

# Canonical equations of Hamilton for the nonlinear Schrödinger equation

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**Abstract.** We define two different systems of mathematical physics: the second order differential system (SODS) and the first order differential system (FODS). The Newton's second law of motion and the nonlinear Schrödinger equation (NLSE) are the exemplary SODS and FODS, respectively. We obtain a new kind of canonical equations of Hamilton (CEH), which exhibit some kind of symmetry in form and are formally different from the conventional CEH without symmetry [H. Goldstein, C. Poole, J. Safko, Classical Mechanics, third ed., Addison-Wesley, 2001]. We also prove that the number of the CEHs is equal to the number of the generalized coordinates for the FODS, but twice the number of the generalized coordinates for the SODS. We show that the FODS can only be expressed by the new CEH, but not introduced by the conventional CEH, while the SODS can be done by both the new and the conventional CEHs. As an example, we prove that the nonlinear Schrödinger equation can be expressed with the new CEH in a consistent way.

## 1. Introduction

The Hamiltonian viewpoint provides a framework for theoretical extensions in many areas of physics. In classical mechanics it forms the basis for further developments, such as Hamilton-Jacobi theory, perturbation approaches and chaos [1, 2]. The canonical equations of Hamilton (CEH) for the continuous system in classical mechanics are expressed as [1]

$$\dot{q}_s = \frac{\delta h}{\delta p_s}, \quad (s = 1, \dots, N), \quad (1)$$

$$-\dot{p}_s = \frac{\delta h}{\delta q_s}, \quad (s = 1, \dots, N), \quad (2)$$

where the subscript  $s$ , which in all cases denotes  $1, \dots, N$  throughout the paper, represents the components of the quantity of the continuous system [1],  $\frac{\delta h}{\delta q_s} = \frac{\partial h}{\partial q_s} - \frac{\partial}{\partial x} \frac{\partial h}{\partial q_{s,x}}$  and  $\frac{\delta h}{\delta p_s} = \frac{\partial h}{\partial p_s} - \frac{\partial}{\partial x} \frac{\partial h}{\partial p_{s,x}}$  denote the functional derivatives of  $h$  with respect to  $q_s$  and  $p_s$  with  $q_{s,x} = \frac{\partial q_s}{\partial x}$  and  $p_{s,x} = \frac{\partial p_s}{\partial x}$ ,  $q_s$  and  $p_s$  are the generalized coordinate and the generalized momentum, respectively, and  $h$  is the Hamiltonian density of the continuous system. The generalized momentum  $p_s$  for the continuous system is defined as  $p_s = \frac{\partial l}{\partial \dot{q}_s}$ , and the Hamiltonian density  $h$  for the continuous system is obtained by the Legendre transformation as

$$h = \sum_{s=1}^N \dot{q}_s p_s - l, \quad (3)$$



where  $l$  is the Lagrangian density. It should be noted that for the continuous system both  $q_s$  and  $p_s$  are not only functions of time  $t$ , but also the spatial coordinate  $x$ , where the spatial coordinate  $x$  is not the generalized coordinate. To distinguish  $t$  from the coordinate  $x$ , we refer to time  $t$  as the evolution coordinate.  $p_s$  and  $q_s$  define the infinite-dimensional phase space.  $h$  is a function of  $q_s, p_s$  and  $q_{s,x}$  but not  $p_{s,x}$  [1], so  $\frac{\delta h}{\delta p_s} = \frac{\partial h}{\partial p_s}$ , then Eq.(1) can be also expressed as  $\dot{q}_s = \frac{\partial h}{\partial p_s}$ .

Up to now, to our knowledge, the CEH appearing in all the literatures are of the form (1) and (2), which are established based on the second order differential system (SODS) (the definition of the SODS will be given in the following). Besides the SODS, there are a number of the first order differential systems (FODS) (the definition of the FODS will also be given in the following) to model physical phenomena. For example, the nonlinear Schrödinger equation (NLSE) is a universal FODS. We will show that the conventional CEH, Eqs. (1) and (2), are not valid for the NLSE, from which it is impossible to obtain the NLSE or its complex-conjugate equation. Attempt was made to deal with the difficulty in Ref.[3], but the CEH for the NLSE they obtained were inconsistent, as will be shown later. In this paper, we obtain a new kind of CEH valid for the FODS, with which the NLSE can be expressed in a consistent way. We prove that the new CEH and the conventional CEH are equivalent for the description of the SODS. But the conventional CEH can not express the FODS.

## 2. First-order differential system and its canonical equations of Hamilton

The Newton's second law of motion in classical mechanics, based on which the Hamiltonian formulation is established, is the second order differential equation about the evolution coordinate (here the evolution coordinate is time). In this paper we define the system described by the second order partial differential equation about the evolution coordinate as the second order differential system (SODS). Similarly, the first order differential system (FODS) is the system described by the first order partial differential equation about the evolution coordinate. For example, the NLSE [4]

$$i\frac{\partial \varphi}{\partial t} + \frac{1}{2}\frac{\partial^2 \varphi}{\partial x^2} + |\varphi|^2 \varphi = 0, \quad (4)$$

is an exemplary FODS, where the evolution coordinate  $t$  is the propagation direction coordinate.

For the FODS, the Lagrangian density must be the linear function of the generalized velocities  $\dot{q}_s$  (see Ref. [5] for details), which can be expressed as

$$l = \sum_{s=1}^N R_s(q_s) \dot{q}_s + Q(q_s, q_{s,x}),$$

Consequently, the generalized momentum  $p_s$ , which is obtained by the definition  $p_s = \frac{\partial l}{\partial \dot{q}_s}$ , as

$$p_s = R_s(q_s), \quad (5)$$

is only a function of  $q_s$ . There are  $2N$  variables,  $q_s$  and  $p_s$ , in Eqs. (5). The number of Eqs. (5) is  $N$ , which also means there exist  $N$  constraints between  $q_s$  and  $p_s$ . So the degree of freedom of the system given by Eqs. (5) is  $N$ . Without loss of generality, we take  $q_1, \dots, q_\nu$  and  $p_1, \dots, p_\mu$  as the independent variables, where  $\nu + \mu = N$ . The remaining generalized coordinates and generalized momenta can be expressed with these independent variables as  $q_\alpha = f_\alpha(q_1, \dots, q_\nu, p_1, \dots, p_\mu)$  ( $\alpha = \nu+1, \dots, N$ ), and  $p_\beta = g_\beta(q_1, \dots, q_\nu, p_1, \dots, p_\mu)$  ( $\beta = \mu+1, \dots, N$ ). We obtained the CEH for the FODS (see Ref. [5] for details), which are

$$\frac{\delta h}{\delta q_\lambda} = \sum_{s=1}^N \left( \dot{q}_s \frac{\partial p_s}{\partial q_\lambda} - \dot{p}_s \frac{\partial q_s}{\partial q_\lambda} \right) + \sum_{\alpha=\nu+1}^N \frac{\partial}{\partial x} \frac{\partial h}{\partial q_{\alpha,x}} \frac{\partial f_\alpha}{\partial q_\lambda}, \quad (6)$$

$$\frac{\delta h}{\delta p_\eta} = \sum_{s=1}^N \left( \dot{q}_s \frac{\partial p_s}{\partial p_\eta} - \dot{p}_s \frac{\partial q_s}{\partial p_\eta} \right) + \sum_{\alpha=\nu+1}^N \frac{\partial}{\partial x} \frac{\partial h}{\partial q_{\alpha,x}} \frac{\partial f_\alpha}{\partial p_\eta} \quad (7)$$

( $\lambda = 1, \dots, \nu$ ,  $\eta = 1, \dots, \mu$ , and  $\nu + \mu = N$ ). The CEH, Eqs. (6) and (7), can be easily extended to the discrete system, which can be expressed as  $\frac{\partial H}{\partial q_\lambda} = \sum_{s=1}^N \left( \dot{q}_s \frac{\partial p_s}{\partial q_\lambda} - \dot{p}_s \frac{\partial q_s}{\partial q_\lambda} \right)$  and  $\frac{\partial H}{\partial p_\eta} = \sum_{s=1}^N \left( \dot{q}_s \frac{\partial p_s}{\partial p_\eta} - \dot{p}_s \frac{\partial q_s}{\partial p_\eta} \right)$ , where  $\lambda = 1, \dots, \nu$ ,  $\eta = 1, \dots, \mu$ , and  $\nu + \mu = N$ .

### 3. Application of the new canonical equations of Hamilton with symmetry to the nonlinear Schrödinger equation

In this part, we will discuss the application of the new CEH with symmetry, Eqs. (6) and (7), to the NLSE. It is known that the Lagrangian density for the NLSE can be expressed as [6]  $l = -\frac{i}{2}(\varphi^* \frac{\partial \varphi}{\partial t} - \varphi \frac{\partial \varphi^*}{\partial t}) + \frac{1}{2}|\frac{\partial \varphi}{\partial x}|^2 - \frac{1}{2}|\varphi|^4$ . The NLSE is complex, and therefore it is an equation with two real functions, the real part of  $\varphi$  and its imaginary part. It is convenient to consider instead the fields  $\varphi$  and  $\varphi^*$  which are treated as independent from each other. Therefore,  $N$  (the components of the quantity) for the NLSE equals two, i.e., there are two generalized coordinates,  $q_1 = \varphi^*$  and  $q_2 = \varphi$ , and two generalized momenta can be obtained as  $p_1 = \frac{i}{2}\varphi$  and  $p_2 = -\frac{i}{2}\varphi^*$ . The Hamiltonian density for the NLSE can be obtained by use of Eq.(3) as [4]

$$h = -\frac{1}{2} \left| \frac{\partial \varphi}{\partial x} \right|^2 + \frac{1}{2} |\varphi|^4. \quad (8)$$

If the generalized coordinate  $q_1$  and the generalized momentum  $p_1$  are taken as the independent variables, the remaining generalized coordinate  $q_2$  and the remaining generalized momentum  $p_2$  can be expressed as  $q_2 = -2ip_1$  and  $p_2 = -\frac{i}{2}q_1$ , respectively. We should also note that the Hamiltonian density  $h$  is also the function of  $q_{s,x}$ , which are independent from  $q_s$  and  $p_s$ . Then for the NLSE, the Hamiltonian density (8) should be expressed with the independent variables  $q_1, p_1, q_{1,x}$  and  $q_{2,x}$  as  $h = -\frac{1}{2}q_{1,x}q_{2,x} - 2q_1^2p_1^2$ . We should note that  $\nu = \mu = 1$  and  $N = 2$  for the NLSE, which means that the equations (6) have only one equation, so do Eqs.(7). Therefore, the CEH (6) and (7) will yield two equations for the NLSE. The left side of Eq.(6) is obtained as  $\frac{\delta h}{\delta q_1} = \frac{1}{2} \frac{\partial^2 \varphi}{\partial x^2} + |\varphi|^2 \varphi$ , and its right side is  $-\dot{p}_1 + \dot{q}_2 \frac{\partial p_2}{\partial q_1} = -i\dot{\varphi}$ . Then the NLSE (4) can be obtained. Using the other CEH, the left side of Eq.(7) is obtained as  $\frac{\delta h}{\delta p_2} = -4q_1^2p_1 = -2i|\varphi|^2\varphi^*$ , and its right side is  $\dot{q}_1 - \dot{p}_2 \frac{\partial q_2}{\partial p_1} + \frac{\partial}{\partial x} \frac{\partial h}{\partial q_{2,x}} \frac{\partial q_2}{\partial p_1} = 2\dot{\varphi}^* + i \frac{\partial^2 \varphi^*}{\partial x^2}$ . Then the complex conjugate of the NLSE is also obtained. Therefore, the CEHs (6) and (7) are consistent in the sense that the NLSE can be expressed with one of the two CEHs, and its complex conjugate can be expressed with the other.

In Ref.[4], the CEH for the NLSE were considered to be the same as those for the SODS, that is, Eqs. (1) and (2). Then, according to the definition  $p_\varphi = \partial l / \partial \dot{\varphi}$ ,  $p_\varphi$  must be  $-i/2\varphi^*$  but not  $-i\varphi^*$ . It was artificially doubled in Ref.[4] so that  $p_\varphi = -i\varphi^*$  in Eq.[5.1.29] (to avoid confusion, we replace the parentheses by the brackets to represent the formulas in the references) to make the NLSE derived from the CEH (2). In fact, substitution of the Hamiltonian density (8) into Eq.(2) only yields  $\frac{i}{2} \frac{\partial \varphi}{\partial t} + \frac{1}{2} \nabla_\perp^2 \varphi + |\varphi|^2 \varphi = 0$ , which in fact is not the NLSE (4). In Ref.[3], the CEH obtained by the authors are Eqs.[3.87] and [3.81], the latter is  $\dot{q}_s = \frac{\partial h}{\partial p_s}$ . Although the NLSE can be derived from Eq.[3.87], its complex conjugation could not be obtained from the other, Eq. [3.81]. We now show this claim. Substituting the Hamiltonian density (8) into the equation  $\dot{q}_s = \frac{\partial h}{\partial p_s}$ , the left side of it is obtained as  $\frac{\partial \varphi^*}{\partial t}$ , and the right side is  $\frac{\partial h}{\partial p_{\varphi^*}} = \frac{\partial h}{\partial \varphi} \frac{\partial \varphi}{\partial p_{\varphi^*}} = -2i|\varphi|^2\varphi^*$ , where  $p_{\varphi^*} = \frac{\partial l}{\partial \dot{\varphi^*}}$ . Then the equation  $-\frac{i}{2} \frac{\partial \varphi^*}{\partial t} + |\varphi|^2 \varphi^* = 0$  can be obtained, which is absolutely not the complex conjugate of the NLSE. Therefore, the CEH for the NLSE obtained in Ref.[3] are inconsistent.

#### 4. Some further discussions about the new canonical equations of Hamilton with symmetry

Now, we know that the CEH valid for the FODS are Eqs. (6) and (7), and the conventional CEH valid for the SODS are Eqs. (1) and (2). We will prove here that the new CEH with symmetry, Eqs. (6) and (7), can also be used to express the SODS. If all the  $N$  generalized coordinates  $q_s$  and  $N$  generalized momenta  $p_s$  in Eqs.(6) and (7) are independent, then the CEH, Eqs. (6) and (7), can be reduced to Eqs.(1) and (2). In fact, this is just the case of the SODS, where all the generalized coordinates and the generalized momenta are independent. Consequently, the new CEH with symmetry obtained in the paper can express not only the FODS but also the SODS. In the other word, the new CEH, Eqs. (6) and (7), and the conventional CEH, Eqs.(1) and (2), are equivalent for the description of the SODS, but the former are with some kind of symmetry in form and the latter are lack of such symmetry. The conventional CEH, Eqs.(1) and (2), can only expresses the SODS.

In addition, the number of Eqs. (6) and (7) is  $N$  ( $N$  is the number of the generalized coordinates) in the case for the FODS, and is half of that of Eqs.(1) and (2). This can be explained in the following way. For the SODS, the Euler-Lagrange equations are the second order partial differential equations about the evolution coordinate, the number of which is  $N$ . It is well known that one second-order differential equation can be reduced to two first-order differential equations [7]. Then  $2N$  CEHs, which are the first order partial differential equations about the evolution coordinate, can be obtained from the  $N$  Euler-Lagrange equations. But it is significantly different for the FODS that the Euler-Lagrange equations are the first order partial differential equations about the evolution coordinate, from which only  $N$  CEHs are obtained.

#### 5. Conclusion

We obtain a new kind of CEH, which are of some kind of symmetry in form. The new CEH with symmetry can express both the FODS and the SODS, while the conventional CEH can only express the SODS but impossibly express the FODS. The number of the CEH for the first order differential system is  $N$  rather than  $2N$  like the case for the second order differential system, where  $N$  is the number of the generalized coordinates. The NLSE can be expressed with the new CEH in a consistent way, but can not be expressed with the conventional CEH. The CEH for the NLSE are two equations, which are consistent in the sense that the NLSE can be expressed with one of the CEH and its complex conjugate can be expressed with the other. The Hamiltonian formulation for the continuous system can also be extended to the discrete system.

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