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Canonical Transformations and Commutators in the Lagrangian Formalism*

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In this paper we clarify a number of questions connected with the Lagrangian formulation of canonical transformations and commutator brackets. We make a distinction between "regular" and "singular" theories, the latter having such a structure that the Euler equations cannot be solved uniquely with respect to the accelerations. For "regular" theories we show that the introduction of the Poisson bracket by Peierls, which is based on a variation of the Lagrangian, and the infinitesimal canonical transformations introduced by Bergmann and Schiller lead to equivalent results. For "singular" theories we show first that constants of the motion do not necessarily generate invariant transformations and that, generally speaking, the relationship between transformations and generators is not unique in either direction. Then we show that by restricting ourselves to invariant transformations and their generators we can define commutators between constants of the motion unambiguously. The resulting bracket expressions vanish whenever at least one of the commuted constants of the motion vanishes (is a secondary constraint). It turns out that these commutator brackets in the Lagrangian formalism are equivalent not to Poisson brackets but to (generalized) Dirac brackets. A possible quantization procedure is sketched in the concluding section.

1. INTRODUCTION

IT is well known that the quantum theoretical reformulation of classical theories frequently meets with difficulties that arise out of ambiguities in the proper order of noncommuting factors as well as out of the cumbersome transformation properties of canonical momentum components in theories that are to be relativistically invariant or gauge invariant. A number of authors have dealt with the possibility of circumventing at least some of these difficulties by basing the quantization procedure on the Lagrangian rather than the Hamiltonian version of a classical (i.e., nonquantum) theory.[1–4] Some of these proposals apply only to linear or quasi-linear theories or to theories in which the velocities (i.e., the time derivatives of the configuration variables) can be expressed as unique functions of the canonical variables. We consider that such restrictions are likely to exclude from consideration just those theories in which the Hamiltonian quantization schemes present serious difficulties. In this paper we shall develop those aspects of classical Lagrangian theories that appear likely to represent the points of departure for subsequent quantization.

In what follows, we shall first prove (Sec. 2) the equivalence of Peierls's definition of canonical transformations and their generators[3] and ours,[4] within the realm in which the Peierls formalism applies. Next, (Sec. 3) we shall show that in a certain sense zero generators may give rise to transformations that change the form of the Lagrangian. Finally (Sec. 4), by restricting ourselves to invariant transformations (i.e., transformations that leave the form of the Lagrangian unchanged) we shall discover commutation brackets ("Dirac brackets" rather than Poisson brackets) that are uniquely determined by the generators of the two commuting infinitesimal transformations. In all that follows we shall rely heavily on the notation and results of our earlier paper.[4]

2. LAGRANGIAN THEORIES BY PEIERLS AND BY BERGMANN AND SCHILLER

We begin with a brief resume of the two theories, assuming, for the sake of simplicity, a finite number of degrees of freedom. We shall also, with Peierls, consider in this section only such Lagrangians in which the original differential equations of motion can be solved with respect to the accelerations. We shall call such Lagrangians "regular," others "singular."

Peierls' approach involves the consideration of small changes in the Lagrangian. If we add to a given Lagrangian $L(q_k,\dot{q}_k,t)$ an infinitesimal change,

$$\delta L(q,\dot{q},t)=B(q,\dot{q},t), \tag{2.1}$$

then the solutions of the modified Euler-Lagrange equations will differ from the original solutions $q_k(t)$ by infinitesimal functions of the time, $\delta q_k(t)$, which in turn will bring about a corresponding change in any dynamical variable A that may be given to us as a specified function of the coordinates q_k, the velocities $\dot{q}_k$, and the time t,

$$\delta A=\partial^k A\delta q_k+\partial^{k\cdot} A\delta\dot{q}_k,\quad \partial^k\equiv\partial/\partial q_k,\quad \partial^{k\cdot}\equiv\partial/\partial\dot{q}_k. \tag{2.2}$$

These variations will be unique with suitable initial conditions. Of these, Peierls considers, in particular, variations that result if we require that for $t=-\infty$ the δq_k are to vanish:

$$Dq_k(-\infty)=0,\quad DA(-\infty)=0, \tag{2.3}$$

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[1] R. P. Feynman, Revs. Modern Phys. 20, 367 (1948).
[2] J. Schwinger, Phys. Rev. 82, 914 (1951).
[3] R. E. Peierls, Proc. Roy. Soc. (London) A214, 143 (1952).
[4] P. G. Bergmann and R. Schiller, Phys. Rev. 89, 4 (1953). Referred to as BS.

and variations that vanish for $t=+\infty$:

$$\mathcal{D}q_k(\infty)=0, \quad \mathcal{D}A(\infty)=0. \tag{2.4}$$

We can now introduce the difference $(DA-\mathcal{D}A)$, which depends linearly on the choice of $B(t)$ at all times. With its help we define an expression $T_P[A(t),B(t')]$, as follows:

$$DA(t)-\mathcal{D}A(t)=-\int_{t'=-\infty}^{\infty} T_P(A(t),B(t'))dt'. \tag{2.5}$$

This definition is unique provided it is agreed that $T_P(\ ,\ )$ is linear in B and independent of $\dot{B}(t')$. Then $T_P(\ ,\ )$ is simply the Poisson bracket.

Bergmann and Schiller consider the change brought about in the form of a Lagrangian by an infinitesimal transformation of the coordinates. The change in the coordinate values of a point in configuration space, $\bar{\delta}q_k(t)$, is permitted to depend not only on the coordinates themselves but also on the velocities $\dot{q}_k$, provided the Lagrangian in terms of the new coordinates is still a function of the coordinates and their first time derivatives only, i.e., independent of all higher derivatives. To achieve this purpose it is permissible to add to the Lagrangian an exact time derivative, $\dot{Q}(q,p,t)$. If one introduces the "generator" C, defined as

$$C=\partial^{k\cdot}L\bar{\delta}q_k-Q, \tag{2.6}$$

it is found that the possible variations of the coordinates are connected with the generator by the conditions

$$\partial^{k\cdot}\partial^{l\cdot}L\bar{\delta}q_l\equiv L^{kl}\bar{\delta}q_l=\partial^{k\cdot}C. \tag{2.7}$$

As for the Lagrangian, we must distinguish between its *change in value* for a given point in configuration space and for a given set of velocities,

$$\bar{\delta}L=\dot{Q}, \tag{2.8}$$

and its *change of form*, i.e., its change as a function of its arguments,

$$\delta' L=\bar{\delta}L-\partial^k L\bar{\delta}q_k-\partial^{k\cdot}L\bar{\delta}\dot{q}_k. \tag{2.9}$$

The latter turns out to be

$$\delta' L=-\dot{C}-L^k\bar{\delta}q_k,$$

where

$$L^k=\partial^k L-\frac{d}{dt}(\partial^{k\cdot}L). \tag{2.10}$$

For the details, see BS. Equations (2.7) and (2.10) together establish a connection between the change in the form of the Lagrangian and an infinitesimal coordinate transformation causing the change.

Peierls produces a change in the *actual* trajectories by adding a term to the Lagrangian; Bergmann and Schiller produce a change in the *form* of the Lagrangian and in the *form* of the trajectories through a coordinate transformation. Formally the two approaches must be equivalent, in that in any event the trajectories remain solutions of the Euler-Lagrange equations, which in turn are determined uniquely by the given form of Lagrangian. We shall now demonstrate this equivalence by actual computation. Though Peierls' change of A, Eq. (2.5), is determined by the additions to the Lagrangian throughout the range of the independent variable t, whereas in the BS approach the change is the result of the simultaneous coordinate transformation, the definitions of the Poisson bracket will be the same.

In the BS theory, the variable A, given as a fixed function of its arguments ($\delta' A=0$), will change its value as follows:

$$\bar{\delta}A=\partial^k A\bar{\delta}q_k+\partial^{k\cdot}A\bar{\delta}\dot{q}_k. \tag{2.11}$$

We shall now calculate that expression on the assumption that the equations of motion, $L^k=0$, are satisfied. Without this assumption the concept of Poisson bracket for two variables at different times [see Eq. (2.5)] would be meaningless.

In order to substitute into the expression (2.11) the value of $\bar{\delta}q_k$ as given by Eq. (2.7), we shall introduce, in addition to the matrix $L^{kl}[=\partial^{k\cdot}\partial^{l\cdot}L$, see Eq. (2.7)], its reciprocal matrix, H_{kl}[5] $(=\partial^2 H/\partial p^k\partial p^l=\partial_k\partial_l H)$, so that

$$\bar{\delta}q_k=H_{kl}\partial^{l\cdot}C=\partial C/\partial p^k\equiv\partial_k C. \tag{2.12}$$

In this manner we obtain the expression

$$\bar{\delta}A=\partial^k A\,\partial_k C+\partial_l A\left[\frac{d}{dt}(\partial^{l\cdot}C)-\dot{L}^{lk}\bar{\delta}q_k\right]. \tag{2.13}$$

We shall now rewrite part of this expression in such a form that the independent variables q_k, $\dot{q}_k$ are replaced by q_k, p^k. For this purpose, we must rewrite the first term on the right-hand side by means of the formula

$$(\partial^k A)_{\dot{q}}=(\partial^k A)_p+\partial^k\partial^{l\cdot}L\partial_l A, \tag{2.14}$$

in which the parentheses around the partial derivatives are to be understood as in thermodynamic equations. We obtain

$$\bar{\delta}A=(\partial^k A)_p\partial_k C+\partial_l A\left[\partial^k\partial^{l\cdot}L\partial_k C+\frac{d}{dt}(\partial^{l\cdot}C)-\bar{\delta}q_k\dot{L}^{kl}\right]. \tag{2.15}$$

Next we use the equality

$$\frac{d}{dt}(\partial^{l\cdot}C)=\partial^{l\cdot}\left(\frac{dC}{dt}\right)-\partial^l C, \tag{2.16}$$

as well as Eq. (2.14) for $\partial^l C$. The result is:

$$\bar{\delta}A=(A,C)+\partial_l A[\partial_k C(\partial^k\partial^{l\cdot}L-\partial^{k\cdot}\partial^l L-\dot{L}^{kl})+\partial^{l\cdot}(dC/dt)]. \tag{2.17}$$

The first term on the right represents an ordinary Poisson bracket; the remainder can be simplified but

[5] H_{kl} exists because of the assumed "regularity" of the Lagrangian.

does not vanish. We shall substitute in the very last term from Eq. (2.10). We have:

$$\partial^{l\cdot}(dC/dt) = -\partial^{l\cdot}[L^k\partial_k C + \delta' L] = -\partial^{l\cdot}(L^k)\partial_k C - \partial^{l\cdot}(\delta' L), \quad (2.18)$$

inasmuch as the undifferentiated L^k vanish by assumption. Aside from the last term, $\partial_k C$ is then a joint factor, and we may bring Eq. (2.17) into the form

$$\bar{\delta}A = (A,C) + \partial_k C \partial_l A(\partial^k\partial^{l\cdot}L - \partial^{k\cdot}\partial^l L - \dot{L}^{kl} - \partial^{l\cdot}L^k) - \partial_l A \partial^{l\cdot}(\delta' L). \quad (2.19)$$

The explicit calculation of $\partial^{l\cdot}L^k$ shows that the parenthesis in the second term on the right vanishes identically. We have, thus,

$$\bar{\delta}A = (A,C) - \partial_l A \partial^{l\cdot}(\delta' L) = (A,C) - \partial_l A \delta' p^l. \quad (2.20)$$

The last term might appear disconcerting, because it is well known that in the Hamiltonian formalism the infinitesimal change in A (considered to be a fixed function of the canonical variables) merely equals the Poisson bracket. However, we have performed our calculation on the assumption that A was a fixed function of the q_k and the $\dot{q}_k$. It is, of course, entirely possible to express the velocities as functions of the momentum coordinates, or vice versa, but this algebraic relationship changes under any transformation that changes the form of the Lagrangian (or Hamiltonian). The last term on the right is a "transport term" which precisely expresses this change in relationship.

In order to obtain a relationship similar to that of Peierls, Eq. (2.5), we shall now endeavor to replace the simultaneous generator C by the changes in the Lagrangian, $\delta' L$, at all times. Assuming that at $t=-\infty$ the generator C vanishes, and furthermore that the equations of motion are satisfied throughout (in other words, that our path of integration is a trajectory), we see from Eq. (2.10) that

$$C(t) = -\int_{t'=-\infty}^{t} \delta' L(t')dt'. \quad (2.21)$$

If we are to substitute this integral into Eq. (6.20), we must first agree that we shall define the Poisson bracket of two variables at different times in such a manner that it will continue to satisfy the principle of linear superposition for either of its two factors, that the Poisson bracket with a numeric (such as a function of t only) vanish, and that if either factor contains higher than first time derivatives, these are to be substituted from the equations of motion. The last requirement is necessary to assure that the Poisson bracket of an equation of motion vanish. We have, with these specifications,

$$DA(t) = -\partial_l A(t)\partial^{l\cdot}[\delta' L(t)] - \int_{-\infty}^{t}(A(t),\delta' L(t'))dt'. \quad (2.22)$$

If instead we consider a situation in which C vanishes in the infinite future, we obtain a similar expression for $\mathcal{D}A(t)$. Combining them, we find

$$DA(t) - \mathcal{D}A(t) = -\int_{-\infty}^{\infty}(A(t),\delta' L(t'))dt', \quad (2.23)$$

which is identical with Eq. (2.5).

For the foregoing discussion it is important that the Lagrangian of the theory is "regular" in the sense that the determinant of the matrix L^{kl} be nonzero. If it is, then the velocities are unique functions of the canonical coordinates, and the Euler-Lagrange equations can be solved for the accelerations. These assumptions have been used explicitly or implicitly in the discussion of both the Peierls and the BS theory. If the Lagrangian is "singular," the Peierls construction requires major modifications: trajectories may not be determined uniquely by initial conditions. But as a singular Lagrangian may be rendered regular by the addition of an arbitrarily small term, we face a situation somewhat similar to the perturbation theory of degenerate levels in quantum mechanics. In the BS theory, Eqs. (2.7) and (2.10) remain valid, without modification. In the following sections we shall not assume regularity but will use those relationships that are independent of regularity.

3. TRANSFORMATIONS GENERATED BY CONSTRAINTS

In theories with "regular" Lagrangians there is a one-to-one relationship between the generators and the canonical transformations in the Hamiltonian formalism, and the generators are unrestricted functions of the canonical variables. Correspondingly, in the Lagrangian formalism the generators are unrestricted functions of the q_k and $\dot{q}_k$, and they determine the $\bar{\delta}q_k$ uniquely; the transformations according to Eq. (2.7) determine the generators only up to an arbitrary function of the q_k. In the canonical formalism a generator $C(q_k,t)$ produces a transformation of the p_k only; in the Lagrangian formalism such a transformation amounts to a redefinition of the momenta in terms of the velocities.

With a "singular" Lagrangian, the relationship between generators and transformations is considerably more involved. In particular, a vanishing generator may generate nontrivial transformations; in the Lagrangian formalism transformations may even be associated with a generator that vanishes *identically*, i.e., not merely *modulo* the equations of motion or the constraints. This section will be devoted to the exhibition of such transformations. We shall show later that the lack of a firm relationship between generator and transformation will be remedied if we restrict ourselves to invariant transformations, i.e., transformations that leave the form of the Lagrangian unchanged. In a "regular" theory an invariant transformation will be generated by any constant of the motion (which is permitted to be explicitly time-dependent), and only constants of the motion will generate invariant transformations. In a "singular" theory, the generators of invariant transformations will still be constants of the motion, but the reverse no longer holds: Vanishing generators will surely be constants of the motion, but they may be associated with noninvariant transformations.

In what follows, we shall classify constraints in the Hamiltonian formalism as *primary* and *secondary* constraints.[6] A primary constraint represents an algebraic relationship in a "singular" theory satisfied by the canonical variables as a direct result of the defining equations of the momentum variables; secondary constraints will be the result of the requirement that the primary constraints remain zero in the course of time. They are the Poisson brackets (or possibly iterated Poisson brackets) of the primary constraints with the Hamiltonian. We shall also distinguish between *first-class* and *second-class* constraints.[7] First-class constraints have vanishing Poisson brackets with all other constraints (*modulo* the constraints), whereas second-class constraints do not. As shown below, first-class constraints indicate the existence of a group of invariant transformations that depend on arbitrary functions of the time (of all four coordinates in the case of field theories), whereas second-class constraints do not.

In a Lagrangian formalism, all primary constraints, first-class or second-class, vanish identically, whereas secondary constraints go over into combinations of equations of motion that are free of second time derivatives. As pointed out by Dirac,[7] higher-order constraints may be obtained in some theories by differentiating secondary constraints with respect to time and by eliminating the accelerations with the help of the equations of motion. However, in most theories normally considered, this iterated procedure leads to no new relations.

We shall begin by considering transformations generated (by means of Poisson brackets) by arbitrary combinations of constraints in the Hamiltonian formalism. In a "singular" theory, the Lagrangian determines the Hamiltonian only *modulo* an arbitrary linear combination of primary first-class constraints.[8] Accordingly an invariant transformation is one that changes the Hamiltonian at most by such a combination.

If a quantity F under an infinitesimal canonical transformation changes its value at a given point of phase space by the amount $\bar{\delta}F$ (which will depend on its transformation law), then its change as a function of the canonical coordinates, $\delta''F$, will be given by the expression

$$\delta''F=\bar{\delta}F-\partial^kF\bar{\delta}q_k-\partial_kF\bar{\delta}p^k=\bar{\delta}F-(F,C). \quad (3.1)$$

[6] J. L. Anderson and P. G. Bergmann, Phys. Rev. 83, 1018 (1951).
[7] P. A. M. Dirac, Can. J. Math. 2, 129 (1950); 3, 1 (1951).
[8] P. G. Bergmann and J. H. M. Brunings, Revs. Modern Phys. 21, 480 (1949).

The transformation law for the Hamiltonian under a canonical transformation generated by C is that $\bar{\delta}H$ equal $(\partial C/\partial t)$; hence

$$\delta''H=\frac{\partial C}{\partial t}+(C,H)=\rho_aC_P{}^a \quad (3.2)$$

is the condition for an invariant transformation, where the symbol C_P stands for first-class primary constraints. ρ_a are arbitrary coefficients. It was shown previously that if there exists a group of invariant transformations with arbitrary functions, then these invariant transformations are generated by suitable constraints.[6] The converse statement is: If a theory contains first-class primary and secondary constraints, then there exist linear combinations generating invariant transformations. To simplify the manipulations, we shall assume that the second-order Poisson bracket of a primary first-class constraint with the Hamiltonian, $(H,(H,C_P))$, produces no further secondary constraints; this assumption is not crucial for the result. With this assumption we have, for any $C_S=(C_P,H)$,

$$(C_S{}^a,H)=\kappa_b{}^aC_S{}^b+\omega_b{}^aC_P{}^b. \quad (3.3)$$

Now we examine the change in the Hamiltonian generated by a combination of constraints:

$$C=\gamma_aC_P{}^a+\beta_aC_S{}^a. \quad (3.4)$$

We find, in accordance with the first half of Eq. (3.2),

$$\begin{aligned}\delta''H&=\dot{\gamma}_aC_P{}^a+\dot{\beta}_aC_S{}^a+\gamma_aC_S{}^a\\&\quad+\beta_a(\kappa_b{}^aC_S{}^b+\omega_b{}^aC_P{}^b)\\&=(\dot{\gamma}_b+\beta_a\omega_b{}^a)C_P{}^b+(\dot{\beta}_b+\gamma_b+\beta_a\kappa_b{}^a)C_S{}^b, \end{aligned}\quad (3.5)$$

if the coefficients γ_a and β_a are free of dynamical variables. The transformation generated by C will be invariant if and only if

$$\gamma_b+\dot{\beta}_b+\beta_a\kappa_b{}^a=0. \quad (3.6)$$

In that case, the functions ρ_a introduced in Eq. (3.2) come out to be

$$\rho_b=\dot{\gamma}_b+\beta_a\omega_b{}^a. \quad (3.7)$$

It should be noted that the generators (3.4) and (3.6) in general do not form a group: Each invariant transformation changes the form of the Hamiltonian in accordance with Eqs. (3.7) and (3.2). Once the form of the Hamiltonian has been changed, the relationship between primary and secondary constraints as well as the form of the Poisson bracket of the secondary constraints with the Hamiltonian (3.3) is modified. Accordingly, the precise form of the conditions (3.6) depends on the values of the coefficients ρ_a, which are changed by each invariant transformation. The group character can be established only if the form of the invariant generators is permitted to depend explicitly on the ρ_a. The details are of no importance for what follows and hence are omitted.

At any rate, all combinations of constraints not obeying the conditions (3.6) will generate noninvariant transformations, even though they are manifestly constants of the motion.

We shall now derive analogous results in the Lagrangian formalism. In configuration space, the primary constraints are identically zero and the secondary constraints are those linear combinations of the Euler equations that are free of second derivatives. Because of the assumed irregularity of the theory, the matrix L^{ij} is singular and possesses null vectors $u_{i(a)}(a=1\cdots n-r$, r is the rank of L^{ij}) such that $L^{ij}u_{j(a)}=0$. If we multiply the Euler equations by $u_{i(a)}$, we see that the acceleration terms drop out, and we are left with just the secondary constraints $C_{S(a)}=L^iu_{i(a)}$. By introducing a set of vectors $v_i^{(A)}$ $(A=1\cdots r)$, which are linearly independent of the $u_{i(a)}$ and of each other, we can construct linear combinations of field equations that *do* contain accelerations, $L^iv_i^{(A)}$. To study invariant transformations generated by the secondary constraints, we choose for the generator

$$C=\beta^aL^iu_{i(a)}\equiv\beta^aC_{S(a)}, \qquad (3.8)$$

and try to find solutions of Eq. (2.7) that satisfy Eq. (2.10). It must be remembered that to any solution of Eq. (2.7) we can add a linear combination of null vectors of L^{ij}. It is this addition of null vectors to $\bar{\delta}q_k$ that takes the place of the primary constraints in the Hamiltonian formalism. Substituting Eq. (3.8) into Eq. (2.7), we get

$$L^{ij}\bar{\delta}q_i=\beta^a\partial^{j\cdot}C_{S(a)}. \qquad (3.9)$$

We can obtain the most general solution of Eq. (3.9) by adding to a particular solution an arbitrary linear combination of the solutions of the homogeneous equation. We shall choose that particular solution which is a linear combination of the $v_i^{(A)}$. The most general solution will then have the form:

$$\bar{\delta}q_i=\beta^aM_{aA}v_i^{(A)}+\gamma^au_{i(a)}, \qquad (3.10)$$

where the coefficients M_{aA} are determined, but the γ^a are arbitrary. We now substitute Eqs. (3.10) and (3.8) into (2.10) and obtain

$$\beta^aM_{aA}L^iv_i^{(A)}+\gamma^aL^iu_{i(a)} +\dot{\beta}^aL^iu_{i(a)}+\beta^a\frac{d}{dt}(L^iu_{i(a)})=0. \qquad (3.11)$$

The assumption in the canonical formalism of no tertiary constraints is equivalent to the statement that the time derivatives of those Euler equations that are free of accelerations are equal to a linear combination of field equations,

$$\dot{C}_{S(a)}=w_{aA}L^iv_i^{(A)}+k_a{}^bL^iu_{i(b)}. \qquad (3.12)$$

We have decomposed the Euler equations into two parts, one free of accelerations, the other containing accelerations, by means of the $(n-r)$ null vectors u and the r vectors v. Now Eq. (3.11) can be written

$$\beta^aM_{aA}L^iv_i^{(A)}+\gamma^aL^iu_{i(a)}+\dot{\beta}^aL^iu_{i(a)} +\beta^aw_{aA}L^iv_i^{(A)}+\beta^ak_a{}^bL^iu_{i(b)}\equiv0. \qquad (3.13)$$

Since this equation must be satisfied identically, the coefficients of the second time derivatives must vanish. These derivatives appear only in the term $L^iv_i^{(A)}$. The coefficients of the remaining terms must also vanish. Hence

$$\gamma^a+\dot{\beta}^a+\beta^bk_b{}^a=0. \qquad (3.14)$$

It can now be seen that among the infinitely many solutions of Eq. (3.9) only one generates an invariant transformation.

Thereby we have demonstrated the contention advanced at the beginning of this section. In general, there is an infinity of transformations $\bar{\delta}q_k$ belonging to any one generator C. Two transformations belonging to the same generator ("the same" *modulo* the equations of motion) may differ from each other, both by an invariant transformation generated by secondary constraints and by an arbitrary (not invariant) combination of null vectors. In the next section, we shall find that by restricting ourselves to invariant transformations we may nevertheless define uniquely a commutator bracket between constants of the motion.

4. DIRAC BRACKET

We have found that in the Lagrangian formalism and in the presence of a "singular" Lagrangian, the relationship between infinitesimal transformations and generators is so tenuous that neither determines the other uniquely. Moreover, the generating functions themselves are not completely arbitrary functions of the q_k and $\dot{q}_k$ but are restricted by the requirement implied by Eq. (2.7):

$$\partial^{k\cdot}Cu_{k(a)}=0, \qquad (4.1)$$

where the $u_{k(a)}$ are the null vectors of L^{kl}. It is, therefore, not at all obvious that the commutators between infinitesimal canonical transformations should give rise to a commutator algebra among the generating dynamical variables that will provide a promising point of departure for the construction of commutation relations of quantum-theoretical observables. In this section we shall find that there exists a transformation group with the desired properties and that the resulting commutator brackets are equivalent to the generalized Dirac brackets.[7,9]

We shall begin with the canonical transformations in configuration space.[4] Let us consider two infinitesimal transformations $\bar{\delta}_1q_k$ and $\bar{\delta}_2q_k$, generated by the generators C_1 and C_2, respectively, and their commutator. Immediately we are confronted by the following difficulty: Eq. (2.7), which relates the generator and the transformation quantities, depends explicitly on the form of the Lagrangian or, at any rate, on the matrix

[9] P. G. Bergmann and I. Goldberg, Phys. Rev. 98, 531 (1955).

L^{kl}, which comprises the second derivatives of the Lagrangian with respect to the velocities. Inasmuch as the first of the two transformations will in general change the form of the Lagrangian and, by implication, the form of L^{kl}, we should have to make a decision as to whether in attempting to fix the "identity" of a given transformation we wish to consider the generator C or the transformation quantities $\bar{\delta}q_k$ as fixed functions of their arguments q_k, $\dot{q}_k$. If we fix the generators, the following difficulty arises: In the case of a "singular" Lagrangian, the generators must satisfy Eq. (4.1). Thus if L^{kl}, and with it the $u_{k(a)}$, change form after the first transformation, the second generator may no longer satisfy (4.1). If, instead, we propose to fix the $\bar{\delta}q_k$ as functions of their arguments, we may violate the integrability conditions implied by (2.7):

$$\partial^{l\cdot}(L^{km}\bar{\delta}q_m)-\partial^{k\cdot}(L^{lm}\bar{\delta}q_m)=0. \tag{4.2}$$

We conclude that it is impossible to define a group either on the basis of fixed (but arbitrary) transformation quantities $\bar{\delta}q_k$ or on the basis of fixed (arbitrary) generators $C(q_k,\dot{q}_k,t)$. We can construct a group if we allow both the generators and the transformation quantities to depend explicitly on the form of the Lagrangian; the generator of the commutator transformation may then be found as follows:

The commutator transformation may be written as

$$\bar{\delta}q_k=\bar{\delta}_2(\bar{\delta}_1q_k)-\bar{\delta}_1(\bar{\delta}_2q_k), \tag{4.3}$$

where

$$\bar{\delta}_2(\bar{\delta}_1q_k)=\partial^l(\bar{\delta}_1q_k)\bar{\delta}_2q_l+\partial^{l\cdot}(\bar{\delta}_1q_k)\bar{\delta}_2\dot{q}_l+\delta_2'(\bar{\delta}_1q_k), \tag{4.4}$$

where $\delta_2'(\bar{\delta}_1q_k)$ is the change in $\bar{\delta}_1q_k$ due to its dependence on the form of the Lagrangian. We must now find the generator C which corresponds to the transformation (4.3) according to Eq. (2.7). We see that we must calculate expressions of the form

$$L^{kl}\bar{\delta}_2(\bar{\delta}_1q_l)=\bar{\delta}_2(\partial^{k\cdot}C_1)-\bar{\delta}_2L^{kl}\bar{\delta}_1q_l, \tag{4.5}$$

where we have made use of (2.7). The first term on the right-hand side of (4.5) may be written as

$$\bar{\delta}_2(\partial^{k\cdot}C_1)=\partial^{k\cdot}(\bar{\delta}_2C_1)-\partial^lC_1\partial^{k\cdot}(\bar{\delta}_2q_l)-\partial^{l\cdot}C_1\partial^{k\cdot}(\bar{\delta}_2\dot{q}_l), \tag{4.6}$$

where

$$\bar{\delta}_2C_1=\partial^lC_1\bar{\delta}_2q_l+\partial^{l\cdot}C_1\bar{\delta}_2\dot{q}_l+\delta_2'C_1. \tag{4.7}$$

The term $\delta_2'C_1$ arises because of the explicit dependence of C_1 on the form of the Lagrangian. Similarly, the second term on the right-hand side of (4.5) may be rewritten by using

$$\bar{\delta}_2L^{kl}=\partial^{k\cdot}(\bar{\delta}_2p^l)-\partial^m\partial^{l\cdot}L\partial^{k\cdot}(\bar{\delta}_2q_m)-L^{lm}\partial^{k\cdot}(\bar{\delta}_2\dot{q}_m), \tag{4.8}$$

where p^l is short for $\partial^{l\cdot}L$ and $\bar{\delta}_2p^l$ is given by

$$\bar{\delta}_2p^l=\partial^m\partial^{l\cdot}L\bar{\delta}_2q_m+L^{lm}\bar{\delta}_2\dot{q}_m+\partial^{l\cdot}(\delta_2'L). \tag{4.9}$$

We eliminate ∂^lC_1 from the second term on the right-hand side of (4.6) by using the following equation, obtained by differentiating Eq. (2.10):

$$\partial^{k\cdot}(\delta'L)=(\partial^k\partial^{l\cdot}L-\partial^l\partial^{k\cdot}L)\bar{\delta}q_l-\partial^kC-L^{kl}\bar{\delta}\dot{q}_l-L^l\partial^{k\cdot}(\bar{\delta}q_l). \tag{4.10}$$

In this manner, after antisymmetrizing (4.5) with respect to 1 and 2, we finally obtain for the commutator the expression

$$L^{kl}\bar{\delta}q_l=\partial^{k\cdot}(\bar{\delta}_2C_1-\bar{\delta}_1C_2-\bar{\delta}_2p^l\bar{\delta}_1q_l+\bar{\delta}_1p^l\bar{\delta}_2q_l)+L^m(\partial^{l\cdot}\bar{\delta}_1q_m\partial^{k\cdot}\bar{\delta}_2q_l-\partial^{l\cdot}\bar{\delta}_2q_m\partial^{k\cdot}\bar{\delta}_1q_l). \tag{4.11}$$

We thus see that, *modulo* the equations of motion, the generator of the commutator is

$$C=\bar{\delta}_2C_1-\bar{\delta}_1C_2-\bar{\delta}_2p^l\bar{\delta}_1q_l+\bar{\delta}_1p^l\bar{\delta}_2q_l. \tag{4.12}$$

This transformation group is much larger than the usual group of generators in the Hamiltonian formalism, because of the great freedom in the choice of the dependence of the generators on the form of the Lagrangian. A similar and equally large transformation group may be constructed in the Hamiltonian formalism if we permit the generators to be functions of the canonical variables and also to depend in some manner on the form of the Hamiltonian. In phase space, of course, there is no need for these more general transformations, since the canonical transformation equations do not involve the Hamiltonian; whereas in the Lagrangian formalism these transformations arise naturally owing to the form of the transformation Eq. (2.7).

We note from Eqs. (4.7) and (4.12) that the generator of the commutator transformation contains the expressions $\delta_1'C_2$ and $\delta_2'C_1$ explicitly. The implied dependence of the generators on the form of the Lagrangian is almost arbitrary, restricted only, in the case of "singular" Lagrangians, by Eq. (4.1). Since this group which we have constructed has very little structural similarity with the group of canonical (or Dirac bracket) transformations usually introduced in phase space, its Lie algebra can hardly be considered a suitable starting point for quantization.

However, this large group contains a subgroup that has the right size. We need not consider the dependence of the generators on the explicit form of the Lagrangian if we restrict ourselves to transformations that leave the form of the Lagrangian unchanged, i.e., to invariant transformations. In this case the generators may be considered as fixed functions of the q_k, $\dot{q}_k$, and t, and the resulting infinitesimal transformations will still form a group. We may then define commutator brackets between the constants of motion that occur as generators within this group. For "regular" Lagrangians, to any dynamical variable, including the q_k and the $\dot{q}_k$, one can find a constant of the motion that assumes the value of that dynamical variable at some fixed time t_0. For "singular" Lagrangians, the same holds at least for all those dynamical variables which possess a meaning that is invariant under the "gauge" transformations of the theory (e.g., the gauge transformations in electromagnetic theory or the coordinate transformations in general relativity).

The commutator in the invariant subgroup is constructed in the same way as in the large group, and again the generator is given by (4.12), where now, however, the quantities $\bar{\delta}_1 C_2$, $\bar{\delta}_2 C_1$, $\bar{\delta}_2 p^k$, and $\bar{\delta}_1 p^k$ do not depend on the form of the Lagrangian. That is, instead of the set of Eqs. (4.7), (4.9), and (4.12), we have

$$C=\bar{\delta}_2 C_1-\bar{\delta}_1 C_2-\bar{\delta}_2 p^k \bar{\delta}_1 q_k+\bar{\delta}_1 p^k \bar{\delta}_2 q_k, \quad (4.13a)$$

where

$$\bar{\delta}_2 C_1=\partial^l C_1 \bar{\delta}_2 q_l+\partial^{l\cdot} C_1 \bar{\delta}_2 \dot{q}_l \quad (4.13b)$$

and

$$\bar{\delta}_2 p^l=\partial^m \partial^{l\cdot} L \bar{\delta}_2 q_m+L^{lm} \bar{\delta}_2 \dot{q}_m. \quad (4.13c)$$

Let us introduce the notation $\{C_1,C_2\}$ for the commutator (4.13).

For the bracket (4.13) to be useful, it must be a unique function of the two commuting generators C_1 and C_2. This property is not trivial but must be demonstrated, because the generators do not determine the infinitesimal transformations uniquely. In particular we must be able to show that the bracket of two generators is not changed if we add to one of them an expression that vanishes *modulo* the equations of motion, e.g., a secondary constraint. Our method of proof is based on the fact that the bracket (4.13) is not only a commutator but also represents the transformation law for the dynamical variable C_1 under any transformation generated by C_2. In other words, though in general more than one transformation is connected with the same generator C_2, the transformation law for C_1 (assumed to be the generator of invariant transformations, though not necessarily only of invariant transformations) is the same under all the invariant transformations generated by C_2. Once we have proven this assertion, the uniqueness of the bracket (4.13) follows as a matter of course.

Let us consider a Lagrangian, $L(q_j,\dot{q}_j)$, and let us assume that there are p constraints. We shall label the constants of the motion C_ν but use italic subscripts (C_a) to denote constraints. We denote by $\bar{\delta}_\lambda C_\nu$ the change produced in C_ν by the transformation generated by C_λ.

We first form $\bar{\delta}_\lambda C_\nu$:

$$\begin{aligned}\bar{\delta}_\lambda C_\nu&=\partial^j C_\nu \bar{\delta}_\lambda q_j+\partial^{j\cdot} C_\nu \bar{\delta}_\lambda \dot{q}_j\\&=\partial^j C_\nu \bar{\delta}_\lambda q_j+L^{jk} \bar{\delta}_\nu q_k \bar{\delta}_\lambda \dot{q}_j.\end{aligned} \quad (4.14)$$

The last term has been rewritten with the aid of Eq. (2.7). Using Eq. (4.10) for $L^{ij}\bar{\delta}_\lambda \dot{q}_i$, we obtain

$$\begin{aligned}\bar{\delta}_\lambda C_\nu=&\partial^j C_\nu \bar{\delta}_\lambda q_j-\partial^j C_\lambda \bar{\delta}_\nu q_j\\&+\partial^j \partial^{k\cdot} L(\bar{\delta}_\lambda q_k \bar{\delta}_\nu q_j-\bar{\delta}_\nu q_k \bar{\delta}_\lambda q_j)=\{C_\nu,C_\lambda\},\end{aligned} \quad (4.15)$$

the bracket defined by Eq. (4.13). This relationship holds only modulo the equations of motion since Eq. (4.10) is only valid under this restriction. However, this remark does not render Eq. (4.15) useless; the commutator (4.13) itself is defined only *modulo* the equations of motion.

Equations (4.14) and (4.15) prove that the bracket (4.13) represents the transformation law of the generator of invariant transformations. We now consider the manner in which the constraints are affected by transformations generated by constants of the motion. Constraints occur in a theory by virtue of the form of the Lagrangian, the primary constraints due to its dependence on the $\dot{q}_j$, and the secondary constraints as a consequence of the equations of motion. Therefore, since the transformations affect neither the dependence of L on the $\dot{q}_j$ nor the form of the equations of motion, they do not change the form of the constraints.

Then:

$$\begin{aligned}\bar{\delta}_\nu C_a&=0,\\\{C_a,C_\nu\}&=0.\end{aligned} \quad (4.16)$$

The second of these expressions holds *modulo* the field equations, and demonstrates that the transformations generated by the constraints form an invariant subgroup. Thus we find that the commutators (4.13) possess all the properties of the generalized Dirac brackets,[7,9] and we may use them to define commutators for the true observables of a quantum theory.

5. CONCLUSION

According to our results, the Lagrangian formalism of a theory based on a Hamiltonian principle contains within itself the possibility for constructing a commutator algebra that is equivalent to the one usually based on the Hamiltonian formalism. True, we must restrict ourselves to invariant transformations and, by implication, to the commutators between constants of the motion. However, this restriction is implicit also in conventional theories considering commutators between observables at different times.

Wherever a theory will permit the construction of a Hamiltonian formalism, Lagrangian quantization appears to offer no possibilities that are not also open within the Hamiltonian quantization. It is conceivable, though, that Lagrangian quantization offers an approach to some types of theories, such as nonlocal theories, for which a Hamiltonian formulation is not known or appears artificial.

As for quantization itself, the Lagrangian formulation of commutators also appears to offer a new possibility. In the past, the action principle seemed to embody a dynamical law primarily through the variational principle; the transfer of the variational principle to a q-number action is, however, beset with serious difficulties, which in our opinion have not yet been fully resolved. Through the consideration of invariant transformations, on the other hand, we may construct a complete set of constants of the motion; such a set is equivalent to the differential equations of motion. It appears not unreasonable that the formulation of the dynamical laws through a complete set of constants of the motion is more nearly germane to quantum theory than the formulation through the Euler-Lagrange equations. We propose to follow up this conjecture in subsequent papers.