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CANONICALIZATION OF CONSTRAINED HAMILTONIAN EQUATIONS IN A SINGULAR SYSTEM Shan Cao 1 , Jing-Li Fu *2 , Hua-Shu Dou 3



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Abstract:

In this paper, the canonicalization of constrained Hamiltonian system is discussed. Because the constrained Hamiltonian equations are non-canonical, they lead to many limitations in the research. For this purpose, variable transformation is constructed that satisfies the condition of canonical equation, and the new variables can be obtained by a series of derivations. Finally, two examples are given to illustrate the applications of the result.

Keywords: Singular Lagrangian System; Constrained Hamiltonian System; Motion Equation; Canonicalization.

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1. Introduction

Under the Legendre transformation, the singular Lagrangian system can be transformed into phase space and described by Hamiltonian canonical variables; there are inherent constraints between canonical variables, namely constrained Hamiltonian system. Many important physical systems belong to this system, such as, quantum electrodynamics (QED), quantum flavor dynamics (QFD), quantum chromodynamics (QCD) and general relativity (GR) which is used to describe the basic interaction of nature. The Lagrangian functions of supersymmetry, supergravity and string theory are singular as well. Therefore, the fundamental theory of constrained Hamiltonian system plays a significant role in theoretical physics, especially in modern quantum field theory [1-4].

There are inherent constraints when the singular Lagrangian system transitions to phase space, but the quantization of the system is usually achieved by the canonical variables of phase space, at the point, the quantum method [5-7] in elementary quantum mechanics is in trouble. When the canonical variables are restrained, new problems arising from the quantization theory, have received extensive attention of people. Furthermore, if the canonicalization of variables (\mathbf{p}, \mathbf{q}) in constrained Hamiltonian system is realized, then we can express constrained Hamiltonian system to normal Hamiltonian system, the existing Hamiltonian system symmetry theory^[8-15] can be

used in constrained Hamiltonian system conveniently. And at this time, the system has the symplectic structure^[16], the symplectic geometry method can be used for giving numerical solutions and numerical simulations of constrained Hamiltonian system. So many important physics systems can be simulated with this method.

Therefore, the canonicalization of constrained Hamiltonian system is a major work. In previous studies, Yifa Tang has studied the canonicalization of gyrocenter system ^[17]. Some researches ^[18-21] only provide canonicalization methods for some special cases, and the calculation process is complicated. On the other hand, according to Dardoux's theorem ^[22], for a non-canonical Hamiltonian system, we can find theoretically the local canonical coordinates by solving differential equations, which is an uneconomic method for numerical purpose. To avoid solving differential equations, we do not follow the steps given in the standard proof of Dardoux's theorem. Instead, we explore another procedure to realize the canonicalization of the constrained Hamiltonian system.

In this paper, we define a variable transformation, new canonical variables for constrained Hamiltonian system can be given through a series of calculation, the purpose of canonicalization can be achieved. This method is more general, and makes the calculation simpler. In the end, two examples are given to illustrate the practicability of this method. After canonicalization, many useful theories and algorithms can be applied more conveniently to the constrained Hamiltonian system. Thus, there is important theoretical significance to carry out this research.

2. Hamiltonian Canonical Equations in a Singluar System

Supposing that the dynamics of a system with finite degrees of freedom is described by the Lagrangian $L = L(t, q_i, \mathcal{A}_i)$, $q_i(i = 1, 2, L, n)$ are generalized coordinates, and $\mathcal{A}_i = Dq_i = dq_i/dt$ are generalized velocities. Assuming the Lagrangian is time-independent, generalized momenta are defined as

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \quad (i = 1, 2, \dots, n), \tag{1}$$

And canonical Hamiltonian is

$$H_{c} = \sum_{i=1}^{n} p_{i} \dot{q}_{i} - L(t, q_{i}, \dot{q}_{i}) = p_{i} \dot{q}_{i} - L,$$
(2)

Where repeated instructions represent summation. Hess matrix of function L is

$$H_{ij} = \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \,, \tag{3}$$

if its rank r < n. Using the Legendre transformation to convert the Lagrangian description to the Hamiltonian description, there are inherent constraints between the canonical variables in the phase space

$$\varphi_i(t, q_i, p_i) = 0 \quad (j = 1, 2, L, n - r).$$
 (4)

Then the canonical equations of singular system are given as

$$\dot{q}_i = \{q_i, H_T\}, \quad \dot{p}_i = \{p_i, H_T\},$$
(5)

Where $\{,\}$ is Poisson bracket, equation $H_T = H_c + \lambda_j \varphi_j$ is the total Hamiltonian. λ_j are Lagrange multipliers, Eq. (5) is equivalent to Euler-Lagrange equation. Therefore, the state of the system in phase space is determined by H_T , due to the existence of constraint equations (4), we have to count the Poisson brackets before using these constraints. Motion equations (2) can be written as

$$\dot{q}_{i} = \frac{\partial H_{c}}{\partial p_{i}} + \lambda_{j} \frac{\partial \varphi_{j}}{\partial p_{i}}, \quad \dot{p}_{i} = -\frac{\partial H_{c}}{\partial q_{i}} - \lambda_{j} \frac{\partial \varphi_{j}}{\partial q_{i}}.$$

$$(i = 1, \dots, n; j = 1, \dots, n - r)$$
(6)

If the singular systems with only second class constraints, that is, assume constraints (4) consist of second class primary constraints and secondary constraints, we have

$$\det \left| \left\{ \varphi_k, \varphi_j \right\} \right|_{\varphi = 0} \neq 0 \qquad (k \neq j; k, j = 1, L, n - r), \tag{7}$$

So all Lagrange multipliers λ_j in Eq. (6) can be completely determined by the compatibility condition of constraints

$$\{\varphi_k, H_T\} = \{\varphi_k, H_c\} + \lambda_j \{\varphi_k, \varphi_j\} = 0,$$
 (8)

We have

$$\lambda_i = \lambda_i(t, q_i, p_i). \tag{9}$$

3. The Canonicalization of Constained Hamiltonian Equations

The motion equations for the constrained Hamiltonian system discussed above are noncanonical, in this section; we transform it into canonical form by means of the variable transformation.

The motion equations for constrained Hamiltonian system are

$$\begin{cases}
\dot{p}_{i} = -\frac{\partial H_{c}}{\partial q_{i}} - \lambda_{j} \frac{\partial \varphi_{j}}{\partial q_{i}}, \\
\dot{q}_{i} = \frac{\partial H_{c}}{\partial p_{i}} + \lambda_{j} \frac{\partial \varphi_{j}}{\partial p_{i}}, (i = 1, \dots, n; j = 1, \dots, n - r)
\end{cases}$$
(10)

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Those can be rewritten as the following matrix form

$$\begin{pmatrix} \dot{p}_{1} \\ \vdots \\ \dot{p}_{i} \\ \dot{q}_{1} \\ \vdots \\ \dot{q}_{i} \end{pmatrix} = \begin{pmatrix} 0_{n} & S_{n} \\ 0_{n} & S_{n} \\ T_{n} & 0_{n} \end{pmatrix} \begin{pmatrix} \frac{\partial H_{e}}{\partial p_{1}} \\ \vdots \\ \frac{\partial H_{e}}{\partial p_{i}} \\ \frac{\partial H_{e}}{\partial p_{i}} \\ \vdots \\ \frac{\partial H_{e}}{\partial q_{i}} \end{pmatrix} = M_{2n \times 2n} \begin{pmatrix} \frac{\partial H_{e}}{\partial p_{1}} \\ \vdots \\ \frac{\partial H_{e}}{\partial p_{i}} \\ \frac{\partial H_{e}}{\partial q_{i}} \\ \vdots \\ \frac{\partial H_{e}}{\partial q_{i}} \end{pmatrix},$$

$$(11)$$

Where

$$S_{n} = \begin{pmatrix} -1 - \lambda_{j} \frac{\partial \varphi_{j}}{\partial H_{c}} & L & 0 \\ M & O & M \\ 0 & L & -1 - \lambda_{j} \frac{\partial \varphi_{j}}{\partial H_{c}} \end{pmatrix}_{n \times n},$$

$$T_{n} = \begin{pmatrix} 1 + \lambda_{j} \frac{\partial \varphi_{j}}{\partial H_{c}} & L & 0 \\ M & O & M \\ 0 & L & 1 + \lambda_{j} \frac{\partial \varphi_{j}}{\partial H_{c}} \end{pmatrix}_{n \times n},$$

$$(12)$$

So $M_{2n\times 2n}$ is an anti-symmetric matrix.

For the convenience of discussion, then the form of (11) can be simplified, expressed it in the form of vectors and gradients. Let $\mathbf{v} = (\mathbf{p}, \mathbf{q})^T$, there, $\mathbf{p} = (p_1, p_2, \mathbf{L}, p_i)$, $\mathbf{q} = (q_1, q_2, \mathbf{L}, q_i)$, and introduce gradient operator $\nabla = (\frac{\partial}{\partial p_1}, \mathbf{L}, \frac{\partial}{\partial q_i}, \frac{\partial}{\partial q_1}, \mathbf{L}, \frac{\partial}{\partial q_i})$. If the condition $\det(M) \neq 0$ holds, hence Eq. (11) can be briefly expressed as

$$\dot{\mathbf{v}} = K(\mathbf{v})^{-1} \nabla H_c(\mathbf{v}), \tag{13}$$

Let $K^{-1} = M$, so

$$K(\mathbf{v}) = \begin{pmatrix} 0_n & T_n^{-1} \\ S_n^{-1} & 0_n \end{pmatrix},\tag{14}$$

Where

$$S_n^{-1} = \begin{pmatrix} \frac{\partial H_c}{\partial H_c + \lambda_j \partial \varphi_j} & L & 0\\ M & O & M\\ 0 & L & \frac{\partial H_c}{\partial H_c + \lambda_j \partial \varphi_j} \end{pmatrix}, \tag{15}$$

$$T_{n}^{-1} = \begin{pmatrix} -\frac{\partial H_{c}}{\partial H_{c} + \lambda_{j} \partial \varphi_{j}} & L & 0 \\ M & O & M \\ 0 & L & -\frac{\partial H_{c}}{\partial H_{c} + \lambda_{j} \partial \varphi_{j}} \end{pmatrix}, \tag{16}$$

The system Eq. (13) is a non-canonical Hamiltonian system. At the same time, a canonical Hamiltonian system, which we struggle to seek, should take the form of

$$\dot{\mathbf{Z}} = J^{-1} \nabla H_{c}(\mathbf{Z}) \qquad J = \begin{pmatrix} 0 & I_{n} \\ -I_{n} & 0 \end{pmatrix}. \tag{17}$$

In order to transform the non-canonical Hamiltonian system to canonical form, we seek the corresponding canonical variables. Let $\mathbf{Z} = \psi(\mathbf{v})$ be a transformation from R^{2n} to R^{2n} , $\mathbf{Z} = (\mathbf{\tilde{p}}, \mathbf{\tilde{q}})^{\mathsf{T}}$ are the new variables after canonicalization. According to the chain rule, Eq. (13) can be written as

$$\dot{\mathbf{Z}} = (\frac{\partial \psi}{\partial \mathbf{v}}) K(\mathbf{v})^{-1} (\frac{\partial \psi}{\partial \mathbf{v}})^{\mathrm{T}} \nabla \tilde{H}(\mathbf{Z}), \tag{18}$$

Where
$$H(\mathbf{Z}) = H_c(\mathbf{v})$$
. If we demand $(\frac{\partial \psi}{\partial \mathbf{v}})K(\mathbf{v})^{-1}(\frac{\partial \psi}{\partial \mathbf{v}})^{\mathrm{T}} = J^{-1}$, i.e.,
$$K(\mathbf{v}) = (\frac{\partial \psi}{\partial \mathbf{v}})^{\mathrm{T}}J(\frac{\partial \psi}{\partial \mathbf{v}}), \tag{19}$$

 $K(\mathbf{v})$ is a known matrix, $\mathbf{v} = (\mathbf{p}, \mathbf{q})^T$ are the old variables, so we can get $\psi(\mathbf{v})$ through this transformation, they are a set of canonical new generalized momenta $\mathcal{V} = (\mathcal{V}_1, \mathcal{V}_2, L, \mathcal{V}_3)$ and generalized coordinates $\mathcal{V} = (\mathcal{V}_1, \mathcal{V}_2, L, \mathcal{V}_3)$. At this time, we have transformed the non-canonical Hamiltonian system into a canonical Hamiltonian system.

The old variables are represented by the new variables and substituted into the original Hamiltonian function, at this time, under the new variables, the Hamiltonian equations of the constrained Hamiltonian system become canonical. On this basis, we can study its various properties and use some useful algorithms to study the numerical solution and numerical

simulation of the constrained Hamilton system. After the results are obtained, the new variables are replaced with the old variables, that is, the results of the original system are obtained.

4. Examples

Example 1

The system's Lagrangian is

$$L = \dot{q}_1 q_2 - q_1 \dot{q}_2 + q_1^2 + q_2^2 , \qquad (20)$$

The generalized momenta of the system are

$$p_1 = \frac{\partial L}{\partial \dot{q}_1} = q_2, \qquad p_2 = \frac{\partial L}{\partial \dot{q}_2} = -q_1, \tag{21}$$

The rank r of the Hess matrix of the Lagrangian can be obtained, r = 0, this is a singular Lagrangian system, so that there are two constraints between canonical variables

$$\varphi_1 = p_1 - q_2 = 0, \qquad \varphi_2 = p_2 + q_1 = 0,$$
 (22)

Canonical Hamiltonian of this system is

$$H_c = p_1 \dot{q}_1 + p_2 \dot{q}_2 - L = -(q_1^2 + q_2^2),$$
(23)

Total Hamiltonian is

$$H_{\rm T} = -(q_1^2 + q_2^2) + \lambda_1(p_1 - q_2) + \lambda_2(p_2 + q_1), \tag{24}$$

The Lagrange multipliers can be obtained by the compatibility condition of constraints, i.e., Eq.

$$\lambda_1 = -q_2, \qquad \lambda_2 = q_1, \tag{25}$$

Here, we define a new variable
$$\mathbf{Z} = \psi(\mathbf{v}) = (\tilde{p}_1, \tilde{p}_2, \tilde{q}_1, \tilde{q}_2)$$
, such that
$$K = \begin{bmatrix}
0 & 0 & -\frac{\partial H_c}{\partial H_c + \lambda_1 \partial \varphi_1 + \lambda_2 \partial \varphi_2} & 0 \\
0 & 0 & 0 & -\frac{\partial H_c}{\partial H_c + \lambda_1 \partial \varphi_1 + \lambda_2 \partial \varphi_2} \\
\frac{\partial H_c}{\partial H_c + \lambda_1 \partial \varphi_1 + \lambda_2 \partial \varphi_2} & 0 & 0 & 0 \\
0 & \frac{\partial H_c}{\partial H_c + \lambda_1 \partial \varphi_1 + \lambda_2 \partial \varphi_2} & 0 & 0
\end{bmatrix}, (26)$$

By means of Eq. (19), we have

$$\begin{cases}
\frac{\partial \tilde{q}_{1}}{\partial p_{1}} \frac{\partial \tilde{q}_{1}}{\partial p_{1}} + \frac{\partial \tilde{q}_{1}}{\partial p_{2}} \frac{\partial \tilde{p}_{1}}{\partial q_{2}} - \frac{\partial \tilde{q}_{1}}{\partial q_{1}} \frac{\partial \tilde{p}_{1}}{\partial p_{1}} - \frac{\partial \tilde{q}_{1}}{\partial q_{2}} \frac{\partial \tilde{p}_{1}}{\partial p_{2}} = \frac{\partial H_{c}}{\partial H_{c} + \lambda_{1} \partial \varphi_{1} + \lambda_{2} \partial \varphi_{2}}, \\
\frac{\partial \tilde{q}_{2}}{\partial p_{1}} \frac{\partial \tilde{p}_{2}}{\partial q_{1}} + \frac{\partial \tilde{q}_{2}}{\partial p_{2}} \frac{\partial \tilde{p}_{2}}{\partial q_{2}} - \frac{\partial \tilde{q}_{2}}{\partial q_{1}} \frac{\partial \tilde{p}_{2}}{\partial p_{1}} - \frac{\partial \tilde{q}_{2}}{\partial q_{2}} \frac{\partial \tilde{p}_{2}}{\partial p_{2}} = \frac{\partial H_{c}}{\partial H_{c} + \lambda_{1} \partial \varphi_{1} + \lambda_{2} \partial \varphi_{2}}, \\
\frac{\partial \tilde{q}_{2}}{\partial p_{1}} \frac{\partial \tilde{p}_{2}}{\partial q_{1}} + \frac{\partial \tilde{q}_{2}}{\partial p_{2}} \frac{\partial \tilde{p}_{2}}{\partial q_{2}} - \frac{\partial \tilde{q}_{2}}{\partial q_{1}} \frac{\partial \tilde{p}_{2}}{\partial p_{1}} - \frac{\partial \tilde{q}_{2}}{\partial q_{2}} \frac{\partial \tilde{p}_{2}}{\partial p_{2}} = \frac{\partial H_{c}}{\partial H_{c} + \lambda_{1} \partial \varphi_{1} + \lambda_{2} \partial \varphi_{2}},
\end{cases} (27)$$

From Eq. (27), we can derive the new canonical variables

$$\begin{cases} \tilde{p}_{1} = p_{1} + q_{1}, \\ \tilde{p}_{2} = p_{2} + q_{2}, \\ \tilde{q}_{1} = p_{1} - q_{1}, \\ \tilde{q}_{2} = p_{2} - q_{2}, \end{cases}$$
(28)

The old variables can be introduced by the upper expression as

$$\begin{cases} p_{1} = \frac{\tilde{p}_{1} + \tilde{q}_{1}}{2}, \\ q_{1} = \frac{\tilde{p}_{1} - \tilde{q}_{1}}{2}, \\ p_{2} = \frac{\tilde{p}_{2} + \tilde{q}_{2}}{2}, \\ q_{2} = \frac{\tilde{p}_{2} - \tilde{q}_{2}}{2}, \end{cases}$$
(29)

When the new variables (29) are substituted into the original Hamiltonian, the canonical Hamiltonian equations can be obtained. On this basis, we can do a series of studies. When we get the results, we need to replace the new variables with the old variables in terms of the equations (28), which are the results of the original system.

Example 2

Next we consider an example with the non-potential generalized force.

The system's Lagrangian and generalized force are

$$L = \frac{1}{2}\dot{q}_1^2 + \dot{q}_1q_2 + \frac{1}{2}(q_1 - q_2)^2, \tag{30}$$

$$Q''_1 = -\dot{q}_2, \qquad Q''_2 = \dot{q}_1,$$
 (31)

The generalized momenta of the system are

$$p_1 = \frac{\partial L}{\partial \dot{q}_1} = \dot{q}_1 + q_2, \quad p_2 = \frac{\partial L}{\partial \dot{q}_2} = 0 \quad , \tag{32}$$

We get the rank of the Hess matrix r=1, so that there is a constraint between canonical variables, as

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial \dot{q}_i} = Q''_i \quad (i = 1, 2) , \tag{33}$$

The motion equations of this system are derived as follows

$$\ddot{q}_1 = q_1 - q_2 - 2\dot{q}_2, \tag{34}$$

$$-2\dot{q}_2 + q_1 - q_2 = 0. ag{35}$$

According to reference [8], Eq. (33) is generalized acceleration; Eq. (35) is the constraint condition φ . Canonical Hamiltonian of the system is

$$H_{c} = p_{1}\dot{q}_{1} + p_{2}\dot{q}_{2} - L = \frac{1}{2}\dot{q}_{1}^{2} - \frac{1}{2}(q_{1} - q_{2})^{2},$$
(36)

And total Hamiltonian is

$$H_{\rm T} = \frac{1}{2}\dot{q}_1^2 - \frac{1}{2}(q_1 - q_2)^2 + \lambda(-2\dot{q}_2 + q_1 - q_2), \tag{37}$$

According to [3], we get the Lagrange multiplier

$$\lambda = \dot{q}_1, \tag{38}$$

Here, we define a new variable $\mathbf{Z} = \psi = (\mathcal{Y}_1, \mathcal{Y}_2, \mathcal{Y}_1, \mathcal{Y}_2)$, we have

$$K = \begin{pmatrix} 0 & 0 & -\frac{\partial H_c}{\partial H_c + \lambda \partial \varphi} & 0 \\ 0 & 0 & 0 & -\frac{\partial H_c}{\partial H_c + \lambda \partial \varphi} \\ \frac{\partial H_c}{\partial H_c + \lambda \partial \varphi} & 0 & 0 & 0 \\ 0 & \frac{\partial H_c}{\partial H_c + \lambda \partial \varphi} & 0 & 0 \end{pmatrix}, \tag{39}$$

By means of Eq. (19), we can get

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$$\begin{cases}
\frac{\partial \tilde{q}_{1}}{\partial p_{1}} \frac{\partial \tilde{q}_{1}}{\partial p_{1}} + \frac{\partial \tilde{q}_{1}}{\partial p_{2}} \frac{\partial \tilde{p}_{1}}{\partial q_{2}} - \frac{\partial \tilde{q}_{1}}{\partial q_{1}} \frac{\partial \tilde{p}_{1}}{\partial p_{1}} - \frac{\partial \tilde{q}_{1}}{\partial q_{2}} \frac{\partial \tilde{p}_{1}}{\partial p_{2}} = \frac{\partial H_{c}}{\partial H_{c} + \lambda \partial \varphi}, \\
\frac{\partial \tilde{q}_{2}}{\partial p_{1}} \frac{\partial \tilde{p}_{2}}{\partial q_{1}} + \frac{\partial \tilde{q}_{2}}{\partial p_{2}} \frac{\partial \tilde{p}_{2}}{\partial q_{2}} - \frac{\partial \tilde{q}_{2}}{\partial q_{1}} \frac{\partial \tilde{p}_{2}}{\partial p_{1}} - \frac{\partial \tilde{q}_{2}}{\partial q_{2}} \frac{\partial \tilde{p}_{2}}{\partial p_{2}} = \frac{\partial H_{c}}{\partial H_{c} + \lambda \partial \varphi}, \\
\frac{\partial \tilde{q}_{2}}{\partial p_{1}} \frac{\partial \tilde{p}_{2}}{\partial q_{1}} + \frac{\partial \tilde{q}_{2}}{\partial p_{2}} \frac{\partial \tilde{p}_{2}}{\partial q_{2}} - \frac{\partial \tilde{q}_{2}}{\partial q_{1}} \frac{\partial \tilde{p}_{2}}{\partial p_{1}} - \frac{\partial \tilde{q}_{2}}{\partial q_{2}} \frac{\partial \tilde{p}_{2}}{\partial p_{2}} = \frac{\partial H_{c}}{\partial H_{c} + \lambda \partial \varphi},
\end{cases} \tag{40}$$

We can derive the new canonical variables

$$\begin{cases} \tilde{p}_{1} = 2p_{1} + q_{1}, \\ \tilde{p}_{2} = p_{2} - 2q_{2}, \\ \tilde{q}_{1} = p_{1} + q_{1}, \\ \tilde{q}_{2} = p_{2} - q_{2}, \end{cases}$$

$$(41)$$

The old variables can be introduced by the upper expression as

$$\begin{cases} p_{1} = \tilde{p}_{1} - \tilde{q}_{1}, \\ q_{1} = 2\tilde{q}_{1} - \tilde{p}_{1}, \\ p_{2} = 2\tilde{q}_{2} - \tilde{p}_{2}, \\ q_{2} = \tilde{q}_{2} - \tilde{p}_{2}, \end{cases}$$

$$(42)$$

When the new variables (42) are substituted into the original Hamiltonian, the canonical Hamiltonian equations can be obtained. On this basis, we can do a series of studies. When we get the results, we need to replace the new variables with the old variables in terms of the equations (41), which are the results of the original system.

5. Conclusions

In this paper, the canonicalization of constrained Hamiltonian system is discussed. Due to the existence of constraints, the constrained Hamiltonian equations are non-canonical. In order to make them canonicalized, a variable transformation is conducted between the old and new variable that satisfies the condition of canonical equations. Through this transformation, a set of new variables can be obtained, and the original constrained Hamiltonian equation becomes canonicalized under the new variables. After the systems of equations are canonicalized, a lot of useful theories and algorithms can be applied more easily to the constrained Hamiltonian system. This result is of great significance to further research.

The canonicalization method can also be applied to electromagnetic fields, quantum fields, regular and irregular fields to realize the canonicalization of the system. Similarly, for nonconservation and nonholonomic systems, this method is also applicable. They will be investigated in future studies.

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