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DIRAC AND HAMILTON

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Abstract. Dirac devised his theory of Quantum Mechanics and recognised that his operators resembled the canonical coordinates of Hamiltonian Mechanics. This gave the latter a new lease of life. We look at what happens to Dirac's Quantum Mechanics if one starts from Hamiltonian Mechanics.

Keywords: Dirac, quantum mechanics, Hamiltonian mechanics.

1. Introduction

When Dirac was developing his theory of Quantum Mechanics, see [1], he observed that the operators he had introduced reminded him of something from Mechanics. He looked to his personal collection in his study and could find nothing suitably advanced, such as Whitaker's Treatise [2] which would contain such information. It was a Sunday afternoon and naturally in those more civilised days the College Library would not be open. Dirac had to wait until Monday morning to find that in fact the very properties he had in his operators, apart from the occasional i, were precisely those of the Poisson Brackets of Hamiltonian Mechanics, which had been established and developed some 120 years before by Poisson and incorporated into the new mechanics some 30 years later.

It is a little difficult to draw a line in the history of the development of Mechanics and to claim what is the *terminus a quo*, but to keep this narrative compact we start with the Mechanics of Newton [3], for it is on his Laws of Motion that the subsequent evolution of Mechanics has been based. One of the problems in practice is the solution of equations and it soon became apparent that the number of problems which could be solved at any particular epoch was rather limited. The theoreticians were always trying to think of a new way to solve the unsolvable.

The Calculus of Variations provided one way to look for solutions from a different direction. Developing upon the work of Euler, Lagrange in his *Mécanique analytique* of 1788 introduced his equations of motion based upon the variation of a functional called the Action Integral. As far as Classical Mechanics was concerned, Lagrange's Equations of Motion were of the second order. In principle these equations reduced to the corresponding Newtonian equations, but Lagrange had introduced the idea of generalised coordinates and generalised forces which always have the possibility of giving equations which look simpler than the naive Newtonian equations.

Then along came Hamilton, who decided to reduce Mechanics to a system of first-order equations. In a sense he was returning to the original formulation of Newton II. As the Hamiltonian, as it came to be called, was derived by introducing a momentum as a derivative of the Lagrangian and then obtained by using a Legendre transformation, it inherited the generalised coordinates and generalised forces of Lagrangian Mechanics except that now there were generalised coordinates and generalised momenta. One of the attractions of Hamilton's approach was the introduction of a theory of transformations whereby one could transform from one Hamiltonian to another by means of transformations which obeyed certain rules.

Hamiltonian Mechanics was and is a marvellous theoretical construct which does have some practical uses. However, as a general tool in elementary mechanics it is not of much practical use and could well have faded into near-oblivion had it not been for the observation of Dirac. Now Hamiltonian Mechanics provided a lodestone to the new Quantum Mechanics.

2. A Problem

We have remarked that the basis of these theoretical constructs can be seen in the Equations of Motion of Newton, particularly in the perturbation theory of orbital mechanics. The construction of an Hamiltonian from a Lagrangian is a quite definite procedure. However, the construction of a Lagrangian which leads to the proper Newtonian Equation of Motion, which in itself begs the question of properness, is by no means unique.

We take a very elementary example, namely the simple harmonic oscillator in one space dimension. The Newtonian Equation of Motion is

$$\ddot{q} + q = 0 \tag{1}$$

in which we have scaled the time to remove a distracting Ω^2.

Equation (1) has a plethora of Lagrangians. For a modest sampling see [4]. Here we consider just three, namely

$$L_1 = \frac{1}{2}\left(\dot{q}^2 - q\right), \tag{2}$$

$$L_2 = \frac{1}{2\sin^2 t\left(\dot{q}\sin t - q\cos t\right)} \quad \text{and} \tag{3}$$

$$L_3 = \frac{1}{2\cos^2 t\left(\dot{q}\cos t + q\sin t\right)}. \tag{4}$$

These Lagrangians share a common property in that they all possess five point Noether Symmetries, which is the maximal number for a one-degree-of-freedom system. In each case the algebra of the symmetries is $sl(2, R) \oplus_s 2A_1$, which is a subalgebra of the $sl(3, R)$ algebra of (1).

The standard formalism leads to three Hamiltonians. These are

$$H_1 = \frac{1}{2}\left(p^2 + q^2\right) \tag{5}$$

$$H_2 = pq\cot t + \frac{i\sqrt{p}}{\sin^3/2t} \quad \text{and} \tag{6}$$

$$H_3 = -pq\tan t + \frac{i\sqrt{2p}}{\cos^{3/2} t} \tag{7}$$

with the canonical momentum in each case being

$$\begin{array}{l|l} L_1 & p = \dot{q} \\ L_2 & p = -\dfrac{\operatorname{cosec} t}{2\left(\dot{q}\sin t - q\cos t\right)^2} \quad \text{and} \\ L_3 & p = -\dfrac{\sec t}{2\left(q\sin t + \dot{q}\cos t\right)^2}. \end{array}$$

The 'quantisation procedure' for H_1 (5) is well known and leads to the equation

$$2iu_t = -u_{qq} - q^2 u \tag{8}$$

about which any competent undergraduate can write at length.

In principle we may follow the same procedure for H_2 and H_3. However, there are two problems. The first is the presence of $\sqrt{p}$, which doubtless makes the process a little complicated. It is true that there exist procedures for dealing with nonstandard forms, but this is not the place to deal with such things as we are considering a very elementary problem. The other difficulty is that, even neglecting the fractional power, the resulting Schrödinger equation would be linear in the spatial derivative.

The question is what to do? There are various possibilities:

(1.) A mistake was made in the calculation of the second and third Hamiltonians. This is unlikely as the algorithm is particularly simple and Mathematica is much better at arithmetic than I am.

(2.) The process was initiated under false pretences. One recalls that the simple harmonic oscillator has three linearly independent quadratic integrals. They are

$$I_1 = \frac{1}{2}\left(\dot{q}^2 + q^2\right),$$
$$I_2 = \frac{1}{2}\mathrm{e}^{2it}\left\{\left(\dot{q}^2 - q^2\right) - 2iq\dot{q}\right\} \quad \text{and}$$
$$I_3 = \frac{1}{2}\mathrm{e}^{-2it}\left\{\left(\dot{q}^2 - q^2\right) + 2iq\dot{q}\right\}.$$

The first integral, I_1, corresponds to the Hamiltonian and equally leads to the Schrödinger Equation given above.
I_2 and I_3 can also be used to construct Schrödinger Equations, but the question is that of meaning [5].

One feature of the Schrödinger Equation for H_1 is that it is a parabolic equation which has the same specific algebra as L_1. One could take the Noether Symmetries of L_2, respectively L_3, and construct the corresponding Schrödinger Equation with the additional requirement that it be linear. The meaning of the outcome could be of interest [6].

One could conclude that the similarity of the operators introduced by Dirac and their identification with those of Hamiltonian Mechanics is an accident and one should read Dirac's book carefully.

3. Conclusion

This simple example already shows that there is the potential for ambiguity in the interpretation of the properties of a classical Hamiltonians, in this case that of the Simple Harmonic Oscillator. A critical aspect is the interpretation of how one should progress from Classical Mechanics to Quantum Mechanics. In the approach adopted by Dirac the Hamiltonian corresponding to the 'standard' Lagrangian, *ie* a Lagrangian of the form $L = T - V$ in the case of simple systems was used to construct an operator which fitted into the expectation for the corresponding quantum mechanical system. If one views the Newtonian equation of motion, (1), as the fundamental source of the problem, that equation has eight Lie point symmetries. Without going into anything fanciful one can construct a large number of Lagrangians using these symmetries, two at a time, with the vector field of the equation of motion to determine Jacobi Last Multipliers and the relationship,

$$\frac{\partial^2 L}{\partial \dot{x}^2} = M,$$

where M is a Last Multiplier, to calculate a whole pile of Lagrangians for the single Newtonian Equation, (1). One can then apply Noether's Theorem to each of these Lagrangians in turn to determine the Noether Symmetries. These vary in number up to a maximum of five. There are three such Lagrangians [7], the L_1, L_2 and L_3 listed above. The first, L_1, is the one which is usually used to construct the Hamiltonian for the Simple Harmonic Oscillator and hence a Schrödinger Equation. Why is it that this Lagrangian should be chosen when there are two other Lagrangians equally well endowed with Noether Symmetries?

One can reasonably claim that this choice leads to physically acceptable results. However, this does not really gel well with the idea of symmetry and operators. Consequently one must argue that the choice of Lagrangian, hence Hamiltonian and corresponding operators for Quantum Mechanics must be predicated on other considerations. In Dirac's book he writes of the energy being the source of the operator to be used for quantisation. It is an accident that in elementary mechanics the energy is the Hamiltonian in the usual meaning of the word. That the operators required for Dirac's Quantum Mechanics had essentially the same properties as the canonically conjugate variables of Classical Hamiltonian Mechanics is perhaps a cause for jumping on a bandwagon without checking to see if the horses had been harnessed.

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