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Classical and quantum dynamics of a particle constrained on a circle

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Abstract

The Dirac method is used to analyze the classical and quantum dynamics of a particle constrained on a circle. The method of Lagrange multipliers is scrutinized, in particular in relation to the quantization procedure. Ordering problems are tackled and solved by requiring the Hermiticity of some operators. The presence of an additional term in the quantum Hamiltonian is discussed. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

The seminal and, so far, most used way to formulate the quantum theory of a particle or a field makes wide use of the Hamiltonian description of classical mechanics [1]. The standard rules for constructing the momenta and the Hamiltonian function, however, cannot be applied when the Lagrangian is singular. In such a case it is not possible to extract the functional dependence of all the velocities on the momenta in order to obtain a Hamiltonian function of coordinates and momenta only. Dirac's method concerns the study of classical systems using the Hamiltonian method when the usual procedure fails due to the singularity of the Lagrangian [2]. Dirac gave very general rules to construct the Hamiltonian and calculate sensible brackets that can be used to describe the classical and, by the canonical quantization procedure, the quantum dynamics.

One of the most interesting situation where Dirac's method of handling singular Lagrangians can be applied is in confining particles on curved manifolds [3,4]. Part of this interest is certainly due to the presence of additional terms which arise in many quantization procedures on curved manifolds [5–7] and is far from being clarified. In this Letter we will focus our attention on the connection between the additional terms which occur in the quantum Hamiltonian and the problem of the operator ordering prescription.

In Section 2 we briefly review Dirac's method of handling singular Lagrangians. In Section 3 we quantize a free particle constrained on a circle following the standard procedure, i.e., reducing from the very beginning the number

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of degrees of freedom. Then we solve the same (classical) problem using Dirac's method, recovering a new set of canonical brackets. Finally, we quantize using this bracket algebra, by focusing our attention on the construction of coordinates, linear momenta, angular momentum and Hamiltonian operators and on related ordering problems and we will finally write the Schrödinger equation. Section 4 contains our conclusions.

2. The Dirac method

Let us start by outlining the Dirac method [2] and introduce notation. Take a consistent Lagrangian $L(x, \dot{x})$ with N coordinates. The classical dynamics is obtained by the least action principle:

$$S[x] = \int_{t_0}^{t_1} dt\, L(x, \dot{x}), \qquad \delta S[x] = 0, \tag{2.1}$$

which in terms of the Lagrangian gives N Euler–Lagrange equations

$$\frac{\partial L}{\partial x_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} = 0. \tag{2.2}$$

We define momenta and Hamiltonian and obtain the usual (Poisson) brackets between momenta and coordinates:

$$p_i = \frac{\partial L}{\partial \dot{x}_i}, \quad i = 1, \ldots, N, \tag{2.3}$$

$$H(x, p) = \sum_i p_i \dot{x}_i(x, p) - L\big(x, \dot{x}(x, p)\big), \tag{2.4}$$

$$[x_i, p_j] = \delta_{ij}, \tag{2.5}$$

and for any function A of x's and p's (not explicitly dependent on time),

$$\dot{A} = [A, H]. \tag{2.6}$$

Two scenarios are possible. In the typical case one can invert $p_i(x, \dot{x})$ to obtain $\dot{x}_i(x, p)$; if this is not possible, not even locally, the Lagrangian is said singular and its Hessian with respect to the velocities vanishes

$$\left\| \frac{\partial L}{\partial \dot{x}_i \partial \dot{x}_j} \right\| = 0. \tag{2.7}$$

In such a case we act differently. We consider those relations in (2.3) which hinder the inversion (this step will be clarified in the example of Section 3) as a series of *constraints*

$$\phi_j \approx 0, \tag{2.8}$$

which must be satisfied "weakly" (namely, their Poisson bracket with any given quantity may not vanish) along the physical trajectory. In this way we obtain a number (say M) of constraints which Dirac called *primary* because of their direct derivation from the Lagrangian. Notice that a Hamiltonian is required to be independent of the velocities. If we are not able to erase the $\dot{x}$ dependence, then the straightforward application of the Hamiltonian method is impossible. To solve our problem we proceed as follows. We add to H all our primary constraints multiplied by arbitrary functions of time u_j, to obtain the total Hamiltonian H_{T}

$$H_{\mathrm{T}} = H + \sum_{j=1}^{M} u_j \phi_j(x, p). \tag{2.9}$$

This could seem to imply an arbitrariness (additional freedoms are introduced) but we require a number of consistency conditions: each constraint must be zero during the whole evolution, if it is initially zero:

$$\dot{\phi}_j = [\phi_j, H_\mathrm{T}] \approx 0, \quad j = 1, \ldots, M. \tag{2.10}$$

If these equations are consistent, three cases are possible: an equation can give an identity; it can give a linear equation for the u_j; it can give an equation containing only p's and x's, in which case it must be considered as another constraint. The constraints that arise from this procedure will be called *secondary*, for obvious reasons. Even for these, we impose consistency conditions and this procedure is continued until we have a set of identities and linear equations for the u's. Now we have enlarged our set of constraints to include the secondary ones and we have a new number of constraints, say K.

We have by now defined a constraint as a quantity which satisfies

$$\phi_j \approx 0, \tag{2.11}$$

$$[\phi_j, H_\mathrm{T}] \approx 0. \tag{2.12}$$

This defines a linear vector space (due to the linearity of the Poisson brackets) and so any linear combination of constraints is again a constraint. It is of great importance for our purposes the distinction between *first class* and *second class* constraints. The first are defined as the constraints which "commute" (i.e., have vanishing Poisson brackets) with all the other constraints. The second ones have at least one non-vanishing bracket with some other constraint. It may happen that we can take linear combinations of second class constraints and obtain some first class constraints. This situation brings to light the presence of some gauge degrees of freedom. Dirac showed the profound difference between this two classes. In fact we can switch to new canonical brackets in order to set all of our *second* class constraints *strongly* equal to zero. This means that in any given quantity, such as the Hamiltonian, we can set them to zero "by hand". The first class ones, however, will "survive" (even in the Hamiltonian with their arbitrary multiplicative functions u). In the following analysis we will not deal with first class constraints and so will not discuss them any further. Every constraint that we will find will be of the second class. In such a case, we can safely change to the new canonical brackets, the so-called *Dirac brackets*, defined as follows: let

$$M_{ij} \equiv [\phi_i, \phi_j], \tag{2.13}$$

and its inverse

$$G_{ij} \equiv \left(M^{-1}\right)_{ij} \tag{2.14}$$

(the invertibility of M is a particular feature of the absence of first class constraints: in general M is defined on the subspace of second class constraints only). Then for any two quantities A and B we define the Dirac bracket:

$$[A, B]_\mathrm{D} = [A, B] - \sum_{i,j=1}^{K} [A, \phi_i] G_{ij} [\phi_j, B]. \tag{2.15}$$

These brackets have all the properties of the Poisson bracket plus one: for any dynamical variable A we have

$$[A, \phi_i]_\mathrm{D} = 0, \tag{2.16}$$

$$\dot{A} = [A, H_\mathrm{T}] \approx [A, H_\mathrm{T}]_\mathrm{D}, \tag{2.17}$$

as is easy to see (for (2.17) use (2.12)).

The very meaning of this redefinition of the canonical brackets is simply a change of variables from the original phase space to the constrained manifold [3]. Having obtained a set of canonical brackets, we can now quantize, by looking for self-adjoint operators which satisfy the canonical commutation relation (each quantity in the right-hand side must be multiplied by $i\hbar$).

Let us now look at an interesting example.

3. Particle on a circle

3.1. The standard approach

We want to quantize the following free particle Lagrangian

$$L = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right), \tag{3.1}$$

subject to the relation

$$r^2 \equiv x^2 + y^2 = r_0^2 \tag{3.2}$$

(r_0 being a positive real constant) which must be satisfied at any time. This describes the motion of a particle of unitary mass in the xy-plane, constrained on a circle of radius r_0. We can make a change of variables, from Cartesian to polar coordinates (r, θ),

$$x = r\cos\theta, \qquad y = r\sin\theta, \tag{3.3}$$

after which, using (3.2), the Lagrangian reads

$$L = \frac{1}{2} r_0^2 \dot{\theta}^2. \tag{3.4}$$

We have now a new Lagrangian with only one degree of freedom θ. We can define the momentum p_θ

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = r_0^2 \dot{\theta}, \tag{3.5}$$

and the Hamiltonian

$$H(\theta, p_\theta) = \dot{\theta} p_\theta - L = \frac{p_\theta^2}{2r_0^2}. \tag{3.6}$$

The radial degree of freedom r disappears (as implicitly did any other non-dynamical degree of freedom, such as the z coordinate in (3.1)). The Poisson bracket is

$$[\theta, p_\theta] = 1. \tag{3.7}$$

Now, let us quantize: define two self-adjoint operators $\hat{\theta}$ and $\hat{p}_\theta$ satisfying the canonical commutation relation (CCR) ($\hbar$=1):

$$\left[\hat{\theta}, \hat{p}_\theta\right] = i \tag{3.8}$$

(we shall use the same notation for Poisson brackets and commutator of operators, since no confusion can arise). We can find such a couple of self-adjoint operators in the Hilbert space $\mathcal{H} = L^2(0, 2\pi)$ and their expression is:

$$\hat{\theta}\psi(\theta) = \theta\psi(\theta), \qquad \hat{p}_\theta \psi(\theta) = \left(-i\frac{\partial}{\partial\theta} - \alpha\right)\psi(\theta). \tag{3.9}$$

We add the constant α in the momentum p_θ to mimic the possible presence of a magnetic field enclosed in the circle (see the discussion after (3.44)). Their domains are chosen to be, respectively, $D_\theta = \mathcal{H}$ and $D_{p_\theta} = \{\psi \in \mathcal{H} \mid \psi(0) = \psi(2\pi),\ \psi' \in \mathcal{H}\}$. These are dense subsets of $\mathcal{H}$. Notice also that we have chosen one of the infinite self-adjoint extensions of the momentum $\hat{p}_\theta$. The Hamiltonian reads

$$H\left(\hat{\theta}, \hat{p}_\theta\right) = \frac{\hat{p}_\theta^2}{2r_0^2} = \frac{1}{2r_0^2}\left(-i\frac{\partial}{\partial\theta} - \alpha\right)^2, \tag{3.10}$$

and is self-adjoint in the domain of p_θ, i.e., D_{p_θ}. The Schrödinger equation is (reinserting m and $\hbar$)

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2mr_0^2}\left(-i\frac{\partial}{\partial\theta} - \alpha\right)^2\psi. \tag{3.11}$$

This is what we expected.

3.2. Dirac's approach

Let analyze the same problem with Dirac's method. We start from classical dynamics. We want to find the extremum of the action with the Lagrangian defined in (3.1), subject to the constraint

$$\phi = x^2 + y^2 - r_0^2 \approx 0. \tag{3.12}$$

We use the method of Lagrange multipliers [8] and search for the extremum of the action with the new Lagrangian

$$L(x, \dot{x}, y, \dot{y}, \lambda) = \frac{1}{2}\dot{x}^2 + \frac{1}{2}\dot{y}^2 - \lambda\left(x^2 + y^2 - r_0^2\right), \tag{3.13}$$

the quantity λ being treated as an additional dynamical variable. This Lagrangian gives rise to an action functional $S[x, y, \lambda]$ which must be varied with respect to x, y and also the "new" degree of freedom λ. If we want to use the Hamiltonian method with this Lagrangian, we must start by calculating the momenta:

$$p_x = \frac{\partial L}{\partial\dot{x}} = \dot{x}, \qquad p_y = \frac{\partial L}{\partial\dot{y}} = \dot{y}, \qquad p_\lambda = \frac{\partial L}{\partial\dot{\lambda}} = 0. \tag{3.14}$$

It is apparent that we are facing the situation discussed in the introduction and in Section 2: one of the momenta disappears. So we proceed as previously sketched: read the relation $p_\lambda \approx 0$ as a primary constraint:

$$\phi_1 = p_\lambda \approx 0. \tag{3.15}$$

This is our only primary constraint. Build up the Hamiltonian

$$H = p_x\dot{x} + p_y\dot{y} + p_\lambda\dot{\lambda} - L = \frac{p_x^2}{2} + \frac{p_y^2}{2} + p_\lambda\dot{\lambda} + \lambda\left(x^2 + y^2 - r_0^2\right). \tag{3.16}$$

We now include ϕ_1 multiplied by an arbitrary function of the time u_1:

$$H_{\mathrm{T}} = \frac{p_x^2}{2} + \frac{p_y^2}{2} + \lambda\left(x^2 + y^2 - r_0^2\right) + u_1 p_\lambda. \tag{3.17}$$

Notice that $\dot{\lambda}$ has been absorbed in the arbitrary function u_1. The consistency condition (2.10) is

$$0 \approx \dot{\phi}_1 = [\phi_1, H_{\mathrm{T}}] = [p_\lambda, H_{\mathrm{T}}] = -\left(x^2 + y^2 - r_0^2\right), \tag{3.18}$$

which is a new constraint, that the Lagrange multipliers had already implicitly imposed (ϕ in (3.12))

$$\phi_2 = \phi = x^2 + y^2 - r_0^2 \approx 0. \tag{3.19}$$

The consistency conditions (2.10) for ϕ_2 yields

$$\phi_3 = xp_x + yp_y \approx 0, \tag{3.20}$$

and by imposing (2.10) also for ϕ_3 we obtain

$$\phi_4 = p_x^2 + p_y^2 - 2\left(x^2 + y^2\right)\lambda \approx 0. \tag{3.21}$$

These are additional constraints. If we impose (2.10) for ϕ_4 we get an equation for u_1:

$$u_1 = -\frac{2\lambda}{x^2+y^2}(xp_x + yp_y) \approx 0. \tag{3.22}$$

Since in the following we shall use only Dirac brackets we regard any constraint as a *strong* equation and drop the term $u_1\phi_1$ from the total Hamiltonian. We can also drop the term containing the Lagrangian multiplier because of ϕ_2. So our Hamiltonian becomes the free one:

$$H_{\mathrm{T}} = \frac{p_x^2}{2} + \frac{p_y^2}{2}. \tag{3.23}$$

The fact that the Hamiltonian function of the constrained dynamics is exactly that of an unconstrained dynamics may seem strange. One could (erroneously) argue that even the equations of motion would be the same. This is not correct because we will change the canonical brackets. All additional information characterizing the constrained dynamics is now contained in these new canonical brackets. One could say that Dirac's method "drains" information from the Lagrangian, where it is contained in the additional degree of freedom λ, giving it to the canonical brackets, where it is contained in a non-trivial algebra. In this process, however, the information on the topology of the problem is made explicit, as we shall see in the short discussion just after the algebra construction. This point of view is very useful in quantum mechanics.

We have four constraints and what we need now is the algebra of the Dirac's brackets. We calculate the matrix ($\boldsymbol{r} = (x, y)$ and $\boldsymbol{p} = (p_x, p_y)$)

$$M = \begin{vmatrix} 0 & 0 & 0 & 2\boldsymbol{r}^2 \\ 0 & 0 & 2\boldsymbol{r}^2 & 4\boldsymbol{p}\cdot\boldsymbol{r} \\ 0 & -2\boldsymbol{r}^2 & 0 & 2\boldsymbol{p}^2 + 4\lambda\boldsymbol{r}^2 \\ -2\boldsymbol{r}^2 & -4\boldsymbol{p}\cdot\boldsymbol{r} & -2\boldsymbol{p}^2 - 4\lambda\boldsymbol{r}^2 & 0 \end{vmatrix}, \tag{3.24}$$

and invert it to get

$$G = \begin{vmatrix} 0 & -\big(\boldsymbol{p}^2 + 2\lambda\boldsymbol{r}^2\big)/2\boldsymbol{r}^4 & \boldsymbol{r}\cdot\boldsymbol{p}/\boldsymbol{r}^4 & -1/2\boldsymbol{r}^2 \\ \big(\boldsymbol{p}^2 + 2\lambda\boldsymbol{r}^2\big)/2\boldsymbol{r}^4 & 0 & -1/2\boldsymbol{r}^2 & 0 \\ -\boldsymbol{r}\cdot\boldsymbol{p}/\boldsymbol{r}^4 & 1/2\boldsymbol{r}^2 & 0 & 0 \\ 1/2\boldsymbol{r}^2 & 0 & 0 & 0 \end{vmatrix}. \tag{3.25}$$

We can now calculate the Dirac brackets of any two quantities and appreciate their physical meaning.

To start off, let us first consider an interesting example of the difference between Poisson and Dirac brackets. We can check whether (2.16) is true for $\phi_1 = p_\lambda$ and $A = \lambda$. The commutation rule between the Lagrange multiplier and its momentum changes from $[\lambda, p_\lambda] = 1$ to

$$[\lambda, p_\lambda]_{\mathrm{D}} = 1 - \sum_{i,j}[\lambda, \phi_i]G_{ij}[\phi_j, p_\lambda] = 1 - [\lambda, \phi_1]G_{14}[\phi_4, p_\lambda] = 1 - 1\left(-\frac{1}{2r^2}\right)\left(-2r^2\right) = 0,$$

which enables one to see how the Dirac brackets work in order to satisfy the constraints strongly. We also find (we have replaced r with r_0 in each quantity by using $\phi_2 = 0$):

$$\begin{aligned} &[x, p_x]_{\mathrm{D}} = 1 - \frac{x^2}{r_0^2}, \qquad [y, p_y]_{\mathrm{D}} = 1 - \frac{y^2}{r_0^2}, \qquad [x, p_y]_{\mathrm{D}} = -\frac{xy}{r_0^2}, \\ &[y, p_x]_{\mathrm{D}} = -\frac{xy}{r_0^2}, \qquad [x, y]_{\mathrm{D}} = 0, \qquad [p_x, p_y]_{\mathrm{D}} = -\frac{1}{r_0^2}(xp_y - yp_x). \end{aligned} \tag{3.26}$$

This brackets have a nice geometric interpretation. According to the Poisson bracket $[x, p_x] = 1$, p_x is the *generator of translations* along the x axis. However this property cannot be preserved in the constrained algebra, because typically we cannot translate in the x direction while remaining on the circle. This can be done only at the points ($x = 0$, $y = \pm r_0$) where the first and fourth equations of (3.26) reduce to the Poisson algebra. Another feature is to be noticed: x and y still commute. We can understand this because x and y are the generators of translations in the corresponding p's directions; however there is no constraint containing *only* momenta so any given point in the $p_x p_y$-plane is allowed, by suitably adjusting the other coordinates x, y and λ. This is not the case of the coordinates x and y, as one can readily see: for example, the point $x = 2r_0$, $y = r_0$ is not allowed even by making additional translations of momenta and λ, because of ϕ_2.

We can write the Hamiltonian in the form (3.10) defining L_z:

$$L_z = x p_y - y p_x. \tag{3.27}$$

Squaring it and using ϕ_2 we obtain

$$L_z^2 = r_0^2\big(p_x^2 + p_y^2\big) - (x p_x + y p_y)^2, \tag{3.28}$$

and using ϕ_3 we obtain

$$H = \frac{1}{2}\big(p_x^2 + p_y^2\big) = \frac{L_z^2}{2r_0^2}. \tag{3.29}$$

One can identify L_z with p_θ by writing coordinates and momenta as functions of θ and L_z. This can be done by solving Eqs. (3.27) and (3.20) for p_x and p_y and using (3.2). We get:

$$x = r_0 \cos\theta, \qquad y = r_0 \sin\theta, \tag{3.30}$$

$$p_x = -\frac{1}{r_0} L_z \sin\theta, \qquad p_y = \frac{1}{r_0} L_z \cos\theta. \tag{3.31}$$

The reader can verify that all the relations obtained by the Dirac brackets algebra are equivalent to the single bracket $[\theta, L_z] = 1$ (e.g., $[x, L_z]_{\mathrm{D}} = -y$ should be read $[\cos\theta, L_z] = -\sin\theta$ and so on).

Eq. (3.26) pave the way to quantization. We shall see that the quantization of the Dirac algebra is not a trivial problem: our recipe will be the requirement that some operators be self-adjoint (or at least Hermitian). This requirement will play a fundamental role in our analysis. We look at an explicit representation of the self-adjoint operators $\hat{x}$, $\hat{y}$, $\hat{p}_x$, $\hat{p}_y$ (notice that we will not deal with the operators $\hat{p}_\lambda$ and $\hat{\lambda}$ because they are completely defined by $\phi_1 = 0$ and $\phi_4 = 0$, respectively) satisfying this algebra. We must, however, impose the (now) strong equalities $\phi_i = 0$ ($i = 1, 2, 3, 4$). So (in the following we will drop all hats on operators), $r^2 \equiv x^2 + y^2 = r_0^2$ and there exists a self-adjoint operator θ on the Hilbert space $\mathcal{H} = L^2(0, 2\pi)$ such that:

$$x = r_0 \cos\theta, \qquad y = r_0 \sin\theta. \tag{3.32}$$

We will determine the momentum operators in order to satisfy the following equations:

$$[x, p_x] = i\left(1 - \frac{x^2}{r_0^2}\right), \qquad [y, p_y] = i\left(1 - \frac{y^2}{r_0^2}\right), \qquad [x, p_y] = -i\frac{xy}{r_0^2},$$
$$[y, p_x] = -i\frac{xy}{r_0^2}, \qquad [x, y] = 0, \qquad [p_x, p_y] = -\frac{i}{r_0^2}(x p_y - y p_x). \tag{3.33}$$

Using the fact that (d_θ stands for the θ-derivative, F for any n-times differentiable function) $[d_\theta^n, F(\theta)]$ contains derivatives of order less than or equal to $n - 1$ and looking at the first two equations in (3.33) (whose right-hand side does not contain momenta) one can infer that the p operators in the θ representation contain only first order

derivatives. Then, in the most general case,

$$p_x = -\frac{i}{r_0} f(\theta)\frac{\partial}{\partial\theta} + \frac{1}{r_0}a(\theta), \tag{3.34}$$

$$p_y = -\frac{i}{r_0} g(\theta)\frac{\partial}{\partial\theta} + \frac{1}{r_0}b(\theta). \tag{3.35}$$

Using these expressions we solve for the unknown functions f, g, a and b. The first equation in (3.33) yields

$$\cos\theta\left(-if(\theta)\frac{\partial}{\partial\theta}\right) - \left(-if(\theta)\frac{\partial}{\partial\theta}\right)\cos\theta = i\sin^2\theta, \tag{3.36}$$

which is solved to give

$$f(\theta) = -\sin\theta. \tag{3.37}$$

Analogously, the solution of the second equation in (3.33) gives

$$g(\theta) = \cos\theta. \tag{3.38}$$

At this stage the third, fourth and fifth equations in (3.33) are identities and yield no information on a and b. However, some insight on their form can be obtained from the last of (3.33), which gives

$$a'\cos\theta + b'\sin\theta = -b\cos\theta + a\sin\theta, \tag{3.39}$$

where the primes denotes derivatives. This yields

$$a' = -b, \qquad b' = a. \tag{3.40}$$

However, there are other equations which must be satisfied:

$$[x, H] = ip_x, \qquad [y, H] = ip_y. \tag{3.41}$$

These are linearly dependent and both equivalent to

$$ia\cos\theta + ib\sin\theta = -\frac{1}{2}. \tag{3.42}$$

By using (3.41) this turns into an equation for a whose solutions, under the additional requirement that p_x and p_y be Hermitian operators (this is a necessary step in order to require their self-adjointness), are:

$$a(\theta) = \frac{i}{2}\cos\theta + \alpha\sin\theta, \qquad b(\theta) = -a' = \frac{i}{2}\sin\theta - \alpha\cos\theta,$$

where α is an arbitrary *real* number. Putting all the results together we obtain

$$p_x = \frac{i}{r_0}\sin\theta\frac{\partial}{\partial\theta} + \frac{i}{2r_0}\cos\theta + \frac{\alpha}{r_0}\sin\theta, \qquad p_y = -\frac{i}{r_0}\cos\theta\frac{\partial}{\partial\theta} + \frac{i}{2r_0}\sin\theta - \frac{\alpha}{r_0}\cos\theta. \tag{3.43}$$

We can put these equations in a compact form by using the anticommutator (for any operators A and B: $\{A, B\} \equiv AB + BA$):

$$p_x = \frac{1}{2r_0}e^{i\alpha\theta}\left\{i\frac{\partial}{\partial\theta}, \sin\theta\right\}e^{-i\alpha\theta}, \qquad p_y = \frac{1}{2r_0}e^{i\alpha\theta}\left\{i\frac{\partial}{\partial\theta}, -\cos\theta\right\}e^{-i\alpha\theta}. \tag{3.44}$$

Written in this form, these equations readily show some properties of these operators. First, they are the Weyl ordered operators of the classical quantities (3.31) but this ordering arises naturally by taking suitable solutions of the algebra equations. Second, these p's are self-adjoint in the domain D_{p_θ} defined after (3.9). Finally, equations (3.44) also show that different p's, corresponding to different α's, are connected to each other by means of gauge

transformations; this interesting property can be easily related to the Aharonov–Bohm effect (see [9]), identifying α with $\frac{e}{2\pi c}\Phi_B$ where Φ_B is the flux of the magnetic field enclosed in the circle.

One can check that all the constraints are satisfied: remember that we have chosen the expressions of x and y to satisfy ϕ_2, set $p_\lambda = 0$ to satisfy ϕ_1, defined λ to satisfy ϕ_4, so we must manage only with ϕ_3. Physically ϕ_3/r_0 is the radial part of the momentum $p_r \equiv (\boldsymbol{r}\cdot\boldsymbol{p})/r_0$ (the vector $\boldsymbol{r}$ being on the circle: $\boldsymbol{r}^2 = r_0^2$) so we choose to represent it with a Hermitian operator. We therefore order it (W stands for 'Weyl ordering' which coincides with any other sufficiently symmetric operator ordering procedure for this simple quantity) in order to get the Hermitian expression

$$\phi_{3,\mathrm{W}} = \frac{1}{2}\big(\{x, p_x\} + \{y, p_y\}\big). \tag{3.45}$$

One can easily see, using the solutions (3.32) and (3.43), that $\phi_{3,\mathrm{W}} = 0$. Conversely, using the algebra relations (3.33) it is possible to show that if a non-Weyl-ordered expression for ϕ_3 is constrained to zero the momentum operators are not Hermitian. In fact using the algebra of commutators (3.33) one readily gets three equivalent expressions for the momenta operators:

$$\begin{aligned} p_x &= \frac{1}{2r_0^2}\{-y, L_z\} + \frac{1}{r_0^2}x\left(-\frac{i}{2} + xp_x + yp_y\right) \\ &= \frac{1}{2r_0^2}\{-y, L_z\} + \frac{1}{r_0^2}x\left(\frac{i}{2} + p_x x + p_y y\right) = \frac{1}{2r_0^2}\{-y, L_z\} + \frac{1}{r_0^2}x\phi_{3,\mathrm{W}}, \end{aligned} \tag{3.46}$$

$$\begin{aligned} p_y &= \frac{1}{2r_0^2}\{x, L_z\} + \frac{1}{r_0^2}y\left(-\frac{i}{2} + xp_x + yp_y\right) \\ &= \frac{1}{2r_0^2}\{x, L_z\} + \frac{1}{r_0^2}y\left(\frac{i}{2} + p_x x + p_y y\right) = \frac{1}{2r_0^2}\{x, L_z\} + \frac{1}{r_0^2}y\phi_{3,\mathrm{W}}. \end{aligned} \tag{3.47}$$

These expression are not Hermitian if we set $xp_x + yp_y = 0$ or $p_x x + p_y y = 0$. On the contrary they are Hermitian if we set $\phi_{3,\mathrm{W}} = 0$. Therefore the Hermiticity of these operators and their Weyl ordering are strictly correlated. We shall come back to this remarkable point in the following.

We can now build up any quantity we need in our quantum theory, for example, the z component of the angular momentum

$$L_z = xp_y - yp_x = -i\frac{\partial}{\partial\theta} - \alpha, \tag{3.48}$$

and the Hamiltonian, from (3.23)

$$\begin{aligned} H &= \frac{1}{2}\big(p_x^2 + p_y^2\big) \\ &= \frac{1}{2r_0^2}\left[\left(i\sin\theta\frac{\partial}{\partial\theta} + \frac{i}{2}\cos\theta + \alpha\sin\theta\right)^2 + \left(-i\cos\theta\frac{\partial}{\partial\theta} + \frac{i}{2}\sin\theta - \alpha\cos\theta\right)^2\right] \\ &= \frac{1}{2r_0^2}\left(-i\frac{\partial}{\partial\theta} - \alpha\right)^2 + \frac{1}{8r_0^2}. \end{aligned} \tag{3.49}$$

One can check that the ground state energy is

$$E_{\mathrm{G}} = \frac{1}{2r_0^2}\left(\frac{1}{2} - \left|\frac{1}{2} - \bar{\alpha}\right|\right)^2 + E_0, \tag{3.50}$$

where (in ordinary units) $E_0 = \frac{\hbar^2}{8mr_0^2}$ and $\bar{\alpha} \in [0, 1[$, $\bar{\alpha} = \alpha \bmod 1$. Notice that we have obtained a constant E_0 which was absent both in the classical Hamiltonians (3.29) and (3.6) and in the quantum Hamiltonian (3.10). Let us now

discuss the domains in which these operators are self-adjoint. We see from L_z that a good domain for its definition is the previously defined $D_{p_\theta} = \{\psi \in L^2(0, 2\pi) \mid \psi(2\pi) = \psi(0),\ \psi' \in L^2(0, 2\pi)\}$. In different domains L_z will not be self-adjoint anymore ad so will not be an observable. The Schrödinger equation (reinserting the mass and $\hbar$) reads

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2mr_0^2}\left(-i\frac{\partial}{\partial\theta} - \alpha\right)^2\psi + E_0\psi, \tag{3.51}$$

which differs from (3.11) for the presence of E_0.

At this point one should focus on the connection between the additional term E_0 and the quantization procedure we have established. First of all, observe that if we had not required that the p's be Hermitian we would not have found such a term. For example, taking $H = L_z^2/2r_0^2$ on the circle in the classical context and *then* substituting L_z with the corresponding quantum operator gives (of course) no additional terms in the Hamiltonian. Another way of getting rid of the additional terms is by Abelian conversion of the algebra [4,10,11], by introducing an additional set of coordinates. In practice, there are many ways of dropping or changing the additional terms without changing the algebra.

Similar terms arise in the quantization on curved manifolds as an effect of the (intrinsic) curvature of the manifold itself, as shown by DeWitt [5] and successively elaborated by Schulman [7]. We stress however that the constant E_0 found in Dirac's procedure *cannot* be put in direct correspondence with such curvature terms. Indeed for the quantization on the circle the scalar curvature is 0, while the additional term in Dirac's procedure is $1/8r_0^2$. However, the fact that no direct proportionality is present between these two energies does not mean that one of them (namely Dirac's one) is unphysical, but rather that the procedures of quantization leading to them reflects different physical processes. While, for example, in the path-integral procedure no mention of the embedding space (for example, the circle as a subset of the plane) is made, in Dirac's procedure this embedding is unavoidable. Moreover a parallel with the classical version of Dirac's procedure hints that the physical evolution it suggests is like making a small step (free evolution) in the embedding space followed by a "projection" on the constraining manifold, obtained by dropping the component of the step orthogonal to the manifold [2]. In order to visualize this way of constraining the particle on the manifold one should follow the procedure we outlined, i.e., should quantize the generators of translations p_x and p_y of the embedding space and *then* calculate the Hamiltonian. On the contrary DeWitt's procedures relies upon the presence of a natural metric on the manifold and the additional term is due to the intrinsic curvature of the manifold itself. This scenario obviously sets aside a possible embedding of our manifold in a bigger one. The choice of a given procedure should depend on the physical process one has in mind.

Additional work is needed in this direction, for the problem is certainly far from being solved, as the physical significance of the additional energies appearing in the different procedures is not completely understood.

4. Conclusions

As we have shown, the Dirac method yields deep insight even in a simple example like the one we considered. The construction of the Dirac algebra of brackets is non-trivial and instructive and even more interesting is the search for an explicit representation of the self-adjoint operators satisfying the algebra and the constraints. One must look at their functional form and identify and interpret any possible freedom inherent to their choice. Then one must look at their domains of definition, facing sometimes ordering problems. Eventually, one gains a better comprehension of the Hamiltonian formalism, the connection between Dirac algebra and the topology of the constrained manifold and the quantization procedure on this manifold. An interesting explicit result we have obtained is the presence of an additional energy term different from the ones present in other quantization procedures. We have discussed this term in connection with the Dirac's quantization procedure arguing that its presence is connected to the (physical) way of constraining the dynamics on a manifold.

In this Letter we have adopted for p_θ and L_z only the domain with periodic boundary conditions. Actually there is an infinity of subsets of $L^2(0, 2\pi)$ where every operator we have considered is self-adjoint, i.e., those with $\psi(2\pi) = e^{i2\pi\beta}\psi(0)$ where $\beta \in [0, 1[$. This issue is clearly exposed in [12,13] and references therein. One can regard the gauge transformation with parameter α in Section 3.2 as a similarity transformation between these subsets of L^2. The (potential) freedom in the choice of the domain of definition of the operators is contained in this gauge transformation.

It would be interesting to elucidate the features of this formalism, in the form explicitly including the Lagrange multipliers, in connection with the Faddeev and Popov functional technique in quantum field theory [14].

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