caution is warranted however, because we have only established the commutivity of quantum observables with the constraint for a particular class of gauge-invariant quantities, not all of them. For example, the classical system may have constants of the motion corresponding to the existence of Killing tensors, which we have not consider. Having said that, we are reasonably satisfied with this state of affairs. The only odd thing is the problem of time and that nothing seems to happen in our system. In the next section, we present the canonical quantization of this system and see that we do get time evolution, but not in terms of the parameter time but rather the coordinate time.

### 4.2.3 Canonical quantization via Hamiltonian gauge-fixing

We now try to quantize our system via a gauge-fixing procedure. Our treatment follows [5, 6, 7]. We will specialize to the static case where the metric can be taken to be

$$ds^2 = \Phi^2(y)dt^2 - h_{ij}(y)dy^i dy^j. \quad (156)$$

Here, lowercase Latin indices run  $1 \dots 3$ . We have written  $x^0 = t$  and  $x^i = y^i$  so that  $t$  is the coordinate time and the set  $y$  contains the spatial coordinates. Notice that the metric functions  $\Phi$  and  $h_{ij}$  are coordinate time independent and without loss of generality, we can take  $\Phi > 0$ . We can then rewrite the system's primary constraint as

$$\phi_1 = p_0 - \xi\Phi\sqrt{m^2 + h^{ij}\pi_i\pi_j} = 0, \quad \xi = \pm 1, \quad (157)$$

where  $\pi = \{\pi_i\}$  with  $p_i = \pi_i$ . Notice that since  $\Phi > 0$ , we have  $\xi = \text{sign } p_0$ . This constraint is essentially a ‘‘square-root’’ version of the constraint used in the last section. That is fine, since  $\psi = 0 \Leftrightarrow \phi_1 = 0$ ; i.e. the two constraints are equivalent. We have written  $\phi_1$  in this way to stress that the constraint only serves to specify one of the momenta, leaving three as degrees of freedom.

To fix a gauge we need to impose an supplementary condition on the system that breaks the gauge symmetry. But since the gauge group produces parameter time translations, we need to impose a condition that fixes the form of  $\tau$ . That is, we need a *time dependent* additional constraint. This is new territory for us because we have thus far assumed that everything in the theory was time independent. But if we start demanding relations between phase space variables and the time, we are introducing explicit time dependence into phase space functions. To see this, let us make the gauge choice

$$\phi_G = \phi_2 = t - \xi\tau. \quad (158)$$

This is a relation between the coordinate time, which was previously viewed as a degree of freedom, and the parameter time. It is a natural choice because it basically picks  $\tau = \pm t$ . We have included the  $\xi$  factor to guarantee that  $\dot{x}^0$  has the same sign

at  $p_0$ , which is demanded by the momentum definition (137). Now, any phase space function  $g$  that previously depended on  $t = x^0$  will have an explicit dependence on  $\tau$ . This necessitates a modification of the Dirac bracket scheme, since

$$\dot{g} = \frac{\partial g}{\partial \tau} + \frac{\partial g}{\partial x^\alpha} \dot{x}^\alpha + \frac{\partial g}{\partial p_\alpha} \dot{p}_\alpha. \quad (159)$$

But all is not lost because we still have Hamilton's equations holding in their constrained form,<sup>9</sup> which yields

$$\dot{g} \sim \frac{\partial g}{\partial \tau} + \{g, H + u^I \phi_I\}. \quad (160)$$

But recall that the simple Hamiltonian function for the current theory is identically zero, so we can put  $H = 0$  in the above. We can further simplify this expression by formally introducing the momentum conjugate to the parameter time  $\epsilon$ . That is, to our previous set of phase space variables, we add the conjugate pair  $(t, \epsilon)$ . When we extend the phase space in this way, we can now write the evolution equation as

$$\dot{g} \sim \{g, u^I \phi_I + \epsilon\}. \quad (161)$$

The effect of the inclusion of  $\epsilon$  in the righthand side of the bracket is to pick up a partial time derivative of  $g$  when the bracket is calculated.

Having obtained the correct evolution equation, it is time to see if the extended set of constraints  $\phi$  is second-class and if any new constraints when we enforce  $\dot{\phi}_I = 0$ . The equation of conservation of the constraints reduces to the following matrix problem:

$$0 = \begin{pmatrix} 0 \\ -\xi \end{pmatrix} + \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u^1 \\ u^2 \end{pmatrix}. \quad (162)$$

The  $\Delta$  matrix is clearly invertible and no new constraints arise, so our choice of  $\phi_G$  was a good gauge fixing condition. The solution is clearly

$$\Delta^{-1} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \begin{pmatrix} u^1 \\ u^2 \end{pmatrix} = \begin{pmatrix} \xi \\ 0 \end{pmatrix}. \quad (163)$$

This gives the time evolution equation as

$$\dot{g} \sim \{g, \epsilon\}_D, \quad (164)$$

where the Dirac bracket is, as usual

$$\{F, G\}_D = \{F, G\} - \{F, \phi_I\} \Delta^{IJ} \{\phi_J, G\}. \quad (165)$$

Now, the only thing left undetermined is  $\epsilon$ . But we actually do not need to solve for  $\epsilon$  explicitly if we restrict our attention to phase space functions independent of

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<sup>9</sup>See Appendix A.

$x^0$  and  $p_0$ . This is completely justified since after we find the Dirac brackets, we can take  $\phi_2 = 0$  as a strong identity and remove  $x^0$  and  $p_0$  from the phase space. Then, for  $\eta = \eta(y, \pi)$ , we get

$$\begin{aligned}\dot{\eta} &= -\left\{\eta, p_0 - \xi\Phi\sqrt{m^2 + h^{ij}\pi_i\pi_j}\right\}\{x^0 - \xi\tau, \epsilon\} \\ &= \left\{\eta, -\Phi\sqrt{m^2 + h^{ij}\pi_i\pi_j}\right\}.\end{aligned}\tag{166}$$

Hence, any function of the independent phase space variables  $(x^i, p_j)$  evolves as

$$\frac{d\eta}{dt} = \{\eta, H_{\text{eff}}\}, \quad H_{\text{eff}} = -\xi\Phi\sqrt{m^2 + h^{ij}p_ip_j}, \quad \xi = \pm 1.\tag{167}$$

If we now assume that the metric functions are independent of time, we have succeeded in writing down an unconstrained Hamiltonian theory on a subspace of our original phase space. Furthermore, the effective Hamiltonian does not vanish on solutions so we do not have a trivial time evolution. Taking this equation as the starting point of quantization, we simply have the problem of quantizing an ordinary Hamiltonian and we do not need to worry about any of the complicated things we met in Section 3. In particular, when we quantize this system we will have real time evolution because the  $\hat{H}_{\text{eff}}$  operator in the Schrödinger equation

$$i\hbar\frac{d}{dt}|\Psi\rangle = \hat{H}_{\text{eff}}|\Psi\rangle\tag{168}$$

will not annihilate physical states. We will, however have operator ordering issues due to the square root in the definition of  $H_{\text{eff}}$ . We do not propose to discuss this problem in any more detail here, we refer the interested reader to references [5, 6, 7].

Just one thing before we leave this section. We have actually derived two different unconstrained Hamiltonian theories; one with  $\xi = +1$  and another with  $\xi = -1$ . This is interesting; it suggests that there are two different sectors of the classical mechanics of the relativistic particle. We know from quantum mechanics that the state space of such systems can be divided into particle and antiparticle states characterized by positive and negative energies. We see that same thing here, we can describe the dynamics with an explicitly positive or negative Hamiltonian. The appearance of such behaviour at the classical level is somewhat novel, as has been remarked upon in references [2, 6, 7].

#### 4.2.4 Canonical quantization via Lagrangian gauge-fixing

While the calculation of the previous section ended up with a simple unconstrained Hamiltonian system, the road to that goal was somewhat treacherous. We had to introduce a formalism to deal with time-varying constraints and manually restrict our phase space to get the final result. Can we not get at this more directly? The

answer is yes, we simply need to fix our gauge in the Lagrangian. Let's adopt the same metric *ansatz* as the last section, and write the action principle as

$$\begin{aligned}
0 &= \delta \int d\tau m \sqrt{g_{\alpha\beta} \dot{x}^\alpha \dot{x}^\beta} \\
&= \delta \int d\tau m \sqrt{\Phi^2 \dot{t}^2 - h_{ij} \dot{y}^i \dot{y}^j} \\
&= \delta \int dt \xi m \sqrt{\Phi^2 - h_{ij} u^i u^j}, \tag{169}
\end{aligned}$$

where

$$u^i = \frac{dy^i}{dt} = \frac{\dot{y}^i}{\dot{t}}. \tag{170}$$

This action is formally independent of the coordinate time, but no longer reparameterization invariant. We have made the gauge choice  $\xi\tau = t$ , which is the same gauge-fixing constraint imposed in the last section.

Treating the above action principle as the starting point, the conjugate momentum is

$$p_k = -\frac{m\xi u_k}{\sqrt{\Phi^2 - h_{ij} u^i u^j}}. \tag{171}$$

This equation is invertible, giving the velocities as a function of the momenta:

$$u^k = -\frac{\xi\Phi p^k}{\sqrt{m^2 + h^{ij} p_i p_j}}. \tag{172}$$

Because there are no inexpressible velocities, we do not expect any constraints in this system. Constructing the Hamiltonian is straightforward:

$$H(x, p) = p_i u^i - L = -\xi\Phi \sqrt{m^2 + h^{ij} p_i p_j}, \tag{173}$$

which matches the effective Hamiltonian of the previous section. Therefore, in this case at least, gauge-fixing in the Hamiltonian is equivalent to gauge-fixing in the Lagrangian. Again, we are confronted with an unconstrained quantization problem that we do not study in detail here.

## 5 Summary

We now give a brief summary of the major topics covered in this paper.

In Section 2 we described the classical mechanics of systems with constraints. We saw how these constraints may be explicitly imposed on a system or may be implicitly included in the structure of the action principle if the mass matrix derived from the Lagrangian is singular. We derived evolution equations for dynamical quantities that are consistent with all the constraints of the theory and introduced a



structure known as the Dirac bracket to express these evolution equations succinctly. The constraints for any system could be divided into two types: first- and second-class. System with first-class constraints were found to be subject to time-evolution that was in some sense arbitrary, which was argued to be indicative of gauge freedoms in the system.

In Section 3, we presented the quantum mechanics of systems with constraints. For systems with only second-class constraints we discussed a relatively unambiguous quantization scheme that involved converting the classical Dirac bracket between dynamical quantities into commutation relations between the corresponding operators. For systems involving first-class constraints we presented two different quantization procedures, known as Dirac and canonical respectively. The Dirac quantization involved imposing the first-class constraints at the quantum level as a restriction on the Hilbert space. The non-trivial problems with this procedure were related to actually finding the physical Hilbert space and operators corresponding to classical observables that do not map physical states into unphysical ones. The canonical quantization scheme involved imposing the constraints at the classical level by fixing the gauge. This necessitated the addition of more constraints to our system to convert it to the second-class case. Once this was accomplished, quantization could proceed using Dirac brackets as discussed earlier.

In Section 4, we specialized to a certain class of theories that are invariant under reparameterizations of the time. That is, their actions are invariant under the transformation  $t \rightarrow \tau = \tau(t)$ . We showed that such theories are necessarily gauge theories with first class constraints. Also, these systems have the peculiar property that their Hamiltonians vanish on solutions, which means that the all dynamical quantities evolve via gauge transformations. This was seen to be the celebrated “problem of time”. We further specialized to the case of the motion of a test particle in general relativity as an example of a reparameterization invariant theory. We worked out the classical mechanics of the particle and confirmed that it is a gauge system with a single first-class constraint. We then presented the Dirac and canonical quantization of the relativistic particle. In the former case we recovered the Klein-Gordon equation and demonstrated that a certain subset of classical observables had a spectrum within the physical state space. In the latter case we showed, using two different methods, that gauge-fixing formally reduces the problem to one involving the quantization of an unconstrained Hamiltonian system.

## A Constraints and the geometry of phase space

We showed in Section 2.2 that for any theory derived from an action principle the following relation holds:

$$\delta(p_A Q^A - L) = \dot{Q}^A \delta P_A - \dot{P}_A \delta Q^A. \quad (174)$$

Among other things, this establishes that the quantity on the left is a function of  $Q$  and  $P$ , which are called the phase space variables, and not  $\dot{Q}$ . It is then tempting to define

$$H(Q, P) = p_A Q^A - L, \quad (175)$$

and rewrite the variational equation as

$$0 = \left( \dot{Q}^A - \frac{\partial H}{\partial P_A} \right) \delta P_A - \left( \dot{P}_A + \frac{\partial H}{\partial Q^A} \right) \delta Q^A. \quad (176)$$

If  $\delta Q$  and  $\delta P$  are then taken to be independent, we can trivially write down Hamilton's equations by demanding that the quantities inside the brackets be zero and be done with the whole problem.

However,  $\delta Q$  and  $\delta P$  can only be taken to be independent if there are no constraints in our system. If there are constraints

$$0 = \phi_I(Q, P), \quad I = 1, \dots, D, \quad (177)$$

then we have  $D$  equations relating variations of  $Q$  and  $P$ ; i.e.,  $0 = \delta\phi_I$ . This implies that we cannot set the coefficients of  $\delta Q$  and  $\delta P$  equal to zero in (176) and derive Hamilton's equations. If we were to do so, we would be committing a serious error because there would be nothing in the evolution equations that preserved the constraints.

What are we to do? Well, we can try to write down the constrained  $\delta Q$  and  $\delta P$  variations in (176) in terms of arbitrary variations  $\overline{\delta Q}$  and  $\overline{\delta P}$ . To accomplish this feat, let us define some new notation. Let

$$X = Q \cup P = \{X^a\}_{a=1}^{2d}, \quad (178)$$

where  $2d$  is the number of degrees of freedom in the original theory. The set  $X$  can be taken to be coordinates in a  $2d$ -dimensional space through which the system moves. This familiar construction is known as phase space. Now, the equations of constraint (177) define a  $2d - D$  dimensional surface  $\Sigma$  in this space, known as the constraint surface. We require that the variations  $\delta X$  seen in equation (176) be tangent to this surface in order to preserve the constraints. The essential idea is to express these constrained variations  $\delta X$  in terms of arbitrary variations  $\overline{\delta X}$ . The easiest way to do this is to construct the projection operator  $h$  that will “pull-back” arbitrary phase space vectors onto the constraint surface.

Luckily, the construction of such an operator is straightforward if we recall ideas from differential geometry. Let us introduce a metric  $g$  onto the phase space. The precise form of  $g$  is immaterial to what we are talking about here, but we will need it to construct inner products and change the position of the  $a, b, \dots$  indices. It is not hard to obtain the projection operator onto  $\Sigma$ :

$$h^a_b = \delta^a_b - q^{IJ} \partial_b \phi_I \partial^a \phi_J. \quad (179)$$

Here,

$$q_{IJ} = \partial^a \phi_I \partial_a \phi_J, \quad q^{IK} q_{KJ} = \delta^I_J; \quad (180)$$

i.e.,  $q^{IK}$  is the matrix inverse of  $q_{KJ}$ , which can be thought of as the metric on the space  $\Sigma^*$  spanned by the vectors  $\partial^a \phi_I$ . It is then not hard to see that any vector tangent to  $\Sigma^*$  is annihilated by  $h^a_b$ , *viz.*

$$\nu_a = \nu^K \partial_a \phi_K \quad \Rightarrow \quad h^a_b \nu_a = 0. \quad (181)$$

Also, any vector with no projection onto  $\Sigma^*$  is unchanged by  $h^a_b$ :

$$\mu^a \partial_a \phi_I = 0 \quad \Rightarrow \quad h^a_b \mu_a = \mu_b. \quad (182)$$

So,  $h^a_b$  is really a projection operator. Now, if we act  $h^a_b$  on an arbitrary variation of the phase space coordinates  $\overline{\delta X}^b$ , we will get a variation of the coordinates within the constraint surface, which is what we want. Hence we have

$$\delta X^a = \overline{\delta X}^a - q^{IJ} \partial_b \phi_I \partial^a \phi_J \overline{\delta X}^b. \quad (183)$$

Now, if we define a phase space vector

$$f_a = \left( -\dot{P} - \frac{\partial H}{\partial Q}, \dot{Q} - \frac{\partial H}{\partial P} \right), \quad (184)$$

Then, equation (176) may be written as

$$f_a \delta X^a = 0. \quad (185)$$

Now, expressing this in terms of an arbitrary variation of phase space coordinates, we get

$$0 = (f_a - u^I \partial_a \phi_I) \overline{\delta X}^a, \quad (186)$$

where

$$u^I = q^{IJ} f_a \partial^a \phi_J. \quad (187)$$

Since we now have that  $\overline{\delta X}^a$  is arbitrary, we can then conclude that

$$0 = f_a - u^I \partial_a \phi_I. \quad (188)$$

Splitting this up into a  $Q$  and  $P$  sector, we arrive at

$$\dot{Q}^A = +\frac{\partial H}{\partial P_A} + u^I \frac{\partial \phi_I^{(1)}}{\partial P_A}, \quad (189a)$$

$$\dot{P}_A = -\frac{\partial H}{\partial Q^A} - u^I \frac{\partial \phi_I^{(1)}}{\partial Q^A}. \quad (189b)$$

This matches equation (37), except that now all the constraints have been included, which demonstrates that all constraints must be accounted in the sum on the right-hand side of equation (189) in order to recover the correct equations of motion. That means that as more constraints are added to the system, Hamilton's equations must be correspondingly modified. This justifies the procedure of Section 2.3, where we kept on adding any secondary constraints arising from consistency conditions to the total Hamiltonian. Notice that we now have an explicit definition of the  $u^I$  coefficient, which we previously thought of as “undetermined”. But we cannot use (187) to calculate anything because we have not yet specified the metric on the phase space. This means the easiest way to determine the  $u$  coefficients is the method that we have been using all along; i.e., using the equations of motion to demand that the constraints be conserved. Finally, notice that our derivation goes through for constraints that depend on time. Essentially, what is happening in this case is that the constraint surface  $\phi$  is itself evolving along with the systems's phase portrait. But we can demand that the variation of  $Q$  and  $P$  in equation (176) be done in an instant of time so that we may regard  $\Sigma$  as static. To define the projection operator, we need to only know the derivatives of the constraints with respect to phase space variables, not time. So the derivation of Hamilton's equations will go through in the same fashion as in the case where  $\phi$  carries explicit time dependence. But our expression for  $\dot{g}$  must be modified as discussed in Section 4.2.3.

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