

# Contribution of planetary electronic structure of atom to molecular interaction and properties of nanocomposites

 M. SIKOŃ<sup>1\*</sup>, E. BIDZINSKA<sup>2</sup>, and J. MARCINOWSKI<sup>3</sup>
<sup>1</sup>Cracow University of Technology

<sup>2</sup>Jagiellonian University

<sup>3</sup>Newag IP Management

**Abstract.** The paper proposes a study of molecular interactions using the planetary model of the atomic structure. The description refers to transfer of the interactions by electrons bonded with an atom in a planetary system. In molecules we refer to analysis of electrons that remain unpaired during the formation of chemical compounds. The planetary electronic state of molecular interactions is defined by considering the action arm for interatomic forces. Then the interaction torque is defined. The problem is studied in a collection of atoms forming a nanoparticle and then analysis is carried on in the entire volume of the nanocomposite, which is defined as a set of the nanoparticles in a field of matrix-nanofiller interactions. As a result, new mechanical, magnetic, and optical properties of the nanocomposite arise and are described herein. The atomic-scale phenomena are described by both classical and quantum mechanics and are then transferred to the nanoparticle scale by applying statistical mechanics. The quantum solutions for the optically active electrons form the basis for the optical properties of the nanocomposite using forced gyrobirefringence and Maxwell equations. The results of the theoretical analysis are confirmed by experiment using an electron paramagnetic resonance spectrometer.

**Key words:** molecular action arm; molecular interaction torque; quantum electronic state of interaction; superparamagnetism; gyrobirefringence.

## 1. Introduction

In the analysis of intermolecular interactions [1], a method of molecular modelling [2] is useful where each atom is simulated as a single nanoparticle using classical mechanics (Newton's law of motion) [3] and quantum mechanics (Schrödinger's equation) [4]. Under currently used models for molecular interactions, electron disturbances are not referenced or described in terms of a planetary system for atomic structure. However, it is the electronic states that are responsible for mechanical, magnetic and optical properties of the material [5–14]. We anticipate that the correct description of electron disturbances in the field of matrix-nanofiller interactions involves referencing the planetary model of the atom [15–16], which will allow us to reveal the new properties of nanocomposites.

In the analysis involving the electron state, recent discoveries led to its division into a spinon (carrier of electron spin) and an orbiton (associated with its orbital motion) [17].

Modern experimental studies at the nanometer level, the structure, morphology, and identification of the nanoparticles are performed with several techniques: scanning electron microscopy (SEM), transmission electron microscopy (TEM), polarization microscopy (PLM), etc. [18–20]. However, the analysis of disturbed planetary electrons states as a result of the intermolecular interactions is still an open question.

When the electron is located at some distance from the mass centre of the atom, we can define the action arm:

$$\rho_e = \rho_o n^2, \quad (1)$$

where  $\rho_o$  is the Bohr radius, and  $n = 1, 2, 3, \dots$  is the principal quantum number.

The action arm of electron  $\rho_e$  generates an electronic interaction torque, whose temporary value reads:

$$\mathbf{M}_e = \rho_e \times \mathbf{P}_e, \quad (2)$$

where  $\mathbf{P}_e$  is part of the molecular force action on the electron.

We write Formula (2) in the form:

$$M_e = \rho_e P_e \sin \varphi_e, \quad (3)$$

where  $\varphi_e$  is the angle between  $\rho_e$  and  $\mathbf{P}_e$  (Fig. 1). The average torque  $\langle M_e \rangle$  is based on the average of the sine function  $\langle \sin \varphi_e \rangle$ :

$$\langle M_e \rangle = \rho_e P_e \langle \sin \varphi_e \rangle. \quad (4)$$

For the angles  $\varphi_e$  of the range  $(0, \pi)$ , we write:

$$\langle M_e \rangle = \frac{2}{\pi} \rho_e P_e. \quad (5)$$

For van der Waals bonds, when the bonding energy is 10 meV, at a distance of 0.16 Å between the atoms, the molecular force is  $P_{van\ der\ Waals} = 10^{-11}$  N, and when the action arm is of

\*e-mail: marek.sikon@mech.pk.edu.pl

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the order of an ångstrom,  $\rho_e = 1 \text{ \AA}$ , we obtain the average interaction torque for a single-electron atom:

$$\langle M_e^{van\ der\ Wals} \rangle \cong \frac{2}{\pi} \cdot 10^{-21} \text{ Nm}. \quad (6)$$

In the case of ionic bonding, the bonding energy is 10 eV. Under the same conditions as above, the molecular force is  $P_{ion} = 10^{-7} \text{ N}$  and the interaction torque is:

$$\langle M_e^{ion} \rangle \cong \frac{2}{\pi} \cdot 10^{-17} \text{ Nm}. \quad (7)$$

The torque  $M_e$  is absorbed by the electron, which creates a disturbance of the electron motion in the form of the precession with an angular speed  $\omega_e^M$ . We distinguish the precession of the electron spin  $\omega_S^M$  (for the spinon) and orbital precession  $\omega_L^M$  (for the orbiton) and write:

$$\omega_J^M = \omega_S^M + \omega_L^M, \quad (8)$$

where  $\omega_J^M$  is the angular speed of precession of the total angular momentum of atom.

When a single electron is in the nuclear charge field  $Ze$ , where  $Z$  is the atomic number and  $e$  is the charge of the electron, we write the action arm using the formula:

$$\rho_Z = \frac{\rho_o \hbar^2}{Z}, \quad (9)$$

For a multi-electron atom, when  $Z > 1$ , we will distinguish part of the molecular force  $P_{el}$  acting on the electrons and we write:  $P_{el} = \sum_{\xi_k}^Z P_{\xi_k}$ ,  $\xi_k = 1, \dots, Z$  is the electron number in the atom  $k$ . Now the atomic interaction torque associate with electrons is given as a sum:

$$M = \sum_{\xi_k=1}^Z \rho_{\xi_k} \times P_{\xi_k}, \quad (10)$$

At the atomic scale, we note the disturbance of symmetry of the atom generated by the fact that the electron shells are not completely filled up. If the number of electrons on the shells is not equal to  $2\hbar^2$ , such an atom has polar properties. In the polar atom, the mass centre and centre of action of the Coulomb forces do not coincide. This disturbance of symmetry results in the generation of the action arm at the atomic scale. The atomic action arm induces the atomic interaction torque and precession of the whole atom can be demonstrated.

Usually, asymmetry of the atom is induced by electrons on the last shell, i.e. those most distant from the nucleus (valence electrons). In this case, the interaction torque is related to the radius of the outer shell. The atomic radius can be determined from the interatomic distance with the use of diffraction methods. This radius depends on the crystal structure, coordination number, bond type, oxidation degree, and on the position of the atom in the periodic table of elements (atomic number  $Z$ ). Therefore, the interaction torque changes periodically. An effective charge of the nucleus  $eZ_{eff}$ , with  $eZ_{eff} < Z$ , has been introduced for multi-electron atom [21]. Taking into account the interactions between electrons on the shells (shielding ef-

fect) and the effective atomic number  $Z_{eff}$ , we will record the effective action arm for interatomic forces:

$$\rho = \frac{\rho_o \hbar^2}{Z_{eff}}. \quad (11)$$

As the valence shell is filled up, the atomic number  $Z_{eff}$  increases and electrons are strongly attracted to the nucleus, which results in a decrease in the value of  $\rho$  and a decrease in the interaction torque. (At the same time, the atomic ionization energy increases.) A further increase in the number of valence electrons for the elements at the end of the period results in a repulsion between the electrons (shielding effect), which results in the growth of  $\rho$  and of the interaction torque. If the outer shell is completely filled, with the number of electrons equal to  $2\hbar^2$ , the value of the resultant interaction torque drops to zero. (Also, the ionization energy for a fully filled outer shell has the greatest value.)

In the chemical compound [22], we analyse the absorption of the interatomic torque by unpaired electrons.

For nanoparticles in the field of mechanical interactions between the matrix and nanofiller, we carry out the analysis for the collection of polar atoms whose random orientation is defined by the set of mechanical quantum numbers *mech* (introduced by analogy to magnetic quantum numbers):

$$mech = -J, -J + 1, \dots, 0, \dots, J - 1, J, \quad (12)$$

where  $J$  is the total atomic quantum number. The result of the statistical calculation is the polarization of the atoms.

As a result of electron precession, atomic magnetization occurs. The total magnetic moment increases from zero to the statistical value  $G^M$  according to the formula:

$$G(t) = G^M \left( 1 - e^{-\frac{t}{\tau}} \right), \quad (13)$$

where  $t$  is the current time, and  $\tau$  is the time of magnetic saturation. During this process, the mechanical energy decreases until the angular momentum of the nanoparticle reaches a statistical value  $J^M$  corresponding to the new state of equilibrium,  $G(t = \tau) \cong 0.63 G^M$ .

The perturbations of optically active electrons in the field generated by intermolecular interaction between the matrix and nanofiller can modulate the passage of a light wave through the material. We can write the angular speed of the precession of the optical electrons related to the mechanical quantum numbers of spin of the electron:

$$mech_S = +1/2, \quad \omega^+ = \omega_o - \frac{\omega^M}{2}, \quad (14)$$

$$mech_S = -1/2, \quad \omega^- = \omega_o + \frac{\omega^M}{2}, \quad (15)$$

where  $\omega_o$  is angular speed which does not result from matrix-nanofiller interaction (Appendix), and  $\omega^M$  is angular speed of the disturbance. The difference in the motions of the

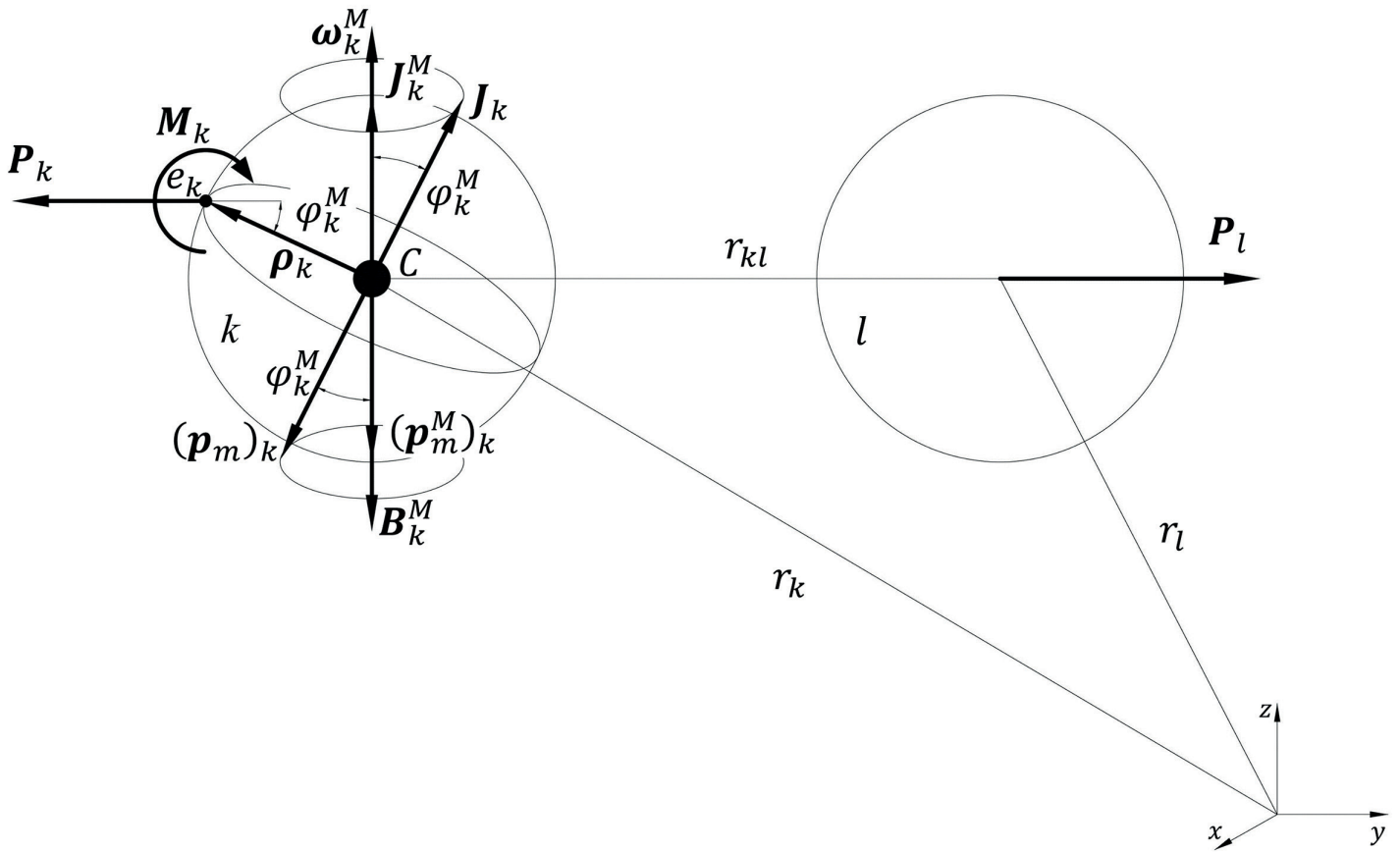


Fig. 1. Transfer of atomic interaction by the planetary system of electron  $e_k$

electrons is described in the form of different directions of the angular velocity:  $\omega^+$  for right-handed, and  $\omega^-$  for left-handed. The two directions split the light wave travelling towards the material into two circular polarization waves: right-handed for  $mech_s = +1/2$  and left-handed for  $mech_s = -1/2$ . These two light waves travel forward with different phase velocities that are proportional to the mechanical state of the material; after interference, the rotation of the azimuth of polarization can be demonstrated.

The EPR signal refers to unpaired electrons. We anticipate that the perturbation of the unpaired electrons by the constant magnetic field of the spectrometer will be modulated by the magnetic field  $B^M$  induced by matrix–nanofiller interactions. As a result, we can obtain a change of the EPR spectrum relative to the spectrum of the free nanofiller.

Nanoparticles act as non-formed crystal structures embedded in an amorphous matrix lacking a crystalline structure. They are randomly oriented and have isotropic properties. We can discuss mechanical, optical and magnetic isotropy and write:

$$P_x = P_y = P_z = P, \quad (16)$$

$$\omega_x^M = \omega_y^M = \omega_z^M = \omega^M, \quad (17)$$

$$B_x^M = B_y^M = B_z^M = B^M, \quad (18)$$

Conditions (16–18) describe the mechanical-optical-magnetic coupling of the nanoparticle loaded in the form of hydrostatic compression in an amorphous matrix.

## 2. Atom

**2.1. Classical mechanics.** In the volume of the nanoparticle, we separate atoms  $k = 1, 2, 3, \dots, n$  with polar properties. We can write the classical parameters of disturbance of the planetary system of the atom  $k$ , in the field of the interatomic interactions, Fig. 1:

$$M_k = \omega_k^M \times J_k, \quad (19)$$

$$U_k^M = -\omega_k^M \cdot J_k, \quad (20)$$

$$J_k^M = J_k \cos \varphi_k^M, \quad (21)$$

$$\varphi_k^M = ar \cos \frac{J_k^M}{J_k}, \quad (22)$$

where:  $M_k$  is the resultant interaction torque from all electrons in the atom  $k$ ,  $\omega_k^M$  is the resultant angular speed of precession,  $J_k$  is the angular momentum of the atom  $k$ ,  $U_k^M$  is the energy

of precession,  $\mathbf{J}_k^M$  is the angular momentum of precession, and  $\varphi_k^M$  is the angle of precession (Fig. 1).

The precession of the electron orbits  $e_k$  generates a magnetic field with induction  $\mathbf{B}_k^M$  for the whole of atom (Fig. 1). We can write the disturbance using  $\mathbf{B}_k^M$  and the magnetic moment  $(\mathbf{p}_m)_k$  of the atom  $k$ :

$$\mathbf{M}_k = (\mathbf{p}_m)_k \times \mathbf{B}_k^M, \quad (23)$$

$$U_k^M = -(\mathbf{p}_m)_k \cdot \mathbf{B}_k^M, \quad (24)$$

$$(\mathbf{p}_m)_k = (\mathbf{p}_m)_k \cos \varphi_k^M, \quad (25)$$

$$\varphi_k^M = ar \cos \frac{(p_m)_k^M}{(p_m)_k}, \quad (26)$$

where  $(\mathbf{p}_k^M)_k$  is the magnetic moment of the disturbance. On the basis of the laws of precession and magneto-mechanical coupling, we write:

$$\mathbf{P}_k \cdot \boldsymbol{\omega}_k^M = 0, \quad (27)$$

$$\mathbf{P}_k \cdot \mathbf{B}_k^M = 0, \quad (28)$$

which means that vectors  $\mathbf{P}_k$  and  $\boldsymbol{\omega}_k^M$  are perpendicular and vectors  $\mathbf{P}_k$  and  $\mathbf{B}_k^M$  are perpendicular.

Considering the precession of the electrons, we can describe the interatomic force  $\mathbf{P}_k$  by combining Eq. (2) and Eq. (19):

$$\mathbf{P}_k = \frac{\omega_k^M}{\rho_k} \mathbf{J}_k, \quad (19.1)$$

or by combining Eq. (2) and Eq. (23):

$$\mathbf{P}_k = \frac{(p_m)_k}{\rho_k} \mathbf{B}_k^M. \quad (23.1)$$

**2.2. Quantum mechanics.** Examining only the part of the electron state (spinon) described by the electron spin  $\mathbf{S}_k$ , on the basis of the classical expression of the intermolecular torque:

$$\mathbf{M}_k^S = \boldsymbol{\omega}_k^S \times \mathbf{S}_k, \quad (29)$$

and according to Formula (17), we write the operator of the interaction torque in the form:

$$\hat{M}_k^S = \sqrt{2} (\omega_{x,y}^S)_k \hat{S}_z^k, \quad (30)$$

where  $z$  is the direction of the quantization and  $(\omega_{x,y}^S)_k$  are the components of the angular speed along the  $x$ - and  $y$ -axes of the Cartesian coordinate system  $(x, y, z)$  as depicted in Fig. 1. We then write the operator equations:

$$\hat{M}_k^S \Phi = M_k^S \Phi, \quad (31)$$

where  $M_k^S$  is the eigenvalue of the operator  $\hat{M}_k^S$ , and  $\Phi$  is the wave function that describes the quantum-mechanical state of

the electron in the field of interactions. Substituting Formula (30) into Formula (31), we write:

$$\sqrt{2} (\omega_{x,y}^S)_k \hat{S}_z^k \Phi = M_k^S \Phi, \quad (32)$$

According to quantum mechanics, the eigenvalue  $M_k^S$  is the physical value of the interaction torque at the nanoscale.

Applying the Pauli operator:

$$\hat{S}_z^k = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (33)$$

where  $\hbar = h/2\pi$  and  $h$  is the Planck constant. We use the wave function in the form:

$$\Phi = \begin{cases} \Phi \uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \text{for } mech_S = \frac{1}{2}, \\ \Phi \downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \text{for } mech_S = -\frac{1}{2}. \end{cases} \quad (34)$$

We write the eigenvalue equation:

$$\frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Phi = \hbar mech_S \Phi, \quad (35)$$

which is satisfied as an identity. Given the analogy between Eqs. (32) and (35), the eigenvalues for both sets of equations are the same. The solution of the unknown quantum value of the interaction torque of the atom  $k$  can be written as:

$$M_k^S = \hbar \sqrt{2} (\omega_{x,y}^S)_k mech_S. \quad (36)$$

We write Formula (36) in the form:

$$(M_k^S)^+ = (M_k^S)^o + \frac{\sqrt{2}}{2} \hbar (\omega_{x,y}^S)_k, \quad mech_S = \frac{1}{2}, \quad (37)$$

$$(M_k^S)^- = (M_k^S)^o + \frac{\sqrt{2}}{2} \hbar (\omega_{x,y}^S)_k, \quad mech_S = -\frac{1}{2}, \quad (38)$$

where  $(M_k^S)^o$  is the torque which does not result from matrix-nanofiller interaction (Appendix). We write the difference in the interatomic torque on the basis of (37) and (38):

$$\Delta(M_k^S) = \sqrt{2} \hbar (\omega_{x,y}^S)_k. \quad (39)$$

The energy contribution due to the electron spin (spinon) in the field of matrix-nanofiller interactions is written in classical mechanics in the following form:

$$U_k^S = -\boldsymbol{\omega}_k^S \cdot \mathbf{S}_k. \quad (40)$$

In the same way as for Eq. (29), we rewrite this in the operator form in the direction of quantization:

$$\hat{U}_k^S = -(\omega_z^S)_k \hat{S}_z^k, \quad (41)$$

and we write the eigenvalue equation for the energy of the atom as follows:

$$-(\omega_z^S)_k \hat{S}_z^k \Phi = U_k^S \Phi. \quad (42)$$

Equation (42) will now correspond to the Schrödinger equation written in the  $z$ -direction. The operators  $\hat{M}_k^S$  and  $\hat{U}_k^S$  comply with the commutation conditions:

$$\hat{M}_k^S \hat{U}_k^S - \hat{U}_k^S \hat{M}_k^S = 0, \quad (43)$$

and eigenvalue Equations (32) and (42) are written for the same wave function  $\Phi$ .

We find the quantum solution of the spinon energy of the precession in the same way as Eq. (36), and finally we write:

$$U_k^S = -(\omega_z^S)_k \hbar \text{mech}_S. \quad (44)$$

We write Formula (44) in the form:

$$(U_k^S)^+ = (U_k^S)^o + \frac{1}{2} (\omega_z^S)_k \hbar, \quad \text{mech}_S = \frac{1}{2}, \quad (45)$$

$$(U_k^S)^- = (U_k^S)^o - \frac{1}{2} (\omega_z^S)_k \hbar, \quad \text{mech}_S = -\frac{1}{2}, \quad (46)$$

where:  $(U_k^S)^o$  is energy which does not result from matrix-nanofiller interaction (Appendix), and we present the difference between the two energy levels from Formula (45) and Formula (46) as:

$$\Delta U_k^S = \hbar (\omega_z^S)_k. \quad (47)$$

Adding the spinon and orbiton state, by analogy to the solutions to Formula (36) and Formula (44), we can write the total atomic interaction torque and total energy of precession in the form:

$$\mathbf{M}_k = \hbar \sqrt{2} (\omega_{x,y}^J)_k \text{mech}_S, \quad (48)$$

$$U_k = -(\omega_z^J)_k \hbar \text{mech}_S, \quad (49)$$

where  $(\omega_{x,y,z}^J)_k$  are components of the angular speed of precession of the total moment of momentum  $\mathbf{J}_k$  in Cartesian coordinate system  $(x, y, z)$ ; see Fig. 1.

We can also write the total polar angle of the atomic precession:

$$\varphi_k^M = ar \cos \frac{J_k^M}{J_k}, \quad (50)$$

where  $J_k = \hbar \sqrt{J(J+1)}$ , and  $J_k^M = \hbar \text{mech}_S$ . Finally, we write the quantum formula for polar rotation of the atom as:

$$\varphi_k^M = ar \cos \frac{\text{mech}_S}{\sqrt{J(J+1)}}. \quad (51)$$

**2.3. Magnetization of atom.** With regard to the magnetic properties of the atom induced by the interaction torque  $\mathbf{M}_k$  (Fig. 1),

we start from the classical formula for the precession energy of the electron spin:

$$U_k^S = -(\mathbf{p}_m^S)_k \cdot \mathbf{B}_k^S, \quad (52)$$

where  $(\mathbf{p}_m^S)_k$  is the magnetic moment of the spinon and  $\mathbf{B}_k^S$  is the magnetic induction generated by the precession of spin. By application of the gyro-magnetic relations  $\gamma^S$  for the spinon:

$$\frac{(\mathbf{p}_m^S)_k}{\mathbf{S}_k} = -\gamma^S, \quad (53)$$

we write the energy of precession in the form:

$$U_k^S = \gamma^S \mathbf{S}_k \cdot \mathbf{B}_k^S, \quad (54)$$

We rewrite Formula (54) in the form of the operator:

$$\hat{U}_k^S = \gamma^S \hat{\mathbf{S}}_k \cdot \mathbf{B}_k^S, \quad (55)$$

and we write the operator equation as:

$$\gamma^S \mathbf{B}_k^S \hat{\mathbf{S}}_k \Phi = U_k^S \Phi. \quad (56)$$

Then we write Eq. (56) on the  $z$ -axis (direction of the quantization):

$$\gamma^S (B_z^S)_k (\hat{S}_z)_k \Phi = (U_k^S)_k \Phi. \quad (57)$$

We find the solution of Eq. (57) in the same way as Eqs. (32) and (42) and finally we write:

$$(U_k^S)_k = \gamma^S \hbar (B_z^S)_k \text{mech}_S. \quad (58)$$

For two spinal mechanical quantum numbers, we write:

$$\text{mech}_S = \frac{1}{2} \quad U_k^+ = U_k^o + \frac{1}{2} \gamma^S \hbar (B_z^S)_k, \quad (59)$$

$$\text{mech}_S = -\frac{1}{2} \quad U_k^- = U_k^o - \frac{1}{2} \gamma^S \hbar (B_z^S)_k. \quad (60)$$

We write the difference between energy levels of the spinon as:

$$\Delta U_k^S = \gamma^S \hbar (B_z^S)_k. \quad (61)$$

Including the formula:

$$\gamma^J \hbar = -g_k \mu_B, \quad (62)$$

where  $g_k$  is the so-called g-factor,  $\gamma^J$  is the gyro-magnetic relation for the total angular momentum  $\mathbf{J}_k$ , and  $\mu_B$  is the Bohr magneton. By analogy to Formula (61), we can write the difference in the energy level of the atom  $k$  (spinon and orbiton together):

$$\Delta U_k = -g_k \mu_B (B_z^J)_k. \quad (63)$$



### 3. Molecule

The description presented in Chapter 2 can be adopted in its entirety to the molecule  $k = 1, 2, 3, \dots, n$ , having  $n$  unpaired electrons.

### 4. Nanoparticle

**4.1. Statistical mechanics.** We describe probabilistic space as a set of the polar atoms/molecules  $k = 1, 2, 3, \dots, n$  in the volume of the nanoparticle. The set of mechanical quantum numbers:  $mech = -J, -J + 1, \dots, 0, \dots, J - 1, J$  forms a set of random numbers. The elementary events are defined as  $M_k, U_k^M, \varphi_k^M$ , and  $J_k^M$ , according to Formulas (48), ..., (51). We will present random variables as functions of the random numbers:

$$M_k = \hbar\sqrt{2}\omega_{x,y}^J mech, \quad (64)$$

$$U_k^M = -\omega_z^J \hbar mech, \quad (65)$$

$$J_k^M = \hbar mech, \quad (66)$$

$$\varphi_k^M = \arccos \frac{mech}{\sqrt{J(J+1)}}. \quad (67)$$

On the basis of the fundamental assumption of the statistical mechanics, we write the canonical distribution:

$$\Pi(mech) = \frac{\exp\left[-\frac{U(mech)}{kT}\right]}{\sum_{mech=-J}^{mech=J} \exp\left[-\frac{U(mech)}{kT}\right]}, \quad (68)$$

where  $k$  is the Boltzmann constant and  $T$  is the temperature. Including assumptions on the hydrostatic state of the matrix-nanofiller interactions, Eqs. (16–18), we can write the average values of the parameter of disturbance in a statistical distribution:

$$\langle M_k \rangle = \sum_{mech=-J}^{mech=J} M_k^J \Pi = \sqrt{2}\hbar\omega_{x,y}^J J B_J, \quad (69)$$

$$\langle U_k^M \rangle = \sum_{mech=-J}^{mech=J} U_k^M \Pi = \hbar\omega_z^J J B_J, \quad (70)$$

$$\langle J_k^M \rangle = \sum_{mech=-J}^{mech=J} J_k^M \Pi = \hbar J B_J, \quad (71)$$

$$\langle \cos_k^M \rangle = \sum_{mech=-J}^{mech=J} \frac{mech}{\sqrt{J(J+1)}} \Pi = \frac{J}{\sqrt{J(J+1)}} B_J, \quad (72)$$

where:

$$B_J = \left[ \frac{2J+1}{2J} \operatorname{ctgh}\left(\frac{2J+1}{2} \frac{\omega_z^J \hbar}{kT}\right) - \frac{1}{2J} \operatorname{ctgh}\left(\frac{\omega_z^J \hbar}{2kT}\right) \right], \quad (73)$$

is the function that is analogous to the Brillouin function. We write the statistical parameters of the matrix-nanofiller interaction in the entire volume of a nanoparticle:

$$\mathbf{m} = n\sqrt{2}\hbar\omega_{x,y}^M J B_J, \quad (74)$$

$$U^M = n\hbar\omega_z^M J B_J, \quad (75)$$

$$J^M = n\hbar J B_J, \quad (76)$$

$$\varphi^M = \arccos \frac{J}{\sqrt{J(J+1)}} B_J. \quad (77)$$

Formulas (74), ..., (77) define the nanoparticle by the matrix-nanofiller interaction as a pseudo-atom characterized by the parameters of disturbance of the planetary electronic system: interaction torque  $\mathbf{m}$ , energy of precession  $U^M$ , moment of momentum of precession  $J^M$ , and angle of precession  $\varphi^M$ .

At a very low temperature where:

$$T < 1K, \quad \frac{\omega_z^M \hbar}{kT} \gg 1, \quad (78)$$

we obtain:

$$\lim_{T < 1K, \frac{\omega_z^M \hbar}{kT} \gg 1} \operatorname{ctgh}\left(\frac{2J+1}{2} \frac{\omega_z^M \hbar}{kT}\right) = 1, \quad (79)$$

$$\lim_{T < 1K, \frac{\omega_z^M \hbar}{kT} \gg 1} \operatorname{ctgh}\left(\frac{\omega_z^M \hbar}{kT}\right) = 1, \quad (80)$$

and we write Formulas (74), ..., (77) in the form:

$$\mathbf{m} = n\sqrt{2}\hbar\omega_{x,y}^M J, \quad (81)$$

$$U^M = n\hbar\omega_z^M J, \quad (82)$$

$$J^M = n\hbar J, \quad (83)$$

$$\varphi_k^M = \frac{J}{\sqrt{J(J+1)}}. \quad (84)$$

Now, for the spinon, when  $J = \frac{1}{2}$ , we write:

$$\mathbf{m} = n \frac{\hbar\omega_{x,y}^M}{\sqrt{2}}, \quad (85)$$

$$U^M = n \frac{\hbar\omega_z^M}{2}, \quad (86)$$

$$J^M = n \frac{\hbar}{2}, \quad (87)$$

$$\varphi^M = \begin{cases} 54,7^\circ \\ 125,3^\circ \end{cases}. \quad (88)$$

## 4.2. Magnetization of the nanoparticle.

**Superparamagnetism by interaction torque.** We write the magnetic moment of the atom in Fig. 1, which is generated by interaction torque  $\mathbf{M}_k$ :

$$\langle p_m^M \rangle_k = -g_k \mu_B m_e h, \quad (89)$$

Applying the canonical distribution, we write the average values of this moment as:

$$\langle \langle p_m^M \rangle_k \rangle = g_k \mu_B J B_{Br}, \quad (90)$$

where  $B_{Br}$  is the Brillouin function. We can describe the magnetization of the nanoparticle in the field of the matrix-nanofiller interaction:

$$G^M = n g_k \mu_B J B_{Br}, \quad (91)$$

relative to the magnetization of the single atom (89). The change in the magnetization direction of the nanoparticle relative to the direction of magnetization of the single atom is described by Eqs. (51) and (77).

## 5. Nanocomposite

**5.1. Formation of equilibrium state.** We define the macroscopic vector of angular momentum in the volume  $dV$  of the nanocomposite:

$$\mathbf{J}^N = \frac{1}{dV} \sum_{k_N=1}^N \mathbf{J}_{k_N}^M, \quad (92)$$

where:  $k_N = 1, \dots, N$  is the number of the nanoparticle,  $\mathbf{J}_{k_N}^M$  is the angular momentum of the nanoparticle number  $k_N$ . For a free nanoparticle, the vectors  $\mathbf{J}_{k_N}^M$ ,  $k_N = 1, \dots, N$ , are oriented in space in a completely disordered way, and the total macroscopic moment of momentum is equal to zero,  $\mathbf{J}^N = 0$ . At the time of the matrix-nanofiller interaction, the vector  $\mathbf{J}^N$  increases. This process lasting for time  $\tau$  is described by the formula:

$$\frac{d\mathbf{J}}{dt} = \frac{\mathbf{J}^N - \mathbf{J}}{\tau}, \quad (93)$$

where:  $\mathbf{J}$  is current in time angular momentum of the nanocomposite.

We write Formula (93) in the form:

$$\frac{d\mathbf{J}}{\mathbf{J}^N - \mathbf{J}} = \frac{dt}{\tau}, \quad (94)$$

By integrating both sides of Eq. (94), we can write the dependence of the macroscopic angular momentum on the time:

$$\mathbf{J}(t) = \mathbf{J}^N \left( 1 - e^{-\frac{t}{\tau}} \right). \quad (95)$$

This means that the macroscopic angular momentum of the nanocomposite is rotated by the angle  $\varphi^N$  and changes in value from  $\mathbf{J} = 0$  to  $\mathbf{J}^N$ . The mechanical energy:

$$U^N(t) = -\mathbf{m}^N \cdot \boldsymbol{\varphi}^N(t), \quad (96)$$

where:  $\mathbf{m}^N = \sum_{k_N=1}^N \mathbf{m}_{k_N}^M$ , decreases until the set of nanoparticles reaches the new state of equilibrium.

**5.2. Mechanical state.** We will refer to the concentration of nanoparticles  $\mathbb{N}_F$  on the elementary surface  $\Delta F$  of the nanocomposite with the number of nanoparticles  $\Delta N$ :

$$\mathbb{N}_F = \lim_{\Delta F \rightarrow 0} \frac{\Delta N}{\Delta F} = \frac{dN}{dF}, \quad (97)$$

The formula is written on the base of Eqs. (74) and (97):

$$\mathbf{m}_F = \mathbb{N}_F \mathbf{m} = \mathbb{N}_F n \sqrt{2} \hbar \boldsymbol{\omega}_{x,y}^M J B_J, \quad (98)$$

can be treated as a vector of polar stress. We can assume that the hydrostatic compression  $p$  of the nanoparticles can be described by the components of the force stress tensor:

$$\sigma_{ij} = -p \delta_{ij}, \quad p > 0, \quad i, j = x, y, z, \quad (99)$$

where  $\delta_{ij}$  is the Kronecker delta. We write the hydrostatic twisting presented by the components of polar stress tensor:

$$\mu_{ij} = -m_F \delta_{ij}, \quad m_F > 0. \quad (100)$$

According to the polar stress tensor  $\mu_{ij}$ , we write the polar strain tensor connected with the vector of rotation  $\boldsymbol{\varphi}^M$ :

$$\varrho_{ij} = \varphi_{j,i}^M. \quad (101)$$

We can write the relation between  $\varrho_{ij}$  and  $\mu_{ij}$  in the form:

$$\varrho_{kk} = -\frac{m_F}{R}, \quad (102)$$

where  $R$  is the material constant associated with rotation of the nanoparticle. Similarly to the stress tensor  $\sigma_{ij}$ , we write the tensor of the strain:

$$\varepsilon_{kk} = -\frac{p}{K}, \quad (103)$$

where  $K$  is equivalent to the compressibility modulus of the nanocomposite.

Formulas (100), (101), and (102) combine the mechanical properties of the nanocomposite in the macroscale, which result from the planetary state of electrons in the atomic scale.

**5.3. Magnetic induction.** On the bases of Eqs. (91) and (97), we can write the magnetic induction generated in nanocomposite and related to the unit of area:

$$\mathbf{B}_F^M = \mathbb{N}_F \frac{\kappa \kappa_o}{\chi} \mathbf{G}^M = \mathbb{N}_F \mathbf{n} \frac{\kappa \kappa_o}{\chi} g \mu_B J \mathbf{B}_{Br}, \quad (104)$$

where  $\kappa$  and  $\kappa_o$  are the dielectric permeabilities of the material and vacuum, while  $\chi$  is the magnetic permeability of the material.

On the basis of Eq. (98) and Eq. (104), we can write the magneto-mechanical coupling association with disturb of the planetary electronic state:

$$\mathbf{B}_F^M = \frac{1}{\sqrt{2}} \frac{\kappa \kappa_o}{\chi} \frac{g \mu_B}{\hbar \omega_{x,y}^M} \mathbf{m}_F. \quad (105)$$

**5.4. Optical activity.** The generalized tensor of the dielectric permittivity is defined in the form:

$$K_{ij} = \kappa_{ij} + i \epsilon_{ijk} \Gamma_k, \quad (106)$$

where  $\Gamma_k = o_{kl} s_l$  is the vector of the optical rotation,  $s_l$  is the unit vector perpendicular to the front of the light wave,  $o_{kl}$  is the tensor of the optical twisting, and  $\epsilon_{ijk}$  is the Levi-Civita symbol.

We describe the optical state of the nanocomposite by matrix representation of the tensor (106) in the form corresponding to hydrostatic state:

$$T_K = \begin{bmatrix} \kappa & -i\Gamma & i\Gamma \\ i\Gamma & \kappa & -i\Gamma \\ -i\Gamma & i\Gamma & \kappa \end{bmatrix}. \quad (107)$$

We separate the matrix (107) into the part that depends on the state of the hydrostatic strain  $\varepsilon$  and the part connected with the polar strain  $\vartheta$ :

$$T_K = \begin{bmatrix} \kappa & 0 & 0 \\ 0 & \kappa & 0 \\ 0 & 0 & \kappa \end{bmatrix} + \begin{bmatrix} 0 & -i\Gamma & i\Gamma \\ i\Gamma & 0 & -i\Gamma \\ -i\Gamma & i\Gamma & 0 \end{bmatrix}. \quad (108)$$

We write the optical-mechanical relations:

$$\kappa = \kappa_o + C_\varepsilon \varepsilon, \quad (109)$$

$$o = o_o + C_\vartheta \vartheta, \quad (110)$$

where  $o_o$  is natural optical twisting (Aragò). The Maxwell equations:

$$\text{rot} \mathbf{E} = -\frac{d\mathbf{B}}{dt}, \quad \text{rot} \mathbf{H} = -\frac{d\mathbf{D}}{dt}, \quad \text{div} \mathbf{D} = 0, \quad \text{div} \mathbf{B} = 0, \quad (111)$$

together with the first approximation of the material equation,

$$\mathbf{D}_k = \chi_o \chi_{kl} \mathbf{E}_l, \quad \mathbf{B}_k = \kappa_o \kappa_{kl} \mathbf{H}_l, \quad k, l = x, y, z, \quad (112)$$

where  $\mathbf{D}_k$  is the vector of the electric induction,  $\mathbf{E}_l$  is the vector of the intensity of the electric field, and  $\mathbf{H}_k$  is the vector of the intensity of the magnetic field, gives the formula:

$$\mathbf{D}_k = \kappa_o n^2 [\mathbf{E}_k - s_k (\mathbf{E} \cdot \mathbf{s})]. \quad (113)$$

which we combine with the basic equation of the gyro-birefringence:

$$\mathbf{D}_k = \kappa_o \kappa_{kl} \mathbf{E}_l + i \kappa_o (\mathbf{\Gamma} \times \mathbf{E})_k, \quad (114)$$

and we write the system of equations for the optical state of the nanocomposite:

$$E_x [\kappa - (1 - s_x^2) n^2] + E_y (n^2 s_x s_y - i\Gamma) + E_z (n^2 s_x s_z + i\Gamma) = 0, \quad (115)$$

$$E_y [\kappa - (1 - s_y^2) n^2] + E_z (n^2 s_y s_z - i\Gamma) + E_x (n^2 s_y s_x + i\Gamma) = 0, \quad (116)$$

$$E_z [\kappa - (1 - s_z^2) n^2] + E_x (n^2 s_z s_x - i\Gamma) + E_y (n^2 s_z s_y + i\Gamma) = 0. \quad (117)$$

Formulas (115), (116), and (117) present the light wave in the gyro-birefringence medium under the action of the hydrostatic compression. We denote the direction of the light path by  $(x)$  and we write the unit vectors as:

$$s_x^{(x)} = 1, \quad s_y^{(x)} = s_z^{(x)} = 0, \quad (118)$$

for the light path parallel to the coordinate  $x$ .

For the chosen direction  $(x)$  of the propagation of the light wave, we write Eqs. (123) and (124) as:

$$E_y (\kappa - n^2) - E_z i\Gamma = 0, \quad (119)$$

$$E_y i\Gamma + E_z (\kappa - n^2) = 0. \quad (120)$$

Then we write the non-zero condition of the solution:

$$\begin{vmatrix} \kappa - n^2 & -i\Gamma_x \\ i\Gamma_x & \kappa - n^2 \end{vmatrix} = 0, \quad (121)$$

and we determine the roots of Eq. (121):

$$n_r^2 = \kappa + \Gamma, \quad (122)$$

$$n_l^2 = \kappa - \Gamma, \quad (123)$$

where  $n_r$  and  $n_l$  are two refractive indexes of the light wave coming toward the  $x$ -direction. We then substitute (122) and (123) into (119) and (120) in order to obtain two independent solutions:



$$\frac{E_z}{E_y} = \pm i, \quad (124)$$

which allow us to describe two light waves:

$$E_I^{(x)} = [0, E_o, iE_o] \exp [i(\omega t - \psi_r^{(x)})], \quad (125)$$

$$E_{II}^{(x)} = [0, E_o, -iE_o] \exp [i(\omega t - \psi_l^{(x)})], \quad (126)$$

where  $E_y = E_o$ , and  $\psi_r^{(x)} = \int_A^B d\psi_r^{(x)}$ ,  $\psi_l^{(x)} = \int_A^B d\psi_l^{(x)}$  are phases of the waves  $E_I^{(x)}$  and  $E_{II}^{(x)}$  from the point  $A$  at which the light enters the material to the output point  $B$ . We take the real part of Formulas (125) and (126) and add mutually perpendicular waves to obtain two pairs of components of the intensity of the electric field:

$$\begin{cases} E_{2I}^{(x)} = E_o \cos(\omega t - \psi_l^{(x)}), \\ E_{3I}^{(x)} = E_o \cos\left(\omega t + \frac{\tau}{2} - \psi_l^{(x)}\right), \end{cases} \quad (127)$$

$$\begin{cases} E_{2II}^{(x)} = E_o \cos(\omega t - \psi_r^{(x)}), \\ E_{3II}^{(x)} = E_o \cos\left(\omega t - \frac{\pi}{2} - \psi_r^{(x)}\right), \end{cases} \quad (128)$$

expressed as:

$$(E_{2I}^{(x)})^2 + (E_{3I}^{(x)})^2 = E_o^2, \quad (129)$$

$$(E_{2II}^{(x)})^2 + (E_{3II}^{(x)})^2 = E_o^2. \quad (130)$$

The solutions (127), (128), (129), and (130) mean that two right- and left-handed circular polarization light waves travel forward in a circular helical path.

We write the elementary increase in the phases of the waves  $E_I^{(x)}$  and  $E_{II}^{(x)}$  relative to the elementary increase in the elementary optical paths  $\Delta_r^{(x)}$  and  $\Delta_l^{(x)}$  of the waves  $E_I^{(x)}$  and  $E_{II}^{(x)}$ :

$$d\psi_r^{(x)} = \frac{2\pi}{\lambda} \Delta_r^{(x)}, \quad (131)$$

$$d\psi_l^{(x)} = \frac{2\pi}{\lambda} \Delta_l^{(x)}, \quad (132)$$

where:

$$\Delta_r^{(x)} = (n_r^{(x)} - n) dx, \quad (133)$$

$$\Delta_l^{(x)} = (n_l^{(x)} - n) dx, \quad (134)$$

$dx$  is the elementary geometrical light way, and  $\lambda$  represents the length of the light wave. So the right- and left-handed circular polarization light waves travel forward in a circular helical path when the path retardations are equal:

$$\Delta^{(x)} = \left[ (n_r^{(x)})_r - (n_l^{(x)})_l \right] dx. \quad (135)$$

The elementary phase retardation for each of the waves  $E_I^{(x)}$  and  $E_{II}^{(x)}$  on the way  $dx$  is written as:

$$d\psi_r^{(x)} = \frac{2\pi}{\lambda} (n_r^{(x)} - n) dx, \quad (136)$$

$$d\psi_l^{(x)} = \frac{2\pi}{\lambda} (n_l^{(x)} - n) dx. \quad (137)$$

The elementary relative phase retardation, (136) and (137), creates the elementary rotation of the azimuth of polarization:

$$d\theta = \frac{(d\psi_r - d\psi_l)}{2}. \quad (138)$$

Using Formulas (122), (123), (136), and (137), we write:

$$d\theta^{(x)} = \frac{\pi}{n\lambda} \Gamma^{(x)} dx. \quad (139)$$

where  $n$  in the denominator of the Formula (139) comes from small optical anisotropy:  $n_r^{(x)} + n_l^{(x)} \cong 2n$ . We introduce the definition of the vector of the optical rotation into Formula (139) and, together with Formula (110), the elementary rotation of the azimuth of polarization is expressed by the components of the polar strain tensor  $\mathcal{G}_{ij}$ :

$$d\theta^{(x)} = \frac{\pi}{n\lambda} (o_o + C_g \mathcal{G}_x) dx, \quad (140)$$

Substituting (101) into (140), we obtain:

$$d\theta^{(x)} = \frac{\pi}{n\lambda} \left( o_o + C_g \frac{\partial \varphi_x^M}{\partial x} \right) dx, \quad (141)$$

By integration on both sides:

$$\int_A^B d\theta^{(x)} = \frac{\pi}{n\lambda} \int_A^B \left( o_o + C_g \frac{\partial \varphi_x^M}{\partial x} \right) dx, \quad (142)$$

we write the expression:

$$\theta^{(x)} = \frac{\pi C_g}{n\lambda} \varphi_x^M, \quad (143)$$

which describes the phenomenon in nanocomposite analogues to the Sagnac effect [23].

## 6. Experiment

The nanocomposite sample was prepared based on a powder of hydrated copper sulfate  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  (nanofiller), epoxy resin E51, and triethylenetetramine as a hardener. The weight of the powder was 0.0295 g. The ratio of powder to epoxy by weight was 1:10 and that of epoxy to hardener was 10:1. The chem-

ical and thermal shrinkage during polymerization of the resin caused hydrostatic compression of the nanoparticles. During the experiment, the paramagnetic ion  $\text{Cu}^{2+}$  with configuration  $3d^9$  was controlled.

The EPR spectrometer was used twice; once for the free powder of  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  and once for the powder mixed with epoxy + hardener. The matrix-nanofiller interaction changed the resonance condition:

$$\Delta U = \hbar(\omega^{EPR} + \omega^M) = g^{(EPR+M)} \mu_B (B^{EPR} + B^M), \quad (144)$$

and absorption power:

$$W = (B^{EPR} + B^M) \frac{d(G^{EPR} + G^M)}{dt}, \quad (145)$$

of the nanocomposite in relation to the free powder:

$$\Delta U = \hbar \omega^{EPR} = g \mu_B B^{EPR}, \quad (146)$$

$$W = B^{EPR} \frac{dG^{EPR}}{dt}, \quad (147)$$

where  $\omega^{EPR}$  is the angular speed of the precession of the unpaired electrons under the action of the magnetic field  $B^{EPR}$  of the spectrometer, and  $G^{EPR}$  is the magnetization induced by magnetic field  $B^{EPR}$ .

EPR measurements were carried on an X-band (9.2 GHz) Bruker ELEXSYS 500 (Karlsruhe) with 100 kHz field modulation.

The spectra were recorded at 293 K with a modulation amplitude of 5 mT, microwave power of 10 mW, and a receiver gain of 30. The EPR parameters of the paramagnetic copper species were determined by a simulation procedure using the software program EPR Sim 32.

The results are presented in the form of the first derivative of the absorption curve. The spectra of the free powder and the nanocomposite sample are significant different Fig. 2. The differences can be interpreted as the influence of interaction between the matrix (epoxy) and the nanofiller ( $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  powder). The spectral parameters for the  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  powder and the nanocomposite sample are collected in Table 1.

Table 1  
Results of EPR investigation

Parameter	Free powder of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$	Nanocomposite
Resonance frequency	$\omega^{EPR} = 61.873592 \cdot 10^9$ Hz	$(\omega^{EPR} + \omega^M) = 60.437608 \cdot 10^9$ Hz
Intensity of spectrum	$I^p = 75000$ units	$I^{nc} = 16000$ units
Resonance magnetic induction	$B^{EPR} = 0,3173$ T	$(B^{EPR} + B^M) = 0,3260$ T
g-factor	$g^{EPR} = 2,217$	$g^{(EPR+M)} = 2,108$
Number of ions $\text{Cu}^{2+}$	$N_V^p = 1,392 \times 10^{21}$	$N_V^{nc} = 1,094 \times 10^{20}$

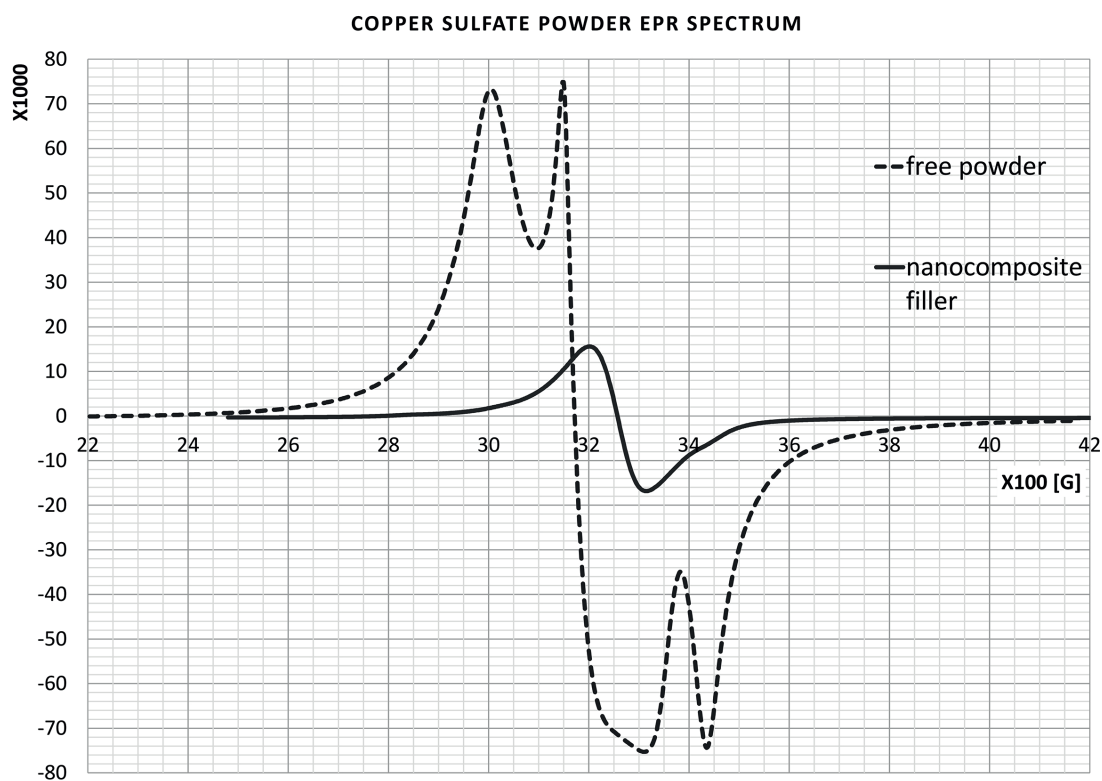


Fig. 2. EPR spectra of the free powder of  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  (green line) and nanocomposite sample (brown line)

Table 2

Parameters of matrix-nanofiller interaction related to unpaired electrons in nanocomposite (CuSO<sub>4</sub> · 5H<sub>2</sub>O powder in epoxy matrix)

State of electron	$\langle M \rangle$ Nm	$\langle U^M \rangle$ J	$\langle J^M \rangle$ kg · m <sup>2</sup> /s	$\langle \cos \varphi^M \rangle$
$J = 5/2$	$2,33(8) \times 10^{-29}$	$1,65(3) \times 10^{-29}$	$1,15(1) \times 10^{-38}$	$3,69(1) \times 10^{-5}$
$J = \ell = 1/2$	$2,00(4) \times 10^{-30}$	$1,41(7) \times 10^{-30}$	$0,98(7) \times 10^{-39}$	$1,08(1) \times 10^{-5}$

Table 3

Parameters of matrix-nanofiller interaction related to the entire volume of the nanocomposite

State of electron	$M$ Nm	$U^M$ J	$J^M$ kg · m <sup>2</sup> /s	$g^M$
$J = 5/2$	$2,55(8) \times 10^{-9}$	$1,80(9) \times 10^{-9}$	$1,25(9) \times 10^{-18}$	1,88
$J = \ell = 1/2$	$2,19(3) \times 10^{-10}$	$1,55(0) \times 10^{-10}$	$1,07(9) \times 10^{-19}$	

The number of Cu<sup>2+</sup> ions in the volume of the free powder  $N_V^p$  and nanocomposite sample  $N_V^{nc}$  were calculate using the comparative method [20]. The number of Cu<sup>2+</sup> ions in the comparative sample CuSO<sub>4</sub>/K<sub>2</sub>SO<sub>4</sub> was  $2.58 \times 10^{18}$ .

From these results, we can determine the spectral parameters of the matrix-nanofiller interaction in the form of the angular speed of the precession  $\omega^M$  and magnetic induction  $B^M$ :

$$\omega^M = 1,435984 \cdot 10^9 \text{ Hz}, \quad (148)$$

$$B^M = 0,0087 \text{ T}, \quad (149)$$

The angular velocity of precession  $\omega^M$  and the magnetic field  $B^M$  induced by the disturbance of non-paired electrons to be regarded as derived from the size of the entire population of the Cu<sup>2+</sup> ions:

$$\omega^M = -\frac{kT}{\hbar} \ln \left( \frac{N_{mech_{j+1}}}{N_{mech_j}} \right)_V, \quad (150)$$

$$B^M = -\frac{kT}{g^M \mu_B} \ln \left( \frac{N_{mech_{j+1}}}{N_{mech_j}} \right)_V, \quad (151)$$

A change in the number of the ions Cu<sup>2+</sup> by a value of  $1.28(3) \times 10^{21}$  for the CuSO<sub>4</sub> · 5H<sub>2</sub>O powder and for the sample may indicate chemical reactions during the formation of a nanocomposite.

We calculate:

$$\frac{\omega_z^M \hbar}{2kT} = 1,871726 \times 10^{-5}. \quad (152)$$

Since  $\frac{\omega_z^M \hbar}{2kT} \ll 1$ , we write the hyperbolic cotangent in the  $B_j$  function (Formula (73)), as a power series. Leaving only the first two terms, we write in the place of Eqs. (69), ... (72):

$$\langle M \rangle = \sqrt{2} \hbar^2 \omega_{x,y}^M J(J+1) \frac{\omega_z^M}{3kT}, \quad (153)$$

$$\langle U^M \rangle = \hbar^2 J(J+1) \frac{(\omega_z^M)^2}{3kT}, \quad (154)$$

$$\langle J^M \rangle = \hbar^2 J(J+1) \frac{\omega_z^M}{3kT}, \quad (155)$$

$$\langle \cos \varphi^M \rangle = \sqrt{J(J+1)} \frac{\omega_z^M \hbar}{3kT}, \quad (156)$$

For the spinon, when  $J = \ell = \frac{1}{2}$ , we write:

$$\langle M \rangle = \sqrt{2} \hbar^2 \omega_{x,y}^M \frac{\omega_z^M}{4kT}, \quad (157)$$

$$\langle U^M \rangle = \hbar^2 \frac{(\omega_z^M)^2}{4kT}, \quad (158)$$

$$\langle J^M \rangle = \hbar^2 \frac{\omega_z^M}{4kT}, \quad (159)$$

$$\langle \cos \varphi^M \rangle = \frac{\sqrt{3}}{6} \frac{\omega_z^M \hbar}{kT}. \quad (160)$$

The results of calculations made on the basis of the Formulas (153), ..., (160) are summarized in Table 2.

Knowing the number of Cu<sup>2+</sup> ions in the nanocomposite sample,  $N_V^{nc} = 1.094 \times 10^{20}$ , we can determine the parameters of a disturbance of non-paired electrons in the entire volume of the nanocomposite (Table 3).

The  $g^M$  - factor in Table 3 was calculated by the dependence:

$$g^M = \frac{\omega^M \hbar}{\mu_B B^M}. \quad (161)$$

We estimate the average of matrix-nanofiller interactions related to the unpaired electron  $\langle P \rangle$  by taking the ionic radius of the  $\text{Cu}^{2+}$  ion according to [24]  $\rho_{\text{Cu}^{2+}} = 0.73 \text{ \AA}$  (Table 4).

Table 4

Matrix-nanofiller interaction related to unpaired electron in the nanocomposite

State of electron	$\langle P \rangle = \frac{\omega^M}{\rho_{\text{Cu}^{2+}}} \hbar \sqrt{J(J+1)}$ N
$J = 5/2$	$6,13(6) \times 10^{-15}$
$J = S = 1/2$	$1,79(7) \times 10^{-15}$

## 7. Conclusion

The disturbance of electrons within a planetary system model used in the context of intermolecular interactions can generate the polar mechanical properties, magnetization, and forced gyrobirefringence of a material. In the atomic scale, intermolecular interactions induce the precession of atoms what causes the whole nanoparticle to rotate. This rotation is the source of new internal stresses in nanocomposites.

The work describes superparamagnetism induced by the matrix-nanofiller interaction.

According to quantum solutions for the optical active electrons, the phenomena analogous to the Sagnac effect can be demonstrated.

The interaction torque combines the mechanical and chemical properties of the atom. It can be concluded that the interaction torque is associated with the chemical reactivity of the elements and is the driving force for the formation of the chemical bonds. The elements are more reactive when their interaction torques are greater. If the interaction torque is zero, the element is mostly unreactive. The moment action depends on the position of the atom in the periodic table of elements. With the presented rules, we can state that the greatest interaction torque in a given period is possessed by atoms in the first group of the periodic table; this influence is smallest for atoms in the middle period.

In the case of van der Waals forces, for an electron cloud that completely fills valance shells, the moment action describes the stochastic fluctuations of the electrons.

According to the description above, the hydrostatic compression of the nanoparticle will produce a condition that known as hydrostatic twisting. When hydrostatic compression changes the distance between the atoms, the hydrostatic twisting manifests by rotation of the nanoparticle.

In the experimental analysis based on EPR spectroscopy, the unpaired electrons can be treated as sensors of the interatomic interaction between matrix and nanofiller. We determined the spectral parameters of these interactions by performing two EPR measurements: once for the free nanoparticles (substrate) and once for the nanoparticles mixed with the matrix (product).

**Appendix.** One should distinguish the angular speed of precession  $\omega_{\zeta_k}^{\text{spinon-orbiton}}$  which does not result from mechanical molecular interactions and is caused by the action of the moment:

$$M_{\zeta_k}^{\text{spinon-orbiton}} = p_{\zeta_k}^{\text{spinon}} \times B_{\zeta_k}^{\text{orbiton}} \quad (\text{A1})$$

coming from the magnetic field  $B_{\zeta_k}^{\text{orbiton}}$  induced by the orbital motion of the electron at the angular momentum  $J_{\zeta_k}^{\text{orbiton}}$ ,  $p_{\zeta_k}^{\text{orbiton}}$  is the magnetic moment of the electron spin. The induction  $B_{\zeta_k}^{\text{orbiton}}$  is obtained from the Biot-Savart law with regard to the effect of the relativistic transformation of the magnetic field (Thomas factor) [25]:

$$B_{\zeta_k}^{\text{orbiton}} = \frac{1}{2} \frac{Z_k e \chi_o}{4\pi \rho_{\zeta_k}^3 m_e} J_{\zeta_k}^{\text{orbiton}} \quad (\text{A2})$$

where:  $\chi_o$  is the magnetic permeability of the vacuum,  $m_e$  is the rest mass of electron. The precession  $\omega_{\zeta_k}^{\text{spinon-orbiton}}$  can be obtained taking into account the relativistic kinematic effect in the system when the acceleration of the electron has a component perpendicular to the velocity vector (Thomas precession) from the formula:

$$\omega_{\zeta_k}^{\text{spinon-orbiton}} = -\frac{e}{2m_e c^2} (\mathbf{v}_{\zeta_k} \times \mathbf{F}_{\zeta_k}) \quad (\text{A3})$$

where:  $\mathbf{v}_{\zeta_k}$  is the speed of the electron  $\zeta_k$ ,  $\mathbf{F}_{\zeta_k}$  is the Coulomb force acting on the electron  $\zeta_k$ ,  $c$  is the speed of light.

The moment  $M_{\zeta_k}^{\text{spinon-orbiton}}$  can be called self-torque of the atom and is not related to the intermolecular interaction and therefore this is not described in this work [26].

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