Quantization of the multidimensional rotor

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Abstract

We reconsider the problem of quantising a particle on the $D$-dimensional sphere. Adopting a Lagrangian method of reducing the degrees of freedom, the quantum Hamiltonian is found to be the usual Schrödinger operator without any boundary term. The equivalence with the Dirac Hamiltonian approach is demonstrated, either in the cartesian or in the curvilinear basis. We also briefly comment on the path integral approach.
1 Introduction and review of the problem

The problem of the quantization of the rotor has been studied since decades, but remains a subject of intense debate.

De Witt\cite{1, 2} studied the path integral quantization, and proposed that a term proportional to the curvature should be included in the Hamiltonian. However, problems connected to the definition of the path integral using curvilinear coordinates, unknown at that time, turns out to invalidate that proposal. This is essentially tied to the fact that for quantisation in curvilinear coordinates, new terms may arise. Such happens even in the quantisation of free particles in curvilinear coordinates. Edwards and Gulyaev\cite{3} carefully considered that problem, and showed that the quantization via path integration may lead to different results, due to problems intrinsically connected to the path integral formulation\cite{4}. Though essential, this last paper has been frequently forgotten in the literature.

Dirac formulation\cite{5} of the problem has also been undertaken\cite{6}. In this case one faces the question of ordering of the quantum operators, a question which can only be tackled using definite ordering prescriptions based on general arguments as hermiticity and general coordinate invariance. The Laplace-Beltrami operator has been obtained using the Dirac quantization procedure without curvature terms in e.g.\cite{6}, for the special case of a three-dimensional rotor.

In the path integral formalism, besides the early developments\cite{3}, there are special definitions of the path integral on the surface of the sphere which do not give rise to the curvature term\cite{7}. A discrepancy with the Dirac formalism has however been reported in several papers\cite{8, 9, 10}, as well as other different results\cite{11, 12}.

In spite of all these developments, the status of the problem is very confusing, and there have been many papers claiming a rejection of the Dirac formalism\cite{8} an intrinsic difference between path integral formulation and operator formalism\cite{9}, or advocating different quantization schemes\cite{11}. The importance of the problem can be appreciated from the fact that it has implications in curved space quantization, when defining the Wheeler-de-Witt equation\cite{13}, and in the quantization of sigma model Lagrangians, important to string theories, where the Wheeler-de-Witt equation has central importance.
The aim of the present paper is to analyse the problem directly in terms of reduced coordinates by solving the constraint, thereby bypassing the ambiguities inherent in either the Dirac or path integral approaches. The classical reduced space is therefore obtained in a straightforward manner. We then pass to the quantum formulation by using the Laplace-Beltrami construction. It leads to a quantum Hamiltonian which is the usual Schrödinger operator without any curvature term. The connection of our results with the Dirac approach is then established. We conclude by briefly mentioning the path integral formulation, where the counterpart of the above approach is the special time slicing of the integral as explained by T. D. Lee [14].

2 Reduced coordinates

The Lagrangian for a particle of unit mass constrained to move on the surface of a $D$-dimensional sphere of radius $R$ is given by the well known expression

$$L = \frac{1}{2} \dot{x}_\alpha \dot{x}_\alpha - \lambda \left( x_\alpha x_\alpha - R^2 \right) \quad \alpha = 1 \cdots D ,$$

(1)

where the constraint

$$\Omega = x_\alpha x_\alpha - R^2 \approx 0 \quad (2)$$

is implemented by the Lagrange multiplier $\lambda$. Since this is a constrained system, the usual canonical approach must be modified. A possible way is to use Dirac’s constraint analysis. It is known that this system presents second class constraints so that the usual Poisson brackets have to be modified to the Dirac brackets. Apart from the fact that these brackets are plagued by ordering ambiguities, the extraction of the physical variables of the system is not very transparent. This has been analysed by several authors [6, 8, 9, 12].

Here we shall adopt an alternative canonical approach developed recently by one of us [15] which is based on a Lagrangian reduction by systemmatically eliminating the unphysical variables using the equations of constraint. From the constraint (2) the coordinate $x_D$ is expressed in terms of the remaining coordinates by

$$x_D = \sqrt{R^2 - \vec{x}^2} = \sqrt{R^2 - x_i^2}, \quad i = 1 \cdots D - 1 \quad (3)$$
Inserting this in equation (1), we obtain the reduced Lagrangian
\[ \mathcal{L}_r = \frac{1}{2} g_{ij} \dot{x}_i \dot{x}_j \]
where the metric is
\[ g_{ij} = \delta_{ij} + \frac{x_i x_j}{R^2 - \vec{x}^2} \]  
(5)
Note that now the Lagrangian is expressed only in terms of the unconstrained variables. Consequently, the conventional canonical formalism is applicable. The canonical momenta are given by
\[ p_i = \frac{\partial \mathcal{L}_r}{\partial \dot{x}_i} = g_{ij} \dot{x}_j \]  
(6)
Since the system is unconstrained the velocities can be obtained unambiguously by inverting (6) to yield
\[ \dot{x}_i = g^{ij} p_j \]
(7)
where \( g^{ij} \) is the inverse of (5), being given by
\[ g^{ij} = \delta_{ij} - \frac{x_i x_j}{R^2} \]
(8)
The canonical Hamiltonian is now obtained by a Legendre transform
\[ \mathcal{H} = p_i \dot{x}_i - \mathcal{L}_r = \frac{1}{2} p_i g^{ij} p_j \]  
(9)
This gives the final expression for the classical reduced Hamiltonian.
In order to perform the quantization the above Hamiltonian is replaced by the corresponding Laplace-Beltrami operator, being defined as
\[ \hat{\mathcal{H}} = \mathcal{O}_{LB} = \frac{1}{2} g^{-1/4} \pi_i g^{1/2} g^{ij} \pi_j g^{-1/4} \]  
(10)
where \( \pi_i \) is the quantum momentum operator, and \( g \) is the determinant of the metric \( g_{ij} \).
As is well known, the above transition from classical to quantum is based of hermiticity and general coordinate invariance. The quantum momentum operator satisfying these conditions is given by the expression
\[ \hat{\pi}_i = -i \hbar g^{-1/4} \partial g^{1/4} \]  
(11)
An essential ingredient is the computation of the determinant of the metric, which is sketched below,

\[ g \equiv \det g_{ij} = \exp \text{tr} \ln \left( \delta_{ij} + \frac{x_i x_j}{R^2 - \vec{x}^2} \right) \]

\[ = \exp \text{tr} \frac{x_i x_j}{\vec{x}^2} \ln \left( 1 + \frac{\vec{x}^2}{R^2 - \vec{x}^2} \right) \]

\[ = \frac{R^2}{R^2 - \vec{x}^2} \]

It is now simple to obtain the quantum Hamiltonian,

\[ \hat{\mathcal{H}} = -\frac{1}{2} \sqrt{R^2 - \vec{x}^2} \partial_i \left( \delta_{ij} - \frac{x_i x_j}{R^2} \right) \left( R^2 - \vec{x}^2 \right)^{-1/2} \partial_j, \quad \partial_i = \frac{\partial}{\partial x_i}. \]

(13)

The arrow above the derivative means that it operates on every element on the right (i.e., it acts as a quantum operator). It is now straightforward to show that the above operator is related to the angular momentum in the reduced space,

\[ L_{ij} = x_i p_j - x_j p_i = -i\hbar (x_i \partial_j - x_j \partial_i) , \quad (14) \]

\[ L_{iD} = -\sqrt{R^2 - \vec{x}^2} p_i = -L_{Di} = i\hbar \sqrt{R^2 - \vec{x}^2} \partial_i . \quad (15) \]

Observe that since the \( x_D \) coordinate has been eliminated, the conjugate momentum \( p_D \) does not exist in the reduced variables. Now it can be verified that,

\[ \hat{\mathcal{H}} = \sum_{\alpha \beta} \frac{L_{\alpha \beta}^2}{2R^2} \]

(16)

We thus find that the quantum Hamiltonian is the conventional Schrödinger operator without any curvature term. This is the central result of the paper.

The above analysis was carried out in the cartesian basis, but it is instructive to repeat it in the curvilinear basis. Apart from serving as a consistency check, this will also illuminate the connection of the present study with the conventional Dirac approach. The mapping from the cartesian to the curvilinear coordinates is given by

\[ x_D = r \cos \varphi_1 \]
\[ x_{D-1} = r \sin \varphi_1 \cos \varphi_2 \]
\begin{align*}
  x_{D-3} &= r \sin \varphi_1 \sin \varphi_2 \cos \varphi_3 \\
  &\quad \cdots = \cdots \\
  x_2 &= r \sin \varphi_1 \cdots \sin \varphi_{D-2} \cos \varphi_{D-1} \\
  x_1 &= r \sin \varphi_1 \cdots \sin \varphi_{D-2} \sin \varphi_{D-1} \\
\end{align*}

In these variables, the Lagrangian is given by

\[ \mathcal{L} = \frac{1}{2} \left( r^2 + r^2 \varphi_1^2 + r^2 \varphi_2^2 \sin^2 \varphi_1 + \cdots + r^2 \varphi_{D-1}^2 \sin^2 \varphi_1 \cdots \sin^2 \varphi_{D-2} \right) + \lambda (r - R) \]

where the Lagrange multiplier \( \lambda \) defines the rotor constraints. The canonical momenta are given by

\[ \begin{align*}
  \pi_\lambda &= 0 , \quad \pi_r = \dot{r} , \\
  \pi_{\varphi_1} &= r^2 \dot{\varphi}_1 \\
  \pi_{\varphi_2} &= r^2 \sin^2 \varphi_1 \dot{\varphi}_2 \\
  &\quad \cdots = \cdots \\
  \pi_{\varphi_{D-1}} &= r^2 \sin^2 \varphi_1 \cdots \sin^2 \varphi_{n-1} \dot{\varphi}_{D-1} \\
\end{align*} \]

In contrast to the cartesian analysis, the solution of the constraint here is trivial and the reduced Hamiltonian obtained by following the previous steps is

\[ \mathcal{H} = \frac{1}{2} \sum g^{ab} \pi_a \pi_b \]

with

\[ g^{ab} = \frac{1}{R^2} \left( \begin{array}{ccccccc}
  1 & 0 & 0 & \cdots & 0 \\
  0 & \frac{1}{\sin^2 \varphi_1} & 0 & \cdots & 0 \\
  0 & 0 & \frac{1}{\sin^2 \varphi_1 \sin^2 \varphi_2} & \cdots & 0 \\
  \cdots & \cdots & \cdots & \cdots & 0 \\
  0 & 0 & 0 & \cdots & \frac{1}{\sin^2 \varphi_1 \sin^2 \varphi_2 \cdots \sin^2 \varphi_{n-2}} \\
\end{array} \right) \]

The quantum Hamiltonian, as usual, is given by the corresponding Laplace-Beltrami operator. The momentum operator \( \Pi \) is given by the expression

\[ \pi_{\varphi_1} = -i \hbar \frac{1}{\sin^2 \varphi_i} \partial_i \sin \frac{\varphi_i}{2} \varphi_i , \]
and in terms of the curvilinear variables for a constant radius the hamiltonian operator (10) reduces to
\[ \hat{H} = -\hbar^2 \sum_{i=1}^{n-1} \prod_{j=1}^{i-1} \frac{1}{\sin^2 \phi_j} \left( \sin^{n-i-1} \phi_i \right) \frac{\partial}{\partial \phi_i} (\sin \phi_i)^{n-i-1} \frac{\partial}{\partial \phi_i} \]
\[ \equiv \frac{\hat{L}^2}{2R^2} \] (23)
which in three dimensions simplifies to the well known expression
\[ \hat{H} = -\hbar^2 \left( \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{(\sin \theta)^2} \frac{\partial^2}{\partial \phi^2} \right) \equiv \frac{\hat{L}^2}{2R^2} \] (24)
which is the expected result and is compatible with our general expression (16) given in the cartesian basis.

To compare with the Dirac formalism we start from the original constrained Lagrangian in curvilinear coordinates given in (18). There is one primary constraint,
\[ \Omega = \pi_\lambda = 0 \] (25)
To check for secondary constraints we construct the total Hamiltonian
\[ \mathcal{H}_T = \mathcal{H}_c + u\pi_\lambda \] (26)
where \( \mathcal{H}_c \) is the canonical Hamiltonian given by
\[ \mathcal{H}_c = \frac{1}{2} \left[ \pi_r^2 + \frac{\pi_{\phi_1}^2}{r^2} + \frac{\pi_{\phi_2}^2}{\sin^2 \phi_1 r^2} + \cdots + \frac{\pi_{\phi_j}^2}{\prod_{j=1}^{n-2} \sin^2 \phi_j r^2} \right] \] (27)
Time conservation of the primary constraint leads to a secondary constraint. Continuing this iterative process, the full set of constraints is obtained.
\[ \Omega_1 = r - R \approx 0 , \quad \Omega_2 = \pi_r \approx 0 \] (28)
The unphysical canonical set \( \lambda, \pi_\lambda \) associated with the Lagrange multiplier is ignored. This leaves us with a pair of second class constraints, \( \Omega_1 \) and \( \Omega_2 \). It is important to point out that they form a canonical set,
\[ \{\Omega_i, \Omega_j\} = \epsilon_{ij} \] (29)
The special form of the constraints allows a straightforward application of the Masakawa-Nakajima theorem\cite{16} to extract the physical variables and the Hamiltonian without the need of any explicit computation of Dirac brackets. Using this theorem, it is simple to show that the canonical pairs are given by $\varphi_i, \pi_{\varphi_i}$. In other words, the Dirac brackets among these variables is equal to their Poisson brackets. The physical Hamiltonian, in terms of these pairs, is now obtained from the canonical Hamiltonian by passing on to the constraint shell. This is found to coincide with the reduced Hamiltonian (20) obtained by our approach. The quantum Hamiltonian is then reobtained from the corresponding Laplace-Beltrami operator.

The Dirac analysis of this problem in the cartesian basis is quite nontrivial. This is essentially tied to the fact that the constraint algebra is no longer canonical. The Dirac Brackets suffer from ordering problems and the extraction of the canonical pairs of variables is quite non-trivial. It is precisely because of these reasons that Dirac analysis has led to much confusion and controversy\cite{6,8,9}. However, by the Masakawa-Nakajima theorem, it is always possible to find the canonical transformation which enables the extraction of the canonical pair of variables without any further ambiguities. To keep our discussion simple we consider below the example of the three dimensional rotator.

The constraint (2) is given by

$$\Omega_1 = x_i x_i - R^2 = 0 \quad (30)$$

The Hamiltonian following from a Legendre transform of the original Lagrangian is simply given by

$$\mathcal{H} = \frac{1}{2} p_i^2 + \lambda \left( x_i x_i - R^2 \right) \quad (31)$$

which leads to the secondary constraint

$$\Omega_2 = x_i p_i = 0 \quad (32)$$

This corresponds to the standard pair of constraints ($\Omega_1, \Omega_2$)\cite{5}. It is straightforward to compute the Dirac Brackets

$$\{x_i, x_j\}^* = 0$$

$$\{x_i, p_j\}^* = \delta_{ij} - \frac{x_i x_j}{R^2} \quad (33)$$

$$\{p_i, p_j\}^* = -\frac{1}{R^2} \left( x_i p_j - x_j p_i \right)$$

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Note that the Dirac Brackets are plagued by ordering ambiguities. This is bypassed by making a canonical transformation to a more convenient set of variables. It is now simple to check that the transformation from cartesian to the curvilinear coordinates given in (17) also defines the canonical transformation from the old to the new set of variables,

\begin{align*}
x_1 &= R \sin \theta \cos \varphi, \quad x_2 = R \sin \theta \sin \varphi, \quad x_3 = R \cos \theta \\
\pi_1 &= \sin \theta \cos \varphi \pi_r + r \cos \theta \cos \varphi \pi_\theta - r \sin \theta \sin \varphi \pi_\varphi \\
\pi_2 &= \sin \theta \sin \varphi \pi_r + r \cos \theta \sin \varphi \pi_\theta + r \sin \theta \cos \varphi \pi_\varphi \\
\pi_3 &= \cos \theta \pi_r - r \sin \theta \pi_\theta
\end{align*} (34)

The canonical pairs are now well defined \((r, \pi_r)\) \((\theta, \pi_\theta)\) and \((\varphi, \pi_\varphi)\). The physical Hamiltonian is obtained from \(H = \frac{1}{2} p_i p_i\) using the canonical change of variables and reads

\[ H_{\text{phys}} = \frac{1}{2 R^2} \left( \pi_\theta^2 + \frac{1}{\sin^2 \theta} \pi_\varphi^2 \right), \quad (35) \]

where we have already pass on to the constraint shell,

\[ x_i p_i = r \pi_r = 0 \quad (36) \]

This completes the classical reduction. Since the above Hamiltonian is expressed in terms of canonical pairs, the Laplace-Beltrami construction goes through and we exactly reproduce the canonical Hamiltonian (24).

This completes our demonstration of the equivalence between the Lagrangian reduction and the Hamiltonian reduction.

## 3 Conclusions

The main conclusion of the present work is that the quantum Hamiltonian for the multidimensional rotor is given by the pure Schrödinger operator without any boundary term, provided we enforce the conditions of hermiticity and general coordinate invariance. This result was obtained in the Lagrangian formalism by directly solving the constraint and reducing the unwanted degrees of freedom. The Lagrangian analysis was done both in cartesian and in the curvilinear basis, following a technique recently suggested by one of us [13].
equivalence with the Hamiltonian formalism of Dirac was also shown in either basis.

Some comments about the path integral are in order. The basic problem here stems from the fact that the definition of the path integral in curvilinear coordinates is rather tricky and subtle. It also appears in the original computation done by de Witt\cite{1} where a curvature term was found. However, the complications of working with path integrals with curvilinear basis was not appreciated at that time. This came to be highlighted only after the work of Edwards and Gulyaev\cite{3}.

Indeed, an apparent clash between the canonical and (a naive) path integral formulation is already seen in the simplest of examples, namely a free non relativistic particle in two dimensions\cite{17}. Using the De Witt path integral prescription it was shown that the free particle propagator obeys the following equation,

\[ i\hbar \frac{\partial}{\partial t} \psi = \left( -\frac{\hbar^2}{2} \nabla^2 + \frac{\hbar^2}{8r^2} \right) \psi \]  

(37)

Surprisingly the above equation differs from the expected free particle Schrödinger equation by an effective potential term. The reason for this discrepancy is subtle. The computation in\cite{17} was done in polar coordinates, but using the naive prescription of De Witt. However, as is well known by now, the passage from the cartesian to the curvilinear basis introduces curvature like terms. This has been explained lucidly in the textbook of Lee\cite{14}. Indeed, for the particular problem at hand the explicit correction term has also been computed. It has been shown that the canonical Hamiltonian $\mathcal{H}_c$ cannot be used to define the path integral, rather it must be $\mathcal{H}_c - \frac{\hbar^2}{8r^2}$\cite{14}. It is now obvious that with this modified Hamiltonian the correct Schrödinger equation will be reproduced from (37). The lesson to be learnt is that the conventional De Witt path integral prescription must be carefully applied for curvilinear coordinates.

Keeping these observations in mind, a clear computation as the one performed by Kleinert\cite{7} leads to the correct result. We however point out that a distinction can be made, so that it is possible to treat the particle either on or near the surface of the sphere. For the former case the boundary term disappears\cite{7} but in the latter, such a term exists. Since in the present analysis the constraints are always strongly enforced, we are confined to the case of the particle exactly
on the sphere. A recent calculation from a more mathematical point of view also confirms our result\[18\].

We conclude therefore that there is no clash between the canonical (either Lagrangian or Hamiltonian) approach and the path integral formalism. Moreover, the Dirac analysis also gives perfectly valid results, as elucidated here.

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References

[1] B. De Witt Phys. Rev. 85 (1952) 653.
[2] B. De Witt Rev. Mod. Phys. 29 (1957) 377
[3] S. F. Edwards and Y. V. Gulyaev Proc. Roy. Soc. A279 (1964) 229.
[4] R. J. Rivers Path integral methods in Quantum Field Theory, Cambridge monographs in Mathematical Physics, 1987.
[5] P. A. M. Dirac Lectures on Quantum Mechanics New York Belfer Graduate School of Sciences, Yeshiva University.
[6] N. K. Falck and A. C. Hirshfeld Eur. J. Phys. 4 (1983) 5.
[7] H. Kleinert Path Integrals in Quantum mechanics Statistical and Polymer Physics, World Scientific 1995.
[8] H. Kleinert and S. V. Shabanov Phys. Lett. A232 (1997) 327.
[9] A. Foerster, H. O. Girotti and P. S. Kuhn Phys. Lett. A 195 (1994) 301.
[10] M. S. Marinov Phys. Rep. 60 (1980) 1.
[11] M. Omote and H. Sato Prog. Theor. Phys. 47 (1972) 1367.
[12] A. Saa Class. Quantum Grav. 14 (1997) 385.
[13] O. Bertolami Phys. Lett. A154 (1991) 225.
[14] T. D. Lee Particle Physics and Introduction to Field Theory Contemporary Concepts in Physics, vol. 1, Harwood Academic Publishers, 1990.

[15] R. Banerjee hep-th/9607199.

[16] T. Maskawa and H. Nakajima Prog. Theor. Phys. 56 (1976) 1295.

[17] A. K. Kapoor Phys. Rev. D29 (1984) 2339.

[18] H. Grundling and C. A. Hurst hep-th/9712052