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Wigner representation of rotational motion

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Abstract. Wigner representations of the rotational motion of a rotator or spherical top, as well as symmetrical and arbitrary tops are presented. The unique form of the transformations to these representations is derived using a set of natural requirements. As a particular case of these representations, a Wigner representation of angular momentum orientation is found. Relations between this representation and those of irreducible tensor operators and coherent states are established. For large angular momentum $l \gg 1$, rough equations for the Wigner functions are derived, and it is shown that they are similar to the well known equation for the Wigner function for translational motion.

1. Introduction

Usually, when describing rotational motion in atomic or molecular physics, we use a quantum mechanical approach, which is based primarily on an lm-representation or an irreducible tensor representation. It is well known that the quantum equations for a density matrix in these representations have a complicated form, and thus are difficult to solve. These difficulties become even greater if the quantum system under consideration has large angular momentum ($l \gg 1$), as is typical for molecules and atomic Rydberg states, where $l \approx 10$–100. On the other hand, it is clear that at this limit the classical description is more suitable and the equations for the density matrix should be essentially simplified. However, there is no direct way to get the classical limit of the quantum equations in these representations. A more appropriate way to approach this limit may be found by the use of coherent state representation [1]. In [1] the theory of the coherent states of an ensemble of two-level atoms [2] was generalized to the description of atomic states degenerate with respect to angular momentum projection, and balanced equations for diagonal elements of the density matrix in zeroth order of the parameter $1/l$ were obtained.

In our opinion, the most suitable and straightforward way to approach the classical limit in a quantum equation is the use of the Wigner representation of rotational motion. It is well known, for example, that for translational motion the classical limit can be easily obtained by the power-series expansion of the quantum equation for the Wigner function with respect to $\hbar$. So, one may expect that by expanding in the corresponding equation for the density matrix in the Wigner representation of rotational motion with respect to powers of $1/l$, it is also possible to get a correct classical limit.

Thus, the problem is to construct a transformation which leads to a Wigner representation of rotational motion and to find a quantum equation for the Wigner function. The rotational Wigner function and the associated correspondence between quantum operators and classical-like functions have already been introduced for a rotator with a fixed axis of revolution and one degree of motional freedom [3, 4]. Dynamic equations for this kind of motion have been discussed previously [5].

In a previous work [6] the following Weyl-like transformation was introduced:

$$\rho(\theta,\phi) = \sum_m \mathrm{e}^{\mathrm{i}\phi m} \rho(l_1, M + \tfrac{1}{2}m | l_2, M - \tfrac{1}{2}m) \qquad \cos\theta = \frac{2M}{l_1 + l_2 + 1} \tag{1.1}$$

where $\rho(l_1, m_1|l_2, m_2)$ are the density matrix elements in the lm-representation. Although the Wigner function $\rho(\theta, \phi)$ is a function of the discrete variable θ, by definition, at $l \gg 1$ this variable may be considered as continuous, where angles ϕ and θ stand for the azimuthal and polar angles of momentum orientation, respectively. By transformation (1.1) the quantum equations for $\rho(\theta, \phi)$ with the correct classical limit were obtained [6]. These equations were applied to a number of problems: polarization phenomena in light spreading in a resonance medium of two-level atoms or molecules [6], resonance excitation exchange between particles [7], and quantum beats in molecules [8].

However, transformation (1.1) only leads to the Wigner representation of angular momentum orientation and not the complete rotational motion.

Therefore, in this paper we construct a transformation providing Wigner representations of complete rotational motion of a rotator or spherical top, as well as symmetrical and arbitrary tops. As a particular result of these transformations the Wigner representation of the angular momentum orientation can be obtained.

To find these transformations we adhere to the method proposed for the determination of the Weyl transformation for the Wigner representation of translational motion [9]. In this method, a set of requirements was formulated (Galilean invariance, reality, normalization, marginal distribution, unitary, free-particle limit, etc) which lead to the unique transformation to the Wigner representation of translational motion. Moreover, this set of conditions was proven to be saturated, and one can use the reduced set of requirements to obtain the unique transformation and some of these requirements may be replaced by others. For example, instead of the requirement of Galilean invariance of uniform translation, we use the free-rotator limit to obtain the unique form of the Wigner representation of rotational motion.

Then, in the following sections, the equations for the Wigner functions are derived, the classical limit of the equations discussed, and the matrix elements of operators in these representations found.

2. Wigner representation for a rotator

First, we consider a quantum rotator, assuming that it is the simplest case to find the transformation leading to the Wigner representation of rotational motion. Later, this transformation is extended to the cases of symmetrical and arbitrary tops.

In coordinate representation the density matrix of the rotator as well as of a spherical top is a function of two pairs of angles, which define the orientation of the rotator in the space: $\rho(\psi_1, \beta_1|\psi_2, \beta_2)$. Here ψ and β are the azimuthal and polar angles of the rotator axis orientation (figure 1). Later on, for brevity, instead of angles ψ, β we use the direction $\boldsymbol{s}$ of the rotator axis.

We also use the 'momentum' or lm-representation for the density matrix. The connection between the coordinate and 'momentum' representations is given by the expansion

$$\begin{aligned} \rho(\boldsymbol{s}_1|\boldsymbol{s}_2) &= \sum_{l_1,l_2=0}^{\infty} \sum_{m_1=-l_1}^{l_1} \sum_{m_2=-l_2}^{l_2} Y_{l_1m_1}(\boldsymbol{s}_1) Y^*_{l_2m_2}(\boldsymbol{s}_2) \rho(l_1, m_1|l_2, m_2) \\ Y_{lm}(\boldsymbol{s}) &= Y_{lm}(\beta, \psi). \end{aligned} \tag{2.1}$$

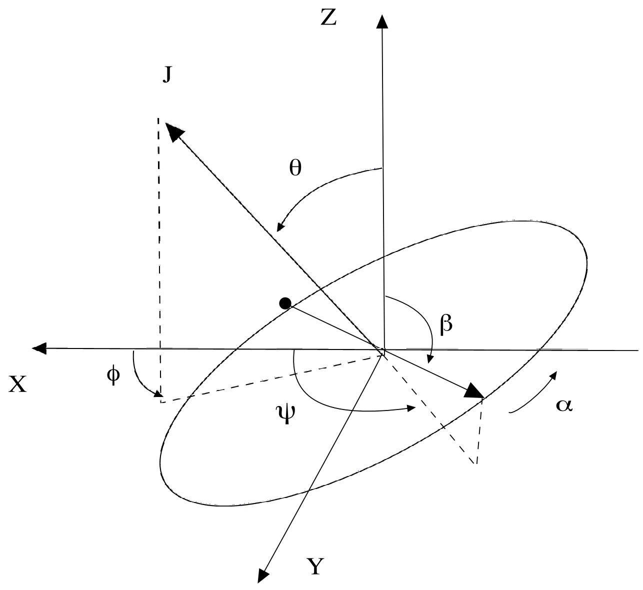

Figure 1. Rotator.

Here $Y_{lm}(\beta, \psi)$ are spherical harmonics. The reciprocal of (2.1) is

$$\rho(l_1, m_1|l_2, m_2) = \int Y^*_{l_1m_1}(s_1)Y_{l_2m_2}(s_2)\rho(s_1|s_2)\,\mathrm{d}s_1\,\mathrm{d}s_2 \qquad \mathrm{d}s = \sin\beta\,\mathrm{d}\beta\,\mathrm{d}\psi. \tag{2.2}$$

The Wigner function of the rotator must depend on the angular momentum of the rotator $\boldsymbol{J}$, and on the orientation of its axis in the space. However, because the rotator axis is orthogonal to angular momentum, it is sufficient to define the angle α indicating the position of the rotator axis in the plane orthogonal to $\boldsymbol{J}$. Thus, we introduce the following Wigner function: $\rho(J, \phi, \theta, \alpha)$. Here J is the value of angular momentum and ϕ and θ are the azimuthal and polar angles of the momentum orientation (figure 1). One may regard ϕ, θ and α as a triplet of Euler angles. Rotating the system of coordinates through these angles in a standard manner, one can bring the z- and x-axes into coincidence with the direction of $\boldsymbol{J}$ and with the rotator axis, respectively.

Let us consider the linear transformation which leads to the Wigner representation

$$\rho(J, \phi, \theta, \alpha) = \int U(J, \phi, \theta, \alpha|s_1; s_2)\rho(s_1|s_2)\,\mathrm{d}s_1\,\mathrm{d}s_2 \tag{2.3}$$

where, at present, the kernel U is an unknown function. Substituting equation (2.1) into (2.3) yields the transformation from the 'momentum' to the Wigner representation

$$\rho(J, \phi, \theta, \alpha) = \sum_{l_1,m_1,l_2,m_2} U(J, \phi, \theta, \alpha|l_1, m_1; l_2, m_2)\rho(l_1, m_1|l_2, m_2). \tag{2.4}$$

The relation between both kernels is given by the equation

$$U(J, \phi, \theta, \alpha|l_1, m_1; l_2, m_2) = \int U(J, \phi, \theta, \alpha|s_1; s_2)Y^*_{l_1m_1}(s_1)Y_{l_2m_2}(s_2)\,\mathrm{d}s_1\,\mathrm{d}s_2.$$

To find an explicit form of the kernel U, we use the same method as Kruger and Poffyn [9] to evaluate the kernel of the Weyl transformation to the Wigner representation for translational motion. Now we formulate a system of requirements; by satisfying these requirements, one can obtain the unique form of the kernel U.

First, because the Wigner function is a real function and the density matrix is a Hermitian matrix, the kernel U should also be Hermitian:

$$U(\boldsymbol{J},\alpha|\boldsymbol{s}_1;\boldsymbol{s}_2)=U^*(\boldsymbol{J},\alpha|\boldsymbol{s}_2;\boldsymbol{s}_1). \tag{2.5}$$

Here, for simplicity, we use the notation $\boldsymbol{J}=(J,\phi,\theta)$.

The kernel U should also be invariant under space reflection. For this transformation the angles are changed as $\alpha\to\alpha+\pi$, $\psi\to\psi+\pi$, $\beta\to\pi-\beta$, whereas the direction of $\boldsymbol{J}$ remains the same. This means that

$$U(\boldsymbol{J},\alpha|\boldsymbol{s}_1;\boldsymbol{s}_2)=U(\boldsymbol{J},\alpha+\pi|-\boldsymbol{s}_1;-\boldsymbol{s}_2). \tag{2.6}$$

Consider the requirement for rotational invariance. It is well known that under infinitesimal rotation of the coordinate system through an angle $\delta\eta$ around an axis $\boldsymbol{b}$, any function A' in a new coordinate system is related to the same function in the initial coordinate system by the equation

$$A'=(1-\mathrm{i}\delta\eta\boldsymbol{b}\hat{\boldsymbol{J}})A \tag{2.7}$$

where $\hat{\boldsymbol{J}}$ is the differential angular operator. If A is a function of the triplet ϕ,θ,α, then the circular components of this operator are [10]

$$\begin{aligned}\hat{J}_0&=-\mathrm{i}\frac{\partial}{\partial\phi}\\ \hat{J}_{\pm1}&=\frac{\mathrm{i}}{\sqrt{2}}\mathrm{e}^{\pm\mathrm{i}\phi}\left[\mp\operatorname{ctg}\theta\frac{\partial}{\partial\phi}+\mathrm{i}\frac{\partial}{\partial\theta}\pm\frac{1}{\sin\theta}\frac{\partial}{\partial\alpha}\right].\end{aligned} \tag{2.8}$$

In the case when A is a function of the angles ψ,β which define the rotator's orientation in the space $\hat{\boldsymbol{J}}\equiv\hat{\boldsymbol{L}}$, $\hat{\boldsymbol{L}}$ is the orbital angular momentum operator with circular components

$$\begin{aligned}\hat{L}_0&=-\mathrm{i}\frac{\partial}{\partial\psi}\\ \hat{L}_{\pm1}&=\frac{\mathrm{i}}{\sqrt{2}}\mathrm{e}^{\pm\mathrm{i}\psi}\left[\mp\operatorname{ctg}\beta\frac{\partial}{\partial\psi}+\mathrm{i}\frac{\partial}{\partial\beta}\right].\end{aligned} \tag{2.9}$$

In the new system of coordinates the Wigner function $\rho'(J,\phi,\theta,\alpha)$ must be related to the density matrix $\rho'(\boldsymbol{s}_1|\boldsymbol{s}_2)$ by the same transformation as (2.3). This requirement gives the equation for the kernel U:

$$(\hat{\boldsymbol{J}}+\hat{\boldsymbol{L}}^{(1)}+\hat{\boldsymbol{L}}^{(2)})U=0. \tag{2.10}$$

Here, the upper index of $\hat{\boldsymbol{L}}$ denotes the angles ψ_1,β_1 or ψ_2,β_2 on which this operator acts.

Further, let us require that the quantum equation for a free rotator

$$\left(\frac{\partial}{\partial t}-\mathrm{i}\frac{1}{2}(\Delta_1-\Delta_2)\right)\rho(\boldsymbol{s}_1|\boldsymbol{s}_2)=0 \tag{2.11}$$

should be transformed into the equation of classical rotation in the Wigner representation

$$\left(\frac{\partial}{\partial t}+J\frac{\partial}{\partial\alpha}\right)\rho(J,\phi,\theta,\alpha)=0. \tag{2.12}$$

Here, we assume that $\hbar=1$ and $I=1$, where I is the rotator inertia moment. In equation (2.11) $\Delta_{1,2}$ are angular Laplacians acting on ψ_1,β_1 and ψ_2,β_2, respectively. This requirement gives the following equation for the kernel U:

$$\left(\frac{1}{2}(\Delta_1-\Delta_2)-\mathrm{i}J\frac{\partial}{\partial\alpha}\right)U(\boldsymbol{J},\alpha|\boldsymbol{s}_1;\boldsymbol{s}_2)=0. \tag{2.13}$$

Finally, we make the requirement that the expected value of any operator $\hat{A}$ is calculated in the Wigner representation as in classical physics:

$$\langle\hat{A}\rangle = \frac{1}{8\pi^2}\int A(\boldsymbol{J},\alpha)\rho(\boldsymbol{J},\alpha)\,\mathrm{d}\boldsymbol{J}\,\mathrm{d}\alpha \qquad \mathrm{d}\boldsymbol{J} = J\,\mathrm{d}J\sin\theta\mathrm{d}\theta\,\phi.$$

This leads to the unitary condition for the kernel U:

$$\frac{1}{8\pi^2}\int U(\boldsymbol{J},\alpha|\boldsymbol{s}_1;\boldsymbol{s}_2)U^*(\boldsymbol{J},\alpha|\boldsymbol{s}_1';\boldsymbol{s}_2')\,\mathrm{d}\boldsymbol{J}\,\mathrm{d}\alpha = \delta(\boldsymbol{s}_1-\boldsymbol{s}_1')\delta(\boldsymbol{s}_2-\boldsymbol{s}_2'). \tag{2.14}$$

It worth noting that in deriving the explicit form for the kernel U, it is more convenient to reformulate the above requirements for the kernel $U(J,\phi,\theta,\alpha|l_1,m_1;l_2,m_2)$. In this way, performing some straightforward algebra, one can find the following unique transformation from the lm-representation to the Wigner representation:

$$\rho(J,\phi,\theta,\alpha) = \sum_{l_1,m_1,l_2,m_2}\sum_{\kappa,q}\frac{\sqrt{2\kappa+1}}{\sqrt{l_1+l_2+1}}\delta_{2J,l_1+l_2+1} \times(-1)^{l_2-m_2}C^{\kappa,q}_{l_1,m_1;l_2,-m_2}D^{\kappa *}_{q,l_1-l_2}(\phi,\theta,\alpha)\rho(l_1,m_1|l_2,m_2) \tag{2.15}$$

where $D^{\kappa}_{q,l_1-l_2}(\phi,\theta,\alpha)$ are Wigner D-functions and $C^{\kappa,q}_{l_1,m_1;l_2,-m_2}$ are Clebsch–Gordan coefficients [10]. Note that according to this transformation, the value J should be discrete: $J=(l_1+l_2+1)/2$.

The reciprocal of (2.15) is

$$\rho(l_1,m_1|l_2,m_2) = \frac{1}{8\pi^2}\sum_{J,\kappa,q}2J\int\frac{\sqrt{2\kappa+1}}{\sqrt{l_1+l_2+1}}\delta_{2J,l_1+l_2+1} \times(-1)^{l_2-m_2}C^{\kappa,q}_{l_1,m_1;l_2,-m_2}D^{\kappa}_{q,l_1-l_2}(\phi,\theta,\alpha)\rho(J,\phi,\theta,\alpha)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}\alpha. \tag{2.16}$$

3. Wigner representation for symmetrical and arbitrary tops

The orientation of an arbitrary and, in particular, a symmetrical top is defined by the triplet of Euler angles ψ,β,ξ. Rotating the coordinate system through these angles in the standard manner [10], one can superimpose the coordinate axes with the main axes of the top. So, the angles ψ,β have the same meaning as for the rotator, i.e. they define the space orientation of one main axis of the top, and the angle ξ defines additional rotation around this main axis. Therefore, the density matrix in the coordinate representation is characterized by six angles: $\rho(\psi_1,\beta_1,\xi_1|\psi_2,\beta_2,\xi_2)$ and in the 'momentum' or lmk-representation by six integer numbers: $\rho(l_1,m_1,k_1|l_2,m_2,k_2)$. The relation between these representations is given by the following expansion in the D-function basis:

$$\rho(\psi_1,\beta_1,\xi_1|\psi_2,\beta_2,\xi_2) = \sum_{l_1m_1k_1,l_2m_2k_2}\sqrt{(2l_1+1)(2l_2+1)} \times D^{l_1 *}_{m_1,k_1}(\psi_1,\beta_1,\xi_1)D^{l_2}_{m_2,k_2}(\psi_2,\beta_2,\xi_2)\rho(l_1m_1k_1|l_2m_2k_2).$$

As we can see, unlike the case of the rotator, here the density matrix elements $\rho(l_1m_1k_1|l_2m_2k_2)$ depend on a new quantum number k—the value of the angular momentum projection on the main axis of the top.

The Wigner representation for a symmetrical top may be constructed in the same way as for a rotator. An additional requirement for deriving the transformation kernel to the Wigner representation is invariance with respect to rotation around the top axis of symmetry. Furthermore, we require that the kinematic term in the quantum equation for the density matrix of a symmetrical top should be transformed to the classical form in the Wigner representation.

Let us define the Wigner function for the symmetrical top as $\rho(J, \theta, \phi, \alpha, K, \gamma)$. Here, the variables J, θ, ϕ, as before, characterize the value and orientation of the angular momentum, angle γ defines the rotation of the top around its axis of symmetry and K is the projection of the moment on this axis. Angle α defines the rotation of the top around $\boldsymbol{J}$.

The invariance with respect to the rotation of the top around its axis of symmetry gives the following additional equation for the kernel U of transformation to the Wigner representation:

$$\left(\frac{\partial}{\partial\gamma} + \frac{\partial}{\partial\xi_1} + \frac{\partial}{\partial\xi_2}\right) U = 0. \tag{3.1}$$

In comparison with the rotator case (see equation (2.11)) the kinematic term in the equation for the symmetrical top's density matrix acquires a new term

$$-\mathrm{i}\epsilon\frac{1}{2}\left(\frac{\partial^2}{\partial\xi_1^2} - \frac{\partial^2}{\partial\xi_2^2}\right)\rho(\psi_1, \beta_1, \xi_1|\psi_2, \beta_2, \xi_2) \tag{3.2}$$

which has to be transformed to the corresponding classical-like term in the Wigner representation

$$\epsilon K\frac{\partial}{\partial\gamma}\rho(J, \phi, \theta, \alpha, K, \gamma). \tag{3.3}$$

Here, the value ϵ indicates the difference between the inertia moment I' and the other two identical inertia moments I: $\epsilon = I/I' - 1$ for a symmetrical top.

The first of these conditions (3.1) for the transformation kernel $U(J, \theta, \phi, \alpha, K, \gamma|l_1, m_1, k_1; l_2, m_2, k_2)$ has the form

$$\left(\frac{\partial}{\partial\gamma} - \mathrm{i}(k_1 - k_2)\right) U = 0.$$

Hence, the kernel U depends on γ as

$$U \sim \mathrm{e}^{\mathrm{i}\gamma(k_1-k_2)}.$$

The second condition gives

$$K = \frac{k_1 + k_2}{2}.$$

Thus K, as well as J, has to be discrete and it may be an integer or half-integer.

So, we can determine the transformation to the Wigner representation from lmk-representation for the symmetrical top:

$$\begin{aligned}\rho(J, \phi, \theta, \alpha, K, \gamma) = &\sum_{l_1m_1k_1,l_2m_2k_2}\sum_{\kappa,q}\sqrt{\frac{2\kappa+1}{l_1+l_2+1}}\delta_{2J,l_1+l_2+1}\delta_{2K,k_1+k_2}\mathrm{e}^{\mathrm{i}\gamma(k_1-k_2)} \\ &\times(-1)^{l_2-m_2}C^{\kappa,q}_{l_1,m_1;l_2,-m_2}D^{\kappa *}_{q,l_1-l_2}(\phi, \theta, \alpha)\rho(l_1, m_1, k_1|l_2, m_2, k_2).\end{aligned} \tag{3.4}$$

It is easy to test that this transformation turns into the corresponding transformation for the rotator equation (2.15) if in (3.4) one puts $k_1 = k_2 = 0$.

The average in the Wigner representation for the symmetrical top is

$$\begin{aligned}\langle A\rangle = &\sum_{l_1m_1k_1,l_2m_2k_2} A(l_1m_1k_1|l_2m_2k_2)\rho(l_2m_2k_2|l_1m_1k_1l_2m_2k_2) = \sum_J J\sum_K\frac{1}{2(2\pi)^3} \\ &\times\int A(J, \phi, \theta, \alpha, K, \gamma)\rho(J, \phi, \theta, \alpha, K, \gamma)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}\alpha\,\mathrm{d}\gamma.\end{aligned} \tag{3.5}$$

The quantum mechanical description of an arbitrary top is the same as for the symmetrical top, so we can suppose that transformation (3.4) is also valid in the case of an arbitrary top.

4. $\phi\theta\alpha$-representation

Let us represent transformation (2.15) as

$$\rho(J,\phi,\theta,\alpha)=\sum_{l_1,l_2}\delta_{2J,l_1+l_2+1}\rho_{l_1,l_2}(\phi,\theta,\alpha) \tag{4.1}$$

where $\rho_{l_1,l_2}(\phi,\theta,\alpha)$ is defined as

$$\rho_{l_1,l_2}(\phi,\theta,\alpha)=\sum_{\kappa,q,m_1,m_2}\frac{\sqrt{2\kappa+1}}{\sqrt{l_1+l_2+1}}(-1)^{l_2-m_2}C^{\kappa,q}_{l_1,m_1;l_2,-m_2}D^{\kappa*}_{q,l_1-l_2}(\phi,\theta,\alpha)\rho(l_1,m_1|l_2,m_2) \tag{4.2}$$

which we call the $\phi\theta\alpha$-function or the $\phi\theta\alpha$-representation for the density matrix. This function depends on the angles θ, ϕ, and α and it also depends on the quantum numbers l_1 and l_2.

Thus, we divide transformation (2.15) into two particular transformations; one of them (4.2) leads to the $\phi\theta\alpha$-representation and the second (4.1) to the complete Wigner representation of rotator motion.

The transformation inverse to (4.2) is

$$\rho(l_1,m_1|l_2,m_2)=\frac{1}{8\pi^2}\int\sum_{\kappa,q}\sqrt{(2\kappa+1)(l_1+l_2+1)}$$
$$\times(-1)^{l_2-m_2}C^{\kappa,q}_{l_1,m_1;l_2,-m_2}D^{\kappa}_{q,l_1-l_2}(\phi,\theta,\alpha)\rho_{l_1,l_2}(\phi,\theta,\alpha)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}\alpha. \tag{4.3}$$

It is easy to find out that the average for the $\phi\theta\alpha$-functions has the form

$$\langle A_{l,l}\rangle=\sum_{l',m,m'}A(lm|l'm')\rho(l'm'|lm)$$
$$=\frac{1}{8\pi^2}\sum_{l'}(l+l'+1)\int A_{l,l'}(\phi,\theta,\alpha)\rho_{l',l}(\phi,\theta,\alpha)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}\alpha.$$

Transformation (4.2) can be written as

$$\rho_{l_1,l_2}(\phi,\theta,\alpha)=\sum_{\kappa,q}\frac{\sqrt{2\kappa+1}}{\sqrt{l_1+l_2+1}}D^{\kappa*}_{q,l_1-l_2}(\phi,\theta,\alpha)\rho_{l_1,l_2}(\kappa,q). \tag{4.4}$$

Here, $\rho_{l_1,l_2}(\kappa,q)$ are the density matrix elements in the irreducible tensor representation

$$\rho_{l_1,l_2}(\kappa,q)=\sum_{m_1,m_2}(-1)^{l_2-m_2}C^{\kappa,q}_{l_1,m_1;l_2,-m_2}\rho(l_1,m_1|l_2,m_2).$$

So, equation (4.4) establishes a relation between the $\phi\theta\alpha$-representation and the irreducible tensor representation. According to equation (4.4), then, the elements of the density matrix in the irreducible tensor representation are the coefficients of the $\phi\theta\alpha$-function expansion in the D-function basis.

Consider the well known equality for D-functions [10]

$$D^{l_1*}_{m_1,l_1}(\phi,\theta,\alpha)D^{l_2}_{m_2,l_2}(\phi,\theta,\alpha)=\sum_{\kappa,q}(-1)^{l_2-m_2}C^{\kappa,q}_{l_1,m_1;l_2,-m_2}D^{\kappa*}_{q,l_1-l_2}(\phi,\theta,\alpha)C^{\kappa,l_1-l_2}_{l_1,l_1;l_2,-l_2}$$

which can be rewritten as

$$D^{l_1*}_{m_1,l_1}(\phi,\theta,\alpha)D^{l_2}_{m_2,l_2}(\phi,\theta,\alpha)$$
$$=\sum_{\kappa,q}P_{l_1,l_2}(\kappa)\sqrt{\frac{2\kappa+1}{l_1+l_2+1}}(-1)^{l_2-m_2}C^{\kappa,q}_{l_1,m_1;l_2,-m_2}D^{\kappa*}_{q,l_1-l_2}(\phi,\theta,\alpha) \tag{4.5}$$

where the factor $P_{l_1,l_2}(\kappa)$ is

$$P_{l_1,l_2}(\kappa) = \sqrt{\frac{l_1+l_2+1}{2\kappa+1}} C^{\kappa,l_1-l_2}_{l_1,l_1;l_2,-l_2} = \left[\frac{(l_1+l_2+1)(2l_1)!(2l_2)!}{(l_1+l_2+\kappa+1)!(l_1+l_2-\kappa)!}\right]^{\frac{1}{2}}.$$

In appendix A it is shown that the factor $P_{l_1,l_2}(\kappa)$ depends on κ in the form $\kappa(\kappa+1)$. Therefore, using the property of the D-function

$$\hat{\boldsymbol{J}}^2 D^{\kappa}_{q,l_1-l_2}(\phi,\theta,\alpha) = \kappa(\kappa+1) D^{\kappa}_{q,l_1-l_2}(\phi,\theta,\alpha) \tag{4.6}$$

this factor in equation (4.5) can be replaced by operator $\hat{P}_{l_1,l_2}$ which is a function of the differential operator $\hat{\boldsymbol{J}}^2$ and can be removed from the sum in equation (4.5):

$$D^{l_1*}_{m_1,l_1}(\phi,\theta,\alpha) D^{l_2}_{m_2,l_2}(\phi,\theta,\alpha) = \hat{P}_{l_1,l_2} \sum_{\kappa,q} \sqrt{\frac{2\kappa+1}{l_1+l_2+1}} (-1)^{l_2-m_2} C^{\kappa,q}_{l_1,m_1;l_2,-m_2} D^{\kappa*}_{q,l_1-l_2}(\phi,\theta,\alpha). \tag{4.7}$$

In the case $l_1+l_2+1 \gg |l_1-l_2|$ we may use the approximation for $P_{l_1,l_2}(\hat{\boldsymbol{J}}^2)$ (see appendix A):

$$\hat{P}_{l_1,l_2} \approx \exp\left[\frac{(l_1-l_2)^2 - \hat{\boldsymbol{J}}^2}{2(l_1+l_2+1)}\right]. \tag{4.8}$$

Using equation (4.7) we can write transformation (4.2) in the form

$$\rho_{l_1,l_2}(\phi,\theta,\alpha) = \hat{P}^{-1}_{l_1,l_2} \sum_{m_1,m_2} D^{l_1*}_{m_1,l_1}(\phi,\theta,\alpha) D^{l_2}_{m_2,l_2}(\phi,\theta,\alpha) \rho(l_1m_1|l_2m_2) \tag{4.9}$$

and instead of (4.3) the reciprocal transformation can be written

$$\rho(l_1m_1|l_2m_2) = \frac{l_1+l_2+1}{8\pi^2} \times \int D^{l_1}_{m_1,l_1}(\phi,\theta,\alpha) D^{l_2*}_{m_2,l_2}(\phi,\theta,\alpha) \hat{P}^{-1}_{l_1,l_2} \rho_{l_1,l_2}(\phi,\theta,\alpha) \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi \, \mathrm{d}\alpha. \tag{4.10}$$

One can present equation (4.9) in the form

$$\rho_{l_1,l_2}(\phi,\theta,\alpha) = \hat{P}^{-1}_{l_1,l_2} \rho^{-}_{l_1,l_2}(\phi,\theta) \mathrm{e}^{\mathrm{i}\alpha(l_1-l_2)} \tag{4.11}$$

where

$$\rho^{-}_{l_1,l_2}(\phi,\theta) = \sum_{m_1,m_2} D^{l_1*}_{m_1,l_1}(\phi,\theta,0) D^{l_2}_{m_2,l_2}(\phi,\theta,0) \rho(l_1,m_1|l_2,m_2) \tag{4.12}$$

is a covariant function in the coherent state representation [1]. Thus, equation (4.11) establishes the relation between the coherent state and the $\phi\theta\alpha$-representation.

Finally, we establish the relation between the $\phi\theta\alpha$-functions and the representation of angular momentum orientation which was introduced in [6] (see equation (1.1)). This relation is valid in the limit $l_1, l_2 \gg 1$. Indeed, using asymptotics for the Clebsch–Gordan coefficients [10]

$$C^{\kappa,q}_{l_1,m_1;l_2,-m_2} = (-1)^{l_2-m_2} \sqrt{\frac{2\kappa+1}{2l_1+1}} \delta_{m_1-m_2,q} D^{\kappa}_{q,l_1-l_2}(0,\theta,0) \qquad \cos\theta = \frac{m_1+m_2}{l_1+l_2+1}$$

which are valid at $l_1, l_2 \gg \kappa$, we can replace the D-function in equation (4.2) by $C^{\kappa,q}_{l_1,m_1;l_2,-m_2}$ and sum over q and κ. In this way it is easy to obtain

$$\bar{\rho}_{l_1,l_2}(\phi,\theta) = \rho_{l_1,l_2}(\phi,\theta,0) = \sum_{m_1,m_2} \delta_{2\bar{M},m_1+m_2} \mathrm{e}^{\mathrm{i}\phi(m_1-m_2)} \rho(l_1,m_1|l_2,m_2)$$

$$\cos\theta = \frac{2\bar{M}}{l_1+l_2+1}.$$

This coincides with the definition of the Wigner representation of angular momentum orientation introduced in [6] (equation (1.1)).

5. Matrix elements of operators in Wigner representations

Here we consider the form acquired by the tensor operators in the Wigner representation.

According to the Wigner–Eckart theorem, any tensor operator T^κ, of rank κ, has the following matrix elements in the lm-representation:

$$T^\kappa_\sigma(l_1, m_1|l_2, m_2) = \frac{T^\kappa_{l_1,l_2}}{\sqrt{2\kappa + 1}}(-1)^{l_2-m_2} C^{\kappa,\sigma}_{l_1,m_1;l_2,-m_2}. \tag{5.1}$$

Here $T^\kappa_{l_1,l_2}$ is the reduced matrix element of the operator T^κ. If T^κ is Hermitian operator the following equation is valid [11]:

$$T^\kappa_{l_1,l_2} = (-1)^{l_1-l_2} T^{\kappa *}_{l_2,l_1}.$$

Applying transformation (4.2) to equation (5.1) and summing over m_1 and m_2, one can obtain the matrix elements in the $\phi\theta\alpha$-representation:

$$T^{\kappa,\sigma}_{l_1,l_2}(\phi, \theta, \alpha) = \frac{T^\kappa_{l_1,l_2}}{\sqrt{l_1 + l_2 + 1}} D^{\kappa *}_{\sigma,l_1-l_2}(\phi, \theta, \alpha). \tag{5.2}$$

Now consider the form of the tensor operator in the Wigner representation of the rotational motion of a top. If, in the coordinate system associated with the top, the operator has components $T^\kappa_{\sigma'}$, then in the laboratory coordinate system the operator's matrix elements in lmk-representation are [12]:

$$T^\kappa_\sigma(l_1, m_1, k_1|l_2, m_2, k_2) = (-1)^{k_2+m_2} \frac{\sqrt{(2l_1 + 1)(2l_2 + 1)}}{2\kappa + 1} C^{\kappa,\sigma}_{l_1,m_1;l_2,-m_2} C^{\kappa,\sigma'}_{l_1,k_1;l_2,-k_2} T^\kappa_{\sigma'}. \tag{5.3}$$

Applying transformation (3.4) to equation (5.3) and summing over m_1, m_2 we obtain

$$T^\kappa_\sigma(J, \phi, \theta, \alpha, K, \gamma) = \sum \delta_{2J,l_1+l_2+1}\delta_{2K,k_1+k_2}(-1)^{l_2+m_2} \frac{\sqrt{(2l_1 + 1)(2l_2 + 1)}}{\sqrt{(l_1 + l_2 + 1)(2\kappa + 1)}} \times D^{\kappa *}_{\sigma,l_1-l_2}(\phi, \theta, \alpha) \mathrm{e}^{\mathrm{i}\sigma'\gamma} C^{\kappa,\sigma'}_{l_1,k_1;l_2,-k_2} T^\kappa_{\sigma'}. \tag{5.4}$$

For $l_1, l_2 \gg 1$ one can use the asymptotic form of the Clebsch–Gordan coefficients

$$C^{\kappa,\sigma'}_{l_1,k_1;l_2,-k_2} \approx (-1)^{l_2-k_2} \sqrt{\frac{2\kappa + 1}{2l_2 + 1}} D^\kappa_{\sigma',l_1-l_2}(0, \vartheta, 0) \qquad \cos\vartheta = \frac{k_1 + k_2}{l_1 + l_2 + 1}$$

which allow one to present equation (5.4) in the form

$$T^\kappa_\sigma(J, \phi, \theta, \alpha, K, \gamma) = \sum_\Delta D^{\kappa *}_{\sigma,\Delta}(\phi, \theta, \alpha) D^{\kappa *}_{\sigma',\Delta}(\gamma, \vartheta, 0) T^\kappa_{\sigma'}.$$

Thus, in the Wigner representation of the top's motion, the components of the tensor operator in the laboratory coordinate system and the components in the coordinate system associated with the top are related by two sequential rotations.

6. Quantum equation in Wigner representation

Usually, the equation for the Wigner function is in integral form and is not convenient for applications. Therefore, instead of this integral equation, we will derive approximate equations in differential form.

To obtain these new equations, we take $l \gg 1$ as the primary condition. Moreover, we stipulate that $|l_1 - l_2| \ll l_1, l_2$ for the matrix elements $\hat\rho_{l_1,l_2}$. This assumption is valid if multipolaricity p of the interaction with the external field is not large. Indeed, the matrix elements of the interaction potential differ from zero if $|l_1 - l_2| \leqslant p$, and for small p (for dipole interaction $p = 1$, for quadrupole one $p = 2$, etc), the interactions bind the states which are not widely spaced from each other in the numbers l_1 and l_2.

6.1. Equation for the $\phi\theta\alpha$-function

Now we deduce the quantum equation for the density matrix in the Wigner representation. We begin by considering how the quantum equation

$$\mathrm{i}\frac{\partial}{\partial t}\hat{\rho} = [\hat{H}, \hat{\rho}] \tag{6.1}$$

is transformed in the $\phi\theta\alpha$-representation.

By using transformations (4.9) and (4.10) we can obtain the integral equation for the $\phi\theta\alpha$-function

$$\mathrm{i}\frac{\partial}{\partial t}\hat{P}_{l_1,l_2}\rho_{l_1l_2}(R) = \frac{(l_1+l_3+1)(l_3+l_2+1)}{(8\pi^2)^2}\int D^{l_1}_{l_1l_1}(R^{-1}R_1)D^{l_2}_{l_2l_2}(R_2^{-1}R)D^{l_3}_{l_3l_3}(R_1^{-1}R_2)$$
$$\times([\hat{P}^{-1}_{l_1l_3}H_{l_1l_3}(R_1)][\hat{P}^{-1}_{l_3l_2}\rho_{l_3l_2}(R_2)] - [\hat{P}^{-1}_{l_1l_3}\rho_{l_1l_3}(R_1)][\hat{P}^{-1}_{l_3l_2}H_{l_3l_2}(R_2)])\,\mathrm{d}R_1\,\mathrm{d}R_2. \tag{6.2}$$

Here, for simplicity, we use the notations

$$\rho_{l_1l_2}(R) = \rho_{l_1l_2}(\phi,\theta,\alpha) \qquad D^l_{m_1m_2}(R) = D^l_{m_1m_2}(\phi,\theta,\alpha) \qquad \mathrm{d}R = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}\alpha \tag{6.3}$$

where R defines the rotation

$$R = \mathrm{e}^{-\mathrm{i}\phi\hat{J}_z}\mathrm{e}^{-\mathrm{i}\theta\hat{J}_y}\mathrm{e}^{-\mathrm{i}\alpha\hat{J}_z}$$

by the triplet of Euler angles $\phi\theta\alpha$ and R^{-1} defines the inverse rotation to R and the relation

$$D^l_{m_1m_2}(R) = D^{l*}_{m_2m_1}(R^{-1}) \tag{6.4}$$

is valid. Two consequent rotations R_1 and R_2, give the new position of the rotator which is defined as R_1R_2 and the following equation is valid:

$$\sum_{m_3} D^l_{m_1m_3}(R_1)D^l_{m_3m_2}(R_2) = D^l_{m_1m_2}(R_1R_2). \tag{6.5}$$

For our purposes the following equality is useful:

$$\hat{P}_{l_1,l_2}\rho_{l_1l_2}(R) = \frac{l_1+l_2+1}{8\pi^2}\int D^{l_1}_{l_1l_1}(R^{-1}R_1)D^{l_2}_{l_2l_2}(R_1^{-1}R)\hat{P}^{-1}_{l_1l_2}\rho_{l_1l_2}(R_1)\,\mathrm{d}R_1 \tag{6.6}$$

which can be deduced by using transformations (4.9) and (4.10). It is also easy to deduce by direct calculation that the following equation is valid:

$$\hat{P}_{l_1,l_2}\hat{\boldsymbol{J}}\rho_{l_1l_2}(R) = \frac{l_1+l_2+1}{8\pi^2}\int D^{l_1}_{l_1l_1}(R^{-1}R_1)D^{l_2}_{l_2l_2}(R_1^{-1}R)\hat{P}^{-1}_{l_1l_2}\hat{\boldsymbol{J}}\rho_{l_1l_2}(R_1)\,\mathrm{d}R_1. \tag{6.7}$$

By acting on equation (6.7) with the operator $\hat{\boldsymbol{J}}$, one can extend equation (6.7) to any degree of $\hat{\boldsymbol{J}}$.

Our aim is to derive the differential equation from equation (6.2). This can be done by using the expansion (see appendix B):

$$D^{l_3}_{l_3,l_3}(R_1^{-1}R_2) = \sum_{k=0}^{2l_3}\frac{2^k(2l_3-k)!}{(2l_3)!k!}[\hat{J}^k_{-1}D^{l_3*}_{l_3,l_3}(R_1)][\hat{J}^k_{+1}D^{l_3}_{l_3,l_3}(R_2)]$$
$$\approx \exp\left[\frac{\hat{J}^{(1)}_{-1}\hat{J}^{(2)}_{+1}}{l_3}\right]D^{l_3}_{l_3,l_3}(R_1^{-1})D^{l_3}_{l_3,l_3}(R_2). \tag{6.8}$$

Here the upper indices of operators $\hat{J}$ indicate in which angles, $\phi_1, \theta_1, \alpha_1$ or $\phi_2, \theta_2, \alpha_2$, they act. To obtain the last equality in equation (6.8) we make some approximations in the sum over k: we expand this sum over the infinite limit and keep only the terms such as

$$\left[\frac{\hat{J}^{(1)}_{-1}\hat{J}^{(2)}_{+1}}{l_3}\right]^k \tag{6.9}$$

of any degree k and neglect all other terms having, in comparison with (6.9), at least one additional factor $1/l_3$.

Next, let us consider the equation (6.2) in the particular system of coordinates where the z and x axes coincide with vector $\boldsymbol{J}$ and the rotator's axis, respectively. Formally, for this we have to put $R = R^{-1} = 1$ in equation (6.2). Applying expansion (6.8) and integrating by parts over R_1 and R_2 while taking into account the following equalities:

$$\hat{J}^{(1)}_{-1} D^{l_1}_{l_1,l_1}(R_1) = 0 \qquad \hat{J}^{(2)}_{+1} D^{l_2}_{l_2,l_2}(R_2^{-1}) = 0$$

one can obtain

$$\begin{aligned} \mathrm{i}\hat{P}_{l_1,l_2}\frac{\partial}{\partial t}\rho_{l_1 l_2}(1) = {} & \frac{(l_1+l_3+1)(l_3+l_2+1)}{(8\pi^2)^2}\int D^{l_1}_{l_1 l_1}(R_1) D^{l_2}_{l_2 l_2}(R_2^{-1}) D^{l_3}_{l_3 l_3}(R_1^{-1}) D^{l_3}_{l_3 l_3}(R_2) \\ & \times \exp\left[\frac{\hat{J}^{(1)}_{-1}\hat{J}^{(2)}_{+1}}{l_3}\right]([\hat{P}^{-1}_{l_1 l_3} H_{l_1 l_3}(R_1)][\hat{P}^{-1}_{l_3 l_2}\rho_{l_3 l_2}(R_2)] \\ & -[\hat{P}^{-1}_{l_1 l_3}\rho_{l_1 l_3}(R_1)][\hat{P}^{-1}_{l_3 l_2} H_{l_3 l_2}(R_2)])\,\mathrm{d}R_1\,\mathrm{d}R_2. \end{aligned} \tag{6.10}$$

If we utilize relations (6.6) and (6.7) the last equation can be rewritten in the form:

$$\begin{aligned} \mathrm{i}\frac{\partial}{\partial t}\rho_{l_1,l_2}(1) = {} & \sum_{l_3}\exp\left[\frac{\hat{J}^{(1)}_{-1}\hat{J}^{(2)}_{+1}}{l_3}\right]([\hat{P}^{-1}_{l_1 l_3} H_{l_1 l_3}(1)][\hat{P}^{-1}_{l_3 l_2}\rho_{l_3 l_2}(1)] \\ & -[\hat{P}^{-1}_{l_1 l_3}\rho_{l_1 l_3}(1)][\hat{P}^{-1}_{l_3 l_2} H_{l_3 l_2}(1)]). \end{aligned} \tag{6.11}$$

The upper indices of the operators $\hat{J}$ represent the number of the function on which they act, i.e.

$$\hat{J}^{(1)}_{-1}\hat{J}^{(2)}_{+1} AB \equiv (\hat{J}_{-1}A)(\hat{J}_{+1}B).$$

Further calculations can be made by using approximation (4.8) for operator $\hat{P}$ and the following well known operator equality

$$\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}} = \mathrm{e}^{\frac{1}{2}[\hat{A},\hat{B}]}\mathrm{e}^{\hat{A}+\hat{B}} = \mathrm{e}^{[\hat{A},\hat{B}]}\mathrm{e}^{\hat{B}}\mathrm{e}^{\hat{A}} \tag{6.12}$$

which is valid if

$$[\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{B},\hat{A}]] = 0. \tag{6.13}$$

Of course, being considered as $\hat{A}$, $\hat{B}$, the operators in the exponents of equations (4.8), (6.11) have non-zero commutators (6.13). However, the commutations (6.13) decrease the power of the operator $\hat{J}$ by at least two and therefore, according to the accepted approximation, we may neglect the terms arising due to commutations such as (6.13). Thus, the use of equality (6.12) in our approximation is justified. Next we make use of the condition that the relations

$$\hat{J}_0 V_{l_1,l_3}(1) = (l_3 - l_1)V_{l_1,l_3}(1)$$
$$\hat{J}_0 \rho_{l_3,l_2}(1) = (l_2 - l_3)\rho_{l_3,l_2}(1)$$

are valid. In this way one can obtain, instead of equation (6.11), the following equation for the $\phi\theta\alpha$-function:

$$\begin{aligned} \mathrm{i}\frac{\partial}{\partial t}\rho_{l_1,l_2}(1) = {} & \sum_{l_3}\exp\left[(\hat{J}^{(1)}_{-1}\hat{J}^{(2)}_{+1} - \hat{J}^{(1)}_{+1}\hat{J}^{(2)}_{-1})\left(\frac{1}{l_1+l_2+1} + \frac{l_1+l_2-2l_3}{2(l_1+l_2+1)^2}\right)\right] \\ & \times[V_{l_1,l_3}(1)\rho_{l_3,l_2}(1) - \rho_{l_1,l_3}(1)H_{l_3,l_2}(1)]. \end{aligned} \tag{6.14}$$

Equation (6.14) is written in the system of coordinates, where the direction of the angular momentum $\boldsymbol{n}(\phi\theta)$ coincides with the z-axis. Obviously, the operator

$$\hat{J}^{(1)}_{-1}\hat{J}^{(2)}_{+1} - \hat{J}^{(1)}_{+1}\hat{J}^{(2)}_{-1} \tag{6.15}$$

is not invariant with respect to coordinate rotation. Therefore, to obtain the equation for the $\phi\theta\alpha$-function which is valid in an arbitrary system of coordinates, one should replace operator (6.15) by another operator which is invariant with respect to rotation (a scalar function) and is equal to (6.15) if $\boldsymbol{n}$ coincides with the z-axis. The unique operator satisfying these conditions and which may be constructed using the vectors $\hat{\boldsymbol{J}}^{(1)}$, $\hat{\boldsymbol{J}}^{(2)}$ and $\boldsymbol{n}$ is

$$\hat{w} = -\mathrm{i}\boldsymbol{n}(\hat{\boldsymbol{J}}^{(1)} \times \hat{\boldsymbol{J}}^{(2)}).$$

The explicit form of this operator is

$$\hat{w}H\rho = -\boldsymbol{n}(\hat{\boldsymbol{J}}^{(1)} \times \hat{\boldsymbol{J}}^{(2)})H\rho = \mathrm{i}\left[\left(\frac{\partial}{\partial\phi} - \cos\theta\frac{\partial}{\partial\alpha}\right)H\frac{\partial}{\partial\cos\theta}\rho - \frac{\partial}{\partial\cos\theta}H\left(\frac{\partial}{\partial\phi} - \cos\theta\frac{\partial}{\partial\alpha}\right)\rho\right]. \tag{6.16}$$

In this notation the final equation for $\phi\theta\alpha$-function can be written as

$$\mathrm{i}\frac{\partial}{\partial t}\rho_{l_1,l_2}(R) = \sum_{l_3}\exp\left[\mathrm{i}\hat{w}\left(\frac{1}{l_1+l_2+1} + \frac{l_1-l_3}{2(l_1+l_2+1)^2} + \frac{l_2-l_3}{2(l_1+l_2+1)^2}\right)\right] \times[H_{l_1,l_3}(R)\rho_{l_3,l_2}(R) - \rho_{l_1,l_3}(R)H_{l_3,l_2}(R)]. \tag{6.17}$$

6.2. Equation for the Wigner function of a rotator

Now, let us derive the quantum equation for the rotator Wigner function $\rho(J,\phi,\theta,\alpha)$. We recall that the relation between $\rho(J,\phi,\theta,\alpha)$ and $\rho_{l_1,l_2}(\phi,\theta,\alpha)$ is established by transformation (4.1). Applying this transformation to equation (6.17), we have:

$$\mathrm{i}\frac{\partial}{\partial t}\rho(J,\phi,\theta,\alpha) = \sum_{l_1,l_2,l_3}\exp\left[\mathrm{i}\hat{w}\left(\frac{1}{2J} + \frac{l_1+l_2-2l_3}{8J^2}\right)\right]\delta_{2J,l_1+l_2+1} \times[H_{l_1,l_3}(\phi,\theta,\alpha)\rho_{l_3,l_2}(\phi,\theta,\alpha) - \rho_{l_1,l_3}(\phi,\theta,\alpha)H_{l_3,l_2}(\phi,\theta,\alpha)]. \tag{6.18}$$

By the transformation reciprocal to (4.1)

$$\rho_{l_1,l_2}(\phi,\theta,\alpha) = \frac{1}{2\pi}\sum_J \delta_{2J,l_1+l_2+1}\int_0^{2\pi} \mathrm{e}^{-\mathrm{i}(\alpha_1-\alpha)(l_1-l_2)}\rho(J,\phi,\theta,\alpha_1)\,\mathrm{d}\alpha_1$$

we express $H_{l_1,l_3}(\phi,\theta,\alpha)$ and $\rho_{l_3,l_2}(\phi,\theta,\alpha)$ in the right-hand side of equation (6.18) in terms of the corresponding Wigner functions. Then, summing over l_1, l_2, l_3, we can obtain the integral equation

$$\mathrm{i}\frac{\partial}{\partial t}\rho(J,\phi,\theta,\alpha) = \sum_{J_1,J_2,}\frac{1}{(2\pi)^2}\exp\left[\mathrm{i}\hat{w}\left(\frac{1}{2J} - \frac{J_1+J_2-2J}{4J^2}\right)\right] \times\int_0^{2\pi}\mathrm{e}^{\mathrm{i}2\alpha(J_1-J_2)+\mathrm{i}2\alpha_1(J_2-J)-\mathrm{i}2\alpha_2(J_1-J)} \times[H(J_1,\phi,\theta,\alpha_1)\rho(J_2,\phi,\theta,\alpha_2) - \rho(J_1,\phi,\theta,\alpha_1)H(J_2,\phi,\theta,\alpha_2)]\,\mathrm{d}\alpha_1\,\mathrm{d}\alpha_2. \tag{6.19}$$

We can then present $H(J_1)$ as

$$H(J_1) = H(J+\Delta J_1) = \exp\left(\Delta J_1\frac{\partial}{\partial J}\right)H(J) \qquad \Delta J_1 = J_1 - J$$

and the same for $\rho(J_2)$. Furthermore, the equalities

$$\Delta J\mathrm{e}^{2\mathrm{i}(\alpha-\alpha')\Delta J} = \frac{\mathrm{i}}{2}\frac{\partial}{\partial\alpha'}\mathrm{e}^{2\mathrm{i}(\alpha-\alpha')\Delta J} = -\frac{\mathrm{i}}{2}\mathrm{e}^{2\mathrm{i}(\alpha-\alpha')\Delta J}\frac{\partial}{\partial\alpha'}$$

(the last of which is obtained by integrating by parts over α') allow us to replace ΔJ_1 and ΔJ_2 in equation (6.19) by the rule

$$\Delta J_1 \to -\frac{\mathrm{i}}{2}\frac{\partial}{\partial\alpha_2} \qquad \Delta J_2 \to \frac{\mathrm{i}}{2}\frac{\partial}{\partial\alpha_1}.$$

Making use of the operator equality (6.12) and the fact that at the limit $J \to \infty$, the sum over integer and half-integer ΔJ

$$\sum_{\Delta J=-J}^{\infty} \mathrm{e}^{\mathrm{i}2(\alpha-\alpha')\Delta J} \to 2\pi\delta(\alpha-\alpha')$$

we can obtain the equation for the Wigner function of a rotator:

$$\mathrm{i}\frac{\partial}{\partial t}\rho = \exp\left[\frac{\mathrm{i}}{2}\hat{W}\right][V\rho - \rho V] \tag{6.20}$$

where the new operator $\hat{W}$ is also represented by Poisson brackets

$$\hat{W}AB = \frac{\partial}{\partial\phi}A\frac{\partial}{\partial M}B + \frac{\partial}{\partial\alpha}A\frac{\partial}{\partial J}B - \frac{\partial}{\partial M}A\frac{\partial}{\partial\phi}B - \frac{\partial}{\partial J}A\frac{\partial}{\partial\alpha}B. \tag{6.21}$$

Here $M = J\cos\theta$. Note that in equation (6.20) ρ and H are functions of J, M, ϕ, α.

Thus, we can see that the pairs ϕ, M and α, J play the role of canonical variables.

6.3. Equation for Wigner function of symmetrical and arbitrary top

The equation for the Wigner function of a symmetrical or an arbitrary top $\rho(J, \alpha, M, \phi, K, \gamma)$ can be obtained in a similar way as was done for the rotator's Wigner function. This equation has the same form as equation (6.20), with only one difference: the operator $\hat{W}$ (6.21) should be generalized as

$$\hat{W}AB = \frac{\partial}{\partial\phi}A\frac{\partial}{\partial M}B + \frac{\partial}{\partial\gamma}A\frac{\partial}{\partial K}B + \frac{\partial}{\partial\alpha}A\frac{\partial}{\partial J}B - \frac{\partial}{\partial M}A\frac{\partial}{\partial\phi}B - \frac{\partial}{\partial K}A\frac{\partial}{\partial\gamma}B - \frac{\partial}{\partial J}A\frac{\partial}{\partial\alpha}B. \tag{6.22}$$

6.4. Classical limit of the quantum equation for Wigner functions

The classical limit of these equations can now be immediately obtained. Let us consider, for example, equation (6.17) for the Wigner function in the $\phi\theta\alpha$-representation. If we replace the exponent in equation (6.17) by one (it corresponds to the limit $l \to \infty$) we obtain

$$\begin{aligned}\mathrm{i}\frac{\partial}{\partial t}\rho_{l_1,l_2}(\phi,\theta,\alpha) &= H^{(0)}_{l_1}\rho_{l_1,l_2}(\phi,\theta,\alpha) - \rho_{l_1,l_2}(\phi,\theta,\alpha)H^{(0)}_{l_2} \\ &\quad + \sum_{l_3}[V_{l_1,l_3}(\phi,\theta,\alpha)\rho_{l_3,l_2}(\phi,\theta,\alpha) - \rho_{l_1,l_3}(\phi,\theta,\alpha)V_{l_3,l_2}(\phi,\theta,\alpha)].\end{aligned} \tag{6.23}$$

Here we put $\hat{H} = \hat{H}^{(0)} + \hat{V}$, where $\hat{H}^{(0)}$ is the Hamiltonian of a free atom or molecule and $\hat{V}$ is the interaction potential of an external field inducing the transitions between the internal states of the quantum system. As can be seen from equation (6.23), in the limit $l \to \infty$ the dynamic term in equation (6.23) does not describe the motion of the angular momentum orientation because the external field causes the transitions between different states without changing the angular momentum orientation. One feature of these equations is that they have the form of the equations of a density matrix in the model of non-degenerate states, and the degeneracy upon projection of angular momentum is included in equation (6.23) as a parametric dependence on ϕ, θ, α in V and ρ. Thus, all the results obtained for non-degenerate states can be generalized by equation (6.23) to the case of degeneracy, and it only remains for us to properly average over ϕ, θ, α in the final formulae obtained in the non-degenerate states model.

We must note that equation (6.23) can also be derived using a coherent state representation [1]. Thus, we may conclude that in the approximation ($l \to \infty$), the Wigner $\phi\theta\alpha$ and the coherent state representations lead to an identical description of the angular momentum orientation of a quantum system.

The next term of the exponential expansion in equation (6.17) gives the new equation for the Wigner function in the $\phi\theta\alpha$-representation

$$
\begin{aligned}
\mathrm{i}\frac{\partial}{\partial t}\rho_{l_1,l_2}(\phi,\theta,\alpha) &= H^{(0)}_{l_1}\rho_{l_1,l_2}(\phi,\theta,\alpha) - \rho_{l_1,l_2}(\phi,\theta,\alpha)H^{(0)}_{l_2} \\
&\quad + \sum_{l_3}[V_{l_1,l_3}(\phi,\theta,\alpha)\rho_{l_3,l_2}(\phi,\theta,\alpha) - \rho_{l_1,l_3}(\phi,\theta,\alpha)V_{l_2,l_2}(\phi,\theta,\alpha)] \\
&\quad + \sum_{l_3}\left(\frac{1}{l_1+l_2+1} + \frac{l_1+l_2-2l_3}{2(l_1+l_2+1)^2}\right)[\hat{w}V_{l_1,l_3}(\phi,\theta,\alpha)\rho_{l_3,l_2}(\phi,\theta,\alpha) \\
&\quad - \hat{w}\rho_{l_1,l_3}(\phi,\theta,\alpha)V_{l_3,l_2}(\phi,\theta,\alpha)]. \qquad (6.24)
\end{aligned}
$$

This equation was derived in [6]. The first dynamic term in equation (6.24) has the same meaning as in equation (6.23), but the second term describes the angular momentum precession caused by an external field. To clarify this picture, we consider the equation for a structureless particle with $V_{l_1,l_2}(\phi,\theta,\alpha) = \delta_{l_1,l_2}V(\boldsymbol{n})$. In this case the equation (6.24) is reduced to

$$
\frac{\partial}{\partial t}\rho(\boldsymbol{n}) = \frac{1}{l}\left[\frac{\partial}{\partial\phi}V(\boldsymbol{n})\frac{\partial}{\partial\cos\theta}\rho(\boldsymbol{n}) - \frac{\partial}{\partial\cos\theta}V(\boldsymbol{n})\frac{\partial}{\partial\phi}\rho(\boldsymbol{n})\right] \qquad (6.25)
$$

which has the form of the Liouville equation for a classical rotator.

The classical limit of the equations for the Wigner functions of a rotator or top can be obtained by the same procedure.

7. Conclusion

We have presented here the Wigner representation of rotational motion. As particular cases, the Wigner representations of angular momentum orientation, rotational motion of a rotator or a spherical top, as well as of a symmetrical and an arbitrary top, were considered. The unique form of transformations which lead to these representations was found on the basis of a set of natural requirements, including rotational and space reflection invariance, the averaging rule, the reality of Wigner functions, and the classical form of equations for free-rotational motion.

The relations were established between the Wigner representation of angular momentum orientation and irreducible tensor operators, coherent states and representation, which was introduced in [6].

In addition, we derived the equations for the Wigner functions, which have forms anologous to the equations of translational motion.

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Appendix A

The factor

$$P_{l_1,l_2}(k) = \sqrt{\frac{l_1+l_2+1}{2\kappa+1}}C^{\kappa,l_1-l_2}_{l_1,l_1;l_2,-l_2} = \left[\frac{(l_1+l_2+1)(2l_1)!(2l_2)!}{(l_1+l_2+\kappa+1)!(l_1+l_2-\kappa)!}\right]^{\frac{1}{2}}$$

can be presented in the following form:

$$\begin{aligned}2\log P_{l_1,l_2}(k) &= \log\frac{\prod_{n=1}^{\kappa}(1-\frac{n}{l_1+l_2+1})}{\prod_{n=1}^{\kappa}(1+\frac{n}{l_1+l_2+1})} - \log\frac{\prod_{n=1}^{l_1-l_2}(1-\frac{n}{l_1+l_2+1})}{\prod_{n=0}^{l_1-l_2-1}(1+\frac{n}{l_1+l_2+1})}\\ &= \sum_{n=0}^{l_1-l_2-1}\log\left(1+\frac{n}{l_1+l_2+1}\right) - \sum_{n=1}^{l_1-l_2}\log\left(1-\frac{n}{l_1+l_2+1}\right)\\ &\quad+\sum_{n=1}^{\kappa}\log\left(1-\frac{n}{l_1+l_2+1}\right) - \sum_{n=1}^{\kappa}\log\left(1+\frac{n}{l_1+l_2+1}\right).\end{aligned}$$

Expanding the logarithms in a Taylor series with respect to the parameter $n/(l_1+l_2+1)$ and summing over n [13], we arrive at

$$\log P_{l_1,l_2}(k) \approx \frac{(l_1-l_2)^2-\kappa(\kappa+1)}{2(l_1+l_2+1)} + \cdots.$$

Appendix B

According to (6.5) $D^l_{l,l}(R_1^{-1}R_2)$ can be expressed as

$$D^l_{l,l}(R_1^{-1}R_2) = \sum_{m=-l}^{l} D^{l*}_{m,l}(\phi_1,\theta_1,\alpha_1)D^l_{m,l}(\phi_2,\theta_2,\alpha_2). \tag{B.1}$$

From the property of the D-functions [10]

$$\hat{J}_{+1}D^l_{m,l}(\phi,\theta,\alpha) = \sqrt{\frac{(l+m)(l-m+1)}{2}}D^l_{m-1,l}(\phi,\theta,\alpha)$$

it follows

$$D^l_{l-k,l}(\phi,\theta,\alpha) = \sqrt{\frac{2^k(2l-k)!}{(2l)!k!}}\hat{J}^k_{+1}D^l_{l,l}(\phi,\theta,\alpha).$$

Using this equation and $\hat{J}_{-1} = \hat{J}^*_{+1}$ one can rewrite equation (B.1) as

$$\begin{aligned}D^l_{l,l}(R_1^{-1}R_2) &= \sum_{k=0}^{2l}\frac{2^k(2l-k)!}{(2l)!k!}(\hat{J}^{(1)}_{-1}\hat{J}^{(2)}_{+1})^k D^{l*}_{l,l}(\phi_1,\theta_1,\alpha_1)D^l_{l,l}(\phi_2,\theta_2,\alpha_2)\\ &= \sum_{k=0}^{2l}\frac{2^k(2l-k)!}{(2l)!k!}(\hat{J}^{(1)}_{-1}\hat{J}^{(2)}_{+1})^k D^l_{l,l}(R_1^{-1})D^l_{l,l}(R_2).\end{aligned}$$

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