THE WAVE FUNCTIONS OF AN ASYMMETRIC TOP

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The solution of the quantum equation of motion of an asymmetric top in a rotating coordinate system is constructed. For the solution, use is made of the fact that the Laplace equation on a sphere admits separation of variables in two coordinate systems, namely in polar and elliptical coordinates.

THE QUANTUM-MECHANICAL PROBLEM OF TOPS

It is well-known that the classical problem of free motion of a rigid body has two constants of the motion, representing the laws of conservation of angular momentum and energy[1,2]:

$$M_1^2+M_2^2+M_3^2=M^2,\quad \frac{M_1^2}{I_1}+\frac{M_2^2}{I_2}+\frac{M_3^2}{I_3}=2\mathscr{E}, \tag{1}$$

where M_1, M_2, M_3 are the components of the angular vector $\mathbf{M}$, $\mathscr{E}$ is the rotational energy, and $I_1 \le I_2 \le I_3$ are the principal moments of inertia of the body. A rigid body is called an asymmetric top if $I_1 \neq I_2 \neq I_3$, it is called a symmetric top if $I_1 = I_2 \neq I_3$ (or $I_1 \neq I_2 = I_3$), and it is called a spherical top if $I_1 = I_2 = I_3$.

In treating the rotations of a rigid body according to quantum mechanics the classical components of the angular momentum in Eq. (1) are usually replaced by the appropriate quantum-mechanical operators. This transforms the system (1) into the system of operator equations

$$M^2/\hbar^2 = L_1^2+\hat{L}_2^2+\hat{L}_3^2,\quad 2\mathscr{E}/\hbar^2 = a\hat{L}_1^2+b\hat{L}_2^2+c\hat{L}_3^2, \tag{2}$$

where $a = 1/I_1$, $b = 1/I_2$, $c = 1/I_3$, $a \ge b \ge c$ and $\hat{L}_1$, $\hat{L}_2$, $\hat{L}_3$ are the components of the angular momentum operator, satisfying the commutation relations

$$[\hat{L}_i,\hat{L}_k] = -ie_{ikl}L_l. \tag{3}$$

Thus, the quantum-mechanical solution of the problem of rotations of a free top reduces to the determination of the eigenfunctions and eigenvalues of the system of operator equations (2). The constants of the motion do not depend on the selection of the reference frame, and for their computation one can use a moving coordinate system which is rigidly tied to the rotating body. It is convenient to direct the axes of this reference frame along the principal axes of inertia of the body.

In the case of a spherical top the two quadratic forms coincide, and with respect to a fixed coordinate system the problem exhibits the symmetry of three-dimensional rotations, i.e., the group O(3). For a symmetric top, two different quadratic forms are conserved. In a fixed coordinate system the wave functions are expressed in terms of the Wigner D-functions, which depend on the Euler angles. These functions are known to form a basis for the representations of the group O(4). It would seem that the asymmetric top should also admit a solution in closed form, since to the symmetric top corresponds a degenerate quadratic form. We show that this is indeed so in a moving coordinate system[1)]. Formally the solution of this problem is related to the fact that the variables in the Laplace operator on the sphere can be separated not only in polar coordinates, but also in elliptic coordinates. Therefore two complete sets of observables exist on the sphere: the first corresponds to the integrals of motion of the symmetric top, whereas the other corresponds to those of the asymmetric top.

In a two-dimensional space of constant positive curvature (i.e., on the sphere $\xi^2+\eta^2+\zeta^2=1$) there exist two coordinate systems which allow for separation of the variables: the polar and the elliptic coordinate systems[4]. It can be shown[5] that in addition to the Laplacian

$$\hat{L} = \hat{L}_1^2+\hat{L}_2^2+\hat{L}_3^2 = -\Delta, \tag{4}$$

in the polar coordinate system

$$\xi=\sin\theta\cos\varphi,\quad \eta=\sin\theta\sin\varphi,\quad \zeta=\cos\theta \tag{5}$$

the second diagonal operator is

$$\hat{L}_S = \hat{L}_3^2, \tag{6}$$

whereas in the elliptic coordinate system[2)]

$$\xi^2=\frac{(a-\rho_1)(a-\rho_2)}{(a-b)(a-c)},\quad \eta^2=\frac{(b-\rho_1)(b-\rho_2)}{(b-a)(b-c)},$$
$$\zeta^2=\frac{(c-\rho_1)(c-\rho_2)}{(c-a)(c-b)} \tag{7}$$
$$(a>\rho_1>b>\rho_2>c)$$

the second diagonal operator is

$$\hat{L}_E = a\hat{L}_1^2+b\hat{L}_2^2+c\hat{L}_3^2. \tag{8}$$

It is obvious that the operator pairs (4), (6) and (4), (8) are the quantum-mechanical operators of the problem of motion of a symmetric and asymmetric top, respectively, in a fixed coordinate system. In order to determine the eigenfunctions and eigenvalues of the pairs (4), (6) and (4), (8) it is necessary to express the

[1)]The wave functions of an asymmetric top in a fixed coordinate system can be obtained by means of a unitary transformation. We shall not dwell upon this here. It should only be mentioned that there exists a beautiful relation between such functions and the wave functions of the three-body problem (a nonrigid top), which has been considered in [3].

[2)]The orthogonal families of lines of a polar coordinate system on the sphere are the family of concentric circumferences (θ = const.) and the pencil of straight lines (ρ_i = const) passing through the pole. For the elliptic coordinates on the sphere the orthogonal lines (ρ_i = const, i = 1, 2) are two families of confocal elipses and convex hyperbolas.

operators $\hat{L}_i$ in terms of the infinitesimal differential operators in the appropriate coordinate systems. It is a priori clear from group-theory considerations that the eigenvalues of the operator (4) are $l(l+1)$, where l is a positive integer or an odd half-integer.

In the polar coordinate system we obtain explicit expressions for the operators $\hat{L}$ and $\hat{L}_S$[6,7]:

$$\hat{L} = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] = l(l+1),$$
$$\hat{L_S} = -\frac{\partial^2}{\partial\varphi^2} = m^2, \quad m = -l, -l+1, \ldots, l-1, l. \tag{9}$$

The eigenfunctions of this system of operators are linear combinations of the well-known spherical functions $Y_{lm}(\theta, \varphi)$:

$$Y_{lm}^{(+)} = \frac{1}{\sqrt{2}}[Y_{lm} + Y_{lm}^*], \quad Y_{lm}^{(-)} = \frac{1}{i\sqrt{2}}[Y_{lm} - Y_{lm}^*], \quad Y_{l0}^{(+)} = Y_{l0}$$
$$Y_{lm}(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}P_l^{|m|}(\cos\theta)e^{im\varphi}. \tag{10}$$

Spherical functions expressed in terms of associated Legendre functions are valid only for integral values of the parameters l and m. In order to obtain expressions for the spherical functions which are valid also for half-integral values of l and m, we transform the Legendre equation, that is satisfied by the associated Legendre functions into a hypergeometric equation, which in turn we subject to a quadratic transformation of the form[8]

$${}_2F_1\left(a, b; \frac{a+b+1}{2}; z\right) = {}_2F_1\left(\frac{a}{2}, \frac{b}{2}; \frac{a+b+1}{2}; 4z(1-z)\right). \tag{11}$$

As a result we obtain

$$P_l^{|m|}(\cos\theta) \approx \sin^{|m|}\theta\, {}_2F_1\left(-l+|m|, l+|m|+1; 1+|m|; \sin^2\frac{\theta}{2}\right)$$
$$= \sin^{|m|}\theta\, {}_2F_1\left(-\frac{l-|m|}{2}, \frac{l+|m|+1}{2}; 1+|m|; \sin^2\theta\right)$$
$$= \cos\theta\sin^{|m|}\theta\, {}_2F_1\left(-\frac{l-|m|-1}{2}, \frac{l+|m|}{2}+1; 1+|m|; \sin^2\theta\right). \tag{12}$$

The hypergeometric functions in (12) can be expressed in terms of Jacobi polynomials $P_n^{(\alpha,\beta)}(\cos 2\theta)$:

$$2^n n! P_n^{(\alpha,\beta)}(x) = (-1)^n(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d^n}{dx^n}[(1-x)^{\alpha+n}(1+x)^{\beta+n}]. \tag{13}$$

Thus we obtained for the normalized spherical functions the following expressions, valid both for integral and half-integral values of l and m:

if $(l - |m|)$ is even, then

$$Y_{lm}(\theta,\varphi) = \left[\frac{2l+1}{4\pi}\Gamma\left(\frac{l-|m|}{2}+1\right)\Gamma\left(\frac{l+|m|+1}{2}\right)\right.$$
$$\left.\times\Gamma^{-1}\left(\frac{l+|m|}{2}+1\right)\Gamma^{-1}\left(\frac{l-|m|+1}{2}\right)\right]^{1/2}\sin^{|m|}\theta P_{(l-|m|)/2}^{(|m|,-1/2)}(\cos 2\theta)e^{im\varphi} \tag{14}$$

if $(l - |m|)$ is odd, then

$$Y_{lm}(\theta,\varphi) = \left[\frac{2l+1}{4\pi}\Gamma\left(\frac{l+|m|}{2}+1\right)\Gamma\left(\frac{l-|m|+1}{2}\right)\right.$$
$$\left.\times\Gamma^{-1}\left(\frac{l-|m|}{2}+1\right)\Gamma^{-1}\left(\frac{l+|m|+1}{2}\right)\right]^{1/2}$$
$$\times\cos\theta\sin^{|m|}\theta P_{(l-|m|-1)/2}^{(|m|,1/2)}(\cos 2\theta)e^{im\varphi}. \tag{15}$$

We construct the explicit expressions for the operators $\hat{L}_i$ in the elliptic coordinate system:

$$\hat{L}_1 = \frac{2i}{\rho_1-\rho_2}\left[\frac{(\rho_1-b)(\rho_1-c)(\rho_2-b)(\rho_2-c)}{(a-b)(c-a)}\right]^{1/2}\times\left[(\rho_1-a)\frac{\partial}{\partial\rho_1}-(\rho_2-a)\frac{\partial}{\partial\rho_2}\right],$$
$$\hat{L}_2 = \frac{2i}{\rho_1-\rho_2}\left[\frac{(\rho_1-c)(\rho_1-a)(\rho_2-c)(\rho_2-a)}{(b-c)(a-b)}\right]^{1/2}\times\left[(\rho_1-b)\frac{\partial}{\partial\rho_1}-(\rho_2-b)\frac{\partial}{\partial\rho_2}\right], \tag{16}$$
$$\hat{L}_3 = \frac{2i}{\rho_1-\rho_2}\left[\frac{(\rho_1-a)(\rho_1-b)(\rho_2-a)(\rho_2-b)}{(c-a)(b-c)}\right]^{1/2}\times\left[(\rho_1-c)\frac{\partial}{\partial\rho_1}-(\rho_2-c)\frac{\partial}{\partial\rho_2}\right].$$

From this we find that the operators $\hat{L}$ and $\hat{L}_E$ have the form

$$\hat{L} = -\frac{4}{\rho_1-\rho_2}\left[\sqrt{-P(\rho_1)}\frac{\partial}{\partial\rho_1}\left(\sqrt{-P(\rho_1)}\frac{\partial}{\partial\rho_1}\right) + \sqrt{P(\rho_2)}\frac{\partial}{\partial\rho_2}\left(\sqrt{P(\rho_2)}\frac{\partial}{\partial\rho_2}\right)\right] = l(l+1),$$
$$\hat{L}_E = -\frac{4}{\rho_1-\rho_2}\left[\rho_2\sqrt{-P(\rho_1)}\frac{\partial}{\partial\rho_1}\left(\sqrt{-P(\rho_1)}\frac{\partial}{\partial\rho_1}\right) + \rho_1\sqrt{P(\rho_2)}\frac{\partial}{\partial\rho_2}\left(\sqrt{P(\rho_2)}\frac{\partial}{\partial\rho_2}\right)\right] = \varepsilon, \tag{17}$$

where $P(\rho)$ denotes the polynomial $P(\rho) = (\rho - a)(\rho - b)(\rho - c)$.

SOLUTION OF THE SYSTEM OF EQUATIONS (SPHERO-CONICAL WAVE FUNCTIONS)

We denote the $(2l + 1)$ eigenfunctions of the system of operator equations (17), corresponding to $2l + 1$ distinct eigenvalues $\epsilon_l^{(S)}$ ($s = 1, 2, \ldots, 2l + 1$, $\epsilon_l^{(1)} < \epsilon_l^{(2)} \ldots < \epsilon_l^{(2l+1)}$) by $E_l^{(S)}(\rho_1, \rho_2)$. We shall designate these eigenfunctions as the wave functions of the asymmetric top (they are also known as sphero-conical functions).

If one assumes that $E(\rho_1, \rho_2) = \Lambda_1(\rho_1)\Lambda_2(\rho_2)$, then from (17) find that each of the functions $\Lambda_1(\rho_1)$ and $\Lambda_2(\rho_2)$ satisfies the differential equation

$$\left[4\sqrt{P(\rho)}\frac{d}{d\rho}\left(\sqrt{P(\rho)}\frac{d}{d\rho}\right) - l(l+1)\rho + \varepsilon\right]\Lambda(\rho) = 0. \tag{18}$$

Equation (18) is the Lamé differential equation in algebraic form[8,9]. It follows from the theory of the Lamé differential equation that for integer values of l its solution consists of $2l + 1$ linearly independent and mutually orthogonal functions, corresponding to $2l + 1$ different values of $\epsilon_1^{(S)}$—the so-called Lamé polynomials[3)]. The solutions of Eq. (18) are represented in the form of the power series

$$\sum_{r=0}^{\infty} A_r(\rho-b)^{l/2-r}, \quad \sqrt{\rho-a}\sum_{r=0}^{\infty} B_r(\rho-b)^{l/2-1/2-r},$$
$$\sqrt{\rho-c}\sum_{r=0}^{\infty} C_r(\rho-b)^{l/2-1/2-r}, \quad \sqrt{(\rho-a)(\rho-c)}\sum_{r=0}^{\infty} D_r(\rho-b)^{l/2-1-r}. \tag{19}$$

Substituting the series (19) into the equation (18) we

[3)]The solutions of Lamé's equation exist also for half-integer values of l. In this case the Lamé equation goes over into a Heun equation [8,9]. According to the Kramers theorem the eigenvalues turn out to be doubly degenerate, since the energy operator of the asymmetric top is equivalent to the operator of quadrupole interaction.

obtain for the coefficients A_r, B_r, C_r, D_r the following recursion relations

$$\begin{aligned}
2r(2l+1-2r)A_r &= [\varepsilon - bl(l+1) + (2b-a-c)(l+2-2r)^2]A_{r-1} \\
&\quad - (a-b)(b-c)(l+4-2r)(l+3-2r)A_{r-2}, \\
2r(2l+1-2r)B_r &= [\varepsilon - bl(l+1) + (b-c)(2l+3-4r) \\
&\quad + (2b-a-c)(l+1-2r)^2]B_{r-1} - (a-b)(b-c)(l+2 \\
&\quad - 2r)(l+3-2r)B_{r-2}, \\
2r(2l+1-2r)C_r &= [\varepsilon - bl(l+1) - (a-b)(2l+3-4r) \\
&\quad + (2b-a-c)(l+1-2r)^2]C_{r-1} - (a-b)(b-c)(l+2 \\
&\quad - 2r)(l+3-2r)C_{r-2}, \\
2r(2l+1-2r)D_r &= [\varepsilon - bl(l+1) + (2b-a-c)(l+1-2r)^2]D_{r-1} \\
&\quad - (a-b)(b-c)(l+2-2r)(l+1-2r)D_{r-2}.
\end{aligned} \tag{20}$$

In Eqs. (20) $A_n = B_n = C_n = D_n = 0$ for $n < 0$. The eigenvalues $\epsilon_l^{(S)}$ are obtained from the condition that the series (20) terminate. In the case of even l we set

$$A_{l/2+1} = B_{l/2} = C_{l/2} = D_{l/2} = 0, \tag{21}$$

and obtain for one equation of degree $l/2+1$ and three equations of degree $l/2$ the solutions of which are $2l+1$ distinct eigenvalues $\epsilon_l^{(S)}$. Similarly, for odd l, setting

$$A_{l/2+1/2} = B_{l/2+1/2} = C_{l/2+1/2} = D_{l/2-1/2} = 0, \tag{22}$$

we obtain for ϵ three equations of degree $l/2 + 1/2$ and one equation of degree $l/2 + 1/2$, which have as solutions again $2l+1$ distinct values of $\epsilon_l^{(S)}$. The coefficients A_0, B_0, C_0, D_0 are determined from the normalization condition of the sphero-conical wave functions

$$\frac{1}{4}\int_b^a\int_c^b [E_l^{(s)}(\rho_1,\rho_2)]^2 \frac{(\rho_1-\rho_2)\,d\rho_1\,d\rho_2}{\sqrt{-P(\rho_1)}\sqrt{P(\rho_2)}} = 1. \tag{23}$$

The energy operator of the asymmetric top, (8), together with the commutation relations (3) is invariant with respect to the simultaneous sign-change of any two of the operators $\hat{L}_1$, $\hat{L}_2$, $\hat{L}_3$, a symmetry which formally coincides with the group D_2. According to this group one can classify the wave functions of the asymmetric top into four classes, transforming according to the irreducible representations A, B_1, B_2, B_3 of this group[6]. In this connection it should be noted that the following relations hold for the eigenvalues $\epsilon_l^{(S)}$, relations which are easily derived from Eqs. (20).

For even l

$$\begin{aligned}
\sum_{s\in A} \varepsilon_l^{(s)} &= {}^1/_6 l(l+1)(l+2)(a+b+c), \\
\sum_{s\in B_1,B_2,B_3} \varepsilon_l^{(s)} &= {}^1/_2 l^2(l+1)(a+b+c)
\end{aligned} \tag{24}$$

and for odd l

$$\sum_{s\in A}\varepsilon_l^{(s)} = {}^1/_6 l(l^2-1)(a+b+c), \qquad \sum_{s\in B_1,B_2,B_3} \varepsilon_l^{(s)} = {}^1/_2 l(l+1)^2(a+b+c). \tag{25}$$

From (24) and (25) also follows the general relation

$$\sum_{s=1}^{2l+1}\varepsilon_l^{(s)} = {}^1/_3 l(l+1)(2l+1)(a+b+c). \tag{26}$$

It is not hard to derive the eigenvalues and the sphero-conical wave functions for the lowest values of the quantum number l. For $l = 0$ we have $\epsilon_0^{(1)} = 0$ and a single sphero-conical function $E_0^{(1)}(\rho_1,\rho_2) = (4\pi)^{1/2}$, belonging to the representation A of the group D_2. For $l = 1$ we have

$$\varepsilon_1^{(1)} = b+c, \quad \varepsilon_1^{(2)} = a+c, \quad \varepsilon_1^{(3)} = a+b \tag{27}$$

and the sphero-conical functions are

$$E_1^{(1)}(\rho_1,\rho_2) = \sqrt{3/4\pi}\,\xi, \quad E_1^{(2)}(\rho_1,\rho_2) = \sqrt{3/4\pi}\,\eta, \quad E_1^{(3)}(\rho_1,\rho_2) = \sqrt{3/4\pi}\,\zeta, \tag{28}$$

belonging respectively to the representations B_3, B_2, B_1 (ξ, η, ζ are defined by (7). For the case $l = 2$ we have two eigenfunctions

$$\begin{aligned}
\varepsilon_2^{(1)} &= 2(a+b+c) - 2\sqrt{(a-c)^2-(a-b)(b-c)}, \\
\varepsilon_2^{(5)} &= 2(a+b+c) + 2\sqrt{(a-c)^2-(a-b)(b-c)},
\end{aligned} \tag{29}$$

to which correspond the sphero-conical functions $E_2^{(1)}(\rho_1,\rho_2)$, $E_2^{(5)}(\rho_1,\rho_2)$ belonging to the representation A. The normalized sphero-conical function $E_2^{(1)}(\rho_1,\rho_2)$ has the form

$$\begin{aligned}
E_2^{(1)}(\rho_1,\rho_2) &= \sqrt{5/16\pi}\,[3\rho_1-(a+b+c)-\sqrt{(a-c)^2-(a-b)(b-c)}] \\
&\times[3\rho_2-(a+b+c)-\sqrt{(a-c)^2-(a-b)(b-c)}]\{2[(a-c)^2-(a-b)(b-c)]^2 \\
&-(2b-a-c)[2(a-c)^2+(a-b)(b-c)]\sqrt{(a-c)^2-(a-b)(b-c)}\}^{-1/2}.
\end{aligned} \tag{30}$$

The function $E_2^{(5)}(\rho_1,\rho_2)$ differs from $E_2^{(1)}(\rho_1,\rho_2)$ only through the sign of the square root $((a-c)^2 - (a-b)(b-c))^{1/2}$. The eigenvalues

$$\varepsilon_2^{(2)} = a+b+4c, \quad \varepsilon_2^{(3)} = a+4b+c, \quad \varepsilon_2^{(4)} = 4a+b+c \tag{31}$$

correspond to the eigenfunctions

$$\begin{aligned}
E_2^{(2)}(\rho_1,\rho_2) &= \sqrt{15/4\pi}\,\xi\eta, \quad E_2^{(3)}(\rho_1,\rho_2) = \sqrt{15/4\pi}\,\eta\zeta, \\
E_2^{(4)}(\rho_1,\rho_2) &= \sqrt{15/4\pi}\,\zeta\xi,
\end{aligned} \tag{32}$$

belonging to the representations B_1, B_2, B_3.

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