

PREQUANTIZATION OF THE ROTATIONAL MOTION

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Abstract. The classical problem of a free rigid body motion is considered within Kostant–Souriau prequantization programme supplemented by the semi-classical Bohr–Sommerfeld quantization rules. The results are two implicit formulae for the energy spectrum which are valid in some intervals defined by the total angular momentum.

1. Introduction

The most studied systems in classical mechanics are those consisting of “material points” and “rigid bodies”. Under transition to quantum mechanics which is primarily a description of the elementary particles like electrons, nucleons and systems composed of them the first category had received much more attention than the second one. Nevertheless it is of the same direct physical importance as the first. For example, in quantizing the rotational motions of molecules they can be regarded as rigid bodies with three principal moments of inertia. When these principal moments of inertia are all equal between themselves the problem reduces to that of the spherical top. The symmetrical case when two of the principal moments of inertia are equal presents no mathematical difficulties in any quantization scheme as well, and yields simple formulae for the rotational energies in terms of the appropriate quantum numbers. The most general asymmetric case when no two of the principal moments of inertia are equal is significantly more difficult and has been treated in various quantization schemes without such definite success. That is why in the applications that involve asymmetric rotor model, the energy eigenvalue spectrum is determined numerically by diagonalizing the matrices representing the rotational energy. Another way to systemize the spectra is offered by a variety of empirical formulae which are successful in different degree when fitting the experimental

data. It is one of the purposes of the present work to supply explicit analytical results based on a mixture of the quasiclassical methods and modern geometrical considerations. The other is to stress on the fact that even though the free rigid body is a classical and well understood mechanical system its quantum-mechanical description still deserves some attention.

2. The Free Rigid Body

Consider a rigid body which is free to rotate in any possible manner about one of its points. Alternatively, the body can be viewed as moving in empty space under no forces. In any of these circumstances one can construct an inertial frame relative which the rotation of the body to be measured. Let Ω is the body angular velocity vector and let $(\Omega_1, \Omega_2, \Omega_3)$ be its components. Then if (I_A, I_B, I_C) are the principal moments of inertia of the body the Euler's equations of motion are accordingly

$$\begin{aligned} I_A \dot{\Omega}_A &= (I_B - I_C) \Omega_B \Omega_C \\ I_B \dot{\Omega}_B &= (I_C - I_A) \Omega_C \Omega_A \\ I_C \dot{\Omega}_C &= (I_A - I_B) \Omega_A \Omega_B. \end{aligned} \quad (2.1)$$

Two first integrals of these equations can be derived immediately. Thus, multiplying the above equations in succession by $\Omega_A, \Omega_B, \Omega_C$, and adding, one finds that

$$I_A \Omega_A \dot{\Omega}_A + I_B \Omega_B \dot{\Omega}_B + I_C \Omega_C \dot{\Omega}_C = 0$$

which integrates at once to give

$$I_A \Omega_A^2 + I_B \Omega_B^2 + I_C \Omega_C^2 = 2E$$

where E is the kinetic energy of the body and therefore this is the energy integral.

Further, multiplication in succession by $I_A \Omega_A, I_B \Omega_B, I_C \Omega_C$, and addition leads respectively to the integral

$$I_A^2 \Omega_A^2 + I_B^2 \Omega_B^2 + I_C^2 \Omega_C^2 = L^2.$$

Introducing angular momentum vector $\mathbf{L} = (L_A, L_B, L_C)$ with components

$$L_A = I_A \Omega_A, \quad L_B = I_B \Omega_B, \quad L_C = I_C \Omega_C, \quad (2.2)$$

these integrals can be rewritten into the form

$$\frac{L_A^2}{I_A} + \frac{L_B^2}{I_B} + \frac{L_C^2}{I_C} = 2E \quad (2.3)$$

$$L_A^2 + L_B^2 + L_C^2 = L^2. \quad (2.4)$$

3. Prequantization

The concept of geometric quantization has been developed by Kostant [4] and Souriau [12]. The starting point is any symplectic manifold (M, ω) . It turns out that in this setting the symplectic form ω generates a Lie algebra structure in the space $R^\infty(M)$ of smooth real-valued functions on M . The problem of describing the representations of $R^\infty(M)$ was approached for the first time by Dirac [1] in the case $(M \equiv R^{2n}, \omega \equiv dp \wedge dq)$. The idea is that if we are able to associate with every classical observable a quantum one, to find a way that the Poisson bracket of two classical observables is represented up to a multiplicative number by the commutator of the respective quantum variables. The scheme has been generalized by Segal [10] for phase spaces which are cotangent bundles and finally Kostant [4] and Souriau [12] transfer it to arbitrary symplectic manifolds. This part of the programme nowadays is called prequantization. Quantum numbers arise in that theory because of the requirement for integrability of ω . By definition the symplectic manifold (M, ω) is pre-quantizable if $[\omega/2\pi\hbar]$ is in the image of the map

$$H_{\text{Cech}}^2(M, \mathbb{Z}) \rightarrow H_{\text{de Rham}}^2(M, \mathbb{R}), \tag{3.1}$$

where $[\]$ denotes the de Rham cohomological class.

When M is a compact manifold this condition is equivalent to

$$\frac{1}{2\pi\hbar} \int_{\sigma} \omega \in \mathbb{Z}, \quad \text{for every two-cycle } \sigma \in H_2(M, \mathbb{Z}). \tag{3.2}$$

The quantization of charge, spin and energy levels of some physical systems exemplify the scheme (for details see [5–8]). A nice introduction to the subject can be found in [11].

If (M, ω) is pre-quantizable, then there exists a complex line bundle $L \rightarrow M$ with a Hermitian metric $h(., .)$ and Chern class $\frac{1}{2\pi\hbar}[\omega]$ which is equipped with a Hermitian connection ∇ that has as a curvature form $R^\nabla \equiv -i\omega/\hbar$ [4]. The irreducibility of the representation which is the second stage (quantization) of the programme is achieved by introducing additionally a new structure called polarization. This step will be not pursued here due to the “no go theorem” of Groenewold and van Hove which states that even the Lie algebra of real-valued polynomials on the flat space \mathbb{R}^{2n} can not be consistently quantized, but nevertheless this is possible for the subalgebra of polynomials up to second degree. This explains also why the quantization of the square of the angular momentum which is a fourth degree polynomial is not so straightforward.

4. Applications

Looking at the second integral of the free rigid body motion (2.4) one can realize immediately that the components of the angular momentum lie on the sphere \mathbb{S}_ℓ^2 of fixed radius ℓ (in units of \hbar). Therefore it seems appropriate to represent them via the spherical polar coordinates in the form

$$L_A = \ell \sin \theta \cos \varphi, \quad L_B = \ell \sin \theta \sin \varphi, \quad L_C = \ell \cos \theta. \quad (4.1)$$

In these coordinates the respective symplectic form ω_ℓ reads

$$\omega_\ell = \ell \sin \theta \, d\theta \wedge d\varphi, \quad (4.2)$$

and the prequantization of the symplectic manifold $(\mathbb{S}_\ell^2, \omega_\ell)$ gives

$$\frac{1}{2\pi\hbar} \int_{\mathbb{S}_\ell^2} \omega_\ell = 2\ell = N \in \mathbb{Z}. \quad (4.3)$$

The Hilbert space of the problem under consideration can be identified with the space of the sections of the line bundle \mathcal{L} over $(\mathbb{S}_\ell^2, \omega_\ell)$ and its dimension is given by the Riemann–Roch theorem [3]

$$\dim \mathcal{H} = \dim \Gamma(\mathbb{S}_\ell^2, \mathcal{L}) = N + 1 = 2\ell + 1. \quad (4.4)$$

The energy spectrum in this space can be obtained by the requirement that the action integral taken along the trajectories of the dynamical system

$$\frac{1}{2\pi\hbar} \oint \Theta_\ell \quad (4.5)$$

should be integer valued function. Here, Θ_ℓ coincides (up to a sign) with the potential one-form of the symplectic two-form ω_ℓ (i. e. $\omega_\ell = -d\Theta_\ell$). Using the local coordinates chosen above, this means that

$$\frac{\ell}{2\pi\hbar} \int_0^{2\pi} \cos \theta \, d\varphi = m, \quad m \in \mathbb{Z}. \quad (4.6)$$

Because θ goes from $-\pi/2$ to $\pi/2$, the corresponding values of $\cos \theta$ are within the interval $[-1, 1]$, and this means that the range of m is specified by the following inequalities

$$-\ell \leq m \leq \ell. \quad (4.7)$$

Besides, one can conclude also that ℓ takes only integer values!

In what follows we will consider the action integral in the most interesting physical cases: (i) an axially symmetric body, and (ii) the asymmetric body.

The Axially Symmetric Body

In this case, two of the three principal moments of inertia (I_A, I_B, I_C) coincide. As the particular choice is inessential, we take $I_A = I_B$, solve (2.3) for L_3 and this gives us

$$L_3^2 = \frac{2E - \frac{\ell^2}{I_A}}{\frac{1}{I_C} - \frac{1}{I_A}} = \ell^2 \cos^2 \theta. \quad (4.8)$$

Entering with

$$\cos \theta = \sqrt{\frac{2EI_A - \ell^2}{\left(\frac{1}{I_C} - \frac{1}{I_A}\right) \ell^2 I_A}}, \quad (4.9)$$

into the Bohr–Sommerfeld condition (4.6) one finally gets the energy spectrum of the axially symmetric rigid body in the form

$$E_{\ell, m} = \frac{\ell^2}{2I_A} \hbar^2 + \frac{m^2}{2} \left(\frac{1}{I_C} - \frac{1}{I_A} \right) \hbar^2, \quad (4.10)$$

$$-\ell \leq m \leq \ell, \quad \ell \in \mathbb{Z}.$$

It is obvious that it is doubly degenerated as $\pm m$ produce the same level.

The Asymmetric Body

In the completely asymmetric case, the three principal moments of inertia are different between themselves, i. e. $I_A \neq I_B \neq I_C$. It is clear that we can re-label the axes so that without any loss of generality (and for definiteness) we will assume that

$$I_A < I_B < I_C, \quad (4.11)$$

and consequently

$$\alpha := 1/I_A > \beta := 1/I_B > \gamma := 1/I_C > 0. \quad (4.12)$$

In the new variables the energy integral takes the form

$$E(\alpha, \beta, \gamma) = (\alpha L_A^2 + \beta L_B^2 + \gamma L_C^2)/2. \quad (4.13)$$

This form suggest to consider the affine transformation of the above variables generated by two arbitrary scalar factors σ and τ which gives

$$E(\sigma\alpha + \tau, \sigma\beta + \tau, \sigma\gamma + \tau) = \sigma E(\alpha, \beta, \gamma) + \frac{\tau}{2} L^2 \quad (4.14)$$

Now, following Ray [9] we will use the freedom in choosing σ and τ and fix them as follows:

$$\sigma\alpha + \tau = 1, \quad \text{and} \quad \sigma\gamma + \tau = -1, \quad (4.15)$$

which means that

$$\sigma = \frac{2}{\alpha - \gamma} \quad \text{and} \quad \tau = -\frac{\alpha + \gamma}{\alpha - \gamma}. \quad (4.16)$$

Under the choices we have made the middle coefficient becomes

$$\sigma\beta + \tau := \varepsilon = \frac{2\beta - \alpha - \gamma}{\alpha - \gamma}. \quad (4.17)$$

In the same spirit it seems appropriate to introduce also

$$E(\varepsilon) = E(1, \varepsilon, -1) = (L_A^2 + \varepsilon L_B^2 - L_C^2)/2, \quad (4.18)$$

and whence

$$E(\alpha, \beta, \gamma) = \frac{1}{\sigma} E(\varepsilon) - \frac{\tau}{2\sigma} L^2. \quad (4.19)$$

The last equation tell us that our quantization problem is equivalent with the problem of finding the spectrum of $E(\varepsilon)$. Another observation is that the geometry of the trajectories this time is determined by the intersection of the sphere (2.4) with the hyperboloid (4.18). This intersection is non-empty in the case when the radius of the sphere ℓ is greater than the smaller semiaxis of the hyperboloid. Further on we will assume that it is larger than the greatest semiaxis as well and this amounts to inequality

$$\frac{2E(\varepsilon)}{\varepsilon} < \ell^2. \quad (4.20)$$

By its very definition it is clear that $\varepsilon \in [-1, 1]$ and that the extreme points correspond to prolate, respectively oblate symmetric rotors. Besides them quite interesting situation is the case $\varepsilon = 0$ which arises under very special relationship among the principal inertia moments, namely

$$\frac{2}{I_B} = \frac{1}{I_A} + \frac{1}{I_C}, \quad (4.21)$$

that will be not pursued furthermore here, but obviously deserves some attention as well. Another useful observation is that we have the general result

$$E(-\varepsilon) = -E(\varepsilon), \quad (4.22)$$

which follows by a simple re-labeling of momentum components and means that we can consider only positive values of ε . Entering with (2.4) into the equation specifying the hyperboloid in question we get

$$\cos \theta = \sqrt{\frac{\cos^2 \varphi + \varepsilon \sin^2 \varphi - 2E(\varepsilon)/\ell^2}{1 + \cos^2 \varphi + \varepsilon \sin^2 \varphi}}. \quad (4.23)$$

The calculation of the action integral will be somewhat easy if we change the variable φ by

$$z = \cos^2 \varphi + \varepsilon \sin^2 \varphi, \quad (4.24)$$

and accordingly

$$d\varphi = -\frac{dz}{2\sqrt{(z-\varepsilon)(1-z)}}, \quad (4.25)$$

so that it becomes

$$\frac{\ell}{\pi \hbar} \int_{\varepsilon}^1 \sqrt{\frac{z - 2E(\varepsilon)/\ell^2}{(1-z)(z-\varepsilon)(z+1)}} dz = m, \quad m \in \mathbb{Z}. \quad (4.26)$$

Introducing

$$a = 1, \quad b = \varepsilon, \quad c = 2E(\varepsilon)/\ell^2, \quad d = -1, \quad (4.27)$$

the above integral can be cast into the general form

$$\int_u^a \sqrt{\frac{z-c}{(a-z)(z-b)(z-d)}} dz \quad (4.28)$$

in which

$$a > u \geq b > c > d, \quad (4.29)$$

and expressed via the complete elliptic integrals of first and third kind as follows (cf. [2])

$$\frac{2}{\sqrt{(a-c)(b-d)}} \left[(d-c)K(k) + (a-d)\Pi\left(\frac{b-a}{b-d} \mid k\right) \right]. \quad (4.30)$$

The modulus of the above elliptic integrals is

$$k^2 = \frac{(a-b)(c-d)}{(a-c)(b-d)} = \frac{(1-\varepsilon)(\ell^2 + 2E(\varepsilon))}{(1+\varepsilon)(\ell^2 - 2E(\varepsilon))}. \quad (4.31)$$

Our study will be incomplete if we do not consider the remaining case when the radius of the sphere lies between the smallest and largest semiaxes of the hyperboloid, namely

$$2E(\varepsilon) < \ell^2 < 2E(\varepsilon)/\varepsilon. \quad (4.32)$$

This case is covered by the following changes: the values of b and c (4.27) exchange their places and the integration in (4.28) have to be performed this time from (the new!) b to a and not from c to a as one can expect. The reason is that in the case under consideration the trajectory does not encircle the north pole of the sphere but the x -axis and this produces the limitation. All this means that now we have to evaluate

$$\int_b^u \sqrt{\frac{x-b}{(a-x)(x-c)(x-d)}} dx \quad (4.33)$$

in which

$$a = 1 > u \geq b = 2E(\varepsilon)/\ell^2 > c = \varepsilon > d = -1. \quad (4.34)$$

As before the result is a linear combination of the first and third kind elliptic integrals, i. e.

$$\frac{2(b-c)}{\sqrt{(a-c)(b-d)}} \left[\Pi\left(\lambda, \frac{a-b}{a-c}, k\right) - F(\lambda, k) \right], \quad (4.35)$$

$$\lambda = \arcsin \sqrt{\frac{(a-c)(u-b)}{(a-b)(u-c)}},$$

where the modulus of the elliptic functions now is

$$k = \sqrt{\frac{(1+\varepsilon)(\ell^2 - 2E(\varepsilon))}{(1-\varepsilon)(\ell^2 + 2E(\varepsilon))}}. \quad (4.36)$$

Taking the limit $u \rightarrow a$ the Bohr–Sommerfeld quantization condition in this case reads

$$\frac{2(b-c)}{\sqrt{(a-c)(b-d)}} \left[\Pi\left(\frac{a-b}{a-c}, k\right) - K(k) \right] = \frac{m}{\ell} \pi \hbar, \quad (4.37)$$

$$m, \ell \in \mathbb{Z}, \quad -\ell \leq m \leq \ell.$$

A few remarks are in order here. First, when solving the implicit equations (4.26) or (4.37) one have to keep in mind the respective inequalities (4.20) and (4.32) which narrow the intervals where $E(\varepsilon)$ can vary. Second, it is obvious that the precise values of $E(\varepsilon)$ can be found only numerically in general. Third,

it could be possible to find some explicit approximate formulae. Finally, it will be quite interesting to test the above results with the huge experimental data available in molecular and nuclear spectroscopy.

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