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Article

New Exact Solutions Describing Quantum Asymmetric Top

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Abstract: In this work, using the noncommutative integration method of linear differential equations, we obtain a complete set of solutions to the Schrodinger equation for a quantum asymmetric top in Euler angles. It is shown that the noncommutative reduction of the Schrodinger equation leads to the Lamé equation. The resulting set of solutions is determined by the Lamé polynomials in a complex parameter, which is related to the geometry of the orbits of the coadjoint representation of the rotation group. The spectrum of an asymmetric top is obtained from the condition that the solutions are invariant with respect to a special irreducible λ -representation of the rotation group.

Keywords: quantum asymmetric top; noncommutative integration method; λ -representation

1. Introduction

The problem of the asymmetric top in quantum mechanics is a standard one, dealt with by a number of authors [1–8]. The quantum asymmetric top has many applications, ranging from quantum information [9] to high-resolution spectroscopy [10], especially in the fields of molecular [11,12] and nuclear [13–15] physics. It should be noted that the problem of scalar waves in a frozen Mixmaster universe is mathematically identical to that of the asymmetric top, except that half-integral angular momenta [16–18].

The stationary Schrodinger equation for a quantum asymmetric top does not allow the separation of variables in the general case [1] because the necessary and sufficient conditions for the theorem on the separation of variables are not satisfied [19]. However, for wave functions that depend on only two variables, the equation admits a separation of variables in an elliptic coordinate system, which makes it possible to find the spectrum of an asymmetric top [20]. In this case, the eigenfunctions in the standard approach are sought in the form of a series of Wigner D -functions.

In this paper, to integrate the Schrodinger equation for a quantum asymmetric top, the noncommutative integration method of linear differential equations [21–24] is used, which, unlike the method of separation of variables, allows us to reduce to an ordinary differential equation in the general case. Note that [25] used this method to study the semiclassical spectrum of an asymmetric top.

The paper is organized as follows. In Section 2, we introduce the basic concepts from the quantum theory of an asymmetric top and describe it in terms of the rotation group $SO(3)$. Section 3 is devoted to finding a complete set of solutions to the Schrodinger equation using the noncommutative integration method. In Section 4, we study the connection between the Wigner D -function and a special irreducible representation (irreps) of the group $SO(3)$, from which the completeness of the obtained set of solutions follows. In the last Section 5, we summarize and discuss the main results. Some useful technical details are placed in the Appendix A.

Here, we are using the natural system of units $c = \hbar = 1$.



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2. The Quantum Asymmetric Top

The Hamiltonian of the quantum top is defined as the operator

$$\hat{H} = A\hat{L}_1^2 + B\hat{L}_2^2 + C\hat{L}_3^2, \quad A \geq B \geq C > 0, \quad (1)$$

where $(2A)^{-1}$, $(2B)^{-1}$ and $(2C)^{-1}$ are the principal moments of inertia, \hat{L}_a are the components of the angular momentum operator along the three principal axes of inertia of the top and satisfying the commutation relations

$$[\hat{L}_a, \hat{L}_b] = \hat{L}_a \hat{L}_b - \hat{L}_b \hat{L}_a = -i\epsilon_{abc} \hat{L}_c,$$

where ϵ_{abc} is the completely antisymmetric tensor with $\epsilon_{123} = 1$. The quantum spherical top corresponds to the case $A = B = C$ and the quantum symmetrical top to the case $A = B \neq C$. A top is called an asymmetric top if $A \neq B \neq C$.

The square of the total angular momentum operator $\hat{L}^2 = \hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2$ commutes with the Hamiltonian \hat{H} , $[\hat{L}^2, \hat{H}] = 0$.

Let us describe quantum top problem in terms of rotation group $SO(3)$. We describe the orientation of the top by Euler angles $g = (\phi, \theta, \psi)$, $\phi \in [0; 2\pi)$, $\theta \in [0; \pi)$, $\psi \in [0; 2\pi)$, referred to as axes fixed in space. We note that Euler angles parameterize the group element $g \in SO(3)$ (see Appendix A). Projections of the angular momentum operator \hat{L} with respect to the axes of the body-fixed reference frame are

$$\hat{L}_1 = i\zeta_1, \quad \hat{L}_2 = i\zeta_2, \quad \hat{L}_3 = i\zeta_3, \quad [\hat{L}_1, \hat{L}_2] = -i\hat{L}_3,$$

where ζ_a are left-invariant vector fields (A2) (see Ref. [16]). Operators for the components of angular momentum along the axes fixed in space (space-fixed reference frame) are given by:

$$\hat{J}_x = i\eta_1, \quad \hat{J}_y = i\eta_2, \quad \hat{J}_z = i\eta_3, \quad [\hat{J}_x, \hat{J}_y] = -i\hat{J}_z,$$

where η_a are right-invariant vector fields (A3). The square of the total angular momentum operator is the Casimir operator of the $SO(3)$ group and the same in both reference frames:

$$\hat{L}^2 = K(-i\zeta) = K(i\eta) = -\frac{1}{\sin^2 \theta} \left(\frac{\partial^2}{\partial \psi^2} + \frac{\partial^2}{\partial \phi^2} - 2 \cos \theta \frac{\partial^2}{\partial \phi \partial \psi} \right) - \frac{\partial^2}{\partial \theta^2} - \cot \theta \frac{\partial}{\partial \theta},$$

where $K(f) = f_1^2 + f_2^2 + f_3^2$.

There are three mutually commuting operators $\mathcal{X} = \{\hat{L}_3, \hat{J}_3, \hat{L}^2\}$. We denote the common eigenfunctions of the set as $|j, m, n\rangle$,

$$\begin{aligned} \hat{L}^2 |j, m, n\rangle &= j(j+1) |j, m, n\rangle, & j &= 1, 2, 3, \dots, \\ -\hat{L}_3 |j, m, n\rangle &= n |j, m, n\rangle, & n &= -j, \dots, j, \\ \hat{J}_z |j, m, n\rangle &= m |j, m, n\rangle, \end{aligned} \quad (2)$$

They correspond to states with a given angular momentum j and its z -projection n , with respect to the axes of the body-fixed reference frame and z -projection m , with respect to the space-fixed reference frame. An explicit form of the states $|j, m, n\rangle$ is given by the Wigner D -functions that are matrix elements of the irreps of the group $SO(3)$ (see Ref. [3,26]):

$$\begin{aligned} \langle g | j, m, n \rangle &= D_{mn}^j(g) = e^{im\phi + in\psi} d_{mn}^j(\theta), \\ d_{mn}^j(\theta) &= (-1)^{m-n} \sqrt{\frac{(j+m)!(j-m)!}{(j+n)!(j-n)!}} \sin^{m-n} \frac{\theta}{2} \cos^{m+n} \frac{\theta}{2} P_{j-m}^{(m-n, m+n)}(\cos \theta), \end{aligned} \quad (3)$$

where $P_n^{(\alpha,\beta)}(z)$ are Jacobi polynomials,

$$P_n^{(\alpha,\beta)}(z) = \frac{(-1)^n}{2^n n!} (1-z)^{-\alpha} (1+z)^{-\beta} \frac{d^n}{dz^n} [(1-z)^{n+\alpha} (1+z)^{n+\beta}].$$

The completeness and orthogonality conditions for the Wigner D -function have the form:

$$\frac{1}{8\pi^2} \int_0^{2\pi} d\psi \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi D_{mn}^j(g) \overline{D_{\tilde{m}\tilde{n}}^j(g)} = \frac{\delta_{j\tilde{j}}}{2j+1} \delta_{m\tilde{m}} \delta_{n\tilde{n}}, \quad (4)$$

$$\sum_{n=-j}^j \overline{D_{mn}^j(g)} D_{\tilde{m}n}^j(g) = \delta_{m\tilde{m}}. \quad (5)$$

Thus, the Hamiltonian (1) is expressed in terms of the left-invariant vector fields on the group $SO(3)$,

$$\hat{H} = H(-i\tilde{\zeta}), \quad H(f) = Af_1^2 + Bf_2^2 + Cf_3^2$$

and commutes with right-invariant vector fields η_a . The states of a quantum top are determined by the wave function, which is a function on the group $SO(3)$.

There is a set of two mutually commuting symmetry operators (the Casimir operator $K(-i\tilde{\zeta})$ and one of the operators ζ_a). The state of the top with a certain value of quantum numbers j and m is described by the system

$$\begin{aligned} \hat{H} |j, m\rangle &= E |j, m\rangle, \\ \hat{L}^2 |j, m\rangle &= j(j+1) |j, m\rangle, \\ \hat{J}_z |j, m\rangle &= m |j, m\rangle. \end{aligned} \quad (6)$$

Note that the system (6) cannot be solved by the separation method variables. In the standard approach [1,16], the solution of Equation (6) is sought as:

$$|j, m\rangle = \sum_{n=-j}^j a_{j,n} |j, m, n\rangle. \quad (7)$$

Substituting (7) in Equation (6), we obtain a $(2j+1)$ -dimensional linear system

$$\sum_{n=-j}^j a_{j,n'} (H_{n,n'} - E\delta_{n,n'}) = 0, \quad H_{n,n'} = \langle j, m, n | \hat{H} | j, m, n' \rangle, \quad (8)$$

for the quantities $a_{j,n}$. The roots of equation

$$\|H_{n,n'} - E\delta_{n,n'}\| = 0 \quad (9)$$

determine the energy levels of the top, after which the system of Equation (8) allows one to determine the wave functions of an asymmetric top with given values j and m .

The secular Equation (9) is of degree $2j+1$. In fact, the eigenvalues E are independent of m . This is so because the Hamiltonian \hat{H} commutes with the raising and lowering operators $\hat{J}_\pm = \hat{J}_1 \pm i\hat{J}_2$. The specialization of the eigenvalue (6) equation to $m=0$,

$$\begin{aligned} \hat{H} |j, 0\rangle &= E |j, 0\rangle, \\ \hat{L}^2 |j, 0\rangle &= j(j+1) |j, 0\rangle, \\ \hat{J}_z |j, 0\rangle &= 0 \end{aligned} \quad (10)$$

admits separation of variables in the elliptic coordinates [20]. The elliptic coordinates (ρ_1, ρ_2) , $\rho_1 \in (B, A)$, $\rho_2 \in (C, B)$ are defined as

$$\begin{aligned}\sin \theta \sin \psi &= \sqrt{\frac{(A - \rho_1)(A - \rho_2)}{(A - B)(A - C)}}, \\ \sin \theta \cos \psi &= \sqrt{\frac{(B - \rho_1)(B - \rho_2)}{(A - B)(A - C)}}, \quad \cos \theta = \sqrt{\frac{(C - \rho_1)(C - \rho_2)}{(C - A)(C - B)}}.\end{aligned}$$

The solution of the system (10) in elliptic coordinates $\psi_j(\rho_1, \rho_2) = \langle \rho_1, \rho_2 \mid j, 0 \rangle$ has the form:

$$\psi_j(\rho_1, \rho_2) = \Lambda_j(\rho_1)\Lambda_j(\rho_2),$$

where function $\Lambda_j(\rho)$ satisfies the differential equation

$$\left\{ 4\sqrt{P(\rho)} \frac{d}{d\rho} \left(4\sqrt{P(\rho)} \frac{d}{d\rho} \right) - j(j+1)\rho + E \right\} \Lambda_j(\rho) = 0, \quad (11)$$

which can readily be identified to be a Lamé equation in algebraic form.

It follows from the theory of the Lamé differential equation that for integers j , there are $2j + 1$ linearly independent and mutually orthogonal functions $\Lambda_{j,s}(\rho)$ (the Lamé polynomials) corresponding to $2j + 1$ different eigenvalues $E_{j,s}$, $s = -j, \dots, j$. Solutions to the Equation (11) are represented as series

$$\begin{aligned}\Lambda_j^{(1)}(\rho) &= \sum_{k=0}^{\infty} a_k (\rho - B)^{j/2-k}, \\ \Lambda_j^{(2)}(\rho) &= \sqrt{\rho - A} \sum_{k=0}^{\infty} b_k (\rho - B)^{(j-1)/2-k}, \\ \Lambda_j^{(3)}(\rho) &= \sqrt{\rho - C} \sum_{k=0}^{\infty} c_k (\rho - B)^{(j-1)/2-k}, \\ \Lambda_j^{(4)}(\rho) &= \sqrt{(\rho - A)(\rho - C)} \sum_{k=0}^{\infty} d_k (\rho - B)^{j/2-k-1}.\end{aligned} \quad (12)$$

From Equation (11), the recurrent relations for the coefficients a_k , b_k , c_k and d_k follow, where $a_l = b_l = c_l = d_l = 0$ for $l < 0$. The eigenvalues of $E_{j,s}$ are obtained from the finiteness conditions for the series (12):

$$a_{\lfloor j/2+1 \rfloor} = b_{\lfloor j/2 \rfloor} = c_{\lfloor j/2 \rfloor} = d_{\lfloor j/2 \rfloor} = 0, \quad (13)$$

where $\lfloor x \rfloor = \max\{m \in \mathbb{N} \mid m \leq x\}$ is the floor function and $\lceil x \rceil = \min\{m \in \mathbb{N} \mid m \geq x\}$ is the ceiling function.

From (13), the eigenvalues $E_{j,s}$ are determined. For even values of j , we have one equation of degree $j/2 + 1$ and three equations of degree $j/2$, whose solution is $2j + 1$ different eigenvalues $E_{j,s}$. For odd values of j , we obtain three equations of degree $(j + 1)/2$ and one equation of degree $j/2$, the solution of which is also $2j + 1$ different eigenvalues $E_{j,s}$.

3. The Noncommutative Integration

In this section, we obtain a complete set of solutions to the stationary Schrodinger equation

$$\hat{H}\Psi(g) = E\Psi(g) \quad (14)$$

with the Hamiltonian (1). Equation (14) can be thought of as the quantum equation on the $SO(3)$ group. To construct solutions of quantum equations on the Lie groups, it is efficient to use the noncommutative integration method [21–23,25,27]. We apply this method to the Equation (14).

First, we must construct a special representation of the Lie algebra $\mathfrak{so}(3)$ of the group $SO(3)$. Following the papers [21,23,25,27–29], we introduce an irreducible λ -representation

(λ -irrep) of the Lie algebra $\mathfrak{so}(3)$, which is parametrized by the parameter $j = 1, 2, \dots$ and acts in the space \mathcal{F}^j functions of the form

$$\Psi(q) = \sum_{n=-j}^j c_n e^{inq}, \quad q \in Q, \quad c_n = \text{const}, \quad (15)$$

where $Q = \{q = \alpha + i\beta \mid \alpha \in [0; 2\pi), \beta \in (-\infty, +\infty)\}$. The λ -irrep of the Lie algebra $\mathfrak{so}(3)$ in space \mathcal{F}^j is given by the operators

$$\begin{aligned} \ell_1(q, \partial_q, j) &= -i \sin q \partial_q + ij \cos q, \\ \ell_2(q, \partial_q, j) &= -i \cos q \partial_q - ij \sin q, \\ \ell_3(q, \partial_q, j) &= \partial_q, \quad [\ell_a(q, \partial_q, j), \ell_b(q, \partial_q, j)] = \epsilon_{abc} \ell_c(q, \partial_q, j). \end{aligned} \quad (16)$$

The operators $\hat{f}_a = -i\ell_a(q, \partial_q, j)$ are Hermitian with respect to the scalar product

$$\begin{aligned} (\Psi_1, \Psi_2)_Q^j &= \int \overline{\Psi_1(q)} \Psi_2(q) d\mu_j(q), \quad \Psi_1, \Psi_2 \in \mathcal{F}^j, \\ d\mu_j(q) &= C_j \frac{dq \wedge d\bar{q}}{(1 + \cos(q - \bar{q}))^{j+1}}, \quad C_j = \frac{(2j+1)!}{2^j(j!)^2}, \end{aligned} \quad (17)$$

and satisfy the commutation relations

$$[\hat{f}_a, \hat{f}_b] = i\epsilon_{abc} \hat{f}_c, \quad K(\hat{f}) = \hat{f}_1^2 + \hat{f}_2^2 + \hat{f}_3^2 = j(j+1).$$

The set of functions $\psi_n(q) = e^{inq}$ is orthogonal with respect to the scalar product (17):

$$(\psi_n, \psi_{\bar{n}})_Q = \frac{1}{B_{nj}} \delta_{n\bar{n}}, \quad B_{nj} = \frac{(j!)^2}{(j-n)!(j+n)!}.$$

This follows the formula for the decomposition coefficients (15):

$$c_n = B_{nj}(\Psi, \psi_n)_Q.$$

Then, the generalized Dirac function in space \mathcal{F}^j ,

$$\Psi(q) = \int_Q \Psi(q') \delta_j(q, \bar{q}') d\mu_j(q'), \quad \Psi \in \mathcal{F}^j$$

is given by the expression

$$\delta_j(q, \bar{q}') = \sum_{n=-j}^j B_{nj} \psi_n(q) \overline{\psi_n(q')} = \frac{2j+1}{C_j} \left(1 + \cos(q - \bar{q}')\right)^j. \quad (18)$$

The λ -irrep (16) corresponds to a non-degenerate integer coadjoint orbit of the group $SO(3)$ that passes through the covector $\lambda(j) = (j, 0, 0)$ (see Ref. [22]),

$$\mathcal{O}_j = \{f \in \mathbb{R}^3 \mid K(f) = j^2, f \neq 0\}. \quad (19)$$

The Kirillov form $\omega_j = (df_1 \wedge df_2)/f_3$ in the orbit \mathcal{O}_j sets a symplectic structure [30]. It is well known that on the symplectic manifold, the Darboux canonical coordinates exist in which the symplectic form is canonical. There is the linear canonical transition

$$\begin{aligned} f_1(p, q, j) &= -ip \sin q + j \cos q, \\ f_2(p, q, j) &= -ip \cos q - j \sin q, \\ f_3(p, q, j) &= p \end{aligned}$$

from the coordinates on the orbit to the Darboux coordinates (p, q) , $\omega_j = dp \wedge dq$. Note that the operators \hat{f}_a can be considered as a result of qp -quantization of the orbit \mathcal{O}_j , $\hat{f}_a = f_a(\hat{p}, \hat{q}, j)$, $\hat{p} = -i\partial_q$, $\hat{q} = q$ (see Ref. [25]), and the set Q is a Lagrangian submanifold to the orbit \mathcal{O}_j .

Within the noncommutative integration method of linear differential equations, wave functions of asymmetric top are sought as a solution system of equations

$$\hat{H}(g)\Psi(q, j; g) = E\Psi(q, j; g), \quad (20)$$

$$[\eta_a(g) + \ell_a(q, \partial_q, j)]\Psi(q, j; g) = 0, \quad (21)$$

where the operators η_a commute with Hamiltonian, $[\hat{H}(g), \eta_a(g)] = 0$. Note that since

$$[\eta_a(g) + \ell_a(q, \partial_q, j), \eta_b(g) + \ell_b(q, \partial_q, j)] = \epsilon_{abc}(\eta_c(g) + \ell_c(q, \partial_q, j)),$$

then the system (21) is consistent. Integration of the system of Equation (21) gives

$$\Psi(q, j; g) = (\cos \theta + i \cos(q + \phi) \sin \theta)^j \Phi_j \left(2 \arctan \left[e^{i\theta} \cot \left(\frac{q+\phi}{2} \right) \right] \right). \quad (22)$$

Substituting (22) into the Equation (20), we obtain the reduced equation

$$H(-i\ell(q', \partial_{q'}, j))\Phi_j(q') = E_j\Phi_j(q'). \quad (23)$$

The Equation (23) describes a quantum asymmetric top in λ -representation. The Hamiltonian $H(-i\ell(q', \partial_{q'}, j)) = H(\hat{f})$ can be considered as the result of qp -quantization of the classic top on the coadjoint orbit (19).

Taking into account the explicit form of the λ -irrep operators (16), we obtain an ordinary differential equation for the function $\Phi_j(q')$:

$$\left\{ (A \sin^2 q' + B \cos^2 q' - C) \frac{d^2}{dq'^2} + (\sin q' \cos q')(1 - 2j)(A - B) \frac{d}{dq'} + (A \cos^2 q' + B \sin^2 q')j^2 + j(A \sin^2 q' + B \cos^2 q') - E_j \right\} \Phi_j(q') = 0. \quad (24)$$

What is remarkable is the fact that by replacing

$$\begin{aligned} \Phi_j(q') &= \left(\frac{2(A - C)(B - C)}{\rho(q') - C} \right)^{j/2} \Lambda_j(\rho(q')), \\ \rho(q') &= \frac{2(A - C)(B - C)}{A + B - 2C - (A - B) \cos 2q'} + C, \end{aligned} \quad (25)$$

we obtain the Lamé equation in algebraic form (11) on the function $\Lambda_j(\rho)$:

$$\left\{ 4\sqrt{P(\rho)} \frac{d}{d\rho} \left(4\sqrt{P(\rho)} \frac{d}{d\rho} \right) - j(j + 1)\rho + E_j \right\} \Lambda_j(\rho) = 0.$$

Thus, we arrive at the same Equation (11) as in the case of separation of variables in the elliptic coordinate system but on a function of the complex variable $\rho = \rho(q')$. As will be shown below, in contrast to the set of solutions $\psi_j(\rho_1, \rho_2)$, the set of solutions $\Psi(q, j; g)$ forms a complete set.

Solutions that respond to Lamé polynomials (12) will be labeled as follows:

$$\Phi_j^{(N)}(q') = \left(\frac{2(A - C)(B - C)}{\rho - C} \right)^{j/2} \Lambda_j^{(N)}(\rho), \quad \rho = \rho(q'), \quad N = 1, 2, 3, 4.$$

Let us write it explicitly:

$$\begin{aligned}
 \Phi_j^{(1)}(q') &= (2(A-B)(B-C))^{j/2} \\
 &\quad \times \sum_{k=0}^{\infty} \frac{a_k}{(B-C)^k} (\cos q')^{j-2k} (a - \cos^2 q')^k, \\
 \Phi_j^{(2)}(q') &= i(2(A-B)(B-C))^{j/2} \sqrt{\frac{A-C}{B-C}} \sin q' \\
 &\quad \times \sum_{k=0}^{\infty} \frac{b_k}{(B-C)^k} (\cos q')^{j-2k-1} (a - \cos^2 q')^k, \\
 \Phi_j^{(3)}(q') &= (2(A-B)(B-C))^{j/2} \sqrt{\frac{A-C}{A-B}} \\
 &\quad \times \sum_{k=0}^{\infty} \frac{c_k}{(B-C)^k} (\cos q')^{j-2k-1} (a - \cos^2 q')^k, \\
 \Phi_j^{(4)}(q') &= i(2(A-B)(B-C))^{(j-1)/2} \sqrt{A-C} \sin q' \\
 &\quad \times \sum_{k=0}^{\infty} \frac{d_k}{(B-C)^k} (\cos q')^{j-2k-2} (a - \cos^2 q')^k,
 \end{aligned}$$

where $a = (A-C)/(A-B)$.

Functions $\Phi_j^{(N)}(q')$ belong to the function space \mathcal{F}^j only when they contain positive powers in $\cos q'$. For this, it is necessary and sufficient that

$$a_{1+j/2} = b_{j/2} = c_{j/2} = d_{j/2} = 0, \quad (26)$$

for even j and

$$a_{(j+1)/2} = b_{(j+1)/2} = c_{(j+1)/2} = d_{(j-1)/2} = 0, \quad (27)$$

for odd values of j . Note that the conditions (26) and (27) coincide with the conditions (13), and they determine the known spectrum $E_{j,s}$ of the quantum asymmetric top.

The coefficients a_0 , b_0 , c_0 and d_0 are defined from the normalization condition for eigenfunctions

$$\Phi_{j,s}(q') = \left(\frac{2(A-C)(B-C)}{\rho-C} \right)^{j/2} \Lambda_{j,s}(\rho)$$

of the operator $H(-i\ell(q', \partial_{q'}, j))$, corresponding to the eigenvalues $E_{j,s}$:

$$(\Phi_{j,s}, \Phi_{j,s'})_Q = (2j+1)\delta_{ss'}. \quad (28)$$

Then, the wave functions

$$\begin{aligned}
 \Psi_{q,j,s}(g) &= \langle g | q, j, s \rangle = (\cos \theta + i \cos(q + \phi) \sin \theta)^j \\
 &\quad \times \Phi_{j,s} \left(\psi + 2 \arctan \left[e^{i\theta} \cot \left(\frac{q+\phi}{2} \right) \right] \right)
 \end{aligned} \quad (29)$$

corresponding to the eigenvalues $E_{j,s}$ satisfy the Equation (20) and the normalization condition

$$\langle q, j, s | q, j, s \rangle = \frac{1}{8\pi^2} \int_0^{2\pi} d\psi \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi |\Psi_{q,j,s}(g)|^2 = \delta_j(q, \bar{q}).$$

We give expressions for the wave functions (29) and the eigenvalues $E_{j,s}$ for the lowest values of the quantum number j . For $j = 0$, we have $E_{0,1} = 0$ and $\Psi_{q,0,1} = 1$. For $j = 1$, we have

$$E_{1,1} = A + C, \quad E_{1,2} = A + B, \quad E_{1,3} = B + C$$

and wave functions

$$\begin{aligned}\Psi_{q,1,1}(g) &= \sqrt{3} \left\{ \frac{1}{2} [\cos(q - \theta + \phi) + \cos(q + \theta + \phi) + 2i \sin \theta] \cos \psi \right. \\ &\quad \left. - \sin(q + \phi) \sin \psi \right\}, \\ \Psi_{q,1,2}(g) &= \sqrt{3} (\cos \theta + i \cos(q + \phi) \sin \theta), \\ \Psi_{q,1,3}(g) &= \sqrt{3} (\cos \psi \sin(q + \phi) + [\cos \theta \cos(q + \phi) + i \sin \theta] \sin \psi),\end{aligned}$$

respectively.

Thus, we have obtained a set of solutions (29), which is parameterized by a set of parameters $\{q, j, s\}$, where j is the quantum number corresponding to the eigenvalue operator \hat{L}^2 , and $q \in Q$ is a complex number that is not an eigenvalue of any integral of motion.

4. Wigner D -Function and λ -Representation of $\mathfrak{so}(3)$ Group

Note that the solution (22) can be represented in the integral form

$$\Psi(q; g) = T^j(g) \Phi(q) = \int_Q \mathcal{D}_{qq'}^j(g) \Phi(q') d\mu(q'), \quad \Phi(q') \in \mathcal{F}^j, \quad (30)$$

where the kernel

$$\mathcal{D}_{qq'}^j(g) = (\cos \theta + i \cos(q + \phi) \sin \theta)^j \delta_j \left(\psi + 2 \arctan \left[e^{i\theta} \cot \left(\frac{q + \phi}{2} \right) \right], \bar{q}' \right) \quad (31)$$

satisfies the system of equations

$$\begin{aligned}(\eta_a(g) + \ell_a(q, \partial_q, j)) \mathcal{D}_{qq'}^j(g) &= 0, \\ (\xi_a(g) + \overline{\ell_a(q', \partial_{q'}, j)}) \mathcal{D}_{qq'}^j(g) &= 0,\end{aligned} \quad (32)$$

with the initial condition $\mathcal{D}_{qq'}^j(0, 0, 0) = \delta_j(q, \bar{q}')$. Using the Equation (18) for the generalized delta function, we obtain

$$\begin{aligned}\mathcal{D}_{qq'}^j(g) &= \frac{2^j (j!)^2}{(2j)!} \left\{ [\cos(\phi + q) \cos(\bar{q}' - \psi) + 1] \cos \theta \right. \\ &\quad \left. + i [\cos(\phi + q) + \cos(\bar{q}' - \psi)] \sin \theta \right. \\ &\quad \left. + \sin(\phi + q) \sin(\bar{q}' - \psi) \right\}^j.\end{aligned} \quad (33)$$

It is shown in [22] that for a generalized function satisfying the system of Equation (32) on some unimodular Lie group, the relations

$$\mathcal{D}_{qq'}^j(g \cdot g') = \int_Q \mathcal{D}_{qq''}^j(g) \mathcal{D}_{q''q'}^j(g') d\mu_j(q''), \quad \overline{\mathcal{D}_{qq'}^j(g)} = \mathcal{D}_{q'q}^j(g^{-1}). \quad (34)$$

From Equation (34), it is implied that the operators $T^j(g)$ in (30) are the operators of the unitary λ -irrep of the group $SO(3)$ in the space \mathcal{F}^j .

Let us find a connection between the Wigner D -function (3) and the $\mathcal{D}_{qq'}^j(g)$ function. Note that the Wigner D -function can be uniquely defined as a solution to the system of

Equation (2), with the initial condition $D_{mn}^j(0, 0, 0) = \delta_{mn}$. Then, we will look for a solution to the system (2) in the form

$$D_{mn}^j(g) = C_{mn}^j \int_Q \overline{F_m(q)} \Phi_n(q') \mathcal{D}_{qq'}^j(g) d\mu_j(q) d\mu_j(q'). \quad (35)$$

Substituting (35) into (2), by the functions $F_m(q)$ and $\Phi_n(q')$, we obtain

$$-i\ell_3(q, \partial_q, j) F_m(q) = m F_m(q), \quad (36)$$

$$-i\ell_3(q', \partial_{q'}, j) \Phi_n(q') = n \Phi_n(q'). \quad (37)$$

Whence $F_m(q) = e^{imq}$, $\Phi_n(q') = e^{inq'}$. The coefficient C_{mn}^j has the form

$$C_{mn}^j = \sqrt{B_{nj} B_{mj}} \exp\left[\frac{i\pi}{2}(m-n)\right].$$

From (4) and (5) and the relation (35), it follows that the functions $\mathcal{D}_{qq'}^j(g)$ are complete and orthogonal:

$$\begin{aligned} \int_G \overline{\mathcal{D}_{qq'}^j(g)} \mathcal{D}_{\tilde{q}\tilde{q}'}^j(g) d\mu(g) &= \frac{1}{2j+1} \delta_j(q, \tilde{q}) \delta_j(q', \tilde{q}') \delta_{jj'}, \\ \sum_{j=0}^{\infty} (2j+1) \int_{Q \times Q} \overline{\mathcal{D}_{qq'}^j(g)} \mathcal{D}_{\tilde{q}\tilde{q}'}^j(g) d\mu_j(q) d\mu_j(q') &= \delta(g \cdot \tilde{g}^{-1}). \end{aligned} \quad (38)$$

The expression (35) can be written in the form

$$|j, m, n\rangle = \sqrt{B_{nj} B_{mj}} e^{i\pi(m-n)/2} \int_{Q \times Q} e^{inq' - im\bar{q}} d\mu_j(q) d\mu_j(q') |j, q, q'\rangle$$

where $\langle g | j, q, q'\rangle = \mathcal{D}_{qq'}^j(g)$. Here is an expression for the expansion of the states $|j, q, q'\rangle$ in terms of Wigner D -functions $|j, m, n\rangle$:

$$|j, q, q'\rangle = \sum_{n=-j}^j \sum_{m=-j}^j \sqrt{B_{nj} B_{mj}} e^{-inq' + im\bar{q} - i\frac{\pi}{2}(m-n)} |j, m, n\rangle. \quad (39)$$

Since the operator $H(-i\ell(q', \partial_{q'}, j))$ is Hermitian in the space \mathcal{F}^j with respect to the inner product (17), then the set of eigenfunctions $\Psi_{q,j,s}(g)$ is complete:

$$\sum_{s=-j}^j \frac{\overline{\Phi_{j,s}(q')} \Phi_{j,s}(q')}{2j+1} = \delta_j(q, \bar{q}'), \quad (40)$$

where the sum over s means the sum over the spectrum of the asymmetric top. From (40) and (38) follows the completeness of the set (29),

$$\begin{aligned} |q, j, s\rangle &= \int_Q d\mu_j(q') \Phi_{j,s}(q') |j, q, q'\rangle, \quad \Psi_{q,j,s}(g) = \langle g | q, j, s\rangle, \\ \sum_{j=0}^{\infty} \sum_{s=-j}^j \int_Q d\mu_j(q) |q, j, s\rangle \langle q, j, s| &= 1. \end{aligned}$$

5. Concluding Remarks

In this article, using the noncommutative integration method, we find the complete system of solutions to the Schrodinger Equation (6) for an asymmetric top. It is shown that the noncommutative reduction of the Schrodinger equation reduces it to the Lamé Equation (11), which arises when separating variables in an elliptic coordinate system for the states $|j, 0\rangle$. In this approach, the spectrum of the asymmetric top arises from the requirement that the solution of the reduced Equation (24) belong to the space \mathcal{F}^j , which is

invariant under the irreducible λ -irrep of the group $SO(3)$. In this case, the set of solutions is expressed by an explicit formula (29), in contrast to the solution in the form of a series (7). It is shown that the complete set of solutions is parametrized by the quantum number q , which takes complex values from the set Q , which has the Lagrangian submanifold to the coadjoint orbit of the $SO(3)$ group.

We also obtained a connection (35) between the kernels λ -irrep and the Wigner D -function, which allowed us to show the completeness of the set (29).

Note that the constructed solutions are not coherent [31–34] since they do not minimize the uncertainty relation $(\Delta K)^2 \geq j$. Since they are in states that correspond to the basis $|q, j, s\rangle$, we have

$$\begin{aligned} (\Delta K)^2 &= j(j+1)\delta_j(q, \bar{q}) \\ &= \frac{2^j(j!)^2}{(2j)!} j(j+1) (\cosh 2\operatorname{Im} q)^j \\ &\geq \frac{4^j(j!)^2}{(2j)!} j(j+1) \geq j^2 \log 4 > j, \quad j > 0. \end{aligned}$$

Therefore, the states $|q, j, s\rangle$ differ significantly from the coherent states of the quantum asymmetric top [35].

By a direct check, one can verify that the set of states

$$\begin{aligned} |j, m, s\rangle &= \sqrt{B_{mj}} \int_Q d\mu_j(q) e^{-im\bar{q}} |q, j, s\rangle \\ &= \sqrt{B_{mj}} \int_{Q \times Q} d\mu_j(q) d\mu_j(q') e^{-im\bar{q}} \Phi_{j,s}(q') |j, q, q'\rangle \end{aligned} \quad (41)$$

are eigenstates for the complete set of operators $\{\hat{H}, \hat{L}^2, \hat{J}_3\}$ and satisfies Equation (6) for $|j, m\rangle = |j, m, s\rangle$. Thus, the states of an asymmetric top with a given value of j and m are determined by the expression (41).

Note that since the rotational energy and rotational terms of a large number of polyatomic molecules are described by quantum asymmetric tops, the new solutions obtained in this work can be used in rotational spectroscopy of molecules. The sets of solutions (29) and (41) can be useful for studying the static mixmaster cosmological model (see Refs. [16–18,36,37]).

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Appendix A. Vector Fields on the Group $SO(3)$

In the Lie algebra $\mathfrak{so}(3)$ of the rotation group $SO(3)$, we introduce some basis $\{e_1, e_2, e_3\}$, with respect to the commutation relations of the algebra that have the form $[e_a, e_b] = C_{ab}^c e_c$, where the structure constant $C_{ab}^c = \epsilon_{abc}$ is the completely antisymmetric tensor, with

$\epsilon_{123} = 1$, $[\cdot, \cdot]$ denoting the Lie brackets; $a, b, c = 1, \dots, 3$. The adjoint representation matrices $(ad_a)_b^c = [e_a, e_b]^c$ have the form

$$ad_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad ad_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad ad_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The group element of the $SO(3)$ will be parametrized using the Euler angles ϕ , θ and ψ :

$$g(\phi, \theta, \psi) = g_z(\phi)g_x(\theta)g_z(\psi) \in SO(3), \quad \phi, \psi \in [0; 2\pi), \quad \theta \in [0; \pi),$$

where $g_x(t)$, $g_y(t)$ and $g_z(t)$ are rotation matrices by the angle t about the axes Ox , Oy and Oz , respectively:

$$\begin{aligned} g_x(t) &= e^{tad_1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos t & -\sin t \\ 0 & \sin t & \cos t \end{pmatrix}, \\ g_y(t) &= e^{tad_2} = \begin{pmatrix} \cos t & 0 & \sin t \\ 0 & 1 & 0 \\ -\sin t & 0 & \cos t \end{pmatrix}, \\ g_z(t) &= e^{tad_3} = \begin{pmatrix} \cos t & -\sin t & 0 \\ \sin t & \cos t & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \quad (A1)$$

To find generators of an arbitrary irrep of $SO(3)$, one has to examine representations in the space of functions $f = f(\phi, \theta, \psi)$ on the group. The left regular representation $T^L(g)$ acts in the space of functions $f(g)$, $g = g(\phi, \theta, \psi) \in SO(3)$ on the group as follows [38]:

$$T^L(g')f(g) = f(g'^{-1} \cdot g), \quad g' \in SO(3),$$

whereas the right regular representation $T^R(g)$ acts in the same space as follows:

$$T^R(g')f(g) = f(g \cdot g'), \quad g' \in SO(3).$$

The decomposition of the left (and right) regular representation contains any irrep of the group.

For generators that correspond to the one-parameter subgroup $\omega(t)$ in the left $T^L(g)$ and right $T^R(g)$ regular representations, we obtain, respectively:

$$\xi_{\omega(t)}f(g) = \left. \frac{d}{dt} T^R(\omega(t))f(g) \right|_{t=0}, \quad \eta_{\omega(t)}f(g) = \left. \frac{d}{dt} T^L(\omega(t))f(g) \right|_{t=0}.$$

Vector fields $\xi_{\omega(t)}$ are called left-invariant vector fields, and $\eta_{\omega(t)}$ are called right-invariant vector fields, corresponding to the subgroup $\omega(t)$. Let us choose one-parameter subgroups as (A1). The straightforward calculations yield the following expressions for generators [35]:

$$\begin{aligned} \xi_1 &= \xi_{g_x(t)} = \frac{\sin \psi}{\sin \theta} \frac{\partial}{\partial \phi} + \cos \psi \frac{\partial}{\partial \theta} - \cot \theta \sin \psi \frac{\partial}{\partial \psi}, \\ \xi_2 &= \xi_{g_y(t)} = \frac{\cos \psi}{\sin \theta} \frac{\partial}{\partial \phi} - \sin \psi \frac{\partial}{\partial \theta} - \cot \theta \cos \psi \frac{\partial}{\partial \psi}, \\ \xi_3 &= \xi_{g_z(t)} = \frac{\partial}{\partial \psi} \end{aligned} \quad (A2)$$

and

$$\begin{aligned}\eta_1 &= \eta_{g_x(t)} = \cot \theta \sin \phi \frac{\partial}{\partial \phi} - \cos \phi \frac{\partial}{\partial \theta} - \frac{\sin \phi}{\sin \theta} \frac{\partial}{\partial \psi}, \\ \eta_2 &= \eta_{g_y(t)} = -\cot \theta \cos \phi \frac{\partial}{\partial \phi} - \sin \phi \frac{\partial}{\partial \theta} + \frac{\cos \phi}{\sin \theta} \frac{\partial}{\partial \psi}, \\ \eta_3 &= \eta_{g_z(t)} = -\frac{\partial}{\partial \phi}.\end{aligned}\tag{A3}$$

The following standard commutation relations hold:

$$[\xi_a, \xi_b] = \epsilon_{abc} \xi_c, \quad [\eta_a, \eta_b] = \epsilon_{abc} \eta_c, \quad [\xi_a, \eta_b] = 0.$$

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