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Quantization of Classical Systems without Lagrangian on Phase Space

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Abstract

The existency conditions of Lagrangian on phase space for general classical dynamical systems are reformulated with symplectic geometry language. For those classical systems that have no Lagrangian discription on phase space, the corresponding quantum systems can not be gained by ordinary quantization methods. To quantize such systems, super-phace-space discriptions of classical systems are introduced and quantization is performed in the super-phase-space with the aid of Dirac's techniques of treating constrained systems.

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[1]

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1. Introduction

A classical dynamical system is determined by a set of differencial equations. In this paper, we will discuss a large class of dynamical systems, Newtonian systems, which cover most of physically interested dynamics. The set of differencial equations determining a Newtonian system can always be expressed as follows:

$$\ddot{x}_i = f_i(x, \dot{x}). \qquad i = 1, 2, ..., d. \tag{1.1}$$

where x_i (i=1,...,d) are coordinates of system's configuration space Q and f_i are some smooth functions over phase space TQ with coordinates $(x_i, \dot{x}_i)$.

For a general Newtonian system, it is not garranteed that the system could get a Lagrangian discription on phase space TQ. That is, for a general Newtonian system, it is usually impossible to find a Lagrangian $L(x, \dot{x})$ on TQ such that its Euler-Lagrange motion equations are equivallent to the given set of equations (1.1). This aspect of interest has been investigated by many people and various forms of existency conditions for Lagrangian on phase space(usually named as Helmhotz conditions) have been proposed[1-5]. However, in order to make this paper self-contained, we will reexamine the problem briefly in section two and give a concice form of Helmhotz conditions in term of symplectic geometry language.

When a given Newtonian system has no Lagrangian discription on phase space TQ, all existing quantization methods can not be directly used. Then, how can we establish the corresponding quantum mechanics for the given system? In section three, we will introduce super-phase-space TTQ and prove that any Newtonian system, whether it has Lagrangian on phase space TQ or not, can always be described via Lagrangian formalism in the super-phase-space TTQ. Since the introduction of TTQ effectively enlarges the number of freedom of the given system, what we have to treat will be some constrained system in the super-phase-space.

When a Newtonian system is viewed as a constrained system in TTQ, its quantum mechanics can be gained with those techniques developed by Dirac. In section four, we will demonstrate the procedure of our super-phase-space quantization with two simple but nontrivial examples.

The last section will be devoted to conclusions and final discussions.

2. Geometric Discription of Helmhotz Conditions

Given a d-dimensional Newtonian system as follows,

$$\ddot{x}_i = f_i(x, \dot{x}) \qquad i = 1, 2, ..., d \tag{2.1}$$

the conditions concerning whether there exist some Lagrangian $L(x, \dot{x})$ on phase space such that the Euler-Lagrangian motion equations coincide with (2.1) are usually named as Helmhotz conditions[1]. In this section, we will derive a geometric discription of the conditions.

Suppose there is a Lagrangian $L(x, \dot{x})$ with its Euler-Lagrangian motion equations as follows:

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{x}_j}) - \frac{\partial L}{\partial x_j} = 0. \tag{2.2}$$

Namely,

$$\frac{\partial^2 L}{\partial \dot{x}_i \partial \dot{x}_j}\ddot{x}_i + \frac{\partial^2 L}{\partial x_i \partial \dot{x}_j}\dot{x}_i - \frac{\partial L}{\partial x_j} = 0. \tag{2.3}$$

In order that equations (2.3) are equivallent to (2.1), following conditions are to be met:

$$Det(\frac{\partial^2 L}{\partial \dot{x}_i \partial \dot{x}_j}) \neq 0. \tag{2.4.a}$$

$$\frac{\partial^2 L}{\partial x_i \partial \dot{x}_j}\dot{x}_j - \frac{\partial L}{\partial x_j} = -\frac{\partial^2 L}{\partial \dot{x}_i \partial \dot{x}_j}f_i. \tag{2.4.b}$$

Now, let us define a 1-form on phase space TQ as,

$$\theta_L = \frac{\partial L}{\partial \dot{x}_i}dx_i. \tag{2.5}$$

The exterior derivative of the 1-form induces a 2-form as follows,

$$\omega_L = d\theta_L = \frac{\partial^2 L}{\partial x_i \partial \dot{x}_j} dx_i \wedge dx_j + \frac{\partial^2 L}{\partial \dot{x}_i \partial \dot{x}_j} d\dot{x}_i \wedge dx_j. \tag{2.6}$$

It is easy to prove that conditions (2.4.a)(2.4.b) can be reexpressed geometrically as:

$$Det(\omega_L) \neq o. \tag{2.7.a}$$

$$i_{\tilde{T}}\omega_L + dh_L = 0. \tag{2.7.b}$$

where $\tilde{T}$ is the vector tangent to the dynamical trajectories in phase space TQ with expression as follows,

$$\tilde{T} = \dot{x}_i \frac{\partial}{\partial x_i} + f_i \frac{\partial}{\partial \dot{x}_i}. \tag{2.8}$$

and h_L is defined as,

$$h_L = \dot{x}_i \frac{\partial L}{\partial \dot{x}_i} - L. \tag{2.9}$$

From its definition (2.6), we know that ω_L is a closed 2-form while condition (2.7.a) implies that it's also nondegenerate. Therefore, ω_L will be a symplectic structure on TQ. Furthermore, from condition (2.7.b), it's easy to prove that this symplectic structure must be vanished by Lie derivative associated with $\tilde{T}$, i.e. $\mathcal{L}_{\tilde{T}}\omega_L = 0$. As a result, we can draw a concice theorem concerning the existency of phase space Lagrangian as follows:

Theorem: *The necessary condition that a given Newtonian system has Lagrangian discription on phase space TQ is that there exist a symplectic structure ω on TQ such that $\mathcal{L}_{\tilde{T}}\omega = 0$, where $\tilde{T}$ is the vector tangent to dynamical trajectories in TQ of the given system.*

Here, a few more words deserve speaking: (i). Above necessary conditions are also sufficient when the foundamental group of the configuration space is trivial. Since if we have found a symplectic struture ω on TQ satisfying $\mathcal{L}_{\tilde{T}}\omega = 0$, we will

have $d(i_{\tilde{T}}\omega) = 0$. According to Poincare theorem[6], when the foundamental group is trivial, any closed form must be exact. As a result, there will exist a function h such that $i_{\tilde{T}}\omega = dh$. Let $\dot{x}_i \frac{\partial L}{\partial \dot{x}_i} - L = h$, we will get a phase space Lagrangian L whose Euler-Lagrangian motion equations coincide with original ones (2.1). This Lagrangian L is called being induced from the symplectic structure ω. (ii). If we have found a symplectic structure ω satisfying $\mathcal{L}_{\tilde{T}}\omega = 0$, then any $\omega' = \alpha\omega$ with α being constants is also a symplectic structure satisfying $\mathcal{L}_{\tilde{T}}\omega' = 0$. The Lagrangians induced from ω and ω' satisfy following relations:

$$L' = \alpha L + \frac{dg}{dt}. \tag{2.10}$$

which are well-known trivially equivallent Lagrangians. (iii). Not all Lagrangians are trivially equivallent. Namely, we might find two or more symplectic strutures, say ω_1 and ω_2, both satisfying $\mathcal{L}_{\tilde{T}}\omega_i = 0$ while $\omega_1 \neq \alpha\omega_2$. In this case, Lagrangians L_1 and L_2 induced from ω_1 and ω_2 have no longer relation like (2.10), though they lead to the same motion equations as (2.1).

As a conclusion of this section, we stress a fact that, for a general Newtonian system, the existency of phase space Lagrangian is not garranteed, but determined by the theorem stated above; on the other hand, in the case that the existency conditions are obeyed, there usually exist many phase space Lagrangians, some of them are trivially equivallent, the others not.

As well-known, quantization starting from different Lagrangians which are equivallent at classical level usually lead to nonequivallent quantum theories. This is one of many ambiguities in quantization procedure which deserve more discussions. However, this paper is devoted to another part of the problem—if a given Newtonian system has no Lagrangian on phase space at all, how can we quantize the system and get a corresponding quantum mechanics system? In next section, we will introduce super-phase-space discription of Newtonian systems, which

makes the problem become tractable.

3. Super-Phase-Space Discription of Newtonian Systems

As discussed last section, it is not unfrequent that a given Newtonian system has no Lagrangian on phase space TQ. Mathematically speaking, this fact is due to that second-order differencial equations generally have no minimum variational principle. However, as point out by Havas[7], a set of first-order differencial equations always has minimum variational principle. This observation make the introduction of super-phase-space a natural attenption. Since through appropriately enlarging the set of variables, second-order differencial equations can be reexpressed as first-order ones under new set of variables. Therefore, according to Havas, any Newtonian system can be described by some Lagrangian on super-phase-space, no matter whether it has Lagrangian on phase space.

Now, let us give the idea a concrete formulation.

Given a general Newtonian system as follows,

$$\ddot{x}_i = f_i(x, \dot{x}) \tag{3.1}$$

where x_i $(i = 1, 2, ..., d)$ are coordinates of system's configuration space Q, f_i's are some smooth functions over system's phase space TQ with coordinates $(x, \dot{x})$.

If we define $q_i = x_i$, $q_{i+n} = \dot{x}_i$, $F_i = q_{i+n}$ and $F_{i+n} = f_i$, equations (3.1) can be rewritten as following first-order forms:

$$\dot{q}_a = F_a(q). \qquad (a = 1, 2, ..., 2d) \tag{3.2}$$

The coordinates of phase space TQ are now represented with q_a's instead of original $(x_i, \dot{x}_i)$. Regarding TQ as a new base manifold, the tangent bundle TTQ over the base manifold will be called super-phase-space with coordinates $(q_a, \dot{q}_a)$.

Now let us look for Lagrangian $\tilde{L}(q, \dot{q})$ on super-phase-space TTQ such that following Euler motion equations coincide with (3.2),

$$\frac{d}{dt}(\frac{\partial \tilde{L}}{\partial \dot{q}_a}) - \frac{\partial \tilde{L}}{\partial q_a} = 0. \tag{3.3}$$

Straightforward comparing of (3.2) with (3.3) shows that $\tilde{L}(q, \dot{q})$ must have forms as,

$$\tilde{L}(q, \dot{q}) = L_a(q)\dot{q}_a + L_0(q). \tag{3.4}$$

while L_a's obey following restrictions,

$$Det\Delta_{ab} \neq 0. \tag{3.5.a}$$

$$\Delta_{ab}F_b = \frac{\partial L_0}{\partial q_a}. \tag{3.5.b}$$

where Δ_{ab} is defined as,

$$\Delta_{ab} = \frac{\partial L_a}{\partial q_b} - \frac{\partial L_b}{\partial q_a}. \tag{3.5.c}$$

According to Koeing's theorem[7], for any $L_0(q)$, we can find a solution for $L_a(q)$ from (3.5). Henceforth, $\tilde{L}(q, \dot{q})$ always exists. This is a main advantage of super-phase-space discription of Newtonian systems over ordinary discription on phase space.

However, the adoption of super-phase-space means that we have hired more variables than necessary. In other words, the Newtonian system must be a constrained system on super-phase-space TTQ. This point will become more apparent if we investigate Hamiltonian formulation of the system.

According to (3.4), we have the conjugated momenta of q_a's and the system's Hamiltonian as follows:

$$p_a = \frac{\partial \tilde{L}}{\partial \dot{q}_a} = L_a(q). \tag{3.6.a}$$

$$H = p_a\dot{q}_a - \tilde{L} = -L_0(q). \tag{3.6.b}$$

where p_a's and q_a's are conjugated in the sence of Poisson bracket defined as,

$$\{A, B\} = \frac{\partial A}{\partial q_a}\frac{\partial B}{\partial p_a} - \frac{\partial B}{\partial q_a}\frac{\partial A}{\partial p_a}. \tag{3.7}$$

From (3.6.a), it is obvious that there are $2d$ primary constrains, *i.e.* $\phi_a = p_a - L_a$. In order to search for other possible constrains, let us use Dirac's techniques[8,9] and modify the Hamiltonian by introducing Lagrangian multiplers as follows,

$$H^* = H + \lambda_a \phi_a. \tag{3.8}$$

The consistency conditions of constrains read as,

$$\dot{\phi}_a = \{\phi_a, H^*\} \approx 0. \tag{3.9}$$

which can be envaluated explicitively as,

$$\Delta_{ab}\lambda_a + \frac{\partial L_0}{\partial q_b} = 0. \tag{3.10}$$

where Δ_{ab} is the one defined previously in (3.5.c).

The fact that no trivial identities appear in (3.10) means the system has no secondary constrains. Therefore, all constrains the system subjects to are those $2d$ primary ones. Further, it is easy to verify that these $2d$ constrains are all belong to second class in the terminology of Dirac, since $\{\phi_a, \phi_b\} = -\Delta_{ab}$ with $Det\Delta \neq 0$.

In this case where all constrains are second class, the Hamiltonian formulation of the system can be most easily described with the aid of Dirac' bracket defined as follows:

$$\begin{aligned}\{A, B\}^* &= \{A, B\} - \{A, \phi_a\}\{\phi_a, \phi_b\}^{-1}\{\phi_b, B\}, \\ &= \{A, B\} + \{A, \phi_a\}\Delta^{-1}_{ab}\{\phi_b, B\}.\end{aligned} \tag{3.11}$$

The time evolution of any quantity on super-phase-space can be generally expressed via Dirac's bracket as,

$$\dot{A} = \{A, H\}^*. \tag{3.12}$$

As a conclusion of this section, we have introduced super-phase-space Lagrangian discription for classical systems, by which any Newtonian system can be viewed as a contrained system in the super-phase-space. The super-phase-space Hamiltonian formulation of the systems has been established with the aid of Dirac's techniques. At this stage, super-phase-space canonical quantization for the systems can be easily realized following Dirac's proposition. In next section, we will demonstrate the quantization procedure with two examples.

4. Super-Phase-Space Quantization of Newtonian Systems

After viewing Newtonian systems as second class contrained systems in super-phase-space, canonical quantization for the systems can be easily achieved, following Dirac's proposition, by replacing Dirac's brackets with commutators of corresponding operators. Namely,

$$\{A, B\}^* \mapsto \frac{i}{\hbar}[\hat{A}, \hat{B}]. \tag{4.1}$$

where $\hat{F}$ represents the operator corresponding to function F.

The quantum evolution equation is Schrodinger-type as follows,

$$i\hbar\frac{\partial}{\partial t}|\psi> = \hat{H}|\psi> \tag{4.2}$$

where Hamiltonian operator $\hat{H} = -L_0(\hat{q})$ according to (3.6.b).

Since there are only $\hat{q}_a$ operators in $\hat{H}$, it is enough to investigate only Dirac brackets and corresponding commutators among q_a's. Referring to (3.11), it is straightforward that,

$$\{q_a, q_b\}^* = \{q_a, q_b\} + \{q_a, \phi_c\}\Delta^{-1}_{cd}\{\phi_d, q_b\} = -\Delta^{-1}_{ab}. \tag{4.3}$$

Henceforth, according to (4.1), the quantum commutators of corresponding operators are as follows,

$$[\hat{q}_a, \hat{q}_b] = i\hbar\Delta^{-1}_{ab}. \tag{4.4}$$

The algebra of commutators (4.4) plus quantum evolution equation (4.2) will determine a quantum system quantized from the given Newtonian system. In fact, all we really need is the expression of $L_0(q)$, since $H = -L_0$ and according to (3.5), Δ_{ab} can be calculated out if L_0 is known.

Since $-L_0$ is the Hamiltonian of the system to be quantized, looking for the expression of L_0 is actually looking for the expression of system's total energy from the given set of motion equations. Generally speaking, this is not a simple work. Anyway, let us demonstrate our super-phase-space quantization procedure with following two simple but nontrivial examples:

Example One: One dimensional conserved systems with motion equation as follows,

$$\ddot{x} = -V'(x). \tag{4.5}$$

This system has Lagrangian discription on phase space and can be easily quantized through ordinary canonical quantization procedure. However, we will demonstrate that the method of super-phase-space quantization will lead to the same result.

Through introducing super-phase-space with coordinates $(q_a, \dot{q}_a)$ where q_a are defined to be $q_1 = x$, $q_2 = \dot{x}$, the motion equations of the system can be rewritten in super-phase-space as:

$$\dot{q}_1 = q_2, \quad \dot{q}_2 = -V'(q_1). \tag{4.6}$$

According to (3.4), the super-phase-space Lagrangian $\tilde{L}(q, \dot{q})$ will has the form as,

$$\tilde{L}(q, \dot{q}) = \dot{q}_1 L_1(q) + \dot{q}_2 L_2(q) + L_0(q). \tag{4.7}$$

where $L_0(q)$ must be the minus of system's total energy, which is obvious for the conserved systems:

$$L_0(q) = -(\frac{q_2^2}{2} + V(q_1)). \tag{4.8}$$

Substituting (4.8) into (3.5) with those F_a's determined by (4.6), the Δ matrix can be calculated out as follows,

$$\Delta^{-1} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{4.9}$$

Therefore, according to (4.4), the quantum commutators between $\hat{q}_a$'s will be,

$$[\hat{q}_1, \hat{q}_2] = i\hbar. \tag{4.10}$$

with others being zero. Or expressed with original variables as,

$$[\hat{x}, \hat{\dot{x}}] = i\hbar. \tag{4.11}$$

with others being zero.

The Hamiltonian operator in Schrodinger equation (4.2) is now,

$$\hat{H} = -L_0(\hat{q}) = \frac{\hat{q}_2^2}{2} + V(\hat{q}_1) = \frac{\hat{\dot{x}}^2}{2} + V(x). \tag{4.12}$$

In coordinate representation $\hat{x}\psi(x) = x\psi(x)$, the differencial realization of $\hat{\dot{x}}$ can be derived from the commutation relation (4.11) as,

$$\hat{\dot{x}} = -i\hbar\frac{\partial}{\partial x}. \tag{4.13}$$

As a result, Schrodinger equation for the system in the coordinate representation will be,

$$i\hbar\frac{\partial}{\partial t}\psi(x) = [\frac{(i\hbar)^2}{2}\frac{\partial^2}{\partial x^2} + V(x)]\psi(x). \tag{4.14}$$

which is the same as the result quantized via ordinary phase space quantization.

Example Two: Let us consider a two dimensional system described by following motion equations:

$$\ddot{x} + \dot{y} = 0, \quad \ddot{y} + y = 0. \tag{4.15}$$

This system, which is belong to case III-b in Douglas' classification[1], has no Lagrangian discription on phase space. If we want to get the quantum mechanics

of this system, the method of super-phase-space quantization discussed above has to be hired.

By tntroducing super-phase-space with coordinates $(q_a, \dot{q}_a)$ where q_a's are defined as $q_1 = x$, $q_2 = y$, $q_3 = \dot{x}$ and $q_4 = \dot{y}$, the motion equations (4.15) can be rewritten in super-phase-space as,

$$\dot{q}_1 = q_3, \quad \dot{q}_2 = q_4, \quad \dot{q}_3 = -q_4, \quad \dot{q}_4 = -q_2. \tag{4.16}$$

According to (3.4), the super-phase-space Lagrangian $\tilde{L}(q, \dot{q})$ will be,

$$\tilde{L}(q, \dot{q}) = \sum_{a=1}^{4} \dot{q}_a L_a(q) + L_0(q). \tag{4.17}$$

where $L_0(q)$ must be the minus of system's total energy.

However, except the cases of conserved systems where systems' total energy are well-defined to be the sum of kinematic energy and conserved potential, the definition of "total energy" of a general Newtonian system is proved to be troublesome. Anyway, following adoption of $L_0(q)$ might be a correct one, since it is the simplest motion integral which looks like energy:

$$L_0(q) = \frac{1}{2}(q_4^2 - q_3^2 - 2q_2q_3). \tag{4.18}$$

It can be readily proven that $\frac{d}{dt}L_0 = 0$, which means that L_0 is indeed a motion intergral.

Now, substituting above expression of $L_0(q)$ into (3.5) with those F_a's determined by (4.16), the Δ matrix can be calculated out as follows:

$$\Delta^{-1} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 \\ 0 & -1 & 1 & 0 \end{pmatrix} \tag{4.19}$$

Therefore, according to (4.4), the quantum commutators between $\hat{q}_a$'s will be,

$$[\hat{q}_1, \hat{q}_2] = i\hbar, \quad [\hat{q}_2, \hat{q}_4] = -i\hbar, \quad [\hat{q}_3, \hat{q}_4] = i\hbar. \tag{4.20}$$

with others being zero.

Expressed with original variables, above commutators become,

$$[\hat{x}, \hat{y}] = i\hbar, \quad [\hat{y}, \hat{\dot{y}}] = -i\hbar, \quad [\hat{\dot{x}}, \hat{\dot{y}}] = i\hbar. \tag{4.21}$$

with others being zero.

The Hamiltonian operator in Schrodinger equation (4.2) is now,

$$\hat{H} = -L_0(\hat{q}) = \frac{1}{2}(\hat{q}_3^2 - \hat{q}_4^2 + 2\hat{q}_2\hat{q}_3). \tag{4.22}$$

or expressed with original variables as,

$$\hat{H} = \frac{1}{2}(\hat{\dot{x}}^2 - \hat{\dot{y}}^2 + 2\hat{y}\hat{\dot{x}}). \tag{4.23}$$

As a result, we have finished the super-phase-space quantization procedure for the given Newtonian system (4.15) under the definition of system's total energy (4.18). The resulting quantum system is completely determined by Schrodinger equation (4.2), Hamiltonian operator (4.23) and commutation relations (4.21).

The differential realization of operators can be achieved by choosing a particular representation. For example, since $[\hat{x}, \hat{\dot{y}}] = 0$, we may choose the representation space to be the one spanned by common eigenstates of $\hat{x}$ and $\hat{\dot{y}}$. Namely,

$$\hat{x}\psi(x, u) = x\psi(x, u), \quad \hat{\dot{y}}\psi(x, u) = u\psi(x, u). \tag{4.24}$$

The differential forms of operators $\hat{y}$ and $\hat{\dot{x}}$ can be easily derived from commutation relations (4.21) as,

$$\hat{y} = -i\hbar(\frac{\partial}{\partial x} + \frac{\partial}{\partial u}), \quad \hat{\dot{x}} = i\hbar\frac{\partial}{\partial u}. \tag{4.25}$$

As a result, Schrodinger equation of the system under the representation chosen above will be,

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{(i\hbar)^2}{2}(\frac{\partial^2\psi}{\partial u^2} + 2\frac{\partial^2\psi}{\partial u\partial x}) - \frac{u^2}{2}\psi. \tag{4.26}$$

5. Conclusions

Motivated by Feynman's idea which was published recently under the name of Dyson[10], we have discussed some problems concerning the quantization procedure from classical dynamical systems which are basically determined by a set of differential equations to corresponding quantum systems.

The existency conditions of phase space Lagrangian are derived in terms of symplectic geometric language. When there exist no phase space Lagrangian for a given classical system, all existing methods of quantization can not be directly used to get the corresponding quantum system. In order to quantize such systems. super-phase-space discription has been introduced, in which any Newtonian system can be viewed as a second class constrained system in the super-phase-space. With the aids of Dirac's algorithm, we have established a formulation of super-phase-space quantization which is applicable to the most general Newtonian systems, no matter whether their phase space Lagrangian exist.

As a final remark, we believe that to generalize the discussions of this paper to more general classical dynamical systems would be an interesting work.

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