Source: P.A.M.Dirac, “Lectrures on Quantum Mechanics”, Chap.1.

Equation labelling follows Dirac’s so they may seem out of sequence at times.

I. The Hamiltonian Method

Conventions:

1. Sum over repeated indices implied.
2. Notations for a vector: $q = (q_1, \ldots, q_N) = (q_n)$

Dirac’s scheme of quantizing a classical system:

Start with an action integral	$S = \int dt\, L$
Obtain the Hamiltonian	$H = \dot{q}_n p_n - L$
Apply quantization rule	$[q_n, p_k] = \delta_{nk}\, i\hbar$

[See source for justification.]

$$S = \int dt\, L(q, \dot{q}) \tag{1.1}$$

$$\delta S = 0 \rightarrow \quad \frac{\partial L}{\partial q_n} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_n} = 0 \tag{1.2}$$

$$p_n = \frac{\partial L}{\partial \dot{q}_n} \qquad n = 1, \ldots, N \tag{1.3}$$

Eq(1.3) is invertible (every $\dot{q}_n$ can be expressed as functions of q & p only) iff

$$\det\left|\frac{\partial^2 L}{\partial \dot{q}_n \partial \dot{q}_k}\right| \neq 0$$

Let R be the rank of the matrix $\frac{\partial^2 L}{\partial \dot{q}_n \partial \dot{q}_k}$. If $R < N$, then only R of the $\dot{q}_n$’s are linearly independent.

In other words, there exists $M = N - R$ relations

$$\phi_m(q, p) = 0 \qquad m = 1, \ldots, M \tag{1.4}$$

so that M of the variables $\{q, p\}$ are not independent. Eq(1.4) are called primary constraints.

If one has a Lagrangian L_F of n degrees of freedom & impose constraints ϕ_m on it, the equations of motion can be obtained by variation on an Lagrangian of $n - M$ degrees of freedom

$$L_E = L_F + u_m \phi_m$$

where u_m are known as Lagrangian multipliers.

In the presence of primary constraints (or deficit of momenta), L already contains ϕ_m and should be identified as L_E. The Hamiltonian principle should therefore be applied to $L_F = L - u_m \phi_m$ so that

$$\delta \int dt\,(L - u_m \phi_m) = \delta \int dt\,(\dot{q}_i p_i - H - u_m \phi_m) = 0$$

$$\rightarrow \quad \int dt \left[\dot{q}_i \delta p_i + p_i \delta \dot{q}_i - \frac{\partial H}{\partial q_i}\delta q_i - \frac{\partial H}{\partial p_i}\delta p_i - u_m \left(\frac{\partial \phi_m}{\partial q_i}\delta q_i + \frac{\partial \phi_m}{\partial p_i}\delta p_i \right) \right] = 0$$

Using

$$\int dt\, p_i \delta \dot{q}_i = p_i \delta q_i \Big|_{\text{ends}} - \int dt\, \dot{p}_i \delta q_i = -\int dt\, \dot{p}_i \delta q_i$$

we have

$$\int dt \left[\left(\dot{q}_i - \frac{\partial H}{\partial p_i} - u_m \frac{\partial \phi_m}{\partial p_i} \right) \delta p_i + \left(-\dot{p}_i - \frac{\partial H}{\partial q_i} - u_m \frac{\partial \phi_m}{\partial q_i} \right) \delta q_i \right] = 0$$

→ $$\dot{q}_i = \frac{\partial H}{\partial p_i} + u_m \frac{\partial \phi_m}{\partial p_i} \qquad (1.7)$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} - u_m \frac{\partial \phi_m}{\partial q_i} \qquad (1.8)$$

Eqs(1.7-8) are the Hamiltonian eqs of motion.

The Poisson bracket between 2 functions $f(q, p)$ & $g(q, p)$ is defined as

$$\{f, g\} = \frac{\partial f}{\partial q_n} \frac{\partial g}{\partial p_n} - \frac{\partial g}{\partial q_n} \frac{\partial f}{\partial p_n} \qquad (1.9)$$

Some properties of the Poisson brackets are

1. Anti-symmetry:

$$\{f, g\} = -\{g, f\} \qquad (1.10)$$

2. Linearity:

$$\{f + h, g\} = \{f, g\} + \{h, g\} \qquad (1.11)$$

$$\{f, h + g\} = \{f, h\} + \{f, g\} \qquad (1.12)$$

3. Jacobi identity:

$$\{f, \{g, h\}\} = \{g, \{h, f\}\} = \{h, \{f, g\}\} = 0 \qquad (1.13)$$

4. Leibniz's rule:

$$\{f, g h\} = \frac{\partial f}{\partial q_n} \frac{\partial (g h)}{\partial p_n} - \frac{\partial (g h)}{\partial q_n} \frac{\partial f}{\partial p_n}$$

$$= \frac{\partial f}{\partial q_n} \left(\frac{\partial g}{\partial p_n} h + \frac{\partial h}{\partial p_n} g \right) - \left(g \frac{\partial h}{\partial q_n} + h \frac{\partial g}{\partial q_n} \right) \frac{\partial f}{\partial p_n}$$

$$= g \{f, h\} + \{f, g\} h \qquad (1.13a)$$

For any function $g(q, p)$, we have

$$\dot{g} = \dot{q}_n \frac{\partial g}{\partial q_n} + \dot{p}_n \frac{\partial g}{\partial p_n} \qquad (1.14)$$

$$= \left(\frac{\partial H}{\partial p_n} + u_m \frac{\partial \phi_m}{\partial p_n} \right) \frac{\partial g}{\partial q_n} - \left(\frac{\partial H}{\partial q_n} + u_m \frac{\partial \phi_m}{\partial q_n} \right) \frac{\partial g}{\partial p_n}$$ [(1.7&8) used.]

$$= \{g, H\} + u_m \{g, \phi_m\} \qquad (1.15)$$

Consider now the bracket

$$\{g, H + u_m \phi_m\} = \{g, H\} + \{g, u_m \phi_m\} \qquad (1.17)$$

$$= \{g, H\} + u_m \{g, \phi_m\} + \{g, u_m\} \phi_m \qquad (1.18)$$

Since (q, p, u) are independent variables, u_m is not a function of q & p. Therefore, the bracket $\{g, u_m\}$ is not defined. However, since $\phi_m = 0$, we can still write

$$\{g, H + \lambda_m \phi_m\} = \{g, H\} + u_m \{g, \phi_m\} \qquad (1.19)$$

$$= \dot{g} \qquad (1.16)$$

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 ≈. For example, eq(1.16) becomes

$$\dot{g} \approx \{g, H_T\} \qquad (1.21)$$

where

$$H_T = H + u_m \phi_m \qquad (1.22)$$

[Obviously, the constraints are to be applied only AFTER all Poisson brackets involving them have been evaluated.]

Note also that

$$A \approx 0 \qquad \rightarrow \qquad A = a_m \phi_m$$

where a_m can be any expression that is not singular as $\phi_m = 0$.

First thing about the equations of motion given by eq(1.21) is the issue of consistency. In particular, since the constraints (1.4) must hold for all times, we have

$$\begin{aligned}\dot{\phi}_m &\approx \{\phi_m, H\} + u_{m'} \{\phi_m, \phi_{m'}\} \\ &\approx 0 \end{aligned} \qquad (1.23)$$

If the equations in (1.23) lead to inconsistencies, then the original Lagrangian does not represent an actual physical system.

Thus, L cannot be an arbitrary function. For example, let $L = q$, then

$$\frac{\partial L}{\partial \dot{q}} = 0 \qquad \frac{\partial L}{\partial q} = 1$$

Lagrange eq(1.2) thus becomes a contradiction

$$1 - 0 = 0$$

For the hamilton eqs,

$$p = \frac{\partial L}{\partial \dot{q}} = 0 = \phi_1$$

$$\rightarrow \qquad H = -q$$

$$\{\phi_1, H\} = -\{p, q\} = 1$$

$$\{\phi_1, \phi_1\} = 0$$

Eq(1.23) thus becomes

$$0 = 1$$

Thus, $L = q$ cannot describe a dynamical system.

There're 3 possible outcomes after $\chi_j = \{\phi_j, H\} + u_m \{\phi_j, \phi_m\}$ for a given j is evaluated.

1. $\chi_j = a_{j\,m} \phi_m \approx 0$.
2. $\chi_j = \chi_j(q, p)$ is independent of u as well as the ϕ_m's.
3. $\chi_j = \chi_j(q, p, u)$ contains some u_m's in it.

For case 1, consistency (1.23) is automatically satisfied.
For case 2, consistency (1.23) introduces a new constraint $\chi_j(q, p) = 0$.
For case 3, consistency (1.23) introduces a condition $\chi_j(q, p, u) \approx 0$ on the u_m's.

The new constraints in case 2 are called secondary constraints. Whereas the primary constraints result from the definition of the momenta (1.3) alone, the secondary constraints, by means of the brackets $\{\phi_m, H\}$, involve the Hamiltonian equations of motion too.

Each secondary constraint comes with another consistency requirement

$$\dot{\chi}_j \approx \{\chi_j, H\} + u_m \{\chi_j, \phi_m\} \approx 0 \qquad (1.25)$$

where $\{\phi_m\}$ includes only primary constraints. The foregoing analysis must be applied anew to this expanded set of constraints. The process must go on until no new independent constraint emerges.

The end result thus takes the form

$$\phi_j \approx 0 \qquad j = 1, \ldots, M + K \qquad (1.27)$$

where K is the number of secondary constraints so that

$$\phi_j = \chi_{j-M} \qquad \forall\ j = M + 1, \ldots M + K = \mathcal{J} \qquad (1.26)$$

Hereafter, we'll assume

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

Once the full set of constraints are found, one can identify all the equations belonging to case 3

$$\chi_j(q, p, u) = \{\phi_j, H\} + u_m \{\phi_j, \phi_m\} \approx 0 \qquad (1.28)$$

Taking (1.28) as a set of linear equations for the unknown u, we can solve it to get a (particular) solution $U_m(q, p)$ so that

$$\{\phi_j, H\} + U_m \{\phi_j, \phi_m\} \approx 0 \qquad (1.29)$$

Such a solution must exist if L is a consistent Lagrangian. Note that this implies there are only $\mu \leq M$ independent eqs in (1.28).

Even if $\mu = M$, the solution to (1.28) is not unique. Let $V_{a\,m}$ be the a^{th} solution to the homogeneous equations

$$u_m \{\phi_j, \phi_m\} = 0$$

i.e.,

$$V_{a\,m} \{\phi_j, \phi_m\} = 0 \qquad \forall \ a = 1, \ldots A \qquad (1.30)$$

the general solution to (1.28) is given by

$$\mathcal{U}_m = U_m + v_a V_{a\,m} \qquad (1.31)$$

where v_a are arbitrary functions of time. This is so since

$$\{\phi_j, H\} + \mathcal{U}_m \{\phi_j, \phi_m\} = \{\phi_j, H\} + U_m \{\phi_j, \phi_m\} + v_a V_{a\,m} \{\phi_j, \phi_m\}$$

$$= \{\phi_j, H\} + U_m \{\phi_j, \phi_m\} \qquad [\ (1.31) \text{ used.}\ ]$$

$$\approx 0 \qquad [\ (1.29) \text{ used.}\ ]$$

Substituting (1.31) into (1.22) gives

$$H_T = H + U_m \phi_m + v_a V_{a\,m} \phi_m \qquad (1.32)$$

$$= H' + v_a \phi_a \qquad (1.33)$$

where

$$H' = H + U_m \phi_m \qquad (1.33')$$

$$\phi_a = V_{a\,m} \phi_m \qquad (1.34)$$

Using (1.32) in the equations of motion (1.21), all the constraints arising from the initial primary contraints will be satisfied. However, the existence of arbitrary functions of time, v_a, 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 $v = (v_1, \ldots, v_A)$. Since the evolution of the (observed) physical states must be unique, all these v-dependent states must correspond to the same physical state.

New terminology is required to describe the situation.

A dynamic variable $R = R(q, p)$ is said to be 1st class if

$$\{R, \phi_j\} \approx 0 \qquad (1.35)$$

Otherwise, it is 2nd class.

By definition, the ϕ_j's are the only independent weakly zero quantities. Therefore, all other weakly zero quantities must be a strong linear combination of the ϕ_j's. Thus, (1.35) implies

$$\{R, \phi_j\} = r_{j j'} \phi_{j'} \qquad (1.36)$$

Theorem:

The Poisson bracket of two 1st class quantities is also 1st class.

Proof:

Let R, S be 1st class.

$$\rightarrow \quad \{R, \phi_j\} = r_{j j'} \phi_{j'} \quad \& \quad \{S, \phi_j\} = s_{j j'} \phi_{j'} \qquad (1.36')$$

Using the Jacobi identity (1.13), we have

$$\{\{R, S\}, \phi_j\} = -\{\{\phi_j, R\}, S\} - \{\{S, \phi_j\}, R\}$$

$= \{ r_{jj'} \phi_{j'}, S \} - \{ s_{jj'} \phi_{j'}, R \}$
$= r_{jj'} \{ \phi_{j'}, S \} + \{ r_{jj'}, S \} \phi_{j'} - s_{jj'} \{ \phi_{j'}, R \} - \{ s_{jj'}, R \} \phi_{j'}$
$= -r_{jj'} s_{j'j''} \phi_{j''} + \{ r_{jj'}, S \} \phi_{j'} + s_{jj'} r_{j'j''} \phi_{j''} - \{ s_{jj'}, R \} \phi_{j'}$
≈ 0 QED

We can divide the constraints into 1st & 2nd class. Coupled with the primary & secondary classification, we have 4 kinds of constraints.

For example, H' in (1.33') & ϕ_a in (1.34) are 1st class.

Proof:

$$\{ H', \phi_j \} = \{ H, \phi_j \} + \{ U_m \phi_m, \phi_j \}$$
$$= \{ H, \phi_j \} + U_m \{ \phi_m, \phi_j \} + \{ U_m, \phi_j \} \phi_m$$
$$\approx -\dot{\phi}_j + \{ U_m, \phi_j \} \phi_m$$
$$\approx \{ U_m, \phi_j \} \phi_m \qquad \text{[Eq(1.28) used.]}$$
$$\approx 0$$

$$\{ \phi_a, \phi_j \} = \{ V_{am} \phi_m, \phi_j \}$$
$$= V_{am} \{ \phi_m, \phi_j \} + \{ V_{am}, \phi_j \} \phi_m$$
$$= \{ V_{am}, \phi_j \} \phi_m \qquad \text{[Eq(1.30) used.]}$$
$$\approx 0 \qquad \text{QED}$$

Since the sum in $V_{am} \phi_m$ is over the primary constraints, ϕ_a is also a primary constraint as well as 1st class.

Hence, H_T is a sum of a 1st class hamiltonian H' & a linear combination of primary, 1st class constraints.

The number of arbitrary functions of time in the general solution is just the number A of the independent 1st class primary constraints.

In practice, these arbitrary functions of time can be deduced from the action integral. Each of these functions then corresponds to a 1st class primary constraint, which is thus obtained expeditiously without working through the official channel via Poisson brackets.

Consider now the infinitesimal evolution from $t = 0$ to $t = \delta t$. For a general dynamic variable g with $g(0) = g_0$, we have

$$g(\delta t) = g_0 + \dot{g}\, \delta t$$
$$= g_0 + \{ g, H_T \} \delta t$$
$$= g_0 + (\{ g, H' \} + v_a \{ g, \phi_a \}) \delta t \qquad (1.37)$$

where v is arbitrary.

Taking the difference with g for $v \to v'$, we have

$$\Delta g(\delta t) = (v_a - v'_a) \{ g, \phi_a \} \delta t \qquad (1.38)$$
$$= \varepsilon_a \{ g, \phi_a \} \qquad (1.39)$$

where

$$\varepsilon_a = (v_a - v'_a) \delta t \qquad (1.40)$$

is small & arbitrary function of time and should be treated as a constant inside a Poisson bracket.

Writing eq(1.39) as

$$g' = g + \varepsilon_a \{ g, \phi_a \} \qquad (1.40a)$$

we can treat it as an infinitesimal canonical transformation by the generating function $\varepsilon_a \phi_a$. The 1st class primary constraints ϕ_a therefore generate a canonical transformation that leaves the physical state unchanged.

If we apply to (1.40a) another infinitesimal canonical transformation with generator $\gamma_a\,\phi_a$, we have

$$\begin{aligned} g'' &= g' + \gamma_a\{g', \phi_a\} \\ &= g + \varepsilon_a\{g, \phi_a\} + \gamma_a\{g + \varepsilon_{a'}\{g, \phi_{a'}\}, \phi_a\} \qquad (1.41) \\ &= g + \varepsilon_a\{g, \phi_a\} + \gamma_a\{g, \phi_a\} + \gamma_a\,\varepsilon_{a'}\{\{g, \phi_{a'}\}, \phi_a\} \end{aligned}$$

If we reverse the order of the transformations, we have

$$\begin{aligned} \tilde{g}' &= g + \gamma_a\{g, \phi_a\} \\ \tilde{g}'' &= \tilde{g}' + \varepsilon_a\{\tilde{g}', \phi_a\} \\ &= g + \gamma_a\{g, \phi_a\} + \varepsilon_a\{g + \gamma_{a'}\{g, \phi_{a'}\}, \phi_a\} \qquad (1.42) \\ &= g + \gamma_a\{g, \phi_a\} + \varepsilon_a\{g, \phi_a\} + \varepsilon_a\,\gamma_{a'}\{g, \phi_{a'}\}, \phi_a\} \end{aligned}$$

$$\begin{aligned} \rightarrow \qquad \Delta g &= g'' - \tilde{g}'' \\ &= \varepsilon_a\,\gamma_{a'}\left(\{\{g, \phi_a\}, \phi_{a'}\} - \{\{g, \phi_{a'}\}, \phi_a\}\right) \qquad (1.43) \\ &= -\varepsilon_a\,\gamma_{a'}\{\{\phi_a, \phi_{a'}\}, g\} \qquad \text{[Jacobi's identity (1.13) used.]} \\ &= \varepsilon_a\,\gamma_{a'}\{g, \{\phi_a, \phi_{a'}\}\} \qquad (1.44) \end{aligned}$$

which is a canonical transformation with generator $\varepsilon_a\,\gamma_{a'}\{\phi_a, \phi_{a'}\}$ that leaves the physical state unchanged.

Since the Poisson bracket of two 1st class variables is still 1st class, $\{\phi_a, \phi_{a'}\}$ remains a 1st class constraint but need not be primary.

In conclusion, we see that the transformations that leave the physical state unchanged are canonical transformations with 1st class (including both primary & secondary) constraints as generators. The converse, that all such constraints can generate transformations that leave the physical state unchanged, will be assumed though not yet proven.