# **Extension of the Dirac-Bergmann theory of constrained systems**

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According to Dirac's and Bergmann's physical ideas, we derive the expression of the finite Dirac contact transformation, propose an extended Dirac conjecture, extend Dirac's original consistency conditions, and obtain the correct definition of physical observables as well as more universal gauge conditions in general singular Lagrangian systems. The difficulties in Cawley's first and second counterexamples of Dirac's conjecture are overcome. Our results are applicable to Hamiltonization of systems with Hessian variable rank and systems with the proper subalgebra of the minimum evolution closed Poisson bracket of first-class constraints, and so provide a correct tool for quantization of these systems.  $[$1050-2947(96)03306-9]$ 

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### **I. INTRODUCTION**

Since Dirac  $[1]$  proposed the algorithm of generation and treatment with constraints and Bergmann and co-workers  $[2]$ clarified the relation between constraints and invariance, the foundation of the dynamics and quantization of constrained systems has been built. The original motivation of their formalism of constrained Hamiltonian dynamics, and also the dynamics of singular Lagrangian systems, was to develop powerful methods that would allow one to put generally covariant or gauge-invariant field theories into canonical form, that is, so-called Hamiltonization  $[1,2]$ . The methods also have been effectively used for a variety of physical systems, often with a finite number of degrees  $[3,4]$ . In particular, Dirac's algorithm was successfully applied to the quantization of the gauge field by Faddeev and Popov  $[5]$  along with the path integral formalism, and was also developed by Batalin, Fradkin, and Vilkovisky along with the Hamiltonian formalism  $[6]$ . Recently, a revival of interest in the theory of constrained systems arose with the superparticle, superstring, and low dimensional physical systems, for example, chiral scalar and two-dimensional gravity  $[7-10]$ ; thereby this theory plays an important role in theoretical physics. In fact, not only is it widely used in various theories with invariance but also its development has become an important elementary subject. There exist a number of excellent reviews  $[3,4,11-15]$  which reflect the present status and methods for dynamics and quantization problems of constrained systems. In a word, the theories of the dynamics and quantization of constrained systems have had a great success and are in a new period of development.

Notwithstanding all these results, there are still some aspects which have not been sufficiently developed and some problems which have not been completely understood. In the classical theory  $[4,16]$ , for some kinds of singular Lagrangian systems whose gauge generators do not exhaust all of the first-class constraints or whose Hessian matrix has varying rank  $[16–19]$ , the Dirac and Bergmann method seems not to work. One is short of a universal algorithm to correctly Hamiltonize such constrained systems. The famous open problem as to whether "Dirac's conjecture" [1], i.e., *that all the secondary first-class constraints were also generators of gauge transformations*, was true still remains. Hence, in order to develop the general theory of the singular Lagrangian and Hamiltonian constraints for general models, a full understanding is necessary of all the ''pathological examples''  $[17–20]$  (always including linear or nonlinear Lagrangian multipliers and often with a Hessian variable rank). Particularly intriguing for us is the cases related with gauge conditions  $[21,22]$ , that is, that the number of gauge conditions or gauge degrees of freedom is not always the same as the number of all the first-class constraints in some general singular Lagrangian systems. This implies that the quantization of these kinds of gauge theories needs restudying on a new footing. Similarly, in quantization of the gauge theories corresponding to the above problems in classical theories, there also exist difficulties  $[15]$ . Some other unsolved and knotty problems in the theory of constrained systems originate from locality and geometry in field theory  $[23]$ , or are connected with the anomalies and their topological aspects  $[24–26]$ .

Faced with one after another difficulty in the Dirac-Bergmann algorithm, a variety of suggestions have been proposed. The recent development is given by Lusanna  $[15]$ , in which he describes and reviews some suggestions. It seems to us that the failure of the Dirac-Bergmann algorithm is not in its physical ideas. But this algorithm does omit some complex situations such as singular systems with the subalgebra of the minimum evolution closed Poisson bracket (MECPB, which is defined in our paper  $[22]$ ; also see Sec. III A) of the first-class constraints, and with Hessian variable rank  $[18]$ . Moreover, this algorithm also has some incomplete proofs and calculations. As a matter of fact, our above views can be supported by analyzing briefly the following three aspects.

First, Dirac and Bergmann thought that the different evolution trajectories with distinct Lagrangian multipliers are equivalent in physical content and they can be transformed into each other by Dirac's contact or gauge transformation. It

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results that the secondary first-class constraints have an obvious contribution in evolution of the system, which implies that the total Hamiltonian can be generalized to the extended Hamiltonian. This is correct. However, Dirac did not obtain the finite expression of his contact transformation but conjectured that all the secondary first-class constraints are generators  $[1]$ . It has been seen that for some examples, Dirac's conjecture seems not to work [17]. Second, Dirac supposed the constrained hypersurface is stable so as to guarantee the full determination of Hamiltonian dynamics in the singular systems. This is natural. But he did not notice that there exists a kind of singular system with Hessian variable rank. For these systems, all the secondary constraints cannot, in general, be fully generated by his original consistency conditions  $[18]$ . Finally, Bergmann pointed out that the physical observables, or gauge invariant quantities, are determined completely by dynamics and initial conditions, in other words, are free of the arbitrary Lagrangian multipliers. This is elementary. Yet the fact is that one does not derive the general and obvious evolution expression of the function on phase space and then does not obtain the correct definition of the physical observable and the universal gauge conditions  $|22|$ .

Therefore, in this paper, our aim is to overcome and solve the difficulties and problems in Hamiltonization, Dirac's conjecture, and the gauge conditions according to Dirac's and Bergmann's physical ideas. This paper is arranged as follows.

In Sec. II, we first recall briefly the Dirac-Bergmann algorithm and then introduce Cawley's two famous counterexamples to Dirac's conjecture. Meanwhile, we express our motivation and aim to overcome the difficulties existing in the two examples.

In Sec. III, we generally discuss the difficulties existing in Dirac and Bergmann's algorithm. Then we point out some causes leading to their appearance and give some notions and formulas used in this paper.

In Sec. IV, after introducing the time translation operator of the constrained system and the calculation technology of the (multi-)Poisson bracket, we derive the obvious expression of the finite Dirac contact transformation and its generators. Moreover, we find, in general, that the generators do not always exhaust all the first-class constraints, but invariably they involve at least all the primary first-class constraints. In other words, the generators have weakly vanishing Poisson brackets not only between themselves but also between them and the total Hamiltonian. Normally, they form a subalgebra of the MECPB of the first-class constraints. This concept was introduced in our paper  $[22]$  and its details can be seen in Sec. III. In order to determine the generalized Hamiltonian, an extended Dirac conjecture is proposed, and it is successfully applied to Cawley's first counterexample to Dirac's conjecture. We conclude that the finite Dirac contact transformation does not change the physical observables and their motions, and that the generators of this finite transformation take the constraints of subalgebra of the MECPB of the first-class constraints, so that the extended Dirac conjecture is reasonably verified. Only if the MECPB takes over all the first-class constraints does it return to the usual Dirac conjecture.

In Sec. V, it is found that in general singular Lagrangian

systems Dirac's original consistency conditions are not enough to generate all secondary constraints and determine all the arbitrary multipliers in front of the second-class constraints. This may lead to the result that the equivalence of Lagrangian and Hamiltonian formalisms is not guaranteed and even the dynamics of the Hamiltonian formalism is not completely determined. In order to overcome the above difficulties and Hamiltonize the general singular Lagrangian system with variable Hessian rank, we propose an extension of Dirac's algorithm of the consistency conditions. In terms of this algorithm of extended consistency conditions, all of the secondary constraints can be generated fully and then the final total Hamiltonian can be obtained correctly. Moreover, the generalized Hamiltonian ought to be constructed by our extended Dirac conjecture. In particular, the algorithm is applicable to Hamiltonization of some more general singular systems with Hessian variable rank. As an application, we study successfully Cawley's second example. For the general cases, we reveal our algorithm in detail and study the validity, application, and presupposition of our algorithm. It is shown that our algorithm connects closely with the Sudarshan-Mukunda (S-M) Lagrangian approach dealing with the constrained system with Hessian variable rank and is a development of S-M's approach along with Hamiltonian formalism.

In Sec. VI, according to Bergmann's physical supplementary conditions, we found that the accustomed conclusion that the number of gauge conditions or gauge degrees of freedom is always equal to the number of all the first-class constraints is not universal in general singular systems. It is shown that the corrected form of physical supplementary conditions is that the physical observables have weakly vanishing Poisson brackets with the elements of the subalgbra of the MECPB of the first-class constraints and also with all of the second-class constraints. A simple Cawley's example is studied. The origin of the gauge conditions is discussed, and the corrected forms and number of the gauge conditions in some general singular Lagrangian systems are given. Our results provide a tool for the quantization of this kind of gauge theories.

In Sec. VII, we summarize our main results, point out some knotty problems, and give the conclusions of this paper. In addition, some details of the derivation and proof of the formulas used in this paper are given in the Appendixes.

## **II. THE DIRAC-BERGMANN ALGORITHM AND CAWLEY'S COUNTEREXAMPLES**

Gauge theories belong to the class of so-called singular Lagrangian theories, which are also theories with constraints. The standard Hamiltonization and quantization methods cannot be directly applied to these theories. In their well-known works [1,2], Dirac and Bergmann gave such an algorithm that one can generate constraints by Dirac's consistency conditions and can construct the extended Hamiltonian by Dirac's conjecture. Although the Dirac-Bergmann algorithm has been successful in many physical systems, it also faces some serious difficulties since Cawley and Frenkel *et al.* proposed several counterexamples  $[17,18]$ . In order to propose our extension of the Dirac-Bergmann theory of constrained systems, it is worth recalling and commenting on their algorithm of constrained dynamics. Meanwhile, we also will review Cawley's two counterexamples so that we can solve their difficulties in the following work.

#### **A. Dirac-Bergmann dynamics of constrained systems**

For a singular system, the rank *r* of its Hessian  $n \times n$ matrix  $[4,16]$ 

$$
W_{ij} \equiv \left\| \partial^2 L(q, \dot{q}) / \partial \dot{q}^i \partial \dot{q}^j \right\| \quad (i, j = 1, \dots, n) \quad (2.1)
$$

is less than *n*. Here  $L(q, \dot{q})$  is Lagrangian in the system. It is always possible to number the coordinates in such a way that in the Hessian matrix *W* the minor of maximum rank *r* is placed in the left corner and consequently

$$
\det \left\|\partial^2 L(q,\dot{q})/\partial \dot{q}^\sigma \partial \dot{q}^\rho\right\| \neq 0 \quad (\sigma,\rho=1,\ldots,r). \tag{2.2}
$$

The other velocities are denoted by  $\dot{q}^A$  and are called the primarily unexpressible velocities  $(A = r + 1, \ldots, n)$  [13]. In Hamiltonian formalism,  $\dot{q}^A$  is replaced by the arbitrary multiplier  $v_A$  which is a function of time. From the definition of canonical momenta

$$
p_{\sigma} \equiv \partial L / \partial \dot{q}^{\sigma} = p_{\sigma}(q, \dot{q}) \tag{2.3}
$$

it is clear that  $dp_{\sigma} = W_{\sigma\rho} dq^{\rho} + (\partial^2 L/\partial \dot{q}^{\sigma} \partial \dot{q}^A) d\dot{q}^A$  $+(\partial^2 L/\partial \dot{q}^\sigma \partial q^i) dq^i$ . Thus it follows from the theorem on implicit functions and Eq.  $(2.2)$  that

$$
\dot{q}^{\sigma} = f^{\sigma}(q, p_{\rho}, \dot{q}^A). \tag{2.4}
$$

 $\dot{q}^{\sigma}$  is called the primarily expressible velocity. One can verify that

$$
p_A = \partial L / \partial \dot{q}^A = \psi_A(q, p_\sigma) \tag{2.5}
$$

and then  $n-r$  primary constraints are expressed as

$$
\phi_A = p_A - \psi_A(q, p_\sigma). \tag{2.6}
$$

So the primary constraints are functions of the variables on phase space. Introducing the Hamiltonian

$$
H = p_{\sigma} \dot{q}^{\sigma} + \psi_A \dot{q}^A - L(q, \dot{q}), \qquad (2.7)
$$

one knows that *H* is only a function of  $q^i$  and  $p_\sigma$ . Making use of the Euler-Lagrange equation one can prove  $[16]$  that the motion equations of *g*, which is a function on phase space, are given by

$$
\dot{g} \approx \{g, H_T\} \tag{2.8}
$$

where  $H_T$  is called the original total Hamiltonian and its definition is

$$
H_T = H + u_A \phi_A \,. \tag{2.9}
$$

Notice that in (2.8) Dirac's symbol of weak equality " $\approx$ " has been used. Following Dirac, the constraints have to preserve an evolution weakly vanishing in time. In other words, the arbitrary order of time derivatives of the constraints should be weakly equal to zero. In terms of this requirement, which is called *the consistency condition*, one can generate the secondary constraints  $\chi_k$  step by step. Therefore Dirac's consistency conditions can be generally expressed as

$$
\{\phi_A, H\} + u_B\{\phi_A, \phi_B\} \approx 0, \quad \{\chi_k, H\} + u_B\{\chi_k, \phi_B\} \approx 0, \tag{2.10}
$$

that is, the Poisson brackets between  $H<sub>T</sub>$  with all constraints are weakly equal to zero. More generally the functions with the above property such as  $H_T$  are called the first-class ones. Otherwise they are called the second-class ones. Dirac has shown that Poisson brackets between two first-class functions are still first class.

Suppose the rank of the coefficient matrix for the unknown multipliers  $u_B$  in (2.10) is *R*. It is always possible to choose the  $n-r-R$  linear combinations of the  $n-r$  primary constraints (Appendix A) in the following way:

$$
\psi_{\alpha} = \xi_{\alpha}^{A} \phi_{A} , \qquad (2.11)
$$

so that they have weakly vanishing Poisson brackets with all the constraints [1,4,16]. Hence  $\phi_{\alpha}$  is called the first-class primary constraint. After dividing all the constraints into the first- and second-class ones, one can rewrite the original total Hamiltonian as its Dirac form,

$$
H^D_T \simeq H^* + u_\alpha \phi_\alpha, \tag{2.12}
$$

where  $u_{\alpha}$  are arbitrary multipliers and  $\phi_{\alpha}$  are the primary first-class constraints, while *H*\*, which is called the firstclass partner of the Hamiltonian, is an evident form of Dirac's first-class Hamiltonian and is defined as

$$
H^* = H - \Omega_s C_{ss'} \{ \Omega_{s'}, H \}. \tag{2.13}
$$

Here  $\Omega_s$  takes over all the second-class constraints.  $C_{ss}$  is the inverse of Dirac's matrix of the second-class constraints, that is,  $C_{ss'}\{\Omega_{s'},\Omega_{s''}\} = \delta_{ss''}$  [1]. In addition, the symbol  $\cdot \cdot \approx \cdot$  in Eq. (2.12) denotes strong equality [16] (Appendix A). In fact, the canonical equations of motion generated are invariant in the weak equality sense when the total Hamiltonian gains or loses a strongly vanishing term. The reason for this is that the Poisson bracket between strongly vanishing terms with a differentiable function on a constrained submanifold is weakly equal to zero.

It is necessary to emphasize that no linear combination of the first-class secondary constraints, which can be denoted by  $\chi_a$ , with the arbitrary multiplier appears in the definition  $(2.12)$  of  $H_T^D$ . So Dirac analyzed the infinitesimal contact transformation from his requirement that the physical states should not depend on arbitrary functions. Then he conjectured that all the first-class constraints, including secondary ones, were the generators of the contact transformation, which did not change the physical states. This means that Dirac's total Hamiltonian is extended as  $[1,4]$ 

$$
H_E = H_T^D + u_a \chi_a = H^* + u_m \phi_m \tag{2.14}
$$

where  $\phi_m = (\phi_\alpha, \chi_a)$ , that is, they take over all the first-class constraints, and  $u_m$  are arbitrary multipliers. It is customary that  $H<sub>E</sub>$  is called the extended Hamiltonian, while the motion equation is given by

$$
\dot{g} \approx \{g, H_E\}.\tag{2.15}
$$

This is just the famous Dirac conjecture.

### **B. Cawley's first example**

Cawley [17] gave his first counterexample of Dirac's conjecture whose Lagrangian is written as

$$
L = \dot{x}\dot{z} + yz^2/2.
$$
 (2.16)

One readily obtains the Euler-Lagrange equations

$$
\ddot{z}=0, \quad z^2/2=0, \quad \ddot{x}=yz.
$$
 (2.17)

From Dirac's algorithm it follows that the primary constraint is

$$
p_y \approx 0. \tag{2.18}
$$

It is straightforward to derive the secondary constraints

$$
z^2/2 \approx 0
$$
,  $p_x z \approx 0$ ,  $p_x^2 \approx 0$ . (2.19)

They can be rewritten as the canonical or linear and functionally independent forms

$$
z \approx 0, \quad p_x \approx 0. \tag{2.20}
$$

Thus, since  $z^2 \approx 0$  (" $\approx$ " means strong equality, see [16]), one can obtain Dirac's total Hamiltonian

$$
H_T^D \simeq p_x p_z + v p_y. \tag{2.21}
$$

From the original Dirac conjecture it follows that the extended Hamiltonian is

$$
H_E = up_x + vp_y + wz. \tag{2.22}
$$

Obviously it generates the following motion equations:

$$
\dot{x} \approx u, \quad \dot{y} \approx v, \quad \dot{z} \approx 0,
$$
\n(2.23a)

$$
\dot{p}_x \approx 0, \quad \dot{p}_y \approx 0, \quad \dot{p}_z \approx -w. \tag{2.23b}
$$

They mean that *x*, *y*, and  $p_z$  are all gauge degrees of freedom. However, *x* is originally physical, viz., *x* has a determined motion free of the arbitrary multiplier  $v$ . Even if we fix the gauge, this system becomes static and does not return to the original physical motion. Consequently, applying Dirac's conjecture to Cawley's counterexample will lead to a change of the physical content of the theory. The result implies that in order to Hamiltonize this kind of singular system, one has to extend or revise the original Dirac conjecture.

#### **C. Cawley's second example**

Let us consider the Lagrangian

$$
L = \dot{x}\dot{z}^2 + yz.\tag{2.24}
$$

It is the Lagrangian of Cawley's second counterexample to Dirac's conjecture [18]. Its Euler-Lagrange equations are

$$
\frac{d}{dt}(\dot{z}^2) = 0, \quad z = 0, \quad \frac{d}{dt}(2\dot{x}\dot{z}) - y = 0.
$$
 (2.25)

Following Sudarshan and Mukunda [16], one has Lagrangian constraints

$$
y=0
$$
,  $y=0$ ,  $z=0$ ,  $\dot{z}=0$ . (2.26)

Defining conjugate momenta

$$
p_x = \dot{z}^2
$$
,  $p_y = 0$ ,  $p_z = 2\dot{x}\dot{z}$ , (2.27)

we have a primary constraint

$$
p_y \approx 0 \tag{2.28}
$$

where Dirac's symbol of weak equality  $[1]$  has been used. The original total Hamiltonian of this example can be written as

$$
H_T = p_x^{1/2} p_z - yz + v p_y, \t\t(2.29)
$$

where  $\nu$  is thought of as a differentiable function on a constrained submanifold. Usually, one uses Dirac's original consistency conditions to generate the secondary constraints  $[1]$ , that is, one requires that the evolution in time of the constraints must be weakly vanishing. In other words, the constraints are preserved in time or the arbitrary-order time derivatives of the constraint equations are still the constraint equations. Consequently, it is straightforwardly derived that there are two secondary constraints,

$$
z \approx 0, \quad p_x \approx 0. \tag{2.30}
$$

Here we have written them in linear form as in Ref.  $[18]$ . The Dirac's algorithm for generation of constraints has ended. There are no more constraints. Now, the set of constraints consists of three constraints  $(2.28)$  and  $(2.30)$ . They determine a Dirac constrained hypersurface  $\Gamma_C^D$ .

Because the constraints in Dirac's algorithm are all first class and the multiplier  $\nu$  is undetermined, the original total Hamiltonian shows, in form, no difference from Dirac's total Hamiltonian

$$
H_T^D = H_T = p_x^{1/2} p_z - yz + vp_y. \tag{2.31}
$$

It follows from it that the canonical motion equations are

$$
\dot{x} \approx p_z/2p_x^{1/2}, \quad \dot{y} \approx v, \quad \dot{z} \approx p_x^{1/2},
$$
 (2.32a)

$$
\dot{p}_x \approx 0, \quad \dot{p}_y \approx z, \quad \dot{p}_z \approx y. \tag{2.32b}
$$

Obviously, they are not equivalent to the original Euler-Lagrange  $(E-L)$  motion equations  $(2.25)$  because the motion in the *x* direction is infinite and the motion in the *y* direction is arbitrary. Thus Dirac's original algorithm gives rise to difficulty. Moreover, Dirac's conjecture proposed by this algorithm also has the same problem, that is, the canonical equations of motion generated by Dirac's extended Hamiltonian

$$
H_E = p_x^{1/2} p_z + u p_x + v p_y + wz \tag{2.33}
$$

are not consistent with the original E-L equations. The reason for this, in our opinion, is that the constraint  $y \approx 0$  and the multiplier  $v = y \approx 0$  are not able to be obtained in terms of Dirac's original consistency conditions. Consequently, the equivalence of the Lagrangian and Hamiltonian formalisms in the physical content is broken. This led us to reconsider an algorithm of Hamiltonization that can be used for the kind of singular systems with Hessian variable rank.

## **III. THE DIFFICULTIES IN THE DIRAC-BERGMANN ALGORITHM**

From the preceding section, we have seen the difficulties in Dirac's original Hamiltonization algorithm by discussing Cawley's first and second examples. For the more general case, we know, in singular systems, that there are mainly two kinds of counterexamples to the Dirac-Bergmann algorithm. One kind is represented by Cawley's first example and it has the feature of the MECPB, that is, there exists a proper subalgebra of the minimum evolution closed Poisson bracket of the first-class constraints within it. Another is represented by Cawley's second example and it has the feature of Hessian variable rank.

### **A. Singular systems with proper subalgebra of the MECPB of first-class constraints**

In order to study the difficulties in the singular systems with proper subalgebra of the MECPB of the first-class constraints, we need to derive the general expression of the evolution in time of the function in phase space. For convenience, let us denote 2*n* phase space variables as  $\eta^{\mu}, \mu = 1,2, \ldots, 2n$ . They are  $q^{i}$  for  $\mu = 1,2, \ldots, n$ ; and  $p_i = \eta^{\mu-n}$  for  $\mu \geq n+1$ . Defining the 2*n*-dimension antisymmetric tensor  $\epsilon^{\mu\nu}$  in the form

$$
\epsilon^{\mu\nu} = \begin{cases}\n0 & \text{if } \mu, \nu \le n \text{ or } \mu, \nu \ge n \\
1 & \text{if } \mu \le n \text{ and } \nu = \mu + n \\
-1 & \text{if } \nu \le n \text{ and } \mu = \nu + n\n\end{cases}
$$
\n(3.1)

and introducing the linear operator *D* which is the Hamiltonian vector field  $[27-30]$ ,

$$
D_f \equiv \epsilon^{\mu\nu} \frac{\partial f}{\partial \eta^{\mu}} \frac{\partial}{\partial \eta^{\nu}} \equiv \frac{\partial f}{\partial q^i} \frac{\partial}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial}{\partial q^i},
$$
(3.2)

we have the Poisson bracket expressed as the operator form  $[31,32]$ 

$$
\{f, g\} = D_f g = -D_g f. \tag{3.3}
$$

Moreover, the multiple Poisson bracket can be expressed as the product of *D* operators

$$
\{f_1, \{f_2, g\}\} = D_{f_1} D_{f_2} g. \tag{3.4}
$$

We can easily verify that the *D* operator has the following properties:

$$
[D_f, D_g] \equiv D_f D_g - D_g D_f = D_{\{f,g\}},\tag{3.5}
$$

$$
D_f^n D_g = \sum_{m=0}^n C_n^m D_{D_f^{n-m}g} D_f^m, \qquad (3.6a)
$$

$$
D_f D_g^n = \sum_{m=0}^n (-1)^m C_n^m D_g^{n-m} D_{D_g^m f},
$$
 (3.6b)

where  $C_n^m$  is the biterm coefficient. The first property of *D*, Eq.  $(3.5)$ , can be called the commutation theorem. It can be shown in terms of the Jacobi identity of the Poisson bracket. The second property of  $D$ , Eq.  $(3.6)$ , can be named the exchange theorem. It is a conclusion of the commutation theorem and can be verified by virtue of the mathematical inductive method (see Appendix B).

By making use of the *D* operator, we obtain the general and explicit expression of the evolution of  $g$  in time (see Appendix C:

$$
g(\eta(t)) \approx e^{-(t-t_0)D_{H^*}(t_0)} g(\eta(t_0))
$$
  
+ 
$$
\sum_{n=1}^{\infty} \frac{1}{n!} (t-t_0)^n \sum_{m=1}^n \sum_{\alpha_1, \alpha_2, \dots, \alpha_m=1}^K
$$
  

$$
\times \left( \prod_{j=1}^m \sum_{k_j=m-j}^{n_{j-1}-1} \sum_{n_j=m-j}^{k_j} (-)^{n_{j-1}-k_j} \right)
$$
  

$$
\times C_{k_j}^{n_j} v_{\alpha_j}^{(n_j-k_j)}(t_0)
$$
  

$$
\times \left\{ (-)^{n_m} D_{H^*}^{n_m} \left( \prod_{s=0}^{m-1} D_{\phi_{\alpha_{m-s}}} D_{H^*}^{n_{m-s-1}-k_{m-s}-1} \right) \right\}
$$
  

$$
\times g(\eta(t)) \Biggr\}_{t=t_0}, \qquad (3.7)
$$

where we have used the consistency condition  $\lfloor 1 \rfloor$  ${H}_T^D, \psi_j$   $\approx$  0, that is, the total Hamiltonian has weakly vanishing Poisson brackets with all of the constraints  $\{\psi_i\}$ . We also assumed that the constraints do not have explicit time dependence and *K* is the number of primary first-class constraints. In addition, in Eq.  $(3.7)$ , we use the notation  $C_0^0 = 1$ ,  $d^0f/dt^0 = f$ ,  $v_\alpha^{(k)} = d^k v_\alpha/dt^k$ , and  $n_0 = n, n_m = 1$ .

Now, we want to know which constraints have contributions to the evolution of *g* in time. It is easy to see that by virtue of the property of the *D* operator the terms related to constraints can be written as

$$
D_{H^{*}}^{a}D_{(D_{H^{*}}^{c_{m}}\phi_{\alpha_{m}})}^{b_{m}}D_{(D_{H^{*}}^{c_{m-1}}\phi_{\alpha_{m-1}})}^{b_{m-1}}\cdots D_{(D_{H^{*}}^{c_{1}}\phi_{\alpha_{1}})}^{b_{1}}g
$$
 (3.8)

with some coefficient functions, in which  $a$ ,  $b_i$ , and  $c_i$  are non-negative integers while each  $\alpha_i$  takes values from 1 to *K*. Obviously, only the constraints generated by any multiple Poisson bracket between the primary first-class constraints and the first-class Hamiltonian *H*\* appear in the evolution expression of *g*. These constraints must be first class, but in general they do not exhaust all the first-class constraints. This is different from the accustomed conclusion. In fact, we can prove that they form the subalgebra of the minimum evolution closed Poisson bracket (MECPB) of the first-class constraints. If one attempts to add the linear combination of the arbitrary multipliers with all the first-class constraints to the extended Hamiltonian, as in Dirac's conjecture, then it is possible, in some general singular systems, to change the physical content of motion. In order to explain it more clearly, let us analyse as follows.

In his well-known work  $[1]$ , Dirac assumed that there is an initial physical state independent of the arbitrary multipliers  $v_{\alpha}$ . Following Bergmann's physical requirement, the physical observables are free of arbitrary multipliers at any time. Hence, in Taylor's expansion of the physical observables at initial time, all of the terms related to the arbitrary multipliers and their derivatives are bound to weakly equal zero. Because  $v_{\alpha}$  is arbitrary and the constrained hypersurface is stable, if and only if

$$
\{ \cdots \{g, H^*\}, \ldots, H^*\}, \phi_\alpha \} \approx 0 \quad (n = 1, 2, \ldots, \infty)
$$
\n
$$
(3.9)
$$

 *is such a physical observable. Then, from Eq.*  $(3.5)$  *and the* first-class property of  $H^*$ , we can see that the validity of Eq.  $(3.9)$  for some *n* generally needs

$$
\{(\underbrace{\{H^*,\ldots,\{H^*,\phi_\alpha\}\cdots\}}_{k},g\} \approx 0 \quad (k=0,1,\ldots,n). \tag{3.10}
$$

**Becaus** 

$$
\longleftarrow{\text{ $\{H^*,\ldots,\{H^*,\phi_\alpha\}^{\ldots}\}^{\infty}$}} 0,
$$

we can write  $[1,16]$ 

$$
\underbrace{\{H^*, \dots, \{H^*, \phi_\alpha\} \cdots\} \simeq f_\alpha^a \phi_a}_{k} \tag{3.11}
$$

where the Einstein summation convention has been used. Denote all of the constraints  $\phi_a$  generated from Eq. (3.11) for  $k=1,2,\ldots,\infty$  by a set  $\{\phi_{J_0}\}\$ . Obviously each  $\phi_{J_0}$  $\in {\phi_{J_0}}$  is a first-class constraint and Eq. (3.10) means generally  $\{\phi_{j_0}, g\} \approx 0$ . By virtue of Eqs. (3.6) and (3.10), we can obtain {{ $\phi_{j_0}, \phi_{j_0},$ },*g*}≈0 and {{ $H^*, \phi_{j_0},$ },*g*}≈0. Moreover,  $\{\phi_{j_0}, \phi_{j_0},\} = C^b_{j_0j_0}, \phi_b$  and  $\{H^*, \phi_{j_0}\} \simeq f^c_{j_0} \phi_c$ . It follows that all the independent constraints among all of the  $\phi_a$ ,  $\phi_b$ , and  $\phi_c$  make up a new set  $\{\phi_{K_0}\}\supseteq \{\phi_{J_0}\}\$ , and for each  $\phi_{k_0}$  $\in \{\phi_{K_0}\}, \{\phi_{k_0}, g\} \approx 0$ . Similarly, in this way, we can obtain, when Eq.  $(3.10)$  is obeyed, that more first-class constraints make up a larger set and each element of this set has weakly vanishing Poisson brackets with *g* in general. This process ends when all of these generating constraints, denoted by a set  $\{\phi_{M_0}\}\text{, form 'the minimum evolution closed subalgebra}$ of the first-class constraints," that is, for each  $\phi_{m_0} \in {\phi_{M_0}}$ 

$$
\{\phi_{m_0}, \phi_{m'_0}\} = C_{m_0 m'_0}^{m''_0} \phi_{m''_0},
$$
\n(3.12a)

$$
\{\phi_{m_0}, H_T^D\} \simeq b_{m_0}^{m_0'} \phi_{m_0}.
$$
 (3.12b)

Generally,  $\{\phi_{M_0}\}\$  always contains all the primary first-class constraints  $\phi_{\alpha}$  but does not always exhaust all the first-class constraints  $\phi_m$ , that is,

$$
\{\phi_P\} \subseteq \{\phi_{M_0}\} \subseteq \{\phi_M\},\tag{3.12c}
$$

where  $\{\phi_p\}$  and  $\{\phi_M\}$  denote respectively the sets of all of the primary first-class and all of the first-class constraints. Cawley's first example above has just this feature. Obviously, Eq.  $(3.7)$  represents a series of trajectories with different choices of  $v_{m_0}$  and they are gauge equivalent. It is worth emphasizing that the number of arbitrary parameters is not equal to one of the first-class constraints but is the same as one of the elements of the subalgebra of the MECPB of the first-class constraints. Therefore for this kind of example, it is not generally correct when construction of the generalized Hamiltonian is given by Dirac's conjecture.

#### **B. Singular systems with Hessian variable rank**

For a singular system, the elements of the Hessian matrix have the relation

$$
W_{Ai} = (\partial \psi_A / \partial p_\sigma) W_{\sigma i}.
$$
 (3.13)

The reason for this is that the primary constraints are expressed as functions of the variables on phase space. Thus the E-L equations can be divided into two systems; the first system consists of the second-order differential equations

$$
W_{\sigma i} \ddot{q}^i = K_{\sigma}, \quad K_i = \partial L / \partial q^i - (\partial^2 L / \partial \dot{q}^i \partial q^j) \dot{q}^j, \tag{3.14}
$$

and the second system consists of the first-order or/and zeroorder differential equations

$$
K_A - (\partial \psi_A / \partial p_\sigma) K_\sigma = \partial L / \partial q^A - d(\partial L / \partial \dot{q}^A) / dt = 0.
$$
\n(3.15)

It can be verified that the second system is just the secondstage constraints,

$$
\chi_A = \{ \phi_A, H \} + \dot{q}_B \{ \phi_A, \phi_B \}
$$
  
=  $[K_A - (\partial \psi_A / \partial p^\sigma) K_\sigma] |_{p_\sigma = \partial L / \partial q^\sigma} \approx 0.$  (3.16)

In Dirac's algorithm, in order to generate the secondary constraints one only requires that Eqs.  $(3.16)$  are preserved in time. Obviously, if the Hessian matrix has variable rank, some of the second-order E-L equations may become firstor/and zero-order ones. Normally, they may, in general, become some new constrained equations independent of those old constraints in Dirac's original algorithm, because those old constraints are only generated by the time derivative of  $\chi_A$  in terms of the consistency conditions. In other words, Dirac's original algorithm may omit in general the new constraints that result from Hessian variable rank.

If the rank of the Hessian matrix decreases in the constrained submanifold  $\Gamma_C^D$  which is given by Dirac's algo-

rithm, it implies that det $\left\|W_{\sigma\rho}\right\|_{\Gamma_C^D} = 0$  or the finite inverse of  $|W_{\sigma\rho}|$  on  $\Gamma_C^D$  does not exist. Thus we cannot find all the primarily expressible velocities  $\dot{q}^{\sigma}$  as finite functions of  $q^{i}$ ,  $p_{\sigma}$ , and  $\dot{q}^{A}$  on  $\Gamma_C^D$  from the relation

$$
dp_{\sigma} = (\partial L/\partial \dot{q}^{\sigma} \partial q^i) dq^i + W_{\sigma \rho} d\dot{q}^{\rho} + W_{\sigma A} d\dot{q}^A. \quad (3.17)
$$

In other words, some of them are infinite on  $\Gamma_C^D$  and consequently  $H_T^D$  is not differentiable on  $\Gamma_C^D$ , viz.,

$$
\dot{q}^a \approx \partial H^D \partial p_a |_{U_D} \to \infty \quad (\dot{q}^a \in {\{\dot{q}^\sigma\}}). \tag{3.18}
$$

It must be emphasized that in the general case for a constrained system with Hessian variable rank, if the number of the primarily expressible velocities decreases, the primary constraints in the Dirac algorithm sense can perhaps not be expressed generally as functions of the phase space variables. The definition and form of Dirac's total Hamiltonian of this kind of system seems not to be suitable. In this kind of system there is difficulty when one passes from Lagrangian formalism to Hamiltonian by directly using Dirac's algorithm. We do not know clearly how to solve this problem in the general case. Future study on this problem would be interesting.

In order to avoid the above difficulty, we assume that the number of primarily expressible velocities does not decrease actually on the final constrained hypersurface in the general case when the Hessian matrix has variable rank. For instance, Cawley's second example is just so. Thus, we still can first compute the rank of the Hessian matrix in *S* which consists of *q* and  $\dot{q}$ , with all *q*'s and  $\dot{q}$ 's being independent, and we can obtain Eq.  $(2.4)$  although some of the  $\dot{q}^{\sigma}$  may tend to infinity on Dirac's constrained hypersurface  $\Gamma_C^D$ . In fact, this poor expression of  $\dot{q}^{\sigma}$  is not intrinsic, it ought to be eliminated in the real and final constrained hypersurface  $\Gamma_C^F$ which is determined by all the constraints. Otherwise, the physical significance of this kind of system is not understandable since there is intrinsically infinite motion.

From Eq.  $(3.17)$  we also see that there is possibly some  $\dot{q}^b \rightarrow \infty$  if there exists some  $\dot{q}^a \rightarrow \infty$ . Thus the above conclusion implies that in the singular system with Hessian variable rank Dirac's total Hamiltonian is not differentiable with respect to some variables on phase space if one only considers the constraints in Dirac's original algorithm. This feature results in the difficulties in Dirac's algorithm.

In particular, although  $(\partial H_T^D/\partial p_a)^{-1} = 0$  on  $\Gamma_C^D$ , one has

$$
d\left[q^a(\partial H_T^D/\partial p_a)^{-1}\right]/dt \approx 1 + q^a \left\{(\partial H_T^D/\partial p_a)^{-1}, H_T^D\right\} \approx 1\tag{3.19}
$$

in which we do not sum for index *a*. Obviously this contradicts the consistency conditions or the stability of the constrained hypersurface. Hence Dirac's algorithm of Hamiltonization is not suitable to such singular systems with Hessian variable rank.

For instance, the Hessian matrix in Cawley's second example is

$$
W_{ij} = \begin{pmatrix} 0 & 0 & 2\dot{z} \\ 0 & 0 & 0 \\ 2\dot{z} & 0 & 2\dot{x} \end{pmatrix} . \tag{3.20}
$$

Its rank is 2 primarily. But in the constrained submanifold  $\Gamma_C^D$  defined by Eqs. (2.28) and (2.30), its rank decreases to 1. According to Dirac's original algorithm, one only claims that the constraint  $p_y \approx 0$  or  $z \approx 0$  is preserved in time. However, this requirement is not enough to generate all of the secondary constraints. The reason is that another second-stage constraint  $y \approx 0$ , which is obtained from the motion equations because of the existence of Hessian variable rank, is omitted.

In fact, in Dirac's algorithm one also assumes that the rank of the Hessian matrix is 2 and then defines the total Hamiltonian. Because some of the primarily expressible velocities tend to infinity on  $\Gamma_C^D$ , the time derivative of some weakly vanishing functions may be nonzero on  $\Gamma_C^D$ . For example,  $2xp_x^{1/2}/p_z \approx 0$  but by differentiating it with respect to time we obtain

$$
d(2xp_x^{1/2}/p_z)/dt \approx 1.
$$
 (3.21)

It implies that the constrained hypersurface  $\Gamma_C^D$  is not stable. In particular, because the equations of motion are weakly equal ones, they should not be changed in the weakly equal sense by adding or dropping a weakly vanishing term. Without loss of generality*,* supposing there is an additional term  $2\lambda xz \approx 0$  ( $\lambda$  is an arbitrary differentiable function) in the right side of the equation for  $g<sub>i</sub>$ ,

$$
\dot{g} \approx \{g, H_T\} + 2\lambda x z,\tag{3.22}
$$

one easily derives

$$
d^{3}g/dt^{3} \approx \{ \{ \{ g, H_{T} \}, H_{T} \}, H_{T} \} + \lambda p_{z}. \tag{3.23}
$$

Since the term  $\lambda p_z$  is not equal to zero but is arbitrary on  $\Gamma_C^D$ , Eq. (3.23) implies that the functions of the variables on phase space at time *t* cannot be expressed by their values at initial time  $t_0$ , or speaking generally, the dynamics of the Hamiltonian formalism is not completely determined.

In a word, from the above analyses and demonstration we see that Dirac's original algorithm is not directly and generally applicable to a certain class of constrained systems.

### **IV. FROM DIRAC'S CONTACT TRANSFORMATION TO THE EXTENDED DIRAC CONJECTURE**

Dirac's conjecture gives a principle of construction for the extended Hamiltonian in constrained systems. As is well known, the crux of the matter is how to construct a correct extended Hamiltonian in the quantization of singular systems. Consequently, in this section we try to overcome the difficulties of Dirac's conjecture, and propose and prove a principle of construction of an extended Hamiltonian. First, the transformations between the various evolution trajectories at any given time are constructed by using the translation operator. Second, the infinitesimal form of trajectory transformation and the relation between this transformation and the canonical transformation are realized. Third, the finite Dirac contact transformation is shown to form a functional group which does not change the physical observables. Thus the generators of the finite Dirac contact transformation, that is, the gauge transformation in constrained systems, are clearly given. They are the constraints in the set of MECPB's of the first-class constraints. Finally, we propose and prove the extended Dirac conjecture. At the same time, it is successfully applied to Cawley's first counterexample to Dirac's conjecture. Our conclusion naturally comes back to the usual Dirac conjecture when Dirac's algorithm is applicable.

#### **A. Time translation operator**

Let us introduce the first-class operator in constrained systems. A so-called first-class operator acts on all the constraints  $\phi_i = (\phi_m, \Omega_s)$  to be weakly equal to zero, viz.,

$$
D\,\phi_j \approx 0.\tag{4.1}
$$

From this it follows that the *D* operator constructed by Dirac's total Hamiltonian is a first-class one. It is easy to show that the *D* operator constructed by first-class functions is first class and the product of first-class operators is also first class. We can derive the motion equation of the firstclass operator as

$$
\dot{D}_f \approx [D_f, D_{H^D_T}] + \partial D_f / \partial t \approx D_{\{f, H^D_T\} + \partial f / \partial t}. \tag{4.2}
$$

For the non-first-class operator its motion equation has an additional nontrivial term  $-c_jD_f\phi_j$  which depends on the function *f.* Actually, even for a non-*D* operator, but a firstclass and linear one, denoted by  $\hat{F}$ , we also have

$$
\dot{\hat{F}} \approx [\hat{F}, D_{H_T^D}] + \partial \hat{F} / \partial t. \tag{4.3}
$$

Its form is the same as Heisenberg's equation and consequently we can use the technology of quantum theories in the sense of classical theories. If we introduce the time ''conjugate momentum''  $\epsilon$  so that

$$
\{t, \epsilon\} = 1 \quad \text{or} \quad D_{\epsilon} = -\frac{\partial}{\partial t},\tag{4.4}
$$

then  $\eta^{\mu}$  and *t*,  $\epsilon$  constitute the extended phase space. Obviously Eq.  $(4.2)$  becomes

$$
\dot{D}_f \approx [D_f, D_{H^D_T + \epsilon}] = -D_{D_{H^D_T + \epsilon}}.\tag{4.5}
$$

It can be used to derive the expression of the time translation operator. As usual, the time translation operator is defined by

$$
g(\eta(t)) = U(t,t_0)g(\eta(t_0)).\tag{4.6}
$$

Its existence is obvious. Because the constrained equations are always obeyed in any time, the time translation operator is first class. In terms of Eq.  $(4.2)$  we can obtain the motion equation of the time translation operator as

$$
\dot{U}(t,t_0) \approx -D_{H_T^D(t)} U(t,t_0). \tag{4.7}
$$

It can be rewritten as an integral equation and thus the successive iteration method is applicable. It follows that the time translation operator for a function which does not relate to time explicitly has the form

$$
U(t,t_0) \approx T \exp\bigg\{-\int_{t_0}^t d\tau \mathcal{D}_{H_T^D(\tau)}\bigg\},\tag{4.8}
$$

$$
U^{-1}(t,t_0) \approx T^* \exp\left\{ \int_{t_0}^t d\tau D_{H_T^D(\tau)} \right\},\tag{4.9}
$$

in which *T* and *T*\* stand for time-ordered and anti-timeordered products, respectively, while the relation between D and *D* can be seen in Appendix D. In particular, when the multipliers  $u_{\alpha}$  do not depend on time explicitly since

$$
\dot{\mathcal{D}}_{H_T^D}(t) \approx 0 \Longrightarrow \mathcal{D}_{H_T^D}(t_1) \approx \mathcal{D}_{H_T^D}(t_2),\tag{4.10}
$$

the operator *T* or  $T^*$  can be dropped and Eq.  $(4.8)$  or  $(4.9)$ becomes simpler,

$$
U(t,t_0) \approx e^{-(t-t_0)\mathcal{D}_{H^D_T}},\tag{4.11}
$$

$$
U^{-1}(t,t_0) \approx e^{(t-t_0)\mathcal{D}_H p}.\tag{4.12}
$$

Therefore the variables  $\eta^{\mu}(t)$  on phase space can be expressed in terms of their initial values  $\eta^{\mu}(t_0)$ , that is,

$$
\eta^{\mu}(t) = U(t,t_0) \,\eta^{\mu}(t_0) \approx T \exp\left(-\int_{t_0}^t d\tau D_{H_T^D}(\tau)\right) \eta^{\mu}(t_0).
$$
\n(4.13)

Equation  $(4.13)$  stands for a set of the evolution trajectories on phase space.

#### **B. The trajectory transformation at any given time**

As is well known, the evolution of the constrained systems is determined by Dirac's total Hamiltonian  $H_T^D$ . However, since  $H_T^D$  involves arbitrary multipliers the system can evolve in various trajectories when various multipliers are chosen. Following Dirac's assumption there exists a definite physical state which does not depend on the arbitrary multipliers. Without loss of generality, we can suppose that the system is in the definite physical state at time  $t<sub>0</sub>$ . Hence the various trajectories intersect at  $t_0$ ,

$$
\eta^{\mu}(t_0) = \tilde{\eta}^{\mu}(t_0). \tag{4.14}
$$

At any time, two trajectories evolve in accordance with the equations

$$
\dot{\eta}^{\mu} \approx -D_{H_T^D(v)} \eta^{\mu} \approx {\eta^{\mu}, H^*} + v_{\alpha} {\eta^{\mu}, \phi_{\alpha}}, \quad (4.15a)
$$

$$
\dot{\widetilde{\eta}}^{\mu} \approx -\widetilde{D}_{\widetilde{H}_{T}^{D}\left(u\right)} \widetilde{\eta}^{\mu} \approx \{ \widetilde{\eta}^{\mu}, \widetilde{H}^{*} \} + \widetilde{u}_{\alpha} \{ \widetilde{\eta}^{\mu}, \phi_{\alpha} \}, \quad (4.15b)
$$

in which we have denoted

$$
\widetilde{f}(\eta) = f(\widetilde{\eta}), \quad \widetilde{D}_{\widetilde{f}} = \epsilon^{\mu\nu} \frac{\partial \widetilde{f}}{\partial \widetilde{\eta}^{\mu}} \frac{\partial}{\partial \widetilde{\eta}^{\nu}}.
$$
 (4.16)

Just as in the above subsection, there are the time translation operators and then



$$
g(t) = V(t, t_0)g(t_0).
$$
 (4.18)

In terms of Eqs.  $(4.14)$  we obtain

$$
\widetilde{g}(t) = G(t, t_0; u, v)g(t),
$$
\n(4.19)

where  $G(t,t_0;u,v)$  is named the trajectory transformation where  $G(t, t_0; u, v)$  is named the trajectory transformation perator from  $\eta^{\mu}$  to  $\tilde{\eta}^{\mu}$  at a given time *t*. Its definition is

$$
G(t,t_0;u,v) = \widetilde{U}(t,t_0)V^{-1}(t,t_0).
$$
 (4.20)

It is convenient to ignore  $t$  and  $t_0$  in the following notation for *G.* It readily is verified that *G* has the following properties:

$$
G(u, u) = G(v, v), \tag{4.21a}
$$

$$
G^{-1}(u,v) = G(v,u), \tag{4.21b}
$$

$$
G(u, v)G(v, w) = G(u, w), \t(4.21c)
$$

Because  $\overline{U}$ , *V* is first class, *G* is also first class. Obviously, there is the relation

$$
\{\tilde{f}_1, \tilde{f}_2\}^{\tilde{\eta}} = G\{f_1, f_2\}^{\eta} \tag{4.22}
$$

in which the upper index  $\eta$ ,  $\widetilde{\eta}$  stands for computation of the In which the upper maex  $\eta$ ,  $\eta$  stands for computation of the Poisson bracket with respect to  $\eta$ ,  $\tilde{\eta}$ , respectively. Equation  $(4.22)$  has the alternative form

$$
\widetilde{D}_{f} = GD_{f}G^{-1}.
$$
\n(4.23)

Thus we can find the motion equation of *G*:

$$
\dot{G}(u,v) \approx -(\tilde{u}_{\alpha} - \tilde{v}_{\alpha}) \tilde{D}_{\tilde{\phi}_{\alpha}} G(u,v) \approx -G(u,v)(u_{\alpha} - v_{\alpha}) D_{\phi_{\alpha}}
$$
\n(4.24)

where  $\tilde{u}_{\alpha} = Gu_{\alpha}$  and  $\tilde{v}_{\alpha} = Gv_{\alpha}$ . By use of the successive iteration method one obtains

$$
G(u,v) \approx T \exp\left\{-\int_{t_0}^t d\tau \left[\tilde{u}_{\alpha}(\tau) - \tilde{v}_{\alpha}(\tau)\right] \tilde{D}_{\phi_{\alpha}}(\tau)\right\}
$$

$$
\approx T^* \exp\left\{-\int_{t_0}^t d\tau \left[u_{\alpha}(\tau) - v_{\alpha}(\tau)\right] D_{\tilde{\phi}_{\alpha}}(\tau)\right\}.
$$
(4.25)

Likewise we have

$$
G^{-1}(u,v) \approx T^* \exp\left\{ \int_{t_0}^t d\tau \left[ \tilde{u}_\alpha(\tau) - \tilde{v}_\alpha(\tau) \right] \tilde{\mathcal{D}}_{\tilde{\phi}_\alpha}(\tau) \right\}
$$

$$
\approx T \exp\left\{ \int_{t_0}^t d\tau \left[ u_\alpha(\tau) - v_\alpha(\tau) \right] \mathcal{D}_{\phi_\alpha}(\tau) \right\}. \tag{4.26}
$$

Equations  $(4.25)$  and  $(4.26)$  are just the obvious forms of the Equations (4.25) and (4.26) are just the obvious forms of the<br>trajectory transformation from  $\eta^{\mu}$  to  $\tilde{\eta}^{\mu}$  at a given time *t*. It is a functional form transformation with transformation pais a functional form transformation with transformation parameters  $u_{\alpha} - v_{\alpha}$  (or  $\tilde{u}_{\alpha} - \tilde{v}_{\alpha}$ ) and generator  $\mathcal{D}_{\phi_{\alpha}}$  (or  $\tilde{\mathcal{D}}_{\phi_{\alpha}}$ )

under the integral for time. Therefore it depends on the values of the multipliers and the forms of the generators not at a given time but in the time interval  $t-t_0$ . In general, the multipliers vary in time. In particular, it is interesting that the evolution in time of the generators  $\mathcal{D}_{\phi_{\alpha}}$  will lead to increase of the numbers of generators, viz., some  $D$  operators constructed by the secondary constraints become new generators.

For some singular systems, if there is the subalgebra of the MECPB of the first-class constraints defined as Eqs.  $(3.12)$ , we can obtain

$$
\dot{\mathcal{D}}_{\phi_{m_0}}(t) \approx b_{m_0}^{m_0'} \mathcal{D}_{\phi_{m_0'}}(t),\tag{4.27}
$$

$$
b_{m_0}^{m_0'} = f_{m_0}^{m_0'} + (D_{\phi_{m_0}} v_\alpha) \delta_{\alpha}^{m_0'} + v_\alpha C_{m_0 \alpha}^{m_0'}.
$$
 (4.28)

Therefore it can be seen that the evolution of the generators  $\mathcal{D}_{\phi_{\alpha}}$  is only interrelated with the operators  $\mathcal{D}_{\phi_{m_0}}$  in which  $\phi_{m_0}$  belongs to the subalgebra of the MECPB of the firstclass constraints. From Eq.  $(4.27)$  it follows that

$$
\mathcal{D}_{\phi_{m_0}}(t) \approx \mathcal{V}_{m_0 m'_0}(t, t_1) \mathcal{D}_{\phi_{m'_0}}(t_1) \tag{4.29}
$$

where  $V$  is a matrix function whose definition is

$$
\mathcal{V}(t,t_1) = T \exp\left\{ \int_{t_1}^t d\tau B(\tau) \right\},\tag{4.30a}
$$

$$
B_{m_0}^{m_0'} = b_{m_0}^{m_0'}.
$$
 (4.30b)

Obviously  $V$  has inverse and unit elements and it can be called the translation function of  $\mathcal{D}_{\phi_{m_0}}$ . It is easy to verify that the product of two successive translation functions is still a translation function. Thus,

$$
\widetilde{\mathcal{D}}_{\widetilde{\phi}_{m_0}}(t) \approx \widetilde{\mathcal{U}}_{m_0 m_0'}(t, t_0) \mathcal{V}_{m_0' m_0''}^{-1}(t, t_0) \mathcal{D}_{\phi_{m_0''}}(t) \qquad (4.31)
$$

where

$$
\widetilde{U}(t,t_0) = T \exp\bigg\{-\int_{t_0}^t d\tau \widetilde{A}(\tau)\bigg\},\qquad(4.32a)
$$

$$
\widetilde{A}_{m_0}^{m'_0} = \widetilde{a}_{m_0}^{m'_0} = \widetilde{f}_{m_0}^{m'_0} + (\widetilde{D}_{\phi_{m_0}} \widetilde{u}_{\alpha}) \delta_{\alpha}^{m'_0} + \widetilde{u}_{\alpha} \widetilde{C}_{m_0 \alpha}^{m'_0},
$$
\n(4.32b)

$$
\mathcal{V}^{-1}(t,t_0) = T^* \exp\Biggl\{-\int_{t_0}^t d\tau B(\tau)\Biggr\},\qquad(4.32c)
$$

and we have used

$$
\widetilde{\mathcal{D}}_{\widetilde{\phi}_{m_0}}(t_0) = \mathcal{D}_{\phi_{m_0}}(t_0). \tag{4.33}
$$

Hence the  $D$  operators constructed by the elements of the subalgebra of the MECPB of the first-class constraints in a given trajectory can be expressed as the linear combinations of their forms in another trajectory.

In terms of the commutation theorem of *D* operators and Eqs.  $(4.29)$  and  $(4.31)$  we can compute the commutators of

 $D_{\phi_{m_0}}$  at various times and the results are still a linear combination of  $\mathcal{D}_{\phi_{m_0}}$ . Of course, our above conclusions are also valid when the subalgebra of the MECPB of the first-class constraints is the whole algebra of the first-class constraint, or the set of the subalgebra of the the MECPB of the firstclass constraints is the complete set of the first-class constraints.

If we make use of the Baker-Hausdorff formula, *G* can be written in the form

$$
G(u,v) \approx e^{-\lambda_{m_0}(u,v;t,t_0)\mathcal{D}_{\phi_{m_0}}(t)}.\tag{4.34}
$$

This form can be seen more clearly in the discussion on infinitesimal transformations in the following section.

Obviously from our above analyses and demonstration whether or not the secondary constraints are the generators of trajectory transformations relies on whether they belong or do not belong to the set of the subalgbra of the MECPB of the first-class constraints.

#### **C. Infinitesimal trajectory transformation**

Let us consider two ''neighboring trajectories,'' viz., the differences of the multipliers in front of the first-class primary constraints tend to zero or are infinitesimal, denoted by  $u_{\alpha}-v_{\alpha}=\epsilon_{\alpha}$ . Hence they are also infinitesimal after integrating over a finite time interval. Thus the infinitesimal transformation  $G_{\epsilon}$  at time *t* of two neighboring trajectories takes the form

$$
G_{\epsilon} \approx 1 - \int_{t_0}^{t} dt_1 \epsilon_{\alpha}(t_1) \mathcal{V}_{\alpha m_0}(t_1, t) \mathcal{D}_{\phi_{m_0}}(t)
$$
  

$$
\approx 1 - \delta \lambda_{m_0}(t, t_0) \mathcal{D}_{\phi_{m_0}}(t).
$$
 (4.35)

Here by use of the method of the change of integration limit,

$$
\int_{t_0}^t dt_1 \int_{t_1}^t dt_2 b_{m_0}^{m_0'}(t_1) b_{m_0'}^{m_0''}(t_2)
$$
\n
$$
= \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 b_{m_0'}^{m_0''}(t_1) b_{m_0}^{m_0'}(t_2), \quad (4.36)
$$

we can rewrite the infinitesimal transformation parameters as

$$
\delta \lambda_{m_0}(t, t_0) = \int_{t_0}^t d\tau \delta \Lambda_{m_0}(\tau, t_0), \qquad (4.37a)
$$

$$
\delta \Lambda_{m_0}(\tau, t_0) = \epsilon_\alpha(\tau) \, \delta_{\alpha m_0} - b_{m'_0}^{m_0}(\tau) \int_{t_0}^\tau \delta \Lambda_{m'_0}(\tau', t_0) d\tau'
$$
  

$$
= \epsilon_\alpha(\tau) \, \delta_{\alpha m_0} - b_{\alpha}^{m_0} \tau \int_{t_0}^\tau dt_1 \epsilon_\alpha(t_1)
$$
  

$$
+ b_{m_0}^{m_0} \sum_{n=2}^\infty (-)^n \int_{t_0}^\tau dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n.
$$
  
(4.37b)

They obey the equations

$$
\frac{d}{dt}\delta\lambda_{m_0}(t) = \epsilon_{\alpha}(t)\delta_{\alpha m_0} - b_{m'_0}^{m_0}(t)\delta\lambda_{m'_0}(t). \tag{4.38}
$$

This means that the infinitesimal transformation parameters are the sums for *n* from 0 to  $\infty$  of the *n*-tuple weighted integrals of  $\epsilon_{\alpha}$  and so their completely independent numbers generally may be different from the  $\phi_{m'_0}$  numbers in the functional sense.

If we introduce the generating function  $F_2$  of the infinitesimal canonical transformation,

$$
F_2(q,\tilde{p}) = q^i \tilde{p}_i + \delta \lambda_{m_0} \phi_{m_0}(q,\tilde{p}), \qquad (4.39)
$$

after dropping the second-order infinitesimal terms we have

$$
\tilde{q}^i = q^i + \delta \lambda_{m_0} \partial \phi_{m_0} / \partial p_i = (1 - \delta \lambda_{m_0} D_{\phi_{m_0}}) q^i,
$$
\n(4.40a)

$$
\tilde{p}_i = p_i - \delta \lambda_{m_0} \partial \phi_{m_0} / \partial q^i = (1 - \delta \lambda_{m_0} D_{\phi_{m_0}}) p_i ,
$$
\n(4.40b)

in which  $\delta\lambda_{m_0}$  is thought of, without loss of generality, as a time function free of dynamics variables. Therefore the infinitesimal trajectory transformation is consistent with the infinitesimal canonical transformation generated by  $F_2$ .

It is easy to verify that Hamiltonian *K* which generates It is easy to verify that Hamiltonian **A** which generates<br>the motion equations of  $\tilde{\eta}^{\mu}$  can be found in terms of the theory of the canonical transformation and  $K$  is equal to theory<br> $\widetilde{H}^D_T(u)$ ,

$$
K = H^*(\eta) + v_\alpha \phi_\alpha + \partial F_2 / \partial t
$$
  
=  $\widetilde{H}^* + u_\alpha \phi_\alpha - b_{m_0}^{m_0'} \delta \lambda_{m_0} \phi_{m_0'}$   
=  $\widetilde{H}^*(\eta) + \widetilde{u}_\alpha \widetilde{\phi}_\alpha = \widetilde{H}_T^D(u).$  (4.41)

Here we have used  $\{\phi_{m_0}, H_T^D\} = b_{m_0}^{m_0'} \phi_{m_0'}$  and dropped the second-order infinitesimal terms.

For the transformation from a given trajectory to another given trajectory at a certain time, one can realize it by a series of successive infinitesimal canonical transformations. Of course it is necessary that  $\delta\lambda_{m_0}$  satisfies Eq. (4.38). The end result is the same as Eq.  $(4.25)$ .

Since the trajectory transformation  $(4.25)$  or  $(4.26)$  is a functional, another form of its infinitesimal transformation can be taken as one in an infinitesimal time interval  $t-t_0=\delta t$ ,

$$
G(\delta t) = 1 - \delta t [u_{\alpha}(t_0 + \delta t) - v_{\alpha}(t_0 + \delta t)] D_{\phi_{\alpha}(t_0 + \delta t)}.
$$
\n(4.42)

It is worth pointing out that a series of successive  $G(\delta t)$ 's do not give rise to trajectory transformations since the trajectories only generally intersect at  $t<sub>0</sub>$ . In his original paper Dirac studied the difference of the product of two arbitrary trajectory transformations in an infinitesimal time interval, which will be seen in the following section.

### **D. Evident Dirac's contact transformation**

In according with physical considerations, the physical observables on the various trajectories should be equal, that is,

$$
g_{\text{ph}}(\eta) \approx g_{\text{ph}}(\tilde{\eta}). \tag{4.43}
$$

Hence the trajectory transformations are ones which do not change the physical observables,

$$
Gg_{\text{ph}}(\eta) \approx g_{\text{ph}}(\eta). \tag{4.44}
$$

In fact Eq.  $(4.44)$  can be shown strictly by the requirement that the physical observables do not depend on arbitrary functions. It is shown in Sec. VI.

Obviously, even when the product of two arbitrary trajectory transformations is not successive, it does not change physical observables,

$$
G_1 G_2 g_{\text{ph}} \approx g_{\text{ph}}.\tag{4.45}
$$

Here invariance is in the sense of weak equality since we derive the trajectory transformations and introduce the physical observables only in the sense of weak equality.

In his original paper Dirac just considered the difference of the products of two such arbitrary infinitesimal trajectory transformations, but he took their forms as Eq.  $(4.42)$  in an infinitesimal time interval, that is,

$$
\beta_{\alpha} = \delta t (u_{\alpha} - a_{\alpha}), \quad \gamma_{\alpha} = \delta t (b_{\alpha} - v_{\alpha}), \quad (4.46)
$$

$$
G_1 \approx 1 - \beta_\alpha D_{\phi_\alpha}, \quad G_2 \approx 1 - \gamma_\alpha D_{\phi_\alpha}, \quad (4.47a)
$$

$$
g' = G_1 G_2 g
$$
,  $g'' = G_2 G_1 g$ . (4.47b)

Hence one has

$$
\Delta g = g' - g'' = [G_1, G_2] g \approx [\beta_\alpha D_{\phi_\alpha}, \gamma_\alpha D_{\phi_\alpha}] g
$$
  

$$
= \{ [\beta_\alpha (D_{\phi_\alpha} \gamma_{\alpha'}) - \gamma_\alpha (D_{\phi_\alpha} \beta_{\alpha'})] D_{\phi_{\alpha'}}
$$
  

$$
+ \beta_\alpha \gamma_{\alpha'} D_{\{\phi_\alpha, \phi_{\alpha'}\}} g.
$$
 (4.48)

The last term may give rise to generators constructed by the secondary constraints because of the closed property of the first-class constraints. But this is not always the case. The shortcoming of such considerations is that one does not obtain secondary constraints derived by  $\{H^*, \phi_{m_0}\}$  as the generators of Dirac's contact transformations in general. This is one of the reasons why Dirac could only make a conjecture.

We think that Dirac's idea of contact transformations in constrained systems refers to the product of two arbitrary trajectory transformations at a given time *t*. Thus we prefer to choose the form of Eq.  $(4.35)$  more definitely and generally, viz.,

$$
G_1 \approx 1 - \delta \lambda_{m_0}^1 D_{\phi_{m_0}}, \quad G_2 \approx 1 - \delta \lambda_{m_0}^2 D_{\phi_{m_0}}, \quad (4.49)
$$

where  $\delta \lambda_{m_0}^1$  and  $\delta \lambda_{m_0}^2$  are independent of each other. Hence

$$
\Delta g = [G_1, G_2] g \approx [\delta \lambda_{m_0}^1 D_{\phi_{m_0}}, \delta \lambda_{m_0}^2 D_{\phi_{m_0}}] g
$$
  
\n
$$
= \{ [\delta \lambda_{m'_0}^1 (D_{\phi_{m'_0}} \delta \lambda_{m_0}^2) - \delta \lambda_{m'_0}^2 (D_{\phi_{m'_0}} \delta \lambda_{m_0}^1)] D_{\phi_{m_0}}
$$
  
\n
$$
+ \delta \lambda_{m_0}^1 \delta \lambda_{m'_0}^2 C_{m_0 m'_0}^m D_{\phi_{m''_0}} g. \qquad (4.50)
$$

Here we have used Eq.  $(3.6)$ . From Eq.  $(4.25)$  we can find more generally the product of two arbitrary trajectory transformations with finite parameters as

$$
G(u,a)G(b,v) \approx T \exp\left\{-\int_{t_0}^t d(\tau)\{[u_{\alpha}(\tau) - a_{\alpha}(\tau)]^{(u)} \times \mathcal{D}_{\phi_{\alpha}^{(u)}}^{(u)}(\tau) + f_{m_0}^{(u)}(\tau)\mathcal{D}_{\phi_{m_0}^{(u)}}^{(u)}(\tau)\}\right\}
$$

$$
= T \exp\left\{-\int_{t_0}^t d(\tau)\Theta_{m_0}^{(u)}\mathcal{D}_{\phi_{m_0}^{(u)}}^{(u)}(\tau)\right\},\tag{4.51}
$$

in which we introduce the notation

$$
A^{(w)}(t) = A(\boldsymbol{\eta}^{(w)}, t), \quad \mathcal{D}_{A^{(w)}}^{(w)} = \epsilon^{\mu\nu} \frac{\partial A^{(w)}}{\partial \boldsymbol{\eta}^{(w)\mu}} \frac{\partial}{\partial \boldsymbol{\eta}^{(w)\nu}},
$$
\n(4.52)

and  $\eta^{(u)\mu}$  evolves in accordance with the equation

$$
\dot{\eta}^{(u)\mu} \approx {\{\eta^{(u)\mu},H^{*(u)}\} + u_{\alpha}^{(u)}{\{\eta^{(u)\mu},\phi_{\alpha}^{(u)}\}}, \qquad (4.53)
$$

while the definition of  $f_{m_0}^{(u)}(t)$  is

$$
f_{m_0}^{(u)}(t) = G(u,a)(b_\alpha - v_\alpha)^{(b)} \mathcal{V}_{\alpha m_0'}^{(b)}(t,t_0) \mathcal{V}_{m_0'm_0}^{(a)}(t,t_0)
$$
\n(4.54)

and the form of  $\Theta_{m_0}$  is given by

$$
\Theta_{m_0}^{(u)}(\tau) = [u_\alpha(\tau) - a_\alpha(\tau)]^{(u)} \delta_{\alpha m_0} + f_{m_0}^{(u)}(\tau). \quad (4.55)
$$

It is worth pointing out that the product of the variables' evolution in the various trajectories or the action of the operators on the other trajectory variables can be calculated by translation of them to the initial values  $\eta^{\mu}(t_0)$ .

By virtue of Eqs.  $(3.12)$  and  $(4.31)$  we see that the products of all the contact transformations are closed and thus they form a functional group, which can be called the contact transformation functional group. Moreover, under the contact transformations all the functional transformation parameters  $\Theta_{m_0}$  are arbitrary and the generators are *D* operators constructed by the elements of the subalgebra of the MECPB of the first-class constraints. The general form of the contact transformation group element is given by

$$
\mathcal{G}(t,t_0) = T \exp \left\{ - \int_{t_0}^t d\tau \Theta_{m_0}(\tau, t_0) \mathcal{D}_{\phi_{m_0}}(\tau) \right\}.
$$
 (4.56)

Here we no longer write the upper index *u* relevant to the trajectory. Because of Eq. (4.31)  $\mathcal{D}_{\phi_m^{(w)}}^{(w)}$  in an arbitrary trajectory can always be expressed as linear combinations of

 $\mathcal{D}_{\phi_{m_0}}$  and this combination coefficient matrix is absorbed into the arbitrary  $\Theta_{m_0}$ . We think that Eq. (4.56) is just what Dirac expected to find as the evident expression of his contact transformations which do not change the physical states. However, it is not the same as the form conjectured by Dirac. Generally, its generators cannot exhaust all the first-class constraints but must involve all primary first-class constraints at least. Normally, its generators should be the elements of the so-called subalgebra of the MECPB of the firstclass constraints, which is defined by Eqs.  $(3.12a)$ – $(3.12c)$ .

By using the Baker-Hausdorff formula and Eqs.  $(4.31)$ and  $(4.35)$  one readily obtains

$$
\mathcal{G}(t,t_0) \approx e^{-\theta_{m_0}(t,t_0)\mathcal{D}_{\phi_{m_0}}(t)}.\tag{4.57}
$$

Of course its infinitesimal form is

$$
\mathcal{G}_{\epsilon}(t,t_0) \approx 1 - \delta \theta_{m_0} D_{\phi_{m_0}}, \tag{4.58}
$$

$$
\frac{d}{dt} [\delta \theta_{m_0}(t)] = \delta \Theta_{m_0}(t) - b_{m_0'}^{m_0}(t) \delta \theta_{m_0'}(t), \quad (4.59)
$$

$$
\delta \theta_{m_0}(t, t_0) = \int_{t_0}^t d\tau \delta \Theta_{m'_0}(\tau, t_0) \mathcal{V}_{m'_0 m_0}(\tau, t)
$$

$$
= \int_{t_0}^t d\tau \overline{\delta \Theta}_{m_0}(\tau, t_0), \qquad (4.60)
$$

$$
\overline{\delta\Theta}_{m_0}(\tau, t_0) = \delta\Theta_{m_0}(\tau, t_0) - b_{m'_0}^{m_0}(\tau) \int_{t_0}^{\tau} d\tau' \overline{\delta\Theta}_{m'_0}(\tau', t_0). \tag{4.61}
$$

Obviously the product of a series of infinitesimal contact transformations such as Eq.  $(4.58)$  will give rise to the finite Dirac contact transformation Eq.  $(4.56)$ .

Likewise, as stated above, the generating function corresponding to the infinitesimal contact transformation is then

$$
\mathcal{F}_2 = q^i \tilde{p}_i + \delta \theta_{m_0} \phi_{m_0}(q, \tilde{p}). \tag{4.62}
$$

It is easy to verify that it generates a transformation consistent with the one given by Eq.  $(4.58)$ .

### **E. Application to Cawley's first example**

In fact, from Eq.  $(4.25)$  it follows that the trajectory transformation operator *G* for Cawley's first example is

$$
G(t) \approx T^* \exp\left\{-\int_{t_0}^t d\tau [u(\tau) - v(\tau)] \mathcal{D}_{p_y}(\tau)\right\}
$$
(4.63)

and the translation function of  $\mathcal{D}_{p_y}$  is

$$
\mathcal{D}_{p_y}(t) \approx \exp\left\{-\int_{t_0}^t dt' \mathcal{D}_{p_y} v(t')\right\} \mathcal{D}_{p_y}(t_0) = \mathcal{V}(t, t_0) \mathcal{D}_{p_y}(t_0). \tag{4.64}
$$

Thus the set of the subalgebra of the MECPB of the firstclass constraints only involves  $p_y$ . Consequently Dirac's contact transformation only has  $D_{p_y}$  as its generator. We also can find *G* from its definition in terms of

$$
\widetilde{\eta}^{\mu}(t) = G(u, v; t, t_0) \eta^{\mu}(t)
$$

$$
\approx \left\{ 1 - \int_{t_0}^t d\tau [\widetilde{u}(\tau) - v(\tau)] \mathcal{D}_{p_y}(t) \right\} \eta^{\mu}(t),
$$
\n(4.65)

in which  $\eta^{\mu}$  takes *x*,*y*,*z* and  $p_x$ , $p_y$ , $p_z$ . It is obvious that except for *y* the other variables do not change. Thus

$$
\widetilde{g}(\eta) = g(\widetilde{\eta}) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n g(\eta)}{\partial y^n} (\widetilde{y} - y)^n
$$

$$
\approx \sum_{n=0}^{\infty} \frac{1}{n!} \left\{ \int_{t_0}^t d\tau [\widetilde{u}(\tau) - v(\tau)] \right\}^n \mathcal{D}_{p_y}^n(t) g(\eta)
$$

$$
= \exp\{-\lambda(t, t_0) \mathcal{D}_{p_y}(t) \} g(\eta), \qquad (4.66)
$$

$$
\lambda(t,t_0) = \int_{t_0}^t d\tau [\tilde{u}(\tau) - v(\tau)], \qquad (4.67)
$$

in which we have made a simplified rule that  $\lambda$  is supposed to be a function only of time *t* and then  $\mathcal{D}_{p_y}$  has no action on it. Therefore

$$
G(u, v; t, t_0) \approx e^{-\lambda(t, t_0) \mathcal{D}_{p_y}(t)}.
$$
\n(4.68)

Dirac's contact transformation operator also has the same form,

$$
\mathcal{G}(t,t_0) \approx e^{-\theta(t,t_0)\mathcal{D}_{p_y}(t)}.\tag{4.69}
$$

This indicates clearly that the Dirac conjecture is not applicable to Cawley's first example. The reason for the absence of the other secondary constraints in Eq.  $(4.69)$  is that the contribution of the strongly vanishing term  $yz^2/2$  to Dirac's contact transformation does not need to be considered. In other words, this strongly vanishing function has strongly vanishing Poisson brackets with the first-class constraints and the *D* operator constructed by the strongly vanishing function has weakly vanishing Poisson brackets with the differentiable (sometimes limited) functions on the constrained hypersurface. Consequently, in the sense of weak equality they at most are some trivial ''generators'' because they have not contributions for the trajectory or contact transformations. Hence they can be dropped.

It is very important and interesting how to determine the correct generalized Hamiltonian. To do this, we will propose an extended Dirac conjecture in the following section.

#### **F. The extended Dirac conjecture**

Under Dirac's contact transformation the physical observables are not changed, which implies

$$
\delta g_{\text{ph}} \approx \delta \theta_{m_0} D_{\phi_{m_0}} g_{\text{ph}} \approx 0. \tag{4.70}
$$

Because  $\delta \theta_{m_0}$  are completely independent one obtains

$$
D_{\phi_{m_0}} g_{\rm ph} {\approx} 0. \tag{4.71}
$$

Notice that

$$
[D_{\phi_{m_0}}, D_{H_T^D}] = D_{\{\phi_{m_0}, H_T^D\}} \approx b_{m_0}^{m_0'} D_{\phi_{m_0'}}.
$$
 (4.72)

Thus it is straightforward to derive

$$
D_{\phi_{m_0}} \dot{g}_{\text{ph}} \approx -D_{\phi_{m_0}} D_{H_T^D} g_{\text{ph}} \approx 0. \tag{4.73}
$$

Therefore the motion equation of the physical observables is also invariant under Dirac's contact transformation. Consequently, sometimes one calls Dirac's contact transformation the gauge transformation.

If we take Eq.  $(4.62)$  as the generating function of the infinitesimal contact transformation, it is easy to derive

$$
\widetilde{q}^i = q^i + \delta \theta_{m_0} \partial \phi_{m_0} / \partial p_i = (1 - \delta \theta_{m_0} D_{\phi_{m_0}}) q^i, \qquad (4.74a)
$$

$$
\widetilde{p_i} = p_i - \delta \theta_{m_0} \partial \phi_{m_0} / \partial q^i = (1 - \delta \theta_{m_0} D_{\phi_{m_0}}) p_i. \tag{4.74b}
$$

Without loss of generality,  $\delta \theta_{m_0}$  is supposed to be a time function and is free of the dynamics variable. Thus it can be verified that the new Hamiltonian under Dirac's infinitesimal contact transformation becomes

$$
H' = H^*(\eta) + v_\alpha \phi_\alpha + \partial F/\partial t = H^*(\eta) + v'_{m_0} \phi_{m_0}.
$$
\n(4.75)

Obviously when  $\delta \theta_{m_0} = \delta \lambda_{m_0}$ , it goes back to Eq. (4.41) and  $H' = H_T^D$ . However, for Dirac's contact transformation, the  $\delta\theta_{m_0}$  are completely independent of each other. This leads to the fact that the generalized Hamiltonian is constructed by only adding the terms of products of the arbitrary multiplier  $v_{m_0}$  and the constraints  $\phi_{m_0}$ :

$$
H_G = H^* + v_{m_0} \phi_{m_0},\tag{4.76}
$$

in which the  $\phi_{m_0}$  belong to the minimum evolution closed subalgebra of the first-class constraints. It is different from the usual extended Hamiltonian because  $\phi_{m_0}$  cannot generally exhaust all the first-class constraints. This is the extended Dirac conjecture proposed by us.

For example, in Cawley's first example, we know that there is only  $ap_y$  in the subalgebra of the MECPB of the first-class constraints. According to the extended Dirac conjecture we can write the generalized Hamiltonian as

$$
H_G = p_x p_z + v p_y. \tag{4.77}
$$

Although Dirac's conjecture fails in the above case, it is still applicable when the set of the minimum evolution closed subalgebra of the first-class constraints is the complete set of the first-class constraints. Many well-known theories belong to such cases. The Christ-Lee's model  $[33]$  is just so (see Appendix  $E$ ).

It is clear that under the above construction of the generalized Hamiltonian the physical sectors of singular systems are invariant or the gauge equivalence between the distinct total Hamiltonians with different multipliers is set up by virtue of Eqs.  $(4.71)$  and  $(4.73)$ .

It is necessary to emphasize that the motion equation is given by  $H_G$  and we need the gauge conditions as well as the gauge fixing conditions so as to return to the physical sector. This is shown in Sec. VI.

Obviously, the extended Dirac conjecture is applicable to Cawley's first example. From our analyses and demonstration the foundation of the extended Dirac conjecture is the finite Dirac contact transformation. We have shown clearly that only the elements of the minimum evolution closed subalgebra of the first-class constraints are able to become the generators of Dirac's contact transformation or the gauge transformation which does not change the physical observables and their motions. As a conclusion the extended Dirac conjecture can be thought to have been proved and is naturally acceptable.

It is worth pointing out that the extended Dirac conjecture is still applicable to those cases in which the Hamiltonian is not differentiable or Dirac's algorithm does not give rise to all the constraints (see Sec. V). But we are bound not to take Dirac's total Hamiltonian but have to use the final Hamiltonian. The latter is given by the extended consistency conditions, as the evolution generating function. Moreover, in these cases, the minimum evolution closed subalgebra involves at least all primary first-class constraints which appear in the final total Hamiltonian together with arbitrary and undetermined multipliers, and it has the closed Poisson bracket algebra between its elements and the final total Hamiltonian. These problems will be dealt with in the following section. If all constraints are generated by our extended consistency conditions, we find that Cawley's second and Frenkel's examples are no longer counterexamples of Dirac's conjecture. In addition, the extended Dirac conjecture is applicable to them.

## **V. FROM DIRAC'S CONSISTENCY CONDITIONS TO HAMILTONIZATION OF THE SINGULAR SYSTEM WITH HESSIAN VARIABLE RANK**

Generally speaking, the stability of the constrained hypersurface is a necessary condition so that the Hamiltonian dynamics in singular systems can be completely determined. In Sec. III, we have seen that, for Cawley's second example, since the term  $\lambda p_z$  is not equal to zero but is arbitrary on  $\Gamma_C^D$ , the functions of the variables on phase space at *t* time are not determined completely by the function value of initial time  $t_0$ . The reason for this is that in singular systems with Hessian variable rank Dirac's primary constraints cannot, in general, be all main branches generating all the secondary constraints. In other words, the new constraints may appear in the other branches and then they may break the requirement of stability of the constrained hypersurface. Hence it seems to us that Dirac's original consistency conditions are not enough to generate all constraints and guarantee the stability of the constraint hypersurface  $\Gamma_C^D$ . It is inconsistent with the origin of Dirac's physical idea of the consistency condition.

In fact, in order to keep the complete determination of Hamiltonian dynamics of singular systems with Hessian variable rank, we have reason to conjecture, or have to assume that, for all the functions which are weakly equal to zero, their evolution in time should preserve the weakly vanishing property. It is a natural conclusion from Dirac's physical idea of the stability of the constrained hypersurface. That is, their arbitrary-order time derivatives are always weakly equal to zero. This is just an extension of Dirac's original consistency conditions.

#### **A. Generation of new constraints in Cawley's second example**

To verify our above point of view, let us start by studying a concrete example—Cawley's second example. In terms of our extended consistency conditions, the second time derivation of the weakly vanishing function 2*xz* is bound to be weakly equal to zero, that is,

$$
\frac{d^2}{dt^2}(2xz) \approx p_z \approx 0. \tag{5.1}
$$

Hence we obtain that  $p<sub>z</sub>$  is a new constraint. Of course, we also have to use the consistency conditions to each new constraint; moreover, again we use them to generate each newer constraint step by step until no more constraints are obtained. So the constraint  $p<sub>z</sub>$  ought to obey

$$
\dot{p}_z \approx \{p_z, H_T\} = y, \quad \dot{y} \approx \{y, H_T\} = v. \tag{5.2}
$$

So another new constraint is then generated and the multiplier *v* is determined as

$$
y \approx 0, \quad v \approx 0. \tag{5.3}
$$

When Eqs.  $(5.1)$  and  $(5.3)$  are satisfied, obviously the canonical equations of motion  $(2.32)$  are equivalent to the original  $E-L$  equations  $(2.25)$ . On the final constrained hypersurface  $\Gamma_C^F$  determined by all constraints  $(2.28)$ ,  $(2.30)$ ,  $(5.1)$ , and  $(5.3)$ , there is no condition which can determine the limit of  $p_z / p_x^{1/2}$ . Thus Eq. (2.32a) indicates that the motion in the *x* direction is undetermined, or arbitrary.

Making use of Eqs.  $(5.2)$  and noting  $v$  to be a differentiable function we have

$$
yz \approx 0, \quad vp_y \approx 0. \tag{5.4}
$$

Therefore we can rewrite the final total Hamiltonian in the form

$$
H_T^F \simeq (p_z p_x^{-1/2}) p_x. \tag{5.5}
$$

It is easy to show that the correct canonical equations of motion are generated by it.

It is interesting that the increase of the number of constraints may result in some first-class constraints changing to second-class ones because these original first-class constraints probably have nonvanishing Poisson brackets with some of the new constraints. For instance, in Cawley's second example, in the new complete set of constraints generated by our algorithm, there is only one first-class constraint,  $p_x \approx 0$ ; the others are second-class ones. According to Dirac's conjecture, this could effect the determination of the extended Hamiltonian; namely, only  $p_x$  is thought to be a generator of gauge transformations. Thus the extended Hamiltonian is

However, since we have not a first-class primary constraint, this conclusion cannot be given by Dirac's infinitesimal contact transformations. Similarly, it cannot be obtained in terms of Dirac's test suggested by Cawley. Formally, Dirac's conjecture does not fail for Cawley's second example since it gives the same motion as that in the Lagrangian formalism. However, Eq.  $(5.6)$  is not fully appropriate when gauge conditions are taken, which can be seen in Sec. VI. In addition, for Frenkel's example we can discuss it similarly and we have the same conclusion. It seems to us that the correct construction of the generalized Hamiltonian ought to be obtained from the extended Dirac conjecture. Obviously, the subalgebra of the MECPB of the first-class constraints is null in Cawley's second example. Hence its final total Hamiltonian is the same as its generalized Hamiltonian.

In his paper, Cawley also gave the above new constraints, which were called ''subsecondary'' ones. But he used the so-called ''sanitization'' method, that is, by imposing a subsecondary constraint  $p_{z} \approx 0$ , so that the motion of *x* is improved [18]. His idea may be acceptable, but limited and incomplete. We need to find the inherent physical causes and the general principle or method.

### **B. The extension of Dirac's algorithm**

For a singular Lagrangian system, without loss of generality*,* the independent weakly vanishing functions on the constrained hypersurface  $\Gamma_C^D$  can be written as [4,13]

$$
C_j^a = A^a(x,p)\phi_j(x,p) \approx 0, \quad A^a(x,p)|_{\Gamma_C} D \neq 0, \infty,
$$
\n(5.7)

where  $\phi_i$  take over all the constraints in Dirac's original algorithm, and  $A^a$  are functionally independent for various indices *a*. Actually, one expands  $C_j^a$  on the constrained hypersurface and uses the property that the various constraints are functionally independent of each other, and then can obtain Eq.  $(5.7)$ . In Ref. [16], this relation is shown in detail by the relation theorem on weak equality and strong equality. It must be emphasized that the higher power terms of constraints need not be considered because they strongly vanish. The reason and argument can be found in Ref.  $|13|$ . Even though one considers the higher power terms of the constraints, the conclusion is the same.

It must be noted that *A<sup>a</sup>* is taken on the constrained hypersurface. According to Ref.  $[13]$ , one can transform all of the old  $2n$  variables on phase space to  $2n$  new variables  $\psi_m$  (*m* = 1,...,*m*) and  $\kappa^{\overline{\mu}}$  ( $\overline{\mu} = \mu + 1, \dots, 2n$ ) in which  $\psi_m$  takes over all the constraints. Thus, without loss of generality, *A*<sup>*a*</sup> can be taken as  $\kappa^{\overline{\mu}}$ .

Suppose that in the system there exist

$$
D_{H_T}^{k+1} A^a |_{\Gamma_C^D} = \infty \quad (k = 0, 1, 2, \dots) \tag{5.8}
$$

where the  $D$  operator is defined as in Eq.  $(3.2)$ . It means that  $\partial^k H_T / \partial \eta^{\mu k}$  is not *k* order differentiable with respect to  $\eta^{\nu}$ . If we only have Dirac's original consistency conditions

$$
d^n \phi_j / dt^n |_{\Gamma_C^D} = 0 \quad (n = 1, 2, ...)
$$
 (5.9)

we cannot guarantee

$$
d^{k+1}C_j^a/dt^{k+1}|\Gamma_C^b(-)^{k+1}(D_{H_T}^{k+1}A^a)\phi_j \qquad (5.10)
$$

vanishing weakly since the right side of Eq.  $(5.9)$  is  $\infty \times 0$ . We also cannot remove the case

$$
d^{k'}C_j^a/dt^k|_{\Gamma_C^D} \neq 0 \quad (k' > k+1). \tag{5.11}
$$

It follows that the weakly vanishing functions  $C_j^a$  on  $\Gamma_C^D$  no longer preserve the weakly vanishing property in time or  $\Gamma_C^D$  is unstable in time. Thus, because the canonical motion equations in the constrained dynamics are written in the form of a weak equality, the Hamiltonian formalism appears inconsistent. In other words, the time higher order derivatives of the function on phase space cannot be calculated exactly and the evolution trajectory in time of the function of the phase space variables cannot be determined completely. This problem has been seen from Cawley's second example in Sec. III B. This inconsistency has to be eliminated. Therefore, we necessarily propose extended consistency conditions, that is, all the weakly vanishing functions also have to preserve the weakly vanishing property in time. This implies that any  $C_j^a$  defined by Eq.  $(5.7)$  obeys

$$
d^{n}C_{j}^{a}/dt^{n} \approx 0 \quad (n=1,2,...).
$$
 (5.12)

But here the ''weakly vanishing'' means to be equal to zero on the final constrained hypersurface. It is similar to the requirement for all the constraints to be weakly equal to zero on  $\Gamma_C^D$  in Dirac's algorithm and thus it is acceptable physically. When the constrained system has no such *A<sup>a</sup>* obeyed by  $(5.8)$ , the extended consistency conditions will return to Dirac's original consistency conditions. However, when the cases  $(5.10)$  occur, the extended consistency conditions will be needed so as to eliminate the inconsistency and generate new constraints. In fact, we have applied the extended consistency conditions successfully to Cawley's second example in Sec. V A by requiring  $2xz$  or  $2xp_x^{1/2}$  to preserve the weakly vanishing property in time. Further discussion can be seen in Sec. V C. Generally speaking, if the right side of Eq.  $(5.10)$  is a function it should vanish weakly in terms of the extended consistency conditions

$$
(D_{H_T}^{k+1}A^a)\phi_j \approx 0. \tag{5.13}
$$

It is a limit of  $0/0$  on  $\Gamma_C^D$  and thus may, generally, generate new constraints. We also have to require all the new constraints to preserve the weakly vanishing property in time and, as usual, this may give rise to more new constraints. If the right side of (5.10) is a constant on  $\Gamma_C^D$ , it implies that the system shows the inconsistency  $0=1$ . Such a system is not interesting according to Dirac  $[1]$ .

Similar to using Dirac's original consistency conditions  $[1]$  we generate constraints in terms of the extended consistency conditions. First, we take  $A^a$  as a constant and require  $C_j^a$  to preserve the weakly vanishing property in time. It is just Dirac's original algorithm. Second, if there exist such phase space variables that the  $k+1$  order partial derivatives of the total Hamiltonian with respect to them are infinite, *A<sup>a</sup>* are respectively taken as their canonical conjugate vari-

ables. We require  $C_j^a = A^a \phi_j$  to satisfy (5.12). Obviously the requirement can generally lead to the generation of new constraints.

This process ends when no more new constraints are generated and/or no more new multiplier equations are given. It is worth pointing out that on the new constrained hypersurface determined by the new complete set of constraints, there is no longer such  $A^a$  so that the cases  $(5.8)$  can appear. Consequently, when the linear combinations of all the constraints, involving the new constraints, are preserved in time, that is, the arbitrary-order time derivatives of the weakly vanishing functions are still weakly equal to zero, the extended consistency conditions are satisfied on the new constrained hypersurface.

More generally, if there still exist the cases such as Eqs.  $(5.12)$ , the process of generation of the constraints does not end generally and we have to require again the higher stage extended consistency conditions. These processes will end at a finite number of steps, at least in systems with finite degrees of freedom and contradictory relations such as  $1 \approx 0$ will not occur. Otherwise the original Lagrangian equations are inconsistent  $[1]$ .

After all the constraints are generated, we have to determine which constraints belong to the first class and which constraints belong to the second class. Then in terms of the well-known Dirac method and extended consistency conditions we can obtain the final Hamiltonian. Moreover, if we need the generalized Hamiltonian, we still must apply the extended Dirac conjecture.

### **C. Study of the general case**

Now, we generally study those systems in which there are some independent  $A^a$  satisfied by  $(5.8)$ . For Cawley's second example such  $A^a$  is only *x*. The existence of such  $A^a$  implies that the total Hamiltonian is not differentiable with respect to some phase space variables. This feature exists in singular Lagrangian system with Hessian variable rank (see Sec.  $III$  B).

In order to Hamiltonize general singular systems with varying rank Hessian matrix we assume all the primarily expressible velocities  $q^{\sigma}$  [13] can be expressed finally as finite functions of the variables  $q, p<sub>\sigma</sub>$  on phase space as well as the multipliers  $(\dot{q}^A)$ , or say their limits always exist on the final constrained submanifold  $\Gamma_C^F$ . The reason for making this assumption is that *the inherently infinite motion has no physical significance*. For example, in the Cawley's example above,  $\dot{x} = p_z/2p_x^{1/2}$  is infinite on  $\Gamma_C^D$  but because there is another constraint  $p_z \approx 0$  one can think its limit, a finite function, exists on  $\Gamma_C^F$ . In fact, this assumption is required so that the primary constraints can be turned to Hamiltonian ones.

Returning to Sec. III B, if det $\|W_{\sigma\rho}\|_{\Gamma_C^D} = 0$ , it implies that some rows or columns of  $(W_{\sigma\rho})$  are either weakly vanishing or linearly dependent on  $\Gamma_C^D$ . For the latter we can make an invertible elementary transformation *P* so that some rows or columns of  $(PW)_{\sigma\rho}$  vanish on  $\Gamma_C^D$ . Without loss of generality, suppose *L* rows of  $PW_{\sigma\rho}$  weakly vanish on  $\Gamma_C^D$ , in which  $L = r - r'$  while *r'* is the rank of  $W_{\sigma \rho}$  on  $\Gamma_C^D$ . Equivalently, there are *L* null eigenvectors  $\lambda_\sigma^{(l)}$  for  $\|\tilde{W}_{\sigma\rho}\|$  on  $\Gamma_C^D$ , that is,

$$
\overline{W}_{l\rho}(q,\dot{q}) \equiv \sum_{\sigma} \lambda_{\sigma}^{(l)}(q,\dot{q}) W_{\sigma\rho}(q,\dot{q}) \big|_{\Gamma_C^{D}} = 0
$$
\n
$$
(l = 1,2, \dots, L). \quad (5.14)
$$

Obviously  $\overline{W}_{l\rho}$  *only* depends on *some* velocities  $\dot{q}^{A'}$  at most Obviously  $W_{l\rho}$  *only* depends on *some* velocities  $q^2$  at most<br>in a weakly dependent sense, that is,  $\partial \overline{W}_{l\rho} / \partial \dot{q}^{A'} \approx 0$ . Otherin a weakly dependent sense, that is,  $\partial W_{l\rho}/\partial q^{\alpha} \approx 0$ . Otherwise  $\overline{W}_{l\rho}$  is not weakly equal to zero if there is no other condition(s). Thus from Eq.  $(5.14)$  we have

$$
\overline{W}_{l\rho} \approx 0, \qquad (5.15a)
$$

$$
\overline{W}_{IA} = \lambda_{\sigma}^{(l)} W_{\sigma A} = \lambda_{\sigma}^{(l)} W_{\sigma \rho} (\partial \psi_A / \partial p_{\rho}) \approx 0 \quad (l = 1, \dots, L).
$$
\n(5.15b)

It is easily seen that  $\overline{W}_{l\rho}$  can be expressed as a function of  $q$ , $p<sub>\sigma</sub>$ , and  $\dot{q}^A$  in terms of Eq. (3.16). Of course, by virtue of the motion equations we obtain

$$
\gamma_l(q,\dot{q}) \equiv \sum_i \lambda_{\sigma}^{(l)}(q,\dot{q}) K_{\sigma}(q,\dot{q}) \big|_{\Gamma_C^{D}} = 0 \quad (l = 1,2,\ldots,L). \tag{5.16}
$$

According to Dirac's idea and the reasons stated above, it is very natural to require them to be preserved in time, that is, we need the extended consistency conditions. In fact, in Ref. 16 Sudarshan and Mukunda did just that in Lagrangian formalism as stated above (see Appendix F). But Sudarshan and Mukunda only required that the constraint equa $tions$   $(5.16)$  were preserved in time. In Lagrangian formalism, in general,  $\overline{W}_{li}q^j$  and  $\overline{W}_{li}q^j$  can be regarded as a linear combination of Lagrangian constraints. Thus in terms of the motion equations generally one cannot get the fact that some velocities  $\dot{q}^a$  tend to infinity. In other words, the time some velocities  $q^u$  tend to infinity. In other words, the time derivatives of  $\overline{W}_{li}$  are finite and thus the evolution of them in time does not give new independent constraints. Therefore, S-M's approach has no problem. However, in Hamiltonian formalism, the case is a little complex because we generally formalism, the case is a little complex because we generally cannot express  $\overline{W}_{li}q^j$  and  $\overline{W}_{li}q^j$  as a linear combination of the Hamiltonian constraints which are defined on  $\Gamma_C^D$ . For instance, in Cawley's second example,  $W_{31}x = 2z\dot{x} = p_z$  is just so. Although in Lagrangian formalism it is zero since the constraint  $\dot{z} = 0$ , in Hamiltonian formalism we do not know it to be zero on  $\Gamma_C^D$  in the Dirac-Bergmann algorithm. It is a little similar to the fact that in general one need not write explicitly the primary constraints in Lagrangian formalism but one needs to clearly give them in Hamiltonian formalbut one needs to clearly give them in Hamiltonian formal-<br>ism. So we have to require generally  $\overline{W}_{li}q^j \approx 0$  to be preserved in time, that is,

$$
\frac{d}{dt}(\overline{W}_{li}q^j) \approx \dot{\overline{W}}_{li}q^j + \overline{W}_{li}\dot{q}^j \approx 0.
$$
 (5.17)

Of course we also have  $\dot{\overline{W}}_{li} \approx 0$ . Because some of the velocities are infinite on  $\Gamma_C^D$  Eq. (5.17) may give rise to new constraints and/or new equations about the  $\dot{q}^A$ . Thus it can be rewritten as

$$
\dot{\overline{W}}_{li} \approx 0, \quad \overline{W}_{li}\dot{q}^j \approx 0. \tag{5.18}
$$

Furthermore, to require similarly

$$
\ddot{W}_{li} \approx 0, \quad \frac{d^2}{dt^2} (\overline{W}_{li} q^j) \approx \ddot{W}_{li} q^j + 2 \dot{\overline{W}}_{li} \dot{q}^j + \overline{W}_{li} \ddot{q}^j \approx 0,
$$
\n(5.19a)

$$
\frac{d}{dt}(\overline{W}_{li}\dot{q}^j) = \dot{\overline{W}}_{li}\dot{q}^j + \overline{W}_{li}\ddot{q}^j \approx 0, \qquad (5.19b)
$$

we have

$$
\dot{\overline{W}}_{li} \approx 0, \quad \overline{\overline{W}}_{li} \dot{q}^j \approx 0, \quad \overline{W}_{li} \ddot{q}^j \approx 0. \tag{5.20}
$$

Obviously they may lead to new constraints and/or multiplier solutions,

$$
\overline{W}_{li}\ddot{q}^i = \gamma_l(q,\dot{q}) \equiv \sum_i \lambda_{\sigma}^{(l)}(q,\dot{q}) K_{\sigma}(q,\dot{q})|_{\Gamma_C^{D}} \approx 0.
$$
\n(5.21)

We have to check continually whether Eqs.  $(5.21)$  are preserved in time. In fact, it is the same as the steps taken by S-M's approach in Lagrangian formalism, that is,  $\gamma_l$  in Eqs.  $(5.21)$  is required to preserve the weakly vanishing property. In other words, all new constraints, which originate from Hessian variable rank, as new main branches generating the secondary constraints, are obtained by our extended consistency conditions. This means that our algorithm of the extended consistency conditions involves the steps of Sudarshan-Mukunda's approach. Therefore, for a singular system with Hessian variable rank, if Sudarshan-Mukunda's approach is applicable our algorithm is also applicable.

For all new constraints generated by the above steps, we have to require them to obey the consistency conditions, namely, their time derivatives are weakly vanishing. As usual, each derivation of them may give rise to more new constraints. This process is ended when no more new constraints are generated and/or no more new multiplier solutions are given. More generally, if there still exists the case of a Hessian matrix with varying rank on  $\Gamma'$  determined by all above new and old constraints, we have to further repeat the above process so that more and newer constraints are generated till the Hessian matrix has no longer a variable rank on the final constrained submanifold  $\Gamma_C^{\bar{F}}$ . These processes must end in finite steps for a system with a finite number of degrees of freedom, and the contradictory relation  $1 \approx 0$  will not occur. Otherwise the original Lagrangian (equations) must be inconsistent.

Comparable with Sudarshan and Mukunda's method  $[16]$ of treating the system with Hessian variable rank in Lagrangian formalism we can say all corresponding Lagrangian constraints are generated by the above processes. It is very important and interesting that the above processes can be determined from the requirement that for each process the determined from the requirement that for each process the constrained functions  $\overline{W}_{li}$  and  $\overline{W}_{li}q^j$  which vanish in the constrained submanifold preserve the weakly vanishing property in time. We call them the extended consistency conditions.

time. We call them the extended consistency conditions.<br>As stated above,  $\overline{W}_{li}$  can be expressed as functions of  $q^i$ and  $p_{\sigma}$  and the multipliers as functions of time, and consequently all the new constraints, which are generated in terms of Hamiltonian (canonical) motion equations and the extended consistency conditions, are Hamiltonian ones. Therefore our algorithm is proposed in Hamiltonian formalism and is a development of Sudarshan-Mukunda's approach along with the Hamiltonian formalism. Of course, the previous assumption in Sec. III B is necessary.

mption in Sec. III B is necessary.<br>Actually, the constrained functions  $\overline{W}_{li}$  and  $\overline{W}_{li}q^j$  can be expanded as a linear combination of the independent weakly vanishing functions  $C_j^a$  defined by (5.7). The higher power of  $C_j^a$  can be absorbed into the combination coefficients [13]. Therefore the extended consistency conditions can also be Therefore the extended consistency conditions can also be expressed as the evolution of the constrained functions  $\overline{W}_{li}$ expressed as the evolution of the constrained functions  $W_{li}$  and  $\overline{W}_{li}q^j$  preserves the weakly vanishing property in time. This is the same as the method proposed in Sec. V B. In addition, in some situations, we can slightly loosen our assumption, that is, we only assume that Dirac's total Hamiltonian of the system with Hessian variable rank is known. Thus we can directly use the algorithm of the extended consistency conditions to generate new constraints and obtain the final total and the generalized Hamiltonian according to the method described in Sec. V B.

## **VI. FROM BERGMANN'S PHYSICAL REQUIREMENT TO THE GAUGE CONDITIONS**

The invariance of the Lagrangian under gauge transformation implies that Lagrangian is singular, i.e., the determinant of its Hessian matrix vanishes  $[4,16]$ . By virtue of the Dirac-Bergmann algorithm  $\lfloor 1,2 \rfloor$ , one can pass from the singular Lagrangian formalism to the Hamiltonian formalism. Since the coordinates and momenta turn out not to be independent in a constrained system, only a submanifold of phase space is relevant to the Hamiltonian description of this system. This submanifold is called the constrained submanifold and it is determined by all of the constrained equations [4,13]. However, the submanifold still contains the gauge variables; one needs to introduce such a reduction process that the gauge variables may be eliminated and then the reduced phase space can be obtained. As is well known, in this process one has to determine the number and form of gauge conditions so as to identify the physical reduced space and give the definition of physical observables on it. In fact, it is necessary for the quantization of constrained systems  $[1-4,13]$ .

#### **A. The definition of physical observables**

It is important that Bergmann proposed a physical requirement  $[2]$ : the physical observables, i.e., the gauge invariant quantities, are determined fully by the dynamics equations and the initial conditions. It means that the physical observables do not depend on the arbitrary functions (Lagrangian multipliers). Only in this sense can they be measured in principle by experiment. Obviously, Bergmann's physical requirement is truly essential and naturally acceptable. However, in systems with constraints or singular Lagrangian systems, one usually thinks that a physical observable *F* is defined implicitly by the conditions  $[4,11-13]$ 

$$
\{F, \psi_j\} \approx 0,\tag{6.1}
$$

where  $\psi_i$  take over all constraints in constrained systems. For a general singular system, the definition  $(6.1)$  seems not to work. In fact, the definition  $(6.1)$  is only a conjecture based on Dirac's algorithm. In Dirac's paper  $[1]$  and the current literature  $[15]$ , the explicit expression of evolution of the phase space function in time is not derived. Only according to the behavior of the second time derivative of the function does one conjecture the definition  $(1)$  of the physical observables.

In his well-known work  $[1]$ , Dirac assumed that there is an initial physical state independent of the arbitrary multipliers  $v_\alpha$ . At time  $t_0$ , suppose the constrained system is at the initial physical state. Thus, if we require that the function  $g(\eta)$  is free of arbitrary multipliers at any time, the coefficients of the terms related to the arbitrary multipliers  $v_{\alpha}$  in Eq.  $(3.7)$  will be weakly equal to zero, that is,

$$
D_{H^{*}}^{n_{m}}\left(\prod_{s=0}^{m-1} D_{\phi_{\alpha_{m-s}}} D_{H^{*}}^{n_{m-s-1}-k_{m-s}-1}\right) g \approx 0.
$$
 (6.2)

This relation shows how the multiple operator *D* acts on *g*. It is always possible that by changing the action order the right side of Eq.  $(6.2)$  could be rewritten as Eq.  $(3.8)$ . It follows, as stated in Sec. III, that *g* satisfies

$$
D_{\phi_{m_0}} g \approx 0 \tag{6.3}
$$

by using the exchange theorem of the  $D$  operator  $(3.6)$  and the first-class property of  $H^*$ . Therefore Eq.  $(6.3)$  is enough to eliminate the dependence of *g* on the arbitrary multipliers at any time. In fact, we also can obtain  $(6.3)$  in terms of the finite Dirac contact transformation or gauge transformation  $(4.56)$  based on the invariance of the physical observables.

In addition, the physical observables should be chosen on the constrained hypersurface and then they have vanishing Poisson brackets with all the second-class constraints since all of the second-class constraints can be expressed as a set of canonical conjugate pairs in the locally equivalent sense [13], that is,

$$
D_{\Omega_s} g \approx 0. \tag{6.4}
$$

Alternatively, Dirac's brackets can be used if one allows the constraints to appear in the physical observables formally  $|13|$ .

Returning to the accustomed definition  $(6.1)$  of the physical observables, we find that it is not appropriate and universal in general singular Lagrangian systems since it may impose too many and too strict restrictions, which may make the physical sector of the constrained system change or even lose the physical observables. This can be seen more clearly in Sec. VI D. Hence, we have to give a corrected definition of the physical observables. As stated above and in Sec. III A, it is shown that the physical observables have weakly vanishing Poisson brackets with  $\phi_{m_0}$ , and also with all the second-class constraints  $\Omega_s$  according to Bergmann's physical requirement,

$$
\{F, \phi_{m_0}\} \approx 0, \quad \{F, \Omega_s\} \approx 0. \tag{6.5}
$$

In fact, the difference between the definitions of physical observables  $(6.1)$  and  $(6.5)$  is not trivial because they result, respectively, in the distinct gauge conditions in some general gauge theories. This can been seen in the following section.

### **B. The gauge conditions**

In order to relate the corrected definition  $(6.5)$  of the physical observables to the origin of gauge conditions, we rewrite Eq.  $(6.5)$  as a system of linear partial differential equations,

$$
A_{m_0\mu} \frac{\partial g}{\partial \eta^{\mu}} \approx 0, \quad A_{m_0\mu} \equiv \{ \phi_{m_0}, \eta^{\mu} \}. \tag{6.6}
$$

Because all of the  $\phi_{m_0}$  are functionally independent of each other,  $A_{m_0\mu}$  has the maximum rank, which is equal to the number of elements of the minimum evolution closed subalgebra of the first-class constraints.

Let us instead of  $\phi_{m_0}$  use  $\Phi_{m_0}$ ,

$$
\Phi_{m_0} \equiv \eta^{m_0} - f(\eta^{\bar{\mu}}) \approx 0, \qquad (6.7)
$$

in which  $\|\partial \phi_{m_0}/\partial \eta^{m_0}\|$  has the maximum rank and  $\eta^{\overline{\mu}}$  takes over the variables on phase space except  $\eta^{m_0}$ .  $\Phi_{m_0}$  is equivalent to  $\phi_{m_0}$  locally [13,34] and can be obtained in terms of the theorem on implicit functions from the constraints  $\phi_{m_0} \approx 0$ . By using the closed property (3.12) of  $\phi_{m_0}$  we have

$$
\{\Phi_{m_0}, \Phi_{m'_0}\} = 0. \tag{6.8}
$$

Thus  $\Phi_{m_0}$  can be chosen as a part of the generalized coordinates, or of the generalized momenta, or the mixing of them (without any pair of canonical conjugates) on phase space. To seek the other new variables on phase space, we can write the system of homogeneous linear partial differential equations of the first order as

$$
\{\Phi_{m_0}, K\} = 0. \tag{6.9}
$$

Obviously, it is a complete system. Therefore this system has  $2n-k$  independent solutions which involve all of the  $\phi_{m_0}$ whose number is supposed to be  $k$  [34]. We again choose a set of such functions  $\chi_{m_0}$  independent of  $\Phi_{m_0}$  so that

$$
\det \left\| \{ \Phi_{m_0}, \chi_{m'_0} \} \right\| \neq 0. \tag{6.10}
$$

It is easy to show that  $\chi_{m_0}$  also does not depend on *K* in Eq.  $(6.9)$ , otherwise Eq.  $(6.10)$  cannot be satisfied. Thus,  $2n$ phase space variables can be replaced by 2*n* new variables  $\kappa^{\mu} = (\Phi_{m_0}, \chi_{m_0}, K^{\sigma}, m_0 = 1, \ldots, k, \sigma = 2k+1, \ldots, 2n)$ . Consequently Eq.  $(6.5)$  becomes

$$
\partial g'(\kappa)/\partial \chi_{m_0} \approx 0, \quad g'(\kappa) = g(\eta). \tag{6.11}
$$

This means that *g*, as a function of new variables  $\kappa^{\mu}$ , is free of  $\chi_{m_0}$  in the weak equality sense. Obviously the general solution of Eq.  $(6.11)$  satisfies

$$
g'( \chi_{m_0} + b_{m_0}, \Phi_{m_0}, K^{\sigma}) \approx g'( \chi_{m_0}, \Phi_{m_0}, K^{\sigma}) \quad (6.12)
$$

because of the first-class property of  $\phi_{m_0}$ . In Eq. (6.12)  $b_{m_0}$  are the arbitrary functions on phase space. From the above Eq.  $(6.12)$ , it follows that the physical observables are invariant under translation transformation of  $\chi_{m_0}$ . Therefore we can choose gauge conditions as

$$
\chi_{m_0} = 0. \tag{6.13}
$$

This is just our corrected form of gauge conditions. Their number is the same as that of the constraints of the subalgebra of the MECPB of the first-class constraints but is not invariably equal to that of all the first-class constraints in general. This conclusion is important and nontrivial. It will result in the well-known difficulties in gauge reduction and quantization of gauge theories because there may be insufficient gauge conditions in general constrained systems. In other words, for the first-class constraint  $\phi_{\overline{m}} (\overline{m} \neq m_0)$  that does not belong to the minimum evolution closed subalgebra of the first-class constraints, one cannot choose such a corresponding gauge condition  $\chi_{m} = 0$  that the equation  $\det \left\{ \left( \phi_{\overline{m}}, \chi_{\overline{m}} \right\} \right\} \neq 0$  exists. In fact, the accustomed physical reduced phase space may no longer be of even dimensions generally and we do not know how to write out the measure in path integral quantization. Cawley's examples  $[17,18]$  discussed in the following are just simple examples.

Therefore a new subject worth studying, the quantization for general singular Lagrangian theories, appears. The quantization of the type of the gauge theories needs restudying on a new footing. We believe that some interesting results will be derived and this is an aim in our future papers.

### **C. A simple example**

A simple case is Cawley's counterexample for Dirac's conjecture  $[1]$ . Let us take the combination of his two examples  $\lceil 17,18 \rceil$  and write the Lagrangian as

$$
L = \dot{x}_1 \dot{z}_1 + y_1 z_1^2 / 2 + \dot{x}_2 \dot{z}_2^2 + y_2 z_2. \tag{6.14}
$$

This example is a singular system with both the proper subalgebra of the MECPB of the first class and Hessian variable rank. One readily obtains the Euler-Lagrange equations

$$
\ddot{z}_1 = 0
$$
,  $z_1^2/2 = 0$ ,  $\ddot{x}_1 = y_1 z_1$ , (6.15a)

$$
\frac{d}{dt}\dot{z}_2^2 = 0, \quad z_2 = 0, \quad \frac{d}{dt}(2\dot{x}_2\dot{z}_2) - y_2 = 0.
$$
 (6.15b)

Hence they describe a motion that is limited to the  $x_1 - y_1$ plane and on the  $x_2$  axis  $(z_1 = y_2 = z_2 = 0)$ . The velocity in the  $x_1$  direction is uniform while the motion in the  $y_1$  and  $x<sub>2</sub>$  directions is arbitrary or undetermined. In terms of Dirac's algorithm, the primary constraint is given by  $p_{y_1} \approx 0$ ,  $p_{y_2} \approx 0$ . It is straightforward to derive secondary constraints similar to Eqs.  $(2.20)$  and  $(2.30)$ . They can be rewritten as the canonical or linearly and functionally independent forms  $z_1 \approx 0$ ,  $p_{x_1} \approx 0$ ,  $z_2 \approx 0$ , and  $p_{x_2} \approx 0$ . Thus since  $z^2 \approx 0$ , one obtains Dirac's total Hamiltonian

$$
H_T^D \simeq p_{x_1} p_{z_1} + v_1 p_{y_1} + p_{x_2}^{1/2} p_{z_2} - y_2 z_2 + v_2 p_{y_2}. \quad (6.16)
$$

Obviously, all the constraints by Dirac's algorithm are first class. If we make use of the accustomed definition  $(6.1)$  of the physical observables, this system has no physical degrees of freedom. In other words, the physical reduced phase space is zero dimensional. In fact, Dirac's conjecture may be coming from the definition  $(6.1)$  to a great extent. Following the original idea of Dirac's conjecture we have the extended Hamiltonian

$$
H_E = u_1 p_{x_1} + v_1 p_{y_1} + w_1 z_1 + p_{x_2}^{1/2} p_{z_2} + u_2 p_{x_2} + v_2 p_{y_2} + w_2 z_2.
$$
\n(6.17)

It follows that the motions of this system in many directions are arbitrary, and particularly the  $x_2$  motion becomes infinite. In other words,  $x_1$ ,  $y_1$ , and  $p_{z_1}$  and  $x_2$ ,  $y_2$ , and  $p_{z_2}$  are all gauge freedoms in Dirac's original algorithm. However,  $x_1$ ,  $p_{z_1}$ ,  $x_2$ ,  $y_2$ ,  $z_2$ ,  $p_{x_2}$ , and  $p_{z_2}$  are originally physical; namely,  $x_1$  has a determined motion and  $x_2$  has an undetermined motion free of the choice of Lagrangian multiplier, while  $p_{z_1}$ ,  $y_2$ ,  $z_2$ ,  $p_{x_2}$ , and  $p_{z_2}$  are also some constants independent of Lagrangian multipliers. If one uses the extended Dirac Hamiltonian to generate the motion equations, even if one fixes the gauge, this system becomes static and does not return to the original physical motion. Consequently, the application of the definitions  $(6.1)$  may result in imposing too many and too strict restrictions on the physical observables. In other words, the physical degrees of freedom may be decreased and the gauge degrees of freedom may be increased unexpectedly in general singular systems. The final result is that the physical content of the theory is changed. Therefore Eq.  $(6.1)$  is not correct and universal.

Actually, because of the Hessian variable rank we have to apply the extended consistency condition. As in Sec. V A, we can obtain the new constraints  $p_{z_2} \approx 0$ ,  $y_2 \approx 0$ , and  $v_2 \approx 0$ . Thus the final total Hamiltonian can be written as

$$
H_T^F \approx p_{x_1} p_{z_1} + v_1 p_{y_1} + p_{x_2}^{1/2} p_{z_2}.
$$
 (6.18)

It is easy to verify that on the final constrained hypersurface the subalgebra of the MECPB of the first-class constraints only has an element  $p_{y_1}$ . From Eq.  $(6.5)$  it follows that the corrected definition of the physical observables is

$$
D_{p_{y_1}}g \approx 0. \tag{6.19}
$$

It implies that this system has only a gauge degree of freedom, and Dirac's contact transformation has only a gauge generator. The corrected generalized Hamiltonian should be constructed by our extended Dirac conjecture. Obviously, it is the same as the final total Hamiltonian in the form

$$
H_G \simeq H_T^F \simeq p_{x_1} p_{z_1} + v_{1} p_{y_1} + p_{x_2}^{1/2} p_{z_2}.
$$
 (6.20)

Of course, a simple choice of the gauge condition is

$$
\chi = y_1 = 0. \tag{6.21}
$$

It gives the same motion as in the Lagrangian formalism.

### **VII. CONCLUSIONS**

In this paper, we try to extend the Dirac-Bergmann theory of constrained systems so that it is applicable to more general singular systems, such as Cawley's first and second counterexamples, which have the feature of the proper subalgebra of the MECPB of the first-class constraints and Hessian variable rank, respectively. We derive the general expression of evolution of the function on phase space in terms the Taylor expansion method and the obvious expression of the finite Dirac contact transformation by virtue of time translation and trajectory transformation. They all indicate that only those first-class constraints belonging to the subalgebra of the MECPB have contributions to the evolution of the system. Therefore the generalized Hamiltonian is constructed by adding the linear combination of the arbitrary Lagrangian multipliers  $v_{m_0}$  and the elements  $\phi_{m_0}$  of the subalgebra of the MECPB of the first-class constraints, that is,  $v_{m_0} \phi_{m_0}$ . This is just the extended Dirac conjecture which is proposed and shown in this paper. For singular systems with Hessian variable rank, we find that, in terms of Dirac's consistency conditions only, the stability of the constrained hypersurface is not guaranteed. In other words, Dirac's original consistency conditions are not enough to generate all the secondary constraints. It seems to us that physically the constrained hypersurface is bound to be stable and so our extended consistency condition is proposed. It leads to generation of new constraints and stability of the constrained hypersurface. Hamiltonization of this kind of system is then realized and its dynamics in Hamiltonian formalism is equivalent to that of Lagrangian formalism. It is worth emphasizing that in many well-known cases, for example, QED and Yang-Mills theory, the minimum evolution closed subalgebra of the first-class constraints is just the complete evolution closed algebra of the first-class constraints, and they have not Hessian variable rank. It is clear that our conclusions are consistent with and go back to the accustomed Dirac-Bergmann algorithm in these cases. It is important and interesting that our results can be used for some more general singular Lagrangian systems with the proper subalgebra of the MECPB of the first-class constraints and/or with Hessian variable rank.

Finally, we would like to point out that in this paper we have finished the Hamiltonization for singular systems with the proper subalgebra of the MECPB of the first-class constraints and/or with Hessian variable rank, and obtained the choice of the gauge condition; however, how to carry out quantization of these singular systems is still an open question. Because, generally speaking, the number of gauge conditions can be less than one of the first-class constraints in these systems, we do not know how to write the correct measurement of path integral quantization. Our algorithm is to provide a tool for quantization of them. We believe that this question is very elementary and some interesting applications of our results can be found. Such work is in progress.

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#### **APPENDIX A**

Suppose the rank of the coefficient matrix for the unknown multipliers  $u_b$  in Eqs. (2.10) is *R*. When *R* is equal to  $n-r$ , which is the number of primary constraints, we can completely determine all multipliers. When  $R \leq n-r$ , there are  $n-r-R$  null eigenvectors  $\xi_A^{\alpha}$  so that

$$
\{\phi_A, \phi_B\} \xi_B^{\alpha} \approx 0, \tag{A1a}
$$

$$
\{\chi_k, \phi_B\} \xi_B^{\alpha} \approx 0, \tag{A1b}
$$

Consequently the  $n-r-R$  linear combinations of primary constraints such as Eq.  $(2.11)$  become the first-class ones, while the other independent linear combinations of primary constraints are secondary ones, denoted by  $\phi_{\beta}$ . We also can recombine linearly the secondary constraints (generally primary constraints may be involved) so that they become first class as far as possible; the remaining independent combinations must be the second class, and we denote them by  $\chi_a$ and  $\chi_b$ , respectively.

In constrained systems, Dirac's total Hamiltonian can only be determined in a strong equality sense. The symbol of the strong equality is denoted by  $\approx$ . If  $f_1 \approx f_2$ , then it means that

$$
\partial f_1 / \partial q^i \approx \partial f_2 / \partial q^i, \quad \partial f_1 / \partial p_i \approx \partial f_2 / \partial p_i. \tag{A2b}
$$

Normally, two functions being strongly equal means that both they and their corresponding partial derivatives with respect to the variables on phase space are weakly equal. Therefore the strongly vanishing term in the total Hamiltonian has no contribution to motion equations with the weak equality form. The following theorem on the relations between weak equality and strong equality can be demonstrated. When the hypersurface is determined by the equations  $\phi_i = 0$ , for the functions f and g whose second derivatives exist and are continuous (sometimes this can be slightly loosened) on the hypersurface, if  $f \approx g$ , then

$$
f(q,p) \approx g(q,p) + c_j \phi_j. \tag{A3}
$$

### **APPENDIX B**

The continuous and differentiable functions *A*, *B*, and *g* satisfy the Jacobi identity of the Poisson bracket,

$$
\{A, \{g, B\}\} = \{\{B, A\}, g\} - \{B, \{A, g\}\}.
$$
 (B1)

Therefore Eq.  $(3.6b)$  is valid for  $n=1$ . Assuming that the equation also is valid for *n*, we have for  $n+1$ 

$$
\{A,\{\cdots\{g,B\},\ldots,B\}\} = \{A,\{(\{\cdots\{g,B\},\ldots,B\}),B\}\}\
$$
  
=  $-\{B,\{A,(\{\cdots\{g,B\},\ldots,B\})\}\} + \{\{B,A\},(\{\cdots\{g,B\},\ldots,B\})\}\}$   
=  $\sum_{m=0}^{n} (-)^{n+1+m} C_n^m \{B,\ldots,\{B,\{(\{B,\ldots,\{B,A\}\cdots\}),g\}\}\cdots\}$   

$$
+\sum_{m=1}^{n+1} (-)^{n+1+m} C_n^{m-1} \{B,\ldots,\{B,\{(\{B,\ldots,\{B,A\}\cdots\}),g\}\}\cdots\}.
$$
 (B2)

In terms of the relation

$$
C_{n+1}^m = C_n^m + C_n^{m-1}
$$
 (B3)

we obtain

$$
\{A,\{\cdots\{g,B\},\cdots,B\}\} = \sum_{m=0}^{n+1} (-)^{n+1+m} C_{n+1}^m \{B,\cdots,B,\{(\{B,\ldots,[B,A\}\cdots\}),g\}\}\ldots\}.
$$
 (B4)

Thus Eq.  $(3.6b)$  is proved.

### **APPENDIX C**

In terms of Eq.  $(3.6)$  we can obtain

$$
\frac{d^n}{dt^n} g(q,p) \approx \frac{d^{n-1}}{dt^{n-1}} (\{g, H^*\} + v_\alpha \{g, \phi_\alpha\})
$$
\n
$$
\approx \{ \cdots \{g, H^*\}, \cdots, H^*\} + \sum_{k=0}^{n-1} \sum_{\alpha=1}^K \frac{d^k}{dt^k} (v_\alpha \{ \{ \cdots \{g, H^*\}, \cdots, H^*\}, \phi_\alpha \})
$$
\n(C1)

in which we have used the consistency condition  $[1]$ 

$$
\{H_T^D, \psi_j\} \approx 0\tag{C2}
$$

and assumed that the constraints do not have explicit time dependence and the number of primary first-class constraints is *K*. Making use of Leibniz's differential formula we continually calculate (C1) and can get

$$
\frac{d^n}{dt^n} g(q,p) \approx \{\cdots \{g,H^*\}, \ldots H^*\} + \sum_{k_1=0}^{n-1} \sum_{\alpha_1=1}^K \sum_{n_1=0}^{k_1} C_{k_1}^{n_1} v_{\alpha_1}^{(n_1-k_1)} \frac{d^{n_1}}{dt^{n_1}} (\{\cdots \{g,H^*\}, \ldots, H^*\}, \phi_{\alpha_1})\}
$$
\n
$$
\approx (-1)^n D_{H^*S}^n + \sum_{k_1=0}^{n-1} \sum_{\alpha_1=1}^K \sum_{n_1=0}^{k_1} C_{k_1}^{n_1} v_{\alpha_1}^{(n_1-k_1)} \frac{d^{n_1}}{dt^{n_1}} [(-)^{n_1-k_1} D_{\phi_{\alpha_1}} D_{H^*}^{n_1-k_1-1} g]
$$
\n
$$
\approx (-1)^n D_{H^*S}^n + \sum_{k_1=0}^{n-1} \sum_{\alpha_1=1}^K \sum_{n_1=0}^{k_1} C_{k_1}^{n_1} v_{\alpha_1}^{(n_1-k_1)} (-1)^{n_1} D_{H^*S}^{n_1} [(-)^{n_1-k_1} D_{\phi_{\alpha_1}} D_{H^*}^{n_1-k_1-1} g]
$$
\n
$$
+ \sum_{k_1=0}^{n-1} \sum_{\alpha_1=1}^K \sum_{n_1=0}^{k_1} \sum_{k_2=0}^{n_1-1} \sum_{\alpha_2=1}^K \sum_{n_2=0}^{k_2} C_{k_1}^{n_1} v_{\alpha_1}^{(n_1-k_1)} C_{k_2}^{n_2} v_{\alpha_2}^{(n_2-k_2)} \frac{d^{n_2}}{dt^{n_2}}
$$
\n
$$
\times [(-1)^{n_2-k_2} D_{\phi_{\alpha_2}} D_{H^*}^{n_2-k_2-1} (-)^{n_1-k_1} D_{\phi_{\alpha_1}} D_{H^*}^{n_1-k_1-1} g]. \tag{C3}
$$

 $\Gamma$ 

Likewise, by the successive iteration method, we can deduce Eq.  $(3.7)$ .

### **APPENDIX D**

Actually the time translation operator can be obtained by the product of a series of successive infinitesimal dynamics transformations,

$$
\eta^{\mu}(t+\delta t) \approx (1-\delta t D_{H_T^{D(t)}}) \eta^{\mu}(t), \qquad (D1)
$$

i.e., the time translation operator has the form

$$
U(t,t_0) \approx \lim_{\substack{t_N = t \\ N \to \infty}} \prod_{\substack{j=1 \\ \longrightarrow}}^N \left[ 1 - (t_j - t_{j-1}) D_{H_T^D(t_{j-1})} \right] \quad (D2)
$$

where  $\rightarrow$  refers to a successive product from left side to right side in turn. It can be written straightforwardly as

$$
U(t,t_0) \approx 1 - \int_{t_0}^t d\tau D_{H_T^{D_{(\tau)}}} U(\tau, t_0).
$$
 (D3)

When making use of the successive iteration method we have to be very careful. It can be shown by the exchange theorem that

$$
D_{f(t)}g(t) \approx \mathcal{D}_f(t)g(t') - \int_{t'}^{t} dt_1 \mathcal{D}_f(t)[D_{H_T^D + \epsilon}g](t_1),
$$
\n(D4a)

$$
\mathcal{D}_{f_1}(t)[D_{f_2(t')}g(t')] \approx \mathcal{D}_{f_1}(t)\mathcal{D}_{f_2}(t')g(t'')
$$

$$
-\int_{t''}^{t'} dt_2 \mathcal{D}_{f_1}(t)\mathcal{D}_{f_2}(t')
$$

$$
\times [D_{H_T^D + \epsilon}g](t_2), \qquad (D4b)
$$

where

$$
\mathcal{D}_f(t)g(t') \equiv \sum_{n=0}^{\infty} \frac{(t-t')^n}{n!} D_{X^n f(t')}g(t'), \quad (D5)
$$

$$
\mathcal{D}_{f_1}(t)\mathcal{D}_{f_2}(t')g(t'') = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(t-t')^n}{n!} \frac{(t'-t'')^n}{m!}
$$

$$
\times D_{X^n f(t'')} D_{X^m f(t'')} g(t'');
$$
 (D6)

similarly for the product of many  $\mathcal{D}'$ 's. The *X* operator is defined as

$$
X \equiv -D_{H^D_T + \epsilon}.\tag{D7}
$$

Obviously the  $D$  operator has the properties

$$
\mathcal{D}_f(t)g(t) = D_{f(t)}g(t), \quad \mathcal{D}_f(t)t' = 0,
$$
 (D8)

$$
\mathcal{D}_f(t) \approx \sum_{n=0}^{\infty} \frac{(t-t')^n}{n!} \mathcal{D}_{X^n f}(t') \approx \mathcal{D}_f(t') + \int_{t'}^t d\tau \mathcal{D}_{Xf}(\tau).
$$
\n(D9)

Thus the successive iteration method is applicable. For a function which does not relate to time explicitly, the time translation operator acting on it has the form of Eqs.  $(4.8)$ and  $(4.9)$ .

### **APPENDIX E**

Let us start from the Christ-Lee model [33]. Its Lagrangian is

$$
L = [r^2 + r^2(\dot{\theta} - \xi)^2]/2 - V(r).
$$
 (E1)

The advantage of this example is that its invariant group has common features with the QCD or QED gauge groups, that is, their elements involve an arbitrary function on *t.* Under such transformations as

$$
\theta \to \theta + \alpha(t), \quad \xi \to \xi + \dot{\alpha}(t), \tag{E2}
$$

Lagrangian  $(E1)$  is invariant.

Defining the conjugate momenta

$$
p_r = \dot{r}, \quad p_\theta = r^2(\dot{\theta} - \xi), \quad p_\xi = 0,
$$
 (E3)

one has a primary constraint

$$
p_{\xi} \approx 0. \tag{E4}
$$

The original total Hamiltonian is

$$
H_T = p_r^2/2 + p_\theta^2/2r^2 + p_\theta \xi + V(r) + v p_\xi.
$$
 (E5)

Obviously the consistency conditions result in a secondary constraint

$$
p_{\theta} \approx 0. \tag{E6}
$$

Because the two constraints are both first class and  $p_{\theta}^2 \approx 0$ , then Dirac's total Hamiltonian has the form

$$
H_T^D \simeq p_r^2 / 2 + p_\theta \xi + V(r) + v p_\xi. \tag{E7}
$$

With the aid of the canonical motion equations one readily obtains

$$
r(t) \approx e^{-(t-t_0)\mathcal{D}_H(t_0)} r(t_0),
$$
 (E8a)

$$
\theta(t) \approx \theta(t_0) + (t - t_0) \xi(t_0) + \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 v(t_2),
$$
\n(E8b)

$$
\xi(t) \approx \xi(t_0) + \int_{t_0}^t dt_1 v(t_1),
$$
 (E8c)

$$
p_r(t) \approx e^{-(t-t_0)\mathcal{D}_H(t_0)} p_r(t_0), \tag{E8d}
$$

$$
p_{\theta}(t) \approx p_{\theta}(t_0), \tag{E8e}
$$

$$
p_{\xi}(t) \approx p_{\xi}(t_0) - (t - t_0) p_{\theta}(t_0),
$$
 (E8f)

in which

$$
H = H^* = p_r^2 / 2 + p_\theta \xi + V(r).
$$
 (E9)

It is easy to see that

$$
\tilde{\eta}^{\mu}(t) = G(u, v; t, t_0) \, \eta^{\mu}(t)
$$
\n
$$
\approx \left\{ 1 - \int_{t_0}^t dt_1 [\, \tilde{u}(t_1) - v(t_1)] \mathcal{D}_{p_{\xi}} \right\}
$$
\n
$$
- \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 [\, \tilde{u}(t_2) - v(t_2)] \mathcal{D}_{p_{\theta}}(t) \right\}
$$
\n
$$
\approx \left\{ 1 - \int_{t_0}^t dt_1 [\, \tilde{u}(t_1) - v(t_1)] \mathcal{D}_{p_{\xi}}(t_1) \right\} \eta^{\mu}(t)
$$
\n
$$
= \exp\{-\lambda_1(t, t_0) D_{p_{\xi}}(t) - \lambda_2(t, t_0) \mathcal{D}_{p_{\theta}}(t) \} \, \eta^{\mu}(t),
$$
\n(E10)

$$
\lambda_1(t, t_0) = \int_{t_0}^t dt_1 [\widetilde{u}(t_1) - v(t_1)], \qquad \text{(E11a)}
$$

$$
\lambda_2(t, t_0) = \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 [\tilde{u}(t_2) - v(t_2)].
$$
 (E11b)

Here  $\mathcal{D}_{p_{\xi}}$  and  $\mathcal{D}_{p_{\theta}}$  are thought not to act on  $\lambda_1$  and  $\lambda_2$  since they are the functions of *t* only. Hence we can write

$$
G(u, v; t, t_0) \approx \exp\{-\lambda_1(t, t_0)\mathcal{D}_{p_{\xi}}(t) - \lambda_2(t, t_0)\mathcal{D}_{p_{\theta}}(t)\}.
$$
\n(E12)

Thus the subalgebra of the MECPB of the first-class constraints has two elements and just exhausts all the first-class constraints. Consequently Dirac's contact transformation operator becomes

$$
\mathcal{G}(t,t_0) \approx e^{-\alpha_1 \mathcal{D}_{p_\xi} - \alpha_2 \mathcal{D}_{p_\theta}}.\tag{E13}
$$

It must be noted that  $\alpha_1$  and  $\alpha_2$  are independent of each other and different from  $\lambda_1$  and  $\lambda_2$ , which satisfy the relation

$$
\dot{\lambda}_2(t, t_0) = \lambda_1(t, t_0). \tag{E14}
$$

It is interesting that the secondary first-class constraint  $p_{\theta}$ becomes a generator of Dirac's contact transformation. This is consistent with Dirac's conjecture. Therefore by using Dirac's conjecture we can determine correctly the generalized Hamiltonian

$$
H_G = p_r^2/2 + V(r) + \alpha_1 p_\theta + \alpha_2 p_\xi
$$
 (E15)

where  $p_{\theta} \xi$  is absorbed into  $\alpha_1 p_{\theta}$ . Consequently, Dirac's conjecture is applicable to the Christ-Lee model since the subalgebra of the MECPB of the first-class constraints is the same as the complete set of the first-class constraints in this model.

### **APPENDIX F**

In order to contrast Sudarshan and Mukunda's method of treating the singular Lagrangian system with Hessian variable rank in Lagrangian formulation  $[16]$  by using our algorithm of the extended consistency conditions in Hamiltonian formalism, let us recall briefly the S-M approach. Because the Hessian matrix is singular and its rank is  $r \leq n$ , there exist  $n-r$  linearly independent null eigenvectors  $\lambda_i^{(a)}(q,\dot{q})$ for this matrix:

$$
\sum_{i} \lambda_i^{(a)}(q, \dot{q}) W_{ij}(q, \dot{q}) = 0 \quad (a = 1, 2, \dots, n-r)
$$
 (F1)

or

$$
\gamma^{(a)}(q,\dot{q}) \equiv \sum_{i} \lambda_i^{(a)}(q,\dot{q}) K_i(q,\dot{q}) = 0. \tag{F2}
$$

(For ease in writing, we omit all explicit time dependence.) Suppose the number of the functionally independent  $\gamma^{(a)}(q,\dot{q})$  is  $k \leq n-r$ . Equation (F2) defines a  $(2n-k)$ -dimensional surface *V* in *S* which consists of *q* and *q*. The rank *r* of  $||W_{ij}||$  was first computed in the space *S*, that is, with all the  $q$ 's and  $\dot{q}$ 's being independent. But the equations of motion have restricted the motion to the surface *V* of lower dimensionality, so that we must go back and recompute the rank of  $||W_{ii}||$  after restricting the variables to the surface *V.* When this is done, although the rank cannot increase, it could, in principle, decrease and we denote its rank as  $r' < r$ . That means that with the variables constrained to *V*, we may find more null eigenvectors for the matrix  $\|W_{i,j}\|$ , and these in turn may introduce more independent constraints among the  $q_i$  and  $\dot{q}_i$ ; the motion then becomes restricted to a surface  $V'$  of lower dimensionality than *V*. The surface *V'* of dimensionality  $(2n-k')$  is defined by  $k'$  ( $\leq r'$ ) independent constraint equations which are obtained by

$$
\gamma^{(b)}(q,\dot{q}) \equiv \sum_{i} \lambda_i^{(b)}(q,\dot{q}) K_i(q,\dot{q})|_V = 0
$$
  
(b = 1,2, ..., n-r') (F3)

in which  $\lambda_i^{(b)}(q, \dot{q})$  are the null eigenvectors for the matrix  $\|W_{ii}(q,\dot{q})\|$  in the surface *V*, that is,

$$
\sum_{i} \lambda_{i}^{(b)}(q, \dot{q}) W_{ij}(q, \dot{q})|_{V} = 0 \quad (b = 1, 2, \dots, n - r'). \quad (F4)
$$

Its functionally independent number is  $k'$ .

Then we have to check whether the constraints  $(F4)$  are preserved in time so that we obtain more secondary constraints. The number of all independent constraints that are generated by the above process is denoted by  $k^{\prime\prime}$ . If the rank of  $|W_{ii}|$  decreases in the surface  $V''$  of dimensionality  $(2n-k'')$  defined by k<sup>*n*</sup> independent constraints involving the secondary constraints, we have to go again through each of the steps described above. For a system with a finite number of degrees of freedom, for which genuine motion is possible, this iterative process must end after a finite number of steps.

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