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Quantization of Classical Systems

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It is shown that classical systems with non-integrable constraints cannot be derivable from a variational principle without invoking subsidiary conditions. Quantization by Dirac's method or by Faddeev-Fradkin's modified path integral method is therefore impossible.

Mostra-se que sistemas clássícos com vínculos não integráveis não podem ser derivados de um principio variacional sem o recurso de condições subsidiárias. A quantização pelo método de Dirac ou pela versão modificada por Faddeev e Fradkin da integral sobre trajetórias torna-se portanto impossivel.

1. INTRODUCTION

If one analyses the development of natural science in this century one immediately perceives two branches which blossomed into theories of natural phenomena with disjoints domains of applications. On the one hand stands quantum theory searching for the fundamental forces of nature and, on the other hand, stands the theory of dynamical systems trying to describe the macroscopic world that surrounds us.

One may place the starting point of the development of quantum theory on the quantization of classical hamiltonians associated to atomic systems. The success of quantum theory followed quickly in the domain of atoms, molecules, crystals and atomic nuclei. But, to develop itself into a consistent theory of nature quantum theory had also to quantize the fundamental fields of forces and contain asymptotically every classycal system.

For systems with a finite number of degrees of freedom two results were of fundamental importance: Dirac's[1] treatment of singular lagrangeans proved that every consistent lagrangean gives, by the use of the variational principle, equations of motion that can be put into the hamiltonian formalism, the singular lagrangeans giving constrained hamiltonian systems. The extension of Feynman integrals to singular lagrangeans, as proposed by Faddeev[2] and extended by Fradkin[4] made the programme for quanírization of equations of motion derived by the variational principle formally well defined. If one might summarize the general approach to a quantized description of the fundamental forcesof nature one would say that it is centered around the ideas of modelling with field lagrangeans and the extension of Faddeev-Fradkin's functional integral to infinite degrees of freedom.

The purpose of this paper is to call attention to the possibility of theoretical development in a diametrically opposed direction to the one considered so far.

If one would have tried to explain the whole spectrum of systems, from simple atoms to large macroscopic objects ininteraction, one would apply quantum theory to the atoms and classical dynamics to the macroscopic objects.

These opposing descriptions would not be in conflict if every classical macroscopic systems could be derived as the asymptotic limit of some quantum system. This is certainly not so. We shall show in this paper that the conflict exists even in the realm of newtonianniechanics, as in the case of particles moving subject to non-integrable constraints.

In the next section we shall discuss the simplest caseof newtonian mechanics with a non-integrable constraint: a particle in three dimensions subject to a single constraint. In section 3 we generalize our results. In section 4 we discuss an example. In section 5 we argue on the impossibility of quantizing such system by any standard method.

2. THE THREE DIMENSIONAL CASE

Consider a non-relativistic particle with mass m and coordinates q_i subject to the ideal constraint given by

$$a_i dq_i = 0 \tag{2.1}$$

summation over repeated indíces beíng meant.

Eq. (2.1) means that at every instant of time the motion of the particle is such that the possible virtual displacements dq_i must be perpendicular to the vector $\vec{a}$ with components a_i. We shall assume, from here on, that $\vec{a}$ is a unit vector:

$$a_i a_i = 1 \tag{2.2}$$

From D'Alembert's principle we must have

$$m\ddot{q}_i dq_i = 0 \tag{2.3}$$

subject to eq.(2.1) from where we easily obtain

$$\begin{aligned} m\ddot{q}_i &= \lambda a_i \\ a_i q_i &= 0 \end{aligned} \tag{2.4}$$

X being a Lagrange multiplier.

Eliminating λ from the above equations we obtain finally

$$\ddot{q}_i + a_i(\partial a_j/\partial q_k)\dot{q}_j\dot{q}_k = 0$$

$$a_i\dot{q}_i = 0 \tag{2.5}$$

as the equations of motion, with X given by

$$\lambda = -m(\partial a_i/\partial q_j)\dot{q}_i\dot{q}_j$$

Let us try to obtain the same equations from the variational principle.

We begin choosing the lagrangean

$$L = 1/2\ m\ \dot{q}_i \dot{q}_i - \lambda\ a_i \dot{q}_i \tag{2.6}$$

where we treat λ as the fourth coordinate of the particle The Euler-Lagrange equations give

$$m\ddot{\vec{q}} = \dot{\lambda}\vec{a} - \lambda\dot{\vec{q}} \wedge \text{rot}\ \vec{a}$$
$$\vec{a}\cdot\dot{\vec{q}} = 0 \tag{2.7}$$

We may decompose rot $\vec{a}$ in its two components one parallel to $\vec{a}$ and the other in the plane perpenticular to $\vec{a}$. We get

$$m\ddot{\vec{q}} = (\dot{\lambda} - \lambda\vec{a}\cdot\dot{\vec{q}} \wedge \text{rot}\ \vec{a})\vec{a} - \lambda(\vec{a}\ \text{rot}\ \vec{a})\dot{\vec{q}} \wedge \vec{a} \tag{2.8}$$

Therefore eq. (2.7) is equivalent to eq. (2.4) if and only if

$$\vec{a}\cdot\text{rot}\ \vec{a} = 0 \tag{2.9}$$

which is the integrability condition for the constraints given by eq. (2.1).

We therefore conclude that the necessary and sufficient condition for the lagrangean given by eq. (2.6) to give the correct eq.(2.4) for the motion of the particle is that the constraint, given by eq.(2.1) be integrable.

This result suggests the question if some lagrangean, not necessarily of the form given by eq. (2.6), may give the correct equation of motion for non-integrable constraints. Before considering this fundamental question we shall generalize the results shown in this section.

3. THE GENERAL CASE

We now consider a generalization of the previous result by considering a free particle moving in a n-dimensional space subject to p ideal constraints ($p \leq n-2$) of the form

$$a_i^\beta\ dq_i = 0 \qquad \beta = 1,2,\ldots,p \tag{3.1}$$

We assume, without loss of generality, that the vectors a^β are of unit length and linearly independent.

Newton's equations are therefore, from D'Alembert's principle, of the form

$$m\ddot{q}_i = \lambda_\beta a_i^\beta \tag{3.2}$$

where λ_β are the Lagrange multipliers. From eqs. (3.1) and (3.2) we obtain

$$\ddot{q}_i + a_i^\beta(\partial a_j^\beta/\partial q_k)\dot{q}_k\dot{q}_j = 0 \tag{3.3}$$

Let us consider

$$L = 1/2\, m\, \dot{q}_i\dot{q}_i - \lambda_\beta a_i^\beta \dot{q}_i \tag{3.4}$$

and let us investigate whether the above lagrangean produces, by the variational principle, Newton's eq. (3.3).

The Euler's equations derived from L are

$$m\ddot{q}_i = \dot{\lambda} a_i + \lambda_\beta(a_i^\beta/\partial q_j - \partial a_j^\beta/\partial q_i)\dot{q}_j$$

$$a_i^\beta\dot{q}_i = 0 \quad , \quad i = 1,2,\ldots n \; . \tag{3.5}$$

It is easy to prove that the condition for eq.(3.5) to be equivalent to eq. (3.3) is that the vector A with components given by

$$A_i = \lambda_\beta(\partial a_i^\beta/\partial q_j - \partial a_j^\beta/\partial q_i)\dot{q}_j \tag{3.6}$$

be a linear combination of the vectors a^β, that is

$$\lambda_\beta(\partial a_i^\beta/\partial q_j - \partial a_j^\beta/\partial q_i)\dot{q}_j = C_\beta a_i^\beta \; . \tag{3.7}$$

We now prove that the condition given by eq. (3.7) is equivalent to say that the system of forms given by eq. (3.1) is integrable.

Let us suppose that the system is integrable. Then, there must exist a non-singular matrix $t^{\beta\beta'}$ and functions $\phi^{\beta}(q)$ such that

$$a_i^{\beta}\, dq_i = t^{\beta\beta'}\ d\phi^{\beta'}$$

Calculating A_i using the above equations we obtain

$$A_i = -\lambda_{\beta}(\partial t^{\beta\beta'}/\partial q_j)(\partial\phi^{\beta'}/\partial q_i)\dot{q}_j$$

Therefore

$$A_i = C_{\beta} a_i^{\beta}$$

where

$$C_{\beta} = -\lambda_{\beta}(\partial t^{\beta\beta'}/\partial q_j)(t^{-1})^{\beta'\ \beta}\dot{q}_j$$

which proves that if the constraints given by eq. (3.1) are integrable eq. (3.7) is valid.

Let us now start from eq. (3.7) assumed valid for every possible value of the λ_{β} compatible with eq. (3.5). From eq. (3.5) we conclude that λ_{β} satisfies a first order linear equation and therefore, for every set of values of q and $\dot{q}$ we can arbitrarily choose the values of λ_{β}. This being so, we conclude from eq. (3.7) that

$$(\partial a_i^{\beta}/\partial q_j - \partial a_j^{\beta}/\partial q_i)\dot{q}_j = (\partial C_{\beta'}/\partial\lambda_{\beta})a_i^{\beta'}$$

Let us interpret the above equation as a relation between forms. We have

$$(\partial a_i^{\beta}/\partial q_j - \partial a_j^{\beta}/\partial q_i)dq_j = (\partial C_{\beta'}/\partial\lambda_{\beta})a_i^{\beta'}\ dt$$

or better

$$(\partial a_i^{\beta}/\partial q_j) - \partial a_j^{\beta}/\partial q_i)dq_j \wedge dq_i = (\partial C_{\beta'}/\partial\lambda_{\beta})dt \wedge a_i^{\beta'}\ dq_i$$

writing $\omega^{\beta} = a_i\ dq_i$ we have

$$d\omega^\beta = 1/2\ (\partial a_i^\beta/\partial q_j - \partial a_j^\beta/\partial q_i)\, dq_j \wedge dq_i$$

and thus, from eq. (3.8)

$$d\omega^\beta = S^\beta_{\beta'}\,\omega^{\beta'}$$

where

$$S^\beta_{\beta'} = 2(\partial C_{\beta'}/\partial\lambda_\beta)\,dt$$

Let us call

$$\Omega = \omega^1 \wedge \omega^2 \wedge \dots \wedge \omega^p$$

We have finally

$$d\omega^\beta \wedge \Omega = 0 \quad , \qquad \beta = 1, 2, \dots, p \ ,$$

and by Froebenius Theorem[3], the system

$$\omega^\beta = 0 \ , \quad \beta = 1,2,\dots,p \ ,$$

is integrable.

4. AN EXAMPLE

In order to make clear the difference of the results of the newtonian and lagrangean approaches to the equation of motion, we consider in this section the simplest case of non-integrability of constraints. We suppose the constraint to be given by

$$d_1 dq_2 + dq_3 = 0 \qquad (4.1)$$

This corresponds to have a_i given by

$$a_1 = 0, \quad a_2 = q_1/(1+q_1^2)^{1/2} \ , \ a_3 = 1/(1+q_1^2)^{1/2} \qquad (4.2)$$

The condition of integrability is

$$\vec{a}\cdot\mathrm{rot}\ \vec{a} = 1/(1+q_1^2) \neq 0$$

everywhere different from zero, exhibiting the non-integrability of the constraint given by eq. (4.1).

Eq. (2.5) take the form (m=1)

$$\begin{aligned}
\ddot{q}_1 &= 0 \\
\ddot{q}_2 &= -q_1\dot{q}_1\dot{q}_2/(1 + q_1^2) \qquad (4.3) \\
\dot{q}_3 &= -q_1\dot{q}_2
\end{aligned}$$

The general solution for the above equations can easily be found

$$\begin{aligned}
q_1 &= q_{10} + \dot{q}_{10}\ t \\
q_2 &= q_{20} + \dot{q}_{20}\frac{\sqrt{1+q^2}}{\dot{q}_{10}}\ \ln\left[\frac{q_1+\sqrt{1+q_1^2}}{q_{10}+\sqrt{1+q_{10}^2}}\right] \qquad (4.4) \\
q_3 &= q_{30} - \frac{q_{20}\sqrt{1+q_{10}^2}}{q_{10}}\left(\sqrt{1+q^2} - \sqrt{1+q_{10}^2}\right)
\end{aligned}$$

where

$$\vec{q}_0 = (q_{10},q_{20},q_{30}) \quad \text{and} \quad \dot{\vec{q}}_0 = (\dot{q}_{10},\dot{q}_{20},\dot{q}_{30})$$

are the initial position and velocity of the particle, respectively. It is interesting to notice the absence of $\dot{q}_{30}$ from eqs. (4.4). This is so because the initial conditions have to be consistent with theconstraint equation and we have the relation

$$\dot{q}_{10}\,\dot{q}_{20} + \dot{q}_{30} = 0$$

from where we eliminate $\dot{q}_{30}$ from the law of motion.

If one considers all the trajectories that start from $\vec{q}_0$, one obtains a surface which in our case has its equation given by the elimination of $\dot{q}_{10}$ and $\dot{q}_{20}$ from eq. (4.4). We obtain

$$(q_2-q_{20})(\sqrt{1+q_1^2}-\sqrt{1+q_{10}^2})+(q_3-q_{30})\ln\left(\frac{q_1+\sqrt{1+q_1^2}}{q_{10}+\sqrt{1+q_{10}^2}}\right)=0 \qquad (4.5)$$

Though the motion which started from the point $\vec{q}_0$ is restricted to the above surface, this surface is not an integral for the constraint as $\vec{a}$ is perpendicular only to the trajectories that pass through the point $\vec{q}_0$ but not to the whole surface. Suppose we proceed along a particular trajectory and take another point $\vec{\tilde{q}}_0$ constructing the surface of the trajectories that start from $\vec{\tilde{q}}_0$. the new surface will be different from the previous one intercepting it along the common trajectory that connects $\vec{q}_0$ to $\vec{\tilde{q}}_0$.

Let us suppose now that $a_i dq_i$ is integrable and $\phi(\vec{q})$ is an integral of the constraint. In this case the trajectories that start from $\vec{q}_0$ lie on the surface given by

$$\phi(\vec{q}) = \phi(\vec{q}_0) \qquad (4.6)$$

and the trajectories that start from $\vec{\tilde{q}}_0$ lie on a similar surface given by

$$\phi(\vec{q}) = \phi(\vec{\tilde{q}}_0) \qquad (4.7)$$

If $\vec{\tilde{q}}$ is on the surface given by equation (4.6) then

$$\phi(\vec{\tilde{q}}_0) = \phi(\vec{q}_0)$$

and the two surfaces, given by eqs. (4.6) and (4.7) are the same. The integrability of the constraint decomposes the configuration space into disjoint classes of points, each class corresponding to a surface of the form given by eq. (4.6). The dynamics of the system is fundamentally in a four dimensional phase space in contrast to the case of non-integrable constraint where the phase space has necessarily five dimensions.

Let us consider the equations derived from the lagrangean given by eq. (2.6) with the constraint given, again, by eq. (4.1). After some algebraic manipulations we have the following set of equations for the description of the motion

$$\ddot{q}_1 = -\lambda\dot{q}_2/(1+q_1^2)^{3/2}$$

$$\ddot{q}_2 = -\frac{q_1\dot{q}_1\dot{q}_2}{1+q_1^2} + \frac{\lambda\,\dot{q}_1}{(1+q_1^2)^{3/2}}$$

$$\dot{\lambda} = -\frac{\dot{q}_1\,\dot{q}_2}{(1+q_1^2)^{1/2}} \tag{4.8}$$

$$\dot{q}_3 = -q_1\,\dot{q}_2$$

What is important to observe is that λ satisfies a first order differential equation and that the equation for $\vec{q}$ depends on λ. Thus, by giving the initial conditions at $\vec{q}$, $(q_{01}, q_{02}, q_{03}, \dot{q}_{01}$ and $\dot{q}_{02})$ the motion of the particle is still undetermined, in contrast to what happens in newtonian mechanics. The natural way to fix the conditions for eq. (4.8) is by specifying the initial and the final points of the trajectory. In this case, the initial values $\dot{q}_{01}$, $\dot{q}_{02}$ and λ_0, for the velocity and λ respectively, can be chosen for the motion to reach the final specified point. It is interesting to observe that in the newtonian case, the initial position restricts the final position of the trajectory to the surface given by eq. (4.5). In the lagrángean case this is not so and even if the final position of the particle is on the surface above, the motion is very much different from the newtonian dynamics as one can easily be checked by inspecting the law of motion for $\vec{q}$.

5. CONCLUSIONS

To quantize a classical system by the general procedures developed by Dirac supplemented by Faddeev and Fradkin one has to start from a lagrangean that contains all the dynamical information of the system, the equations of motion being Euler's equations derived from the vanishing of the first variation of the action. To quantize classical systems with constraints one has to obtain a lagrangean which gives, by the variational principle, not only the standard equations of motion but also the constraint equations.

If we consider a non-relativistic free particle subject to the constraint

$$a_i dq_i = 0 \tag{5.1}$$

then the lagrangean

$$L = 1/2\, m\, \dot{q}_i \dot{q}_i - \lambda\, a_i \dot{q}_i$$

gives the correct equations of motion if we treat λ as the fourth coordinate of the particle and if $\omega = a_i dq_i$ is completely integrable. This result can easily be generalized when the particle moves in a n-dimensional space with the constraints of the form given by eq. (5.1) as we have done in section 3. Both results can be further generalized when the system contain applied forces. If the constrained motion of the particle is described by the lagrangean $L_0(q,\dot{q})$ then, the lagrangean

$$L = L_0(q,\dot{q}) - \lambda_\beta a^\beta_i \dot{q}_i$$

gives the correct equations of motion and constraint if we treat $\lambda^\beta(\beta = 1,2,\ldots,p)$ as additional coordinates and if the system of forms

$$\omega^\beta \equiv a^\beta_i dq_i \ , \quad \beta = 1,2,\ldots,p \ ,$$

is completely integrable. In case the systems of forms is not completely integrable the Euler's equations derived from the lagrangean given by eq. (5.2) are not the correct equations obtained by D'Alembert's principle which is fulfilled by every classical system with ideal constraints.

The question one can ask immediately is whether there is a more general lagrangean than these considered so far that reproduces the correct equations of motion. Let us try to answer this question in the case of a particle (free) moving in three dimensional euclidean space subject to a single non-integrable constraint. We suppose that there is a lagrangean defined in a four dimensional manifold that exhibits the correct equations of motion as given by eq. (2.4). If one of these equations is first degree in derivatives, the lagrangean is necessarily singular and its hamiltonian system has constraints. The total number of constraints and gauge conditions (associated to each first class constraint) is necessarily even (see, for example, Fradkin[4] and therefore, by the general theorem of constrained hamiltonians, upon elimination of the constraints, we end up with an unconstrained hamiltonian H^* with phase space of dimension $2(n-p)$, where $2p$ is the total number of constraints and gauge conditions. In our case, as the phase space of H^* has to contain the phase space of the system given by eq. (2.4) we conclude that $p=1$ and H* describe the motion of a system in six dimensional phase space. Now, the phase space of the system given by eq. (2.4) hasonly five dimensions and, therefore, it must be constrained in a five dimensional manifold of the space of H*. Let us assume this manifold to be given by the equation

$$\chi(p^*,q^*) = 0$$

Because the system under consideration does not move out of this manifold we also have

$$\dot{\chi}(p^*,q^*) = \{\chi,H\} = 0$$

and it follows that χ is a constraint for the system described by H* which, by construction, is uncostrained. As the contradictions camefrom the assumption of the existence of a lagrangean for the system given by eq. (2.4) we conclude that it is impossible to construct a lagrangean that completely describes the motion of a system subject to non-integrable constraints.

We therefore conclude that there is a fundamental conflict between the quantum description of the microscopic level and the classical description at the macroscopic level. This conflict is not only between quantum and classical mechanics but also with thetraditional methods of doing statistical mechanics which is based on the existence of a hamiltonian for the elementary systems subject to statistical analysis.

However, there is a difference between the conflict in statistical mechanics and quantum theory. Statistical mechanics makes use of hamiltonian dynamics only to assure the invariance of the density of phase space. This does not require, by itself, that the classical system be necessarily hamiltonian. On the other hand, if one takes the quantization rule as given by Feynman path integral in its hamiltonian form, one observes that it requires two invariants: the phase space density and the Poincaré-Cartan invariant

$$\int (pdq - H\, dt) = \text{invariant}$$

It is an important result of mechanics[5] that the invariance of the integral above is equivalent to impose that the system is hamiltonian what shows once again that one is able to quantize only classical hamiltonian systems.

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