Optical activity tensor for radiating atomic and molecular systems

Alexei M. Frolov and David M. Wardlaw

Department of Chemistry
University of Western Ontario,
London, Ontario N6H 5B7, Canada

(Dated: October 26, 2010)

Abstract

The optical activity tensor (OAT) is explicitly derived. It is shown that to evaluate a large number of effects related to optical activity of some atomic/molecular system at arbitrary frequency $\omega$ of the incident light, one needs to know only four optical activity tensors which have twelve irreducible (tensor) components. An additional amplification factor contains one $3 \times 3$ tensor of light scattering with three irreducible components. The explicit dependence of all irreducible components of OAT upon $\omega$ and some molecular parameters is derived and discussed. We apply OAT to explain the dispersion of optical rotation in dilute solutions of organic molecules. This study opens a new avenue in application of methods of modern Quantum Electrodynamics to the optical activity.

PACS number(s): 33.55.+b and 33.20.Ni

*E–mail address: afrolov@uwo.ca
†E–mail address: dwardlaw@uwo.ca
I. INTRODUCTION

Our goal in this study is to derive the explicit expression for the optical activity tensor \( \mathbf{OAT} \) (below, OAT, for short) and for all its irreducible components. It is shown that this tensor depends upon some molecular parameters and the frequency \( \omega \) of the incident light. In general, the optical activity tensor must describe a large number of optical phenomena directly related to the optical activity in various molecules, quasi-molecules and many-atomic clusters. Furthermore, if we know the OAT for some molecule, then we can predict the dispersion of molecular optical rotation and the circular dichroism for this molecule. It is clear a priori that such a tensor describes the corrections to ‘regular’ light scattering \[2\].

These corrections correspond to the lowest order approximation in terms of an expansion in the fine structure constant \( \alpha \). In high order approximations one needs to apply mathematical constructions which are significantly more complicated than regular \( 3 \times 3 \) tensors. In this study we perform a detailed analysis of the tensor of optical activity \[1\]. In particular, we derive the formulas for each of the irreducible components of the tensor of optical activity and discuss their \( \omega \)--dependencies.

The following approach is taken here. We consider the scattering of a photon by a system of electrons, which is referred below as a molecule. The molecule has two (discrete) energy levels designated below as state 1 and state 2. The scattering of the photon means that the initial photon \((k, \omega)\) is absorbed by the molecule. Simultaneously another photon \((k', \omega')\) is emitted by this molecule. Finally, the molecule may either stay in the same (initial) state, or it can be transferred into a state which is different from its initial state. In the first case we are dealing with the non-shifted light scattering (or Rayleigh scattering). In the second case the light frequency changes by the value \( \omega' - \omega = E_1 - E_2 \), where \( E_1 \) and \( E_2 \) are the initial and final energies of the molecule. It is clear that in this case we consider the shifted light scattering (also called the Raman scattering).

As is well known from quantum-electrodynamics (see, e.g., \[3\], \[4\]) the operator of electromagnetic perturbation has no matrix elements for transitions in which two photon occupation numbers change simultaneously. The scattering effects appear only in the second approximation of perturbation theory. The exact formulas will be given below, but here we want to describe the general features of our solution. In second order perturbation theory we need to determine the matrix element \( V_{21} \) of the transition \( 1 \rightarrow 2 \), i.e. from the inci-
dent molecular state 1 into the final molecular state 2. The explicit formula for this matrix elements is

$$V_{21} = \sum' \left( \frac{V_{2n} V_{n1}}{\mathcal{E} - E_n} + \frac{V_{2n} V'_{n1}}{\mathcal{E} - E_n - \omega - \omega'} \right)$$

(1)

where $\mathcal{E} = E_1 + \omega$ is the total energy of the system which consists of the molecule and radiation quanta $(k, \omega)$. Also, in this formula $V_{\ldots}$ are the matrix elements for the absorption of the photon $(k, \omega)$, while $V'_{\ldots}$ are the matrix elements for the emission of the photon $(k', \omega')$. By computing the matrix element $V_{21}$ we can determine the differential cross-section

$$d\sigma = |V_{21}|^2 \frac{(\omega')^2 d\omega'}{4\pi}$$

(2)

where $d\omega'$ is a solid-angle element for the direction of the final photon $(k', \omega')$. Our first goal below is to derive the analytical formulas for the differential cross-section $d\sigma$. At the next step we want to investigate the dependencies of this cross-section upon different parameters of the system and the frequency of the incident light.

II. THE TENSOR OF LIGHT SCATTERING

In this study we develop an approach which is based on the method used earlier by G. Placzek [2]. In [2] Placzek introduced the tensor of light scattering $(C_{ik})_{21}$ and derived the following formula for the differential scattering cross-section of light by an atomic/molecular system

$$d\sigma = \frac{\omega(\omega + \omega_{12})^3}{\hbar^2 c^4} \left| (C_{ik})_{21}(e'_i)^* e_k \right|^2 d\omega'$$

(3)

where $(C_{ik})_{21}$ is the $3 \times 3$ tensor of light scattering, while $e'_i$ and $e_k$ are the polarization vectors of the incident and final photons, respectively. The angular variables $d\omega'$ in Eq.(3) are the angular variables of the final photon which is designated by the superscript $'$, i.e. $d\omega' = \sin \theta d\theta d\phi$. The light scattering tensor $(C_{ik})_{21}$ in Eq.(3) is

$$(C_{ik})_{21} = \sum_n \left[ \frac{(d_l)_{2n}(d_k)_{n1}}{\omega_n - \omega - \nu} + \frac{(d_k)_{2n}(d_l)_{n1}}{\omega_n + \omega - \nu} \right]$$

(4)

where $\omega' = \omega + \omega_{12}$, while $d_l$ and $d_k$ are the corresponding components of the vector of the dipole moment $d$. The infinitesimal imaginary increments in the denominators correspond to the regular rule for pole avoidance in quantum-mechanical perturbation theory (for more detail, see, e.g., [4]). Note that the differential cross-section $d\sigma$, Eq.(3), corresponds to the
lowest order approximation in terms of an expansion in the fine structure constant $\alpha \approx \frac{1}{137}$ and contains only contributions from the electric dipole-dipole interaction.

The tensor of light scattering $(C_{ik})_{21}$ in Eq. (3) can be written as the sum of its irreducible components $(C_{ik})_{21} = C^0_{21} + (C^s_{ik})_{21} + (C^a_{ik})_{21}$, where $C^0_{21}$ is the scalar component, $(C^s_{ik})_{21}$ is the symmetric tensor component with zero trace and $(C^a_{ik})_{21}$ is the antisymmetric tensor component. The expressions for these irreducible components are:

$$C^0_{21} = \frac{1}{3} \sum_{i=1}^{3} (C_{ii})_{21} = \frac{1}{3} \sum_n \frac{(\omega_{n1} + \omega_{n2})(d_{2n} \cdot d_{n1})}{(\omega_{n1} - \omega)(\omega_{n2} + \omega)}$$

$$\frac{1}{2} \sum_n \frac{\omega_{n1} + \omega_{n2}}{(\omega_{n1} - \omega)(\omega_{n2} + \omega)}[(d_{2n})_i(d_{n1})_k + (d_{2n})_k(d_{n1})_i] - C^0_{21} \delta_{ik}$$

$$\frac{2\omega + \omega_{12}}{2} \sum_n \frac{[(d_{2n})_i(d_{n1})_k - (d_{2n})_k(d_{n1})_i]}{(\omega_{n1} - \omega)(\omega_{n2} + \omega)}$$

where $a_i$ is the $i$-th (Cartesian) component of the $a$ vector. The formulas Eqs. (5) - (7) allow one to consider the $\omega$-dependence (or dispersion, for short) of many properties related to light scattering. Note that these expressions follow the work of Placzek [2] which was a fundamental contribution to the Quantum-Mechanical Dispersion Theory (QMDT) developed earlier by Kramers and Heisenberg [5] and Dirac [6]. Since 1934 the approach proposed by Placzek [2] was widely and successfully used in applications to various atoms and molecules. In this study we consider the lowest order correction (in terms of the expansion in $\alpha$) to the leading (Placzek) term defined in QMDT.

III. THE PLANE WAVES WITH ZERO SPATIAL DISPERSION

The Placzek approach for atoms suggests attempting to derive an analogous method for molecules which would describe their optical activity. In this Section this problem is considered in detail and it is shown that, in the lowest order approximation, the optical activity can be described by product of the tensor $(C_{ik})_{21}$ of light scattering and the four (or two in some cases) new tensors. These tensors are called the tensors of molecular optical activity, or optical activity tensors (OAT), for short. For a regular atom in its ground state such a product of the $(C_{ik})_{21}$ tensor with the tensor of molecular optical activity equals zero identically, and this explains the word ‘molecular’ in the old definition of such a tensor. Note that in some actual cases the four/two tensors of optical activity are reduced to one tensor only.
To produce the closed analytical expressions for the optical activity tensors in this study we shall assume that the electromagnetic field is represented as a combination of plane waves. Each of these plane waves has its own frequency $\omega$ and polarization which is represented by the vector $e$. The wave functions of the incident and final photons can be taken in the form (see, e.g., [4])

$$A_{e\omega} = \sqrt{\frac{2\pi}{\omega}} \exp(-i\omega t + ik \cdot r)e, \quad A_{e'\omega'} = \sqrt{\frac{2\pi}{\omega'}} \exp(-i\omega't + ik' \cdot r)e'$$

where $\omega$ and $\omega'$ are the corresponding frequencies, while vectors $e$ and $e'$ represent the polarization of the incident (absorbed) and final (emitted) photons, respectively. Note that for the emitted photon we need its conjugate wave function, i.e. $A_{e^*\omega'}$, rather than the wave function defined in Eq.(8). Below, we shall consider the plane waves in the transverse (or radiation) gauge, where $\text{div} A = 0$. In this gauge one finds $k \cdot e = 0$ and $k' \cdot e' = 0$. As follows from these equations the electric $E$ and magnetic $H$ fields are

$$E_{e\omega} = -\frac{\partial}{\partial t} A_{e\omega} = -i\sqrt{2\pi\omega}e \exp(-i\omega t + ik \cdot r)$$

$$H_{e\omega} = \text{curl} A_{e\omega} = i\sqrt{\frac{2\pi}{\omega}} (k \times e) \exp(-i\omega t + ik \cdot r)$$

By introducing the unit vector $n = \frac{k}{\omega}$ we can re-write the last equation in the form

$$H_{e\omega} = i\sqrt{2\pi\omega}(n \times e) \exp(-i\omega t + ik \cdot r)$$

Analogous expressions can be obtained for the $E_{e'\omega'}$ and $H_{e'\omega'}$ fields

$$E_{e'\omega'} = \frac{\partial}{\partial t} A_{e^*\omega'} = i\sqrt{2\pi\omega'}e^* \exp(i\omega't - ik' \cdot r')$$

$$H_{e'\omega'} = \text{curl} A_{e^*\omega'} = -i\sqrt{2\pi\omega'}(n \times e^*) \exp(i\omega't - ik' \cdot r')$$

From these equations one finds the following expressions for the electric dipole and magnetic dipole interactions. In fact, for each of the $(e, \omega)$-components of the $E$ and $H$ vectors we have

$$V^e_{e\omega} = -d \cdot E_{e\omega} = i\sqrt{2\pi\omega}(d \cdot e) \exp(-i\omega t + ik \cdot r)$$

and

$$V^m_{e\omega} = -m \cdot H_{e\omega} = -i\sqrt{2\pi\omega}m \cdot (n \times e) \exp(-i\omega t + ik \cdot r)$$

where $d$ and $m$ are the vectors of the electric and magnetic dipole moments, respectively. For the emitted photon we have analogously

$$(V^e)_{e'\omega'} = -d \cdot E_{e'\omega'} = -i\sqrt{2\pi\omega'}(d \cdot (e')^*) \exp(i\omega't - ik' \cdot r')$$
and
\[(V^m)'_{e'\omega'} = -\mathbf{m} \cdot \mathbf{H}_{e'\omega'} = i\sqrt{2\pi\omega'}\{\mathbf{m} \cdot [\mathbf{n} \times (\mathbf{e'} *)]\} \exp(i\omega' t - i\mathbf{k'} \cdot \mathbf{r}')\] (17)

In derivation of these formulas we have assumed that the vector of dipole moment \(\mathbf{d}\) is real. Note that such an assumption corresponds to the case of classical mechanics. In quantum mechanics the vector \(\mathbf{d}\) is always real (in the coordinate representation), while the vector \(\mathbf{m}\) is a complex vector, since it contains an imaginary unit \(i\) as a factor. Furthermore, in applications of perturbation theory in quantum electrodynamics one finds a number of additional advantages if the following identities are obeyed \((V^e)' = (V^e)^*\) and \((V^m)' = (V^m)^*\) for the interactions which involve the emitted photon(s). In our case, this means that Eq.(16) does not change its form, while in Eq.(17) one finds the \(\mathbf{m}^*\) vector instead of \(\mathbf{m}\) vector
\[(V^m)'_{e'\omega'} = i\sqrt{2\pi\omega'}\{\mathbf{m}^* \cdot [\mathbf{n} \times (\mathbf{e'} *)]\} \exp(i\omega' t - i\mathbf{k'} \cdot \mathbf{r}')\] (18)

Now, we can introduce an approximation that the wavelengths \(\lambda\) of the incident and final photons are significantly larger than a typical linear size \(a\) of the molecule (our light scatterer). In this case we have \(k \cdot r \leq |k| |r| \approx \frac{\lambda}{\lambda} \approx 0\). In this approximation one finds from Eqs.(9) and (10)
\[E_{e\omega} = -i\sqrt{2\pi\omega e} \exp(-i\omega t) \quad \text{and} \quad H_{e\omega} = i\sqrt{2\pi\omega}(n \times e) \exp(-i\omega t)\] (19)

Analogous expressions for the \((e',\omega')\) components are
\[E_{e'\omega'} = i\sqrt{2\pi\omega'}(e')^* \exp(i\omega' t) \quad \text{and} \quad H_{e'\omega'} = -i\sqrt{2\pi\omega'[n \times (e')^*] \exp(i\omega' t)}\] (20)

Plane waves with zero spatial dispersion are often used for analysis of interactions between light (with relatively large wavelengths \(\lambda\)) and matter. In particular, below, we shall use only these plane waves with zero spatial dispersion. In general, this approximation is very useful for studying of light scattering \((\lambda \geq 2000 \text{ Å})\) on atoms and relatively small molecules with \(a_{max} \leq 500 - 800 \text{ Å}\). For our present purposes the use of this approximation is crucial, since only this approximation allows one to derive the closed analytical expressions for all matrix elements required in our procedure (see below).

**IV. PERTURBATION THEORY**

As we mentioned above the scattering effects in an electromagnetic field appear only in the second order perturbation theory. In this second order approximation the matrix
element $V_{21}$ for the transition between states 1 and 2 is written in the following form:

$$V_{21} = \sum_n \left( \frac{V'_{2n} V_{n1}^e}{\mathcal{E}_1 - \mathcal{E}_n^I} + \frac{V_{2n} V'_{n1}^e}{\mathcal{E}_1 - \mathcal{E}_n^{II}} \right)$$  \( (21) \)

where the notation $\mathcal{E}$ designates the total energy of the system (‘molecule + photons’), i.e. in the case considered here we have $\mathcal{E}_n^I = E_n$ and $\mathcal{E}_n^{II} = E_n + \omega + \omega'$, where $E_n$ is the energy of an intermediate atomic state, $\omega$ is the frequency of the incident light and $\omega' = \omega + \omega_2 = E_2 - E_1 + \omega$ is the frequency of the final photon. The matrix element $V_{ab}$ represents absorption of the photon with the wave vector $k$. Analogously, the matrix element $V'_{ab}$ represents emission of the photon with the wave vector $k'$. In the general case, in Eq. (21) the $V_{ab}$ and $V'_{ab}$ interactions are represented in the forms $V = V^e + V^m + V^{qe} + V^{qm} + \ldots$ and $V' = (V^e)' + (V^m)' + (V^{qe})' + (V^{qm})' + \ldots$, respectively. Here $V^e, V^m, V^{qe}$ are the electric dipole, magnetic dipole and electric quadruple interactions, respectively. Keeping only lowest order terms in the fine structure constant expansion of $V$, we can write for these interactions $V \approx V^e + V^m$ and $V' \approx (V^e)' + (V^m)'$. In this case one finds from Eq. (21)

$$V_{21} = \sum_n \left[ \frac{(V^e)'_{2n} V_{n1}^e}{\mathcal{E}_1 - \mathcal{E}_n^I} + \frac{V_{2n} (V^m)'_{n1}}{\mathcal{E}_1 - \mathcal{E}_n^{II}} \right] + \sum_n \left[ \frac{(V^e)'_{2n} V_{n1}^e}{\mathcal{E}_1 - \mathcal{E}_n^I} + \frac{V_{2n} (V^m)'_{n1}}{\mathcal{E}_1 - \mathcal{E}_n^{II}} \right] + \frac{V_{2n} V_{n1}^e}{\mathcal{E}_1 - \mathcal{E}_n^I} \right] + \sum_n \left[ \frac{(V^m)'_{2n} V_{n1}^m}{\mathcal{E}_1 - \mathcal{E}_n^I} + \frac{V_{2n} (V^m)'_{n1}}{\mathcal{E}_1 - \mathcal{E}_n^{II}} \right] + \ldots$$  \( (22) \)

By neglecting here by all terms $\sim V^m V^m$ and other terms of higher order in the fine structure constant $\alpha$, we obtain the following formula for the differential cross-section of light scattering $d\sigma$

$$d\sigma = |V_{21}|^2 \frac{(\omega')^2 d\omega'}{4\pi^2} \approx \left\{ \sum_n \left[ \frac{(V^e)'_{2n} V_{n1}^e}{\mathcal{E}_1 - \mathcal{E}_n^I} + \frac{V_{2n} (V^m)'_{n1}}{\mathcal{E}_1 - \mathcal{E}_n^{II}} \right] \right\}^2 \frac{(\omega')^2 d\omega'}{4\pi^2}$$

$$+ \left\{ \sum_n \left[ \frac{(V^e)'_{2n} V_{n1}^e}{\mathcal{E}_1 - \mathcal{E}_n^I} + \frac{V_{2n} (V^m)'_{n1}}{\mathcal{E}_1 - \mathcal{E}_n^{II}} \right] \right\} \cdot \left\{ \sum_n \left[ \frac{(V^e)'_{2n} V_{n1}^e}{\mathcal{E}_1 - \mathcal{E}_n^I} + \frac{V_{2n} (V^m)'_{n1}}{\mathcal{E}_1 - \mathcal{E}_n^{II}} \right] \right\} \frac{(\omega')^2 d\omega'}{4\pi^2} = d\sigma_{ee} + d\sigma_{em}$$  \( (23) \)

where $d\sigma_{ee}$ is the part of the total cross-section which is reduced to the expression given above (see Eq. (3)). This part of the cross-section is not related to the optical activity. The second term in the right-hand side of Eq. (23) is significantly smaller, in the general case, than the first term, i.e. $d\sigma_{em} \ll d\sigma_{ee}$. However, the second term in Eq. (23) is of great interest, since it represents new physical effects, including effects directly related to the optical activity.
As follows from Eq. (23) in order to determine the part of the total cross-section responsible for molecular optical activity in the lowest order approximation we need to obtain the explicit formulas for the matrix elements of $V_e(V_e)'$, $V_e(V_m)'$, $V_m(V_e)'$ and other similar products. For the plane waves with non-zero spatial dispersion the arising expressions are extremely complicated, since each of the $V_e$ and/or $V_m$ interactions contains an infinite number of $V_e\omega$ and $V_m\omega$ components. In general, in $V_e(V_m)'$, $V_m(V_e)'$ and other similar products one finds an infinite number of cross-terms which explicitly depend upon coordinates. These terms cannot be computed without a complete and accurate knowledge of the molecular electron density $\rho_e(r)$. In turn, this problem is almost unsolvable in the general case. However, in the approximation $\lambda \gg a$ mentioned above we do not need to know the molecular electron density $\rho_e(r)$ in each spatial point. Briefly, this means that we can use only the two ‘molecular’ vectors $d$ and $m$, which are assumed to be constant in any spatial point inside of the molecule. These two vectors $d$ and $m$ are the vectors of electric dipole and magnetic dipole moment, respectively. The vector of the electric dipole moment $d$ is a polar vector, while the magnetic dipole moment $m$ is a axial vector (or pseudo-vector).

The approximation $\lambda \gg a$ corresponds to the use of the plane waves with zero spatial dispersion defined in the end of previous Section. By using these plane waves we can write for $V^e, (V^e)', V^m$ and $(V^m)'

\begin{align*}
V^e_{\omega} &= i\sqrt{2\pi\omega}(d \cdot e)exp(-i\omega t) \quad , \quad (V^e)'_{\omega} = -i\sqrt{2\pi\omega}(d \cdot e^*)exp(i\omega t) \quad (24) \\
V^m_{\omega} &= -i\sqrt{2\pi\omega}[m \cdot (n \times e)]exp(-i\omega t) \quad , \quad (V^m)'_{\omega} = i\sqrt{2\pi\omega}[m^\ast \cdot (n \times (e')^\ast)]exp(i\omega t) \quad (25)
\end{align*}

where $d$ and $m$ are the corresponding vectors of the dipole and magnetic moments of the molecule.

The next step of our procedure is to derive the explicit formula for the cross-section from which the formula for the optical activity tensor (OAT) will follow directly. This is our goal in the next Section.

8
V. THE TENSOR OF MOLECULAR OPTICAL ACTIVITY

By using the expressions derived in the previous Sections we can write the following formula for the differential cross-section \( d\sigma_{em} \) (defined above in Eq. (23))

\[
d\sigma_{em} = \frac{\sum_n (d_{2n} \cdot e') (d_{n1} \cdot e)}{\omega_1 - \omega - i0} + \frac{(d_{2n} \cdot e) (d_{n1} \cdot e')}{\omega_1 + \omega' - i0} \bigg| \sum_n \frac{(d_{2n} \cdot e') (|m_{n1} \times n \rangle \cdot e)}{\omega_1 - \omega - i0} + \frac{(d_{2n} \cdot e) (|m_{n1} \times n \rangle \cdot e')}{\omega_1 + \omega' - i0}
\]

\[
\frac{[(m_{2n}^* \times n) \cdot e'] (d_{n1} \cdot e)}{\omega_1 - \omega - i0} + \frac{(d_{2n} \cdot e) (|m_{n1}^* \times n \rangle \cdot e')}{\omega_1 + \omega' - i0} + \frac{[(m_{2n} \times n) \cdot e'] (d_{n1} \cdot e')}{\omega_1 + \omega' - i0} \bigg| \frac{\omega(\omega')^3}{\hbar^2 c^4} d\omega'
\]

where the notation \( e' \) designates the vector \( (e')^* \). This system of notation is also used in the two following equations. The equation Eq. (26) can be re-written as

\[
d\sigma_{em} = \frac{\sum_n (d_{2n} \cdot e') (d_{n1} \cdot e)}{\omega_1 - \omega - i0} + \frac{(d_{2n} \cdot e) (d_{n1} \cdot e')}{\omega_1 + \omega' - i0} \bigg| \sum_n \frac{(d_{2n} \cdot e') (|m_{n1} \cdot (n \times e)\rangle)}{\omega_1 - \omega - i0} + \frac{(d_{2n} \cdot e) (|m_{n1} \cdot (n \times e')\rangle)}{\omega_1 + \omega' - i0}
\]

\[
\frac{[m_{2n}^* \cdot (n \times e')] (d_{n1} \cdot e)}{\omega_1 - \omega - i0} + \frac{(d_{2n} \cdot e) [m_{n1}^* \cdot (n \times e')] (d_{n1} \cdot e')}{\omega_1 + \omega' - i0} + \frac{(m_{2n} \cdot (n \times e)) (d_{n1} \cdot e')}{\omega_1 + \omega' - i0} \bigg| \frac{\omega(\omega')^3}{\hbar^2 c^4} d\omega'
\]

Note that the vector \( n \) in these equations corresponds to the direction of the scattered light. Formally, this vector can be oriented in an arbitrary spatial direction, but in almost all modern experiments on optical activity in homogeneous solutions the direction of the scattered light always coincides with the direction of the incident light. This means that our differential cross-section must be multiplied by a delta-function \( \delta(n_m - n) \) and integrated over the angular variables \( \omega' = (\theta', \phi') \) of the unit vector \( n = (\cos \theta' \cos \phi', \cos \theta' \sin \phi', \sin \theta') \) which represents the direction of the final photon. The unit vector \( n_m \) describes the direction of the incident photon. This produces the following expression for the cross-section \( \sigma_{em} \)

\[
\sigma_{em} = \frac{4\pi \omega(\omega + \omega_1)^2}{\hbar^2 c^4} \cdot \left| \sum_n \frac{(d_{2n} \cdot e') (d_{n1} \cdot e)}{\omega_1 - \omega - i0} + \frac{(d_{2n} \cdot e) (d_{n1} \cdot e')}{\omega_1 + \omega' - i0} \right| \times \left| \sum_n \frac{(d_{2n} \cdot e') (|m_{n1} \cdot (n_m \times e)\rangle)}{\omega_1 - \omega - i0} + \frac{|m_{2n}^* \cdot (n_m \times e')\rangle (d_{n1} \cdot e)}{\omega_1 - \omega - i0} + \frac{(d_{2n} \cdot e) |m_{n1}^* \cdot (n_m \times e')\rangle (d_{n1} \cdot e')}{\omega_1 + \omega' - i0} \right| \frac{\omega(\omega')^3}{\hbar^2 c^4} d\omega'
\]

where \( \omega' = \omega + \omega_1 \) and unit-vector \( n_m \) designates the direction of propagation of the incident photon.

The expression, Eq. (28), can be cast in the following form

\[
\sigma_{em} = \frac{4\pi \omega(\omega + \omega_1)^2}{\hbar^2 c^4} \cdot |(C_{ik})_{21} (e')^* e_k| \cdot |(S_{ik})_{21} (e')^* (n_m \times e)_k + (T_{ik})_{21} (n_m \times (e')^*)_l (e)_k + (U_{ik})_{21} (n_m \times (e')^*)_k + (V_{ik})_{21} (n_m \times e)_l (e')^*_k|
\]
where \((S_{ik})_{21}, (T_{ik})_{21}, (U_{ik})_{21}\) and \((V_{ik})_{21}\) are \(3 \times 3\) electro-magnetic dipole-dipole tensors, while the electric dipole-dipole tensor \((C_{ik})_{21}\) is defined above in Eq.\((3)\). The explicit formulas for these tensors are

\[
(S_{ik})_{21} = \frac{(d_{2n})_i(m_{n1})_k}{\omega_{n1} - \omega} = \frac{(d_{i})_{2n}(m_{k})_{n1}}{\omega_{n1} - \omega} \tag{30}
\]

\[
(U_{ik})_{21} = \frac{(m_{2n})_i(d_{n1})_k}{\omega_{n1} - \omega} = \frac{(m_{i})_{2n}(d_{k})_{n1}}{\omega_{n1} - \omega} \tag{31}
\]

\[
(T_{ik})_{21} = \frac{(d_{2n})_i(m_{n1}^*)_k}{\omega_{n1} + \omega'} = \frac{(d_{i})_{2n}(m_{k}^*)_{n1}}{\omega_{n1} + \omega'} \tag{32}
\]

\[
(V_{ik})_{21} = \frac{(m_{2n})_i(d_{n1}^*)_k}{\omega_{n1} + \omega'} = \frac{(m_{i})_{2n}(d_{k}^*)_{n1}}{\omega_{n1} + \omega'} \tag{33}
\]

Here we assume that, in the general case, the vectors \(e'\) and \(e\) which represent the polarization of light are complex. Note that in the last equations and everywhere below we drop the infinitesimal imaginary increments in the denominators which indicate the avoidance of the poles in the \(\omega\)-plane. Each of these tensors can be represented as a sum of its irreducible components, e.g.,

\[
S_{ik} = S^0 \delta_{ik} + S^s_{ik} + S^a_{ik}, \quad (34)
\]

are the scalar, symmetric tensor and antisymmetric tensor components of the tensor \(S_{ik}\), respectively. The scalar, symmetric and antisymmetric tensor components of the \(T_{ik}, U_{ik}, V_{ik}\) tensors are defined analogously. Note that all components of these irreducible \(S^0, T^0, U^0, V^0, S^s_{ik}, T^s_{ik}, U^s_{ik}, V^s_{ik}, S^a_{ik}, T^a_{ik}, U^a_{ik}\) and \(V^a_{ik}\) tensors contain the products of different components of the \(d\) and \(m\) vectors, which are the vectors of the electric dipole moment and magnetic dipole moment, respectively. The vector-operator which represents the electric dipole moment is assumed to be self-conjugate. In general, this is true only in the coordinate representation. For instance, the explicit expressions for the \(S^0, T^0, U^0\) and \(V^0\) scalars (they are also called the scalar-components of the \(S, T, U\) and \(V\) tensors) are

\[
(S^0)_{21} = \frac{1}{3} \sum_n \frac{d_{2n} \cdot m_{n1}}{\omega_{n1} - \omega}, \quad (T^0)_{21} = \frac{1}{3} \sum_n \frac{m_{2n} \cdot d_{n1}}{\omega_{n1} - \omega}, \tag{35}
\]

\[
(U^0)_{21} = \frac{1}{3} \sum_n \frac{d_{2n} \cdot m_{n1}^*}{\omega_{n2} + \omega}, \quad (V^0)_{21} = \frac{1}{3} \sum_n \frac{m_{2n} \cdot d_{n1}^*}{\omega_{n2} + \omega},
\]

respectively. The formulas for the symmetric and antisymmetric parts of the \(S, T, U\) and \(V\) tensors are slightly more complicated. For instance, for the \((S^s_{ik})_{21}\) and \((S^a_{ik})_{21}\) tensors one
finds the following formulas

\[(S^s_{ik})_{21} = \frac{1}{2} \sum_n \frac{(d_i)_{2n}(m_k)_{n1} + (d_k)_{2n}(m_i)_{n1}}{\omega_{n1} - \omega} - (S^0)_{21} \delta_{ik} \]  
\[(S^a_{ik})_{21} = \frac{1}{2} \sum_n \frac{(d_i)_{2n}(m_k)_{n1} - (d_k)_{2n}(m_i)_{n1}}{\omega_{n1} - \omega} \]  

The symmetric and antisymmetric tensor components of the $T$, $U$ and $V$ tensors have can be written in a very similar form

\[(T^s_{ik})_{21} = \frac{1}{2} \sum_n \frac{(m_i)_{2n}^* (d_k)_{n1} + (m_k)_{2n}^* (d_i)_{n1}}{\omega_{n1} - \omega} - (T^0)_{21} \delta_{ik} \]  
\[(T^a_{ik})_{21} = \frac{1}{2} \sum_n \frac{(m_i)_{2n}^* (d_k)_{n1} - (m_k)_{2n}^* (d_i)_{n1}}{\omega_{n1} - \omega} \]  
\[(U^s_{ik})_{21} = \frac{1}{2} \sum_n \frac{(d_i)_{2n}(m_k)_{n1}^* + (d_k)_{2n}(m_i)_{n1}^*}{\omega_{n2} + \omega} - (U^0)_{21} \delta_{ik} \]  
\[(U^a_{ik})_{21} = \frac{1}{2} \sum_n \frac{(d_i)_{2n}(m_k)_{n1}^* - (d_k)_{2n}(m_i)_{n1}^*}{\omega_{n2} + \omega} \]  
\[(V^s_{ik})_{21} = \frac{1}{2} \sum_n \frac{(m_i)_{2n}(d_k)_{n1} + (m_k)_{2n}(d_i)_{n1}}{\omega_{n2} + \omega} - (V^0)_{21} \delta_{ik} \]  
\[(V^a_{ik})_{21} = \frac{1}{2} \sum_n \frac{(m_i)_{2n}(d_k)_{n1} - (m_k)_{2n}(d_i)_{n1}}{\omega_{n2} + \omega} \]  

These expressions explicitly define each of the components of the optical activity tensor (OAT). The formulas derived in this Section allow one to describe a large number of optical phenomena related to the optical activity in various molecular, atomic and quasi-atomic systems. Some applications of these formulas in the case of Rayleigh light scattering are discussed in the next Section.

VI. RAYLEIGH LIGHT SCATTERING. DISPERSION OF THE OPTICAL ROTATION

In the case of Rayleigh light scattering the formulas given above are simplified substantially, since the incident state is identical with the final state, i.e. in these formulas we need to use $1 = 2, \omega_{12} = 0, \omega' = \omega$, etc. The tensor of light scattering, Eq. \[4\], now has only two irreducible components: (1) the scalar component

\[C^0_{11} = \frac{2}{3} \sum_n \frac{\omega_{n1}}{\omega_{n1}^2 - \omega^2} (d_{1n} \cdot d_{n1}) \]  
\[\]
and symmetric (tensor) component

\[(C_{ik}^{a})_{11} = \frac{1}{3} \sum_n \frac{\omega_{n1}}{\omega_{n1} - \omega} [ (d_{1n})_i (d_{n1})_k + (d_{1n})_k (d_{n1})_i ] - C_{11}^0 \delta_{ik} \] (45)

The third (or antisymmetric) irreducible component of the tensor of light scattering \((C_{ik}^{a})_{11}\) equals zero identically, since the vector-operator of the dipole moment \(d\) is self-conjugate and each of its components is real, i.e. we can write \((d_i)_{1n} (d_k)_{n1} = (d_k)_{1n} (d_i)_{n1}\) and, therefore, \((C_{ik}^{a})_{11} = 0\).

The irreducible components of the tensor of molecular optical activity take the following form

\[(S^0)_{11} = \frac{1}{3} \sum_n \frac{d_{1n} \cdot m_{n1}}{\omega_{n1} - \omega} , \quad (T^0)_{11} = \frac{1}{3} \sum_n \frac{m_{1n} \cdot d_{n1}}{\omega_{n1} - \omega} , \quad (U^0)_{11} = \frac{1}{3} \sum_n \frac{d_{1n} \cdot m_{n1}}{\omega_{n1} + \omega} , \quad (V^0)_{11} = \frac{1}{3} \sum_n \frac{m_{1n} \cdot d_{n1}}{\omega_{n1} + \omega} \] (46)

for the scalar components, and

\[(S_{ik}^s)_{11} = \frac{1}{2} \sum_n \frac{(d_i)_{1n} (m_k)_{n1} + (d_k)_{1n} (m_i)_{n1}}{\omega_{n1} - \omega} - (S^0)_{11} \delta_{ik} \] (47)

\[(T_{ik}^s)_{11} = \frac{1}{2} \sum_n \frac{(m_i)_{1n}^* (d_k)_{n1} + (m_k)_{1n}^* (d_i)_{n1}}{\omega_{n1} - \omega} - (T^0)_{11} \delta_{ik} \] (48)

\[(U_{ik}^s)_{11} = \frac{1}{2} \sum_n \frac{(d_i)_{1n} (m_k)_{n1}^* + (d_k)_{1n} (m_i)_{n1}^*}{\omega_{n1} + \omega} - (U^0)_{11} \delta_{ik} \] (49)

\[(V_{ik}^s)_{11} = \frac{1}{2} \sum_n \frac{(m_i)_{1n} (d_k)_{n1}^* + (m_k)_{1n} (d_i)_{n1}^*}{\omega_{n1} + \omega} - (V^0)_{11} \delta_{ik} \] (50)

\[(U_{ik}^a)_{11} = \frac{1}{2} \sum_n \frac{(d_i)_{1n} (m_k)_{n1}^* + (d_k)_{1n} (m_i)_{n1}^*}{\omega_{n1} + \omega} \] (51)

\[(V_{ik}^a)_{11} = \frac{1}{2} \sum_n \frac{(m_i)_{1n} (d_k)_{n1}^* + (m_k)_{1n} (d_i)_{n1}^*}{\omega_{n1} + \omega} \] (52)

for the symmetric and anti-symmetric tensor components, respectively. These formulas determine each component of the optical activity tensor in the case of Rayleigh light scattering, i.e. for non-shifted light scattering \(\omega_{12} = 0\).

Let us apply these formulas to the dilute solution of organic substances. In modern organic chemistry the researcher routinely measures the so-called optical rotation, i.e. the
angle by which the plane of linearly polarized light is turned about the direction of light propagation as the light travels through dilute solutions of organic substances. Theory of optical rotation by chiral organic molecules is a well developed area of theoretical chemistry (see, e.g., [8]). The fundamental formulas and results in this theory were derived to the middle of 1940’s [9], [10] (more references and discussion can be found in [8] and [11]). In all these works the approach based on the direct solution of Maxwell equations have been used. The optical activity tensor for radiating atomic and/or molecular systems was not constructed. If our new approach is correct, then we must obtain the same formulas and results. We consider the optical rotation by chiral organic molecules as an example for application of our theory.

In general, the optical rotation is measured by comparing orientation of the plane of linearly polarized light before and after its propagation through a solution which contains chiral organic molecules. In such experiments the directions of propagation of the incident and final light coincide with each other. Therefore, we can apply the formulas derived above. Formally, the rotation of the plane of linearly polarized light is described by the factor (or scalar product) \( n \cdot (e_i \times e'_i) = e'_i \cdot (n \times e_i) \), where the unit vector \( n \) determines the direction of light propagation, while the unit vectors \( e_i \) and \( e'_i \) are the vectors which describe polarization of the incident and final light. In the case of linearly polarized light all these vectors are real. The angle between these two vectors (\( e_i \) and \( e'_i \)) determines the ‘optical rotation’ of the plane of linearly polarized light. If there are no chiral molecules in the solution, then we have \( n \cdot (e_i \times e'_i) = n \cdot (e_i \times e_i) = 0 \), i.e. no optical rotation at all.

The expression for the cross-section, Eq. (29) in the case of pure optical rotation is modified to the form

\[
\sigma_{em} = \frac{4\pi \omega^4}{\hbar^2 c^4} \cdot \left| \left( (C^0)_{21} (e' \cdot e) \right) \cdot \left( (S^0)_{21} n_m \cdot (e \times e') - (T^0)_{21} n_m \cdot (e \times e') \right) \right| - \left( (U^0)_{21} n_m \cdot (e \times e') + (V^0)_{21} n_m \cdot (e \times e') \right) \right| \]  

(55)

This formula can be re-arranged to the form

\[
\sigma_{em} = \frac{4\pi \omega^4}{\hbar^2 c^4} \cdot \left| \left( (C^0)_{21} \right) \cdot \left( (S^0)_{21} - (T^0)_{21} - (U^0)_{21} + (V^0)_{21} \right) \cdot \left| (e' \cdot e) \right| \right| \cdot \left| n_m \cdot (e \times e') \right| \]  

(56)

By using the known expressions for all scalar components of the tensors (see, Eqs. (44) and (46) above) one finds

\[
\sigma_{em} = \frac{4\pi \omega^4}{\hbar^2 c^4} \left| \sum_n \frac{\omega_{n1}}{\omega_{n1}^2 - \omega^2} (d_{1n} \cdot d_{n1}) \right| \cdot \left| \sum_n \frac{1}{\omega_{n1} - \omega} Im(m_{1n} \cdot d_{n1}) \right| \]  

13
\[ + \frac{2}{3} \sum_n \frac{1}{\omega_{n1} + \omega} Im(d_{1n} \cdot m_{n1}) \left| (e' \cdot e) \right| \cdot \left| n_{in} \cdot (e \times e') \right| \] (57)

where the notation \( Im \) designates the imaginary part of the terms written in the following brackets.

Assuming that always \( d_{1n} \cdot m_{n1} = m_{1n} \cdot d_{n1} \), we obtain the final formula for the \( \sigma_{em} \) cross-section

\[ \sigma_{em} = \frac{32\pi\omega^4}{9\hbar^2 c^4} \sum_n \frac{\omega_{n1}}{\omega_{n1}^2 - \omega^2} (d_{1n} \cdot d_{n1}) \left| \sum_n \frac{\omega_{n1}}{\omega_{n1}^2 - \omega^2} Im(d_{1n} \cdot m_{n1}) \left| (e' \cdot e) \right| \cdot \left| n_{in} \cdot (e \times e') \right| \] (58)

Note that the factor \( n_{in} \cdot (e \times e') \) is the optical rotation itself. Furthermore, the scalar product \( (e' \cdot e) \) is a constant factor if the two unit vectors \( e \) and \( e' \) are known (they describe polarization of the incident and final light waves). Therefore, instead of the \( \sigma_{em} \) cross-section we can consider the coefficient of optical rotation (or optical rotation, for short) \( R \)

\[ R = \frac{32\pi\omega^4}{9\hbar^2 c^4} \sum_n \frac{\omega_{n1}}{\omega_{n1}^2 - \omega^2} (d_{1n} \cdot d_{n1}) \left| \sum_n \frac{\omega_{n1}}{\omega_{n1}^2 - \omega^2} Im(d_{1n} \cdot m_{n1}) \right| \] (59)

This formula follows from rigorous QED analysis and it describes the dispersion of optical rotation \( R(\omega) \) in various solutions of different organic molecules. As follows from the formula, Eq. (59), that the optical rotation \( R(\omega) \to 0 \), if the frequency \( \omega \to 0 \). Note that the formula Eq. (59) formally works at arbitrary light frequencies, including frequencies which correspond to the optical transitions, i.e. to the absorbtion and/or emission of light quanta. However, in such cases one needs to operate with the complete formulas, which include small imaginary increments in the denominators, for the light scattering tensor and optical activity tensor(s). For frequencies which correspond to the optical transitions (or resonance frequencies) and for frequencies close to them the explicit expressions for these small imaginary increments become important. This essentially makes impossible to conclude our universal analysis, since such increments depend upon the natural widths of spectral lines \( \Gamma_{1n} (= \Gamma_{n1}) \). For different molecular systems such natural widths are very different and they also depend on some other factors.

In actual experiments in organic chemistry chemists measure the optical rotatory parameter \( \beta \) (angle) which is also called the chiral response parameter (see, e.g., [7], [8])

\[ \beta = \frac{c}{6\pi\hbar} \sum_n \frac{Im(d_{1n} \cdot m_{n1})}{\nu_{n1}^2 - \nu^2} \] (60)

where the summation is taken over all intermediate states. In this equation we use the linear frequencies \( \nu \) instead of circular frequencies \( \omega \), where \( \omega = 2\pi\nu \). Note that in some works
the definition of $\beta$ contains an additional factor $\sim \nu^2$ (see, e.g., [9]). The formula, Eq. (60), is based on the semi-classical analysis of optical rotation performed by Rosenfeld in [10]. In actual cases this formula can be applied only in very limited intervals of light frequencies $\nu$ or wavelengths $\lambda$. In general, it cannot be used in the ‘resonance areas’, i.e. at the frequencies where the absorption/emission of light is very high. Furthermore, to describe the results of real experiments, even at regular frequencies, the formula Eq. (60) is often modified with the use of some additional ‘empirical’ parameters.

The piece which corresponds to Eq. (60) can easily be recognized in our Eq. (59). Note that the formula Eq. (60) represents the optical rotation, but some additional (and important) factors are missing from Eq. (60). In particular, Eq. (60) does not contain any component of the tensor of light scattering. Therefore, based only on this equation we cannot conclude that frequencies, for which the absorption of light is high, are also responsible very large optical rotations of polarized light. This fact is well known from numerous experiments and it follows from Eqs. (28) and (29). This means that Eq. (60) cannot correctly describe the dispersion of optical rotation at arbitrary light frequencies. Finally, we want to emphasize that optical rotation is only one of a large number of phenomena related to the optical activity in various atomic and molecular systems. In this Section we have applied our method to the solutions of chiral organic molecules. The goal of this application was to show that it produces formulas and results which are similar (but more complete and general) to the expressions found in earlier studies [9], [10] (see also [8], [11] and references therein) based on the direct solution of the Maxwell equations.

However, we want to emphasize that there are many other atomic and molecular systems which have a great interest for solution of many important physical problems. Recently, a large number of such problems was discovered in Stellar Astrophysics (see, e.g. [12], [13] and references therein). Currently, there are many various Stars and other Stellar Objects that emit light with noticeable partial linear and/or circular polarization, e.g., the hot Be-stars and Herbig Ae-stars [13], [14], the Wolf-Rayet Stars [12], [15], etc. For many of these problems even preliminary expressions and results were never derived due to their extremely high complexity. The formulas derived in this study allow one to describe the emission of polarized light by some Stellar objects. It will be considered in our future studies.
VII. THE POLARIZATION PARAMETERS FOR THE ELEMENTARY LIGHT SCATTERING

Let us assume that the incident light has a linear polarization which is described by the unit polarization vector $e$, Eq.(19). After the scattering the light also has a linear polarization which is represented by the unit vector $e'$, Eq.(20). In order to describe the change of the polarization of light during its scattering we can define the three following parameters

$$s_0 = |e \cdot e'|^2 + |e_\perp \cdot e'|^2 = |e \cdot e'|^2 + |(e \times n) \cdot e'|^2$$  \hspace{1cm} (61)

$$s_1 = |e \cdot e'|^2 - |e_\perp \cdot e'|^2 = |e \cdot e'|^2 - |(e \times n) \cdot e'|^2$$  \hspace{1cm} (62)

$$s_2 = 2(e \cdot e')(e_\perp \cdot e') = 2(e \cdot e')[(n \times e) \cdot e']$$  \hspace{1cm} (63)

where $e_\perp = (n \times e)$ is the unit vector which represents another polarization vector which is orthogonal to the vector $e$ and $n$ is the direction of the incident light propagation. Let us introduce the angle $\theta$ such that

$$(e \cdot e') = \cos \theta$$  \hspace{1cm} (64)

In this case, one finds

$$(e_\perp \cdot e') = \sin \theta = (n \times e) \cdot e' = n \cdot (e \times e')$$  \hspace{1cm} (65)

With these expressions we can write for the $s_0, s_1$ and $s_2$ parameters $s_0 = 1, s_1 = \cos(2\theta)$ and $s_2 = \sin(2\theta)$. It is clear that $s_0^2 + s_1^2 + s_2^2 = 2$. These three parameters describe polarization of an arbitrary linearly polarized light which is represented as a combination of plane waves with zero spatial dispersion. In some sense, the $s_0, s_1$ and $s_2$ parameters can be considered as the Stokes parameters (see, e.g., [12]) defined for plane waves with zero spatial dispersion. Note also that the absolute value of the $s_2$ parameter is included in our formula for the $\sigma_{em}$ cross-section, Eq.(58).

VIII. CONCLUSION

We have shown that all phenomena related to the optical activity can completely be described with the use of only four tensors: $S_{21}, T_{21}, U_{21}$ and $V_{21}$. The fifth tensor $C_{21}$
(the tensor of electric-dipole light scattering) is included in the formula for the cross-section $\sigma_{em}$ as an amplification factor. These five tensors have fifteen irreducible tensor-components $C^0, C^s_{ik}, C^a_{ik}, S^0, U^0, V^0, S^s_{ik}, T^s_{ik}, U^s_{ik}, V^s_{ik}, S^a_{ik}, T^a_{ik}, U^a_{ik}$ and $V^a_{ik}$. The first three tensors $C^0, C^s_{ik}, C^a_{ik}$ here have nothing to do with the optical activity itself. Instead they determine the amplification factor which also depends upon $\omega$. The optical activity is described by the twelve tensors ($S^0, T^0, U^0, V^0, S^s_{ik}, T^s_{ik}, U^s_{ik}, V^s_{ik}, S^a_{ik}, T^a_{ik}, U^a_{ik}$ and $V^a_{ik}$). In many real applications, however, the total number of independent tensors can be reduced. For instance, if the 1- and 2-states are identical and $\omega_{21} = 0$ (Rayleigh scattering), then to describe optical activity one needs only two tensors (not four!) with six irreducible components. Furthermore, if the polarization vectors are chosen as real (not complex), then to describe the optical activity one needs only one $3 \times 3$ tensor with three irreducible components. However, the explicit $\omega$—dependence of such a tensor will be quite complicated.

In conclusion, we wish to note that the intensity of the scattered light $I'$ is uniformly related to the intensity of the incident light $I$ by the relation

$$I' = \left(\frac{\omega'}{\omega}\right)\sigma I$$

(66)

where $\omega' = \omega + \omega_{12}$. As follows from the formula for the cross-section $\sigma$, Eq. (28), in any optically active solution the direction of maximal light intensity of the (scattered) light will always be rotated during its propagation along the direction $\mathbf{n}_{in}$. The factor $\left(\frac{\omega'}{\omega}\right)\sigma$ in the last formula can be considered as the rotation power. As follows from Eq. (66) and Eq. (29) the uniform combination of the twelve irreducible tensors mentioned above multiplied by the amplification factor $\sim |(C_{ik})_{21}|$ allows one to determine the so-called rotation power of any given optically active solution. It is also clear that the approach described above produces the complete (and correct) formula for the $\omega$—dependence of the rotation power. Thus, we have shown that our method produces the correct results for dilute solutions of chiral organic molecules. Our next goal is to apply this method to various problems from Stellar Astrophysics which are related with the emission of polarized light [16]. In general, these problems are significantly more complicated than analysis of the optical rotation in dilute solutions of chiral organic molecules. Very likely, that our approach developed in this study will be modified and improved before its applications to the problems from Stellar Astrophysics. In particular, it can be necessary to replace the plane waves with zero spatial dispersion by some more complicated functions.
Acknowledgments

It is a pleasure to acknowledge the University of Western Ontario for financial support.

[1] A.M. Frolov and D.M. Wardlaw, *On the theory of molecular optical activity*, ArXiv: 1009.0889 [ph.at-ph] (2010).

[2] G. Placzek, in: *Handbuch der radioologie* Ed. E. Marx, (Academishe, Leipzig, (1934)), 6, 205.

[3] W. Greiner and J. Reinhart, *Quantum Electrodynamics*, (3rd Ed., Springer, Berlin, (2003)).

[4] V.B. Beresteskkii, E.M. Lifshitz and L.P. Pitaevskii, *Quantum Electrodynamics*, (2nd Ed., Pergamon Press, New York, (1984)).

[5] H.A. Kramers and W. Heisenberg, Z. Phys., 31, 681 (1925).

[6] P.A.M. Dirac, Proc. Royal Soc., 114, 710 (1927).

[7] C. Djerassi, *Optical Rotatory Dispersion*, (McGraw-Hill, New York, (1960)).

[8] S.F. Mason, *Molecular Optical Activity and Chiral Discrimination*, (Cambridge University Press, London, (1982)).

[9] H. Eyring, J. Walter and G. Kimball, *Quantum Chemistry*, (J. Willey and Sons Inc., New York, (1944)).

[10] L. Rosenfeld, Z. Phys. 52, 161 (1928).

[11] L.D. Barron, *Molecular Light Scattering and Optical Activity* (Cambridge University Press, Cambridge, 1982).

[12] D. Clarke, *Stellar Polarimetry*, (Wiley-VCH Verlag GmbH & Co, Berlin, (2010)).

[13] F.E. MacKay, N.M. Elias II, C.E. Jones and T.A.A. Sigut, Astrophys. J. (ApJ) 704, 591 (2009).

[14] N.N. Petrova and V.S. Shevchenko, Sov. Astron. Lett. 13, 289 (1987).

[15] A. Moffat and V. Piirola, Astrophys. J. (ApJ) 413, 724 (1993).

[16] A.M. Frolov and C.E. Jones, *Radiation of polarized light from hot Be stars* (2010), in preparation.