4.6. Constraints

Ref: P.A.M.Dirac, “Lectures on Quantum mechanics”.
Detailed mathematical derivations can be found in
“ 1._TheHamiltonianMethod.pdf ” & “ 2._The ProblemOfQuantization.pdf ’’.

Caution

Dirac’s treatment for constraints is meant for systems with a deficit of independent momenta, i.e., systems with built-in constraints. The signature of such systems is that the dynamical variables are not observables, e.g., the electromagnetic potentials. [See Dirac’s “Lectures on Quantum mechanics”.]

Classical Systems

Consider a set of r scleronomous (time-independent) constraints given by

$$f_i(q, \dot{q}) = 0 \qquad \frac{\partial f_i(q, \dot{q})}{\partial t} = 0 \qquad i = 1, \ \ldots, r \tag{4.126}$$

or, in variational form, by

$$\delta f_i(q, \dot{q}) = \frac{\partial f_i(q, \dot{q})}{\partial q_j} \delta q_j + \frac{\partial f_i(q, \dot{q})}{\partial \dot{q}_j} \delta \dot{q}_j = 0 \tag{4.127}$$

At the classical level, the problem can be solved by the method of Lagrange multipliers. One replaces the original Lagrangian $\mathcal{L}_0$ by

$$\mathcal{L}_f(q, \dot{q}, \lambda) = \mathcal{L}_0 (q, \dot{q}) + \sum_{i=1}^{r} \lambda_i f_i(q, \dot{q}) \tag{4.128}$$

Treating (q_j, λ_i) as generalized coordinates, the corresponding Euler eqs become

q_j: $$\frac{\partial \mathcal{L}_0}{\partial q_j} - \frac{d}{dt} \frac{\partial \mathcal{L}_0}{\partial \dot{q}_j} + \sum_{i=1}^{r} \lambda_i \left(\frac{\partial f_i}{\partial q_j} - \frac{d}{dt} \frac{\partial f_i}{\partial \dot{q}_j} \right) = 0 \tag{4.128a}$$

λ_i: $$f_i = 0$$

Likewise the Hamiltonian:

$$\begin{aligned} H_f(p, q, \lambda) &= \sum_j \frac{\partial \mathcal{L}_f}{\partial \dot{q}_j} \dot{q}_j - \mathcal{L}_f \\ &= \sum_j \frac{\partial \mathcal{L}_0}{\partial \dot{q}_j} \dot{q}_j - \mathcal{L}_0 - \sum_{i=1}^{r} \lambda_i f_i(q, \dot{q}) \\ &= H_0 (p, q) - \sum_{i=1}^{r} \lambda_i f_i(p, q) \end{aligned} \tag{4.128b}$$

where in the last expression, we have made use of the fact that

$$p_j = \frac{\partial \mathcal{L}_f}{\partial \dot{q}_j} = \frac{\partial \mathcal{L}_0}{\partial \dot{q}_j}$$

is invertible so that every $\dot{q}_j$ can be written as a function of q & p only.

The $2(n + r)$ Hamiltonian equations become

$$\dot{q}_j = \frac{\partial H_f}{\partial p_j} = \frac{\partial H_0}{\partial p_j} - \sum_{i=1}^{r} \lambda_i \frac{\partial f_i}{\partial p_j}$$

$$\dot{p}_j = -\frac{\partial H_f}{\partial q_j} = -\frac{\partial H_0}{\partial q_j} + \sum_{i=1}^{r} \lambda_i \frac{\partial f_i}{\partial q_j} \qquad (4.129)$$

and

$$\dot{\lambda}_i = \frac{\partial H_f}{\partial p_{\lambda_i}} = 0$$

$$\dot{p}_{\lambda_i} = -\frac{\partial H_f}{\partial \lambda_i} = f_i = 0$$

where we've used

$$p_{\lambda_i} = \frac{\partial \mathcal{L}_f}{\partial \dot{\lambda}_i} = 0 \quad \to \qquad \dot{p}_{\lambda_i} = 0$$

Note that the constraints $f_i = 0$ are now members of the set of equations of motion so that they hold for all times automatically for any solutions to eq(128a) or eq(4.129). In other words, since $f_i = 0$ for all times, $\dot{f}_i = 0$.

Consider now a Lagrangian $\mathcal{L}$ whose momenta

$$p_j = \frac{\partial \mathcal{L}}{\partial \dot{q}_j} \qquad j = 1, \ ..., \ n \qquad (4.129a)$$

are not invertible, i.e., $\dot{q}_j$ cannot be solved & expressed in terms of q & p only. This is so if

$$\det \left| \frac{\partial^2 \mathcal{L}}{\partial \dot{q}_j \partial \dot{q}_k} \right| = 0 \qquad (4.129b)$$

Let R be the rank of the matrix $\frac{\partial^2 \mathcal{L}}{\partial \dot{q}_n \partial \dot{q}_k}$. If $R < n$, then only R of the $\dot{q}_j$'s are linearly independent. In other words, there exists $m = n - R$ relations

$$\phi_m(q, p) = 0 \qquad m = 1, \ ..., \ M \qquad (4.126a)$$

so that M of the variables $\{q, p\}$ are not independent. Eq(4.126a) are called primary constraints.

Note that one can still use $p_j = \frac{\partial \mathcal{L}}{\partial \dot{q}_j}$ to re-write eq(4.126a) as

$$\phi_m (q, \dot{q}) = 0 \qquad (4.126b)$$

In the presence of primary constraints (or deficit of momenta), $\mathcal{L}$ already contains ϕ_m and should be identified as $\mathcal{L}_f$. We next apply the Hamiltonian principle to the "free" Lagrangian $\mathcal{L}_0 = \mathcal{L} - \sum_m \lambda_m \phi_m$. "Free" here means free of constraints so that

$$p_j = \frac{\partial \mathcal{L}_0}{\partial \dot{q}_j}$$

is invertible.

The Hamilton principle then gives (see Dirac)

$$\delta \int d\,t \left(\mathcal{L} - \sum_m \lambda_m \phi_m \right) = \delta \int d\,t \left(\sum_j \dot{q}_j p_j - H - \sum_m \lambda_m \phi_m \right) = 0$$

$$\to \qquad \dot{q}_j = \frac{\partial H_0}{\partial p_j} = \frac{\partial H}{\partial p_j} + \sum_m \lambda_m \frac{\partial \phi_m}{\partial p_i}$$

$$\dot{p}_j = -\frac{\partial H_0}{\partial q_j} = -\frac{\partial H}{\partial q_j} - \sum_m \lambda_m \frac{\partial \phi_m}{\partial q_j} \qquad (4.129c)$$

where the independent dynamic variables include only q & p so that λ & ϕ are just parameters. The dynamics of $\mathcal{L}$ is recovered by imposing the constraints (4.126a) to the solutions of eq(4.129c).

The major difference between ϕ_m and f_i is that $\phi_m = 0$ are not members of the set of equations of motion and must be treated as auxiliary equations to eq(4.129c). The evolution of ϕ_m is thus governed by the Poisson brackets as

$$\dot{\phi}_m = \{\phi_m, H_0\}_{p\,q}$$

Following Dirac, we'll call equations that are true only after the constraints $\phi_m = 0$ are applied weak equations & denote any equality in them with ≈. This means a quantity is weakly zero if it equals to the linear combination of the ϕ_m's.

If $\phi_m = 0$ is to hold for all times, we must have $\dot{\phi}_m = 0$ so that $\gamma_m = \{\phi_m, H_0\}$ should be at least weakly zero. Otherwise, we must impose a new condition

$$\gamma_m = 0$$

This leads to two possibiities. First, if γ_m is independent of the λ_m's, then $\gamma_m(q, p) = 0$ is called a secondary constraint. Otherwise, $\gamma_m(q, p, \lambda) = 0$ is a condition on the Lagrange multipliers λ_m.

Obviously, γ_m itself should be subjected to the same analysis. The process then goes on until the time derivatives of all constraints and conditions on λ are at least weakly zero.

The end result thus takes the form

$$\phi_j = 0 \qquad j = 1, \ \ldots, \ M + K \tag{4.130a}$$

where K is the number of secondary constraints ξ_k so that

$$\phi_{M+k} = \xi_k \qquad \forall \ j = M + 1, \ \ldots M + K = \mathcal{J} \tag{4.130b}$$

Hereafter, we'll assume

$$j = 1, \ \ldots, \mathcal{J} \qquad m = 1, \ \ldots, M \qquad k = 1, \ \ldots, K$$

Besides the constraints, we may also have some conditions on λ

$$\{\phi_j, H\} + \sum_m \lambda_m \{\phi_j, \phi_m\}_{p\,q} \approx 0 \tag{4.130c}$$

In order for a solution to exist, the number of independent equations in (4.130c) should be less than or equal to M.

The general solution to eq(4.130c) is (see Dirac)

$$\lambda_m = U_m + \sum_a v_a V_{a\,m} \tag{4.130d}$$

where U_m is a particular solution so that

$$\{\phi_j, H\}_{p\,q} + \sum_m U_m \{\phi_j, \phi_m\}_{p\,q} \approx 0$$

and $V_{a\,m}$ is the a^{th} homogeneous solution so that

$$\sum_m V_{a\,m} \{\phi_j, \phi_m\}_{p\,q} \approx 0 \qquad a = 1, \ \ldots, A$$

Finally, v_a are arbitrary functions of t. Validity of eq(4.130d) can be easily verified by direct substitution into eq(4.130c).

Using eq(4.130d), we can write the "free" Hamiltonian

$$H_0 = H + \sum_m \lambda_m \phi_m$$

as

$$\begin{aligned} H_0 &= H + \sum_m U_m \phi_m + \sum_{m,a} v_a V_{a\,m} \phi_m \\ &= H' + \sum_a v_a \phi_a \end{aligned}$$

where

$$H' = H + \sum_m U_m \phi_m$$

$$\phi_a = \sum_m V_{a\,m} \phi_m$$

[Incidentally, Dirac called H_0 the “total” hamiltonian and denoted it as H_T.]

The presence of the arbitrary functions of time, v_a, in H_0 means that there’re arbitrary features in the mathematical formulism. In particular, a given initial state $(q(0), p(0))$ can evolve into different states $(q(t; v), p(t; v))$ depending on the choice of $v = (v_1, \ ..., v_A)$. Since the evolution of the (observed) physical states must be unique, all these v-dependent states must correspond to the same physical state.

One notable system with such characteristics is the electromagnetic fields for which the “coordinates” are the vector potentials while the observables are the electromagnetic fields [see Lecture 2 of Dirac].

Following Dirac, we call function $R(q, p)$ a 1st class quantity if it commutes weakly with all constraints,

$$\{ R, \phi_j \}_{p,q} \approx 0 \qquad \forall j \qquad (4.131)$$

Quantities that violate (4.131) belong to the 2nd class.

Let $\{\theta_s ;\ s = 1, \ ..., S\}$ be the set of all 2nd class constraints and set

$$\{ \theta_s , \theta_{s'} \}_{p,q} = t_{s\,s'} \qquad (4.132)$$

$$= -t_{s'\,s}$$

It can be proved that [see 2nd lecture of Dirac]

$$\det (t_{s\,s'}) \neq 0$$

so that the inverse $(c_{s\,s'})$ of the matrix $(t_{s\,s'})$ exists, i.e.,

$$c_{s\,s''}\, t_{s''\,s'} = \delta_{s\,s'}$$

One then define the Dirac bracket as

$$\{ A, B \}_D = \{ A, B \}_{p,q} - c_{s\,s'} \{ A, \theta_s \}_{p,q} \{ \theta_{s'}, B \}_{p,q} \qquad (4.133)$$

It can be shown [see Dirac] that the Dirac bracket behaves like the Poisson bracket, i.e., it is antisymmetric, obeys the Leibniz rule & the Jacobi identity. Furthermore, since H_0 is 1st class,

$$\{ \theta_{s'}, H_0 \}_{p,q} \approx 0$$

$\therefore \qquad \{ g, H_0 \}_D = \{ g , H_0 \}_{p\,q} \qquad (4.133a)$

$\rightarrow \qquad \dot{g} \approx \{ g, H_0 \}_D \qquad (4.133b)$

i.e., the dynamics can be studied using Dirac brackets.

More importantly,

$$\{ g, \ \theta_s \}_D = 0 \qquad (4.133c)$$

so that all 2nd class constraints become strong equations that can be applied before the brackets are evaluated.

Quantum Systems

The 1st step of quantization is to turn the relevant classical dynamic functions f into operators. When f is a function of both p & q, we are confronted with the problem of operator ordering. To evade such complications, we restrict our attention to only 2 types of classical constraints, namely

1. the p-type

$$\phi_m(p_1, \ldots p_n) \equiv \phi_m(p) = 0 \qquad (4.134)$$

2. the q-type

$$\phi_m(q_1, \ldots q_n) \equiv \phi_m(q) = 0 \qquad (4.134a)$$

Furthermore, we'll assume all primary constraints belong to a single type..

Classically, the constraints are enforced only on the actual path of motion. This means in the quantized system, they should apply only to the physical (or solution) subspace of the Hilbert space. Thus, the quantum version of (4.134a) should be written as

$$\phi_m(Q) \mid \psi\rangle = 0 \qquad (4.135)$$

Only states $\mid \psi\rangle_P$ that satisfy (4.135) will be a member of the physical subspace.

If one takes into account that the only measurable quantities are the matrix elements, we can quantize (4.134a) as

$$\langle \psi' \mid \phi_m(Q) \mid \psi\rangle = 0 \qquad (4.136)$$

which is known as the weak implementation. In contrast, (4.135) is known as the strong implementation.

Exercise 4.20 asks you to show that the physical subspace determined by the weak implementation is always larger or equal to that by the strong one.

As in the classical case, consistency requires at least

$$i\hbar\left\langle \psi' \mid \dot{\phi}_m \mid \psi\right\rangle = \langle \psi' \mid [\phi_m, H] \mid \psi\rangle = 0 \qquad (4.137)$$

In case

$$\gamma_m(P, Q) = [\phi_m, H] \neq 0$$

we must impose the secondary constraint

$$\langle \psi' \mid \gamma_m(P, Q) \mid \psi\rangle = 0 \qquad (4.138)$$

As in the classical case, the process may go on until, hopefully, we get a final set of secondary constraints.

According to the quantization rule

$$\{a, b\} \quad \to \quad \frac{1}{i\hbar}[A, B]$$

the quantized version of eqs(131-3) is

$$[A, B]_D = [A, B] - c_{s s'}[A, \theta_s][\theta_{s'}, B] \qquad (4.141)$$

$$[g, H_0]_D = [g, H_0] \qquad (4.139)$$

$$\to \quad \dot{g} \approx [g, H_0]_D \qquad (4.139a)$$

$$[g, \theta_s]_D = 0 \qquad (4.140)$$

so that the 2nd class constraints become operator equations that are always true.

Example

Swanson's discussion of a free particle constrainted to move in a circle is erronous.

First of all, eq(4.142) should read [See " MomentumOperatorInGeneralCoordinates.pdf ".]

$$H = \frac{1}{2m}\left(p_r^+ p_r + \frac{1}{r^2} p_\theta^2\right)$$

where

$$p_r = \frac{\hbar}{i}\frac{\partial}{\partial r} \qquad p_r^+ = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r} r \qquad p_\theta = \frac{\hbar}{i}\frac{\partial}{\partial \theta}$$

Secondly, the constraint $r = a$ is applied externally so that it is guaranteed to hold for all times. Thus, one simply deals with the constrained hamiltonian

$$H = \frac{1}{2\,m\,a^2}\,p_\theta^2$$