Gyroscopic effect in intermolecular collision with the $C_{60}$ fullerene molecule

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Abstract. The work is devoted to the study of the gyroscopic phenomena of a rotating $C_{60}$ fullerene molecule on interaction with a moving particle. To determine the precession characteristics of the $C_{60}$ fullerene molecule, the pairwise interaction model of nonpolar Lennard-Jones molecules was used. The rotational motion of fullerene was described by the dynamic Euler equations. The influence of the angular velocity and direction of rotation of the fullerene molecule on the deviation from the initial position is investigated.

1. Introduction
In this work, to study the gyroscopic phenomena arising from the interaction of a rotating fullerene molecule with an incident particle, we used the methods of classical molecular physics: the intermolecular potential method and Newton's method to describe the motion of a particle. For the numerical solution of the system of ordinary differential equations, the fourth-order Runge–Kutta method \cite{1} was used. A model is presented for describing the rotation of fullerene with frequencies lying in the range of $10^{12}–10^{14}$ Hz and velocities of incident test particles of 200–2000 m/s. For such parameters of the problem, the Debris wavelength of the incident atom, and especially the fullerene molecule, becomes smaller than the diameter of the atomic nucleus and, therefore, this problem is well described using the Newtonian approach, without the need for quantum mechanics. The particles used were carbon and xenon atoms, as well as a fullerene molecule. To determine the precession characteristics of the $C_{60}$ fullerene molecule, we used the Lennard-Jones pair interaction potential, which is well applicable for nonpolar molecules.

2. Problem state
We introduce the Cartesian coordinate system $0xyz$, at the beginning of which we place the center of the rotating fullerene $C_{60}$ (figure 1) as well as the Cartesian coordinate system $0\xi\eta\zeta$, tightly connected with this molecule. Let the particle at the initial moment of time be at a certain distance from the fullerene $C_{60}$, at which the Van der Waals interaction forces are small, and move with velocity $v_a$ in its direction (see figure 2). The dynamic Euler equations are used to describe the rotational motion of fullerene molecules around their centers of mass \cite{2}:

\[
A \frac{dp}{dt} + (C - B)qr = M^{(e)}_\zeta, \quad B \frac{dq}{dt} + (A - C)pr = M^{(e)}_\eta, \quad C \frac{dr}{dt} + (B - A)pq = M^{(e)}_\zeta.
\]

(1)

To describe the motion of the center of mass of a fullerene molecule, the equation (2)
Here \( p, q, r \) are the projections of the angular velocity on the axis of the moving reference frame; \( A, B, C \) are the main moments of inertia of the molecule for its center of mass; \( v_C \) is the velocity of the fullerene molecule center; \( U \) is the interaction potential of carbon atoms, \( \nabla \) is the gradient operator, \( r_k \) is the distance between the particle and the \( k \)-th atom of \( C_{60} \), \( S = 60 \) is the number of carbon atoms in the \( C_{60} \) molecule.

The projections of the moments of forces in formulas (1) on the axis of the connected coordinate system \( 0\xi\eta\zeta \) are defined as follows

\[
M_x^{(e)} = c_1 M_x^{(e)} + c_i M_x^{(e)} + c_1 M_x^{(e)},
\]

\[
M_y^{(e)} = c_4 M_y^{(e)} + c_5 M_y^{(e)} + c_6 M_y^{(e)},
\]

\[
M_z^{(e)} = c_7 M_z^{(e)} + c_8 M_z^{(e)} + c_9 M_z^{(e)},
\]

where \( c_i (i = 1, 9) \) are the direction cosines connecting the Cartesian coordinate systems \( 0xyz \) and \( 0\xi\eta\zeta \) through Euler angles: rotation \( \phi \), precession \( \psi \), and nutation \( \theta \) defined by kinematic relations connecting projections of the instantaneous angular velocity vector with Euler angles and their derivatives:

\[
p = \dot{\psi} \sin \theta \sin \phi + \dot{\theta} \cos \phi, \quad q = \dot{\psi} \sin \theta \cos \phi - \dot{\theta} \sin \phi, \quad r = \psi \cos \theta + \dot{\phi}.
\]

The force effect on each atom of the \( C_{60} \) molecule can be determined by the following formulas:

\[
X_k = -\frac{\partial U}{\partial x}(r_k), \quad Y_k = -\frac{\partial U}{\partial y}(r_k), \quad Z_k = -\frac{\partial U}{\partial z}(r_k).
\]
Here $X_k$, $Y_k$, $Z_k$ are the projections of the forces acting on the $k$-th atom of the C$_{60}$ molecule from the side of the moving carbon atom, on the axis of the fixed reference frame, $r_j$ is the distance between the $k$-th atom of the molecule and the moving atom.

The initial conditions ($t = 0$) for solving the system of differential equations (1)–(2):

$$
\psi = \psi_0, \quad \theta = \theta_0, \quad \varphi = \varphi_0; \quad p = p_0, \quad q = q_0, \quad r = r_0, \quad v_{C} = 0, \quad r_{C} = 0.
$$

The calculation error was estimated using the energy balance equation for the particle-fullerene system

$$
\frac{mv_{C,0}^2}{2} + \frac{1}{2} A\omega^2 + \frac{m_a v_a^2}{2} + U = \frac{mv_{C,0}^2}{2} + \frac{1}{2} A\omega^2 + \frac{m_a v_a^2}{2} + U_0,
$$

where \( \omega = \left( p^2 + q^2 + r^2 \right)^{0.5} \) is the angular velocity C$_{60}$\[2\]. The maximum error of the calculations results presented in this paper is 0.028%.

3. Numerical solution results and their analysis

We consider fullerene C$_{60}$ at the initial instant of time ($t = 0$ s), rotating with an angular velocity $\omega_0$. Let the axis of rotation be oriented in the direction of the axis 0$y$, i.e. angular velocity components $(p, q, r) = (0, \omega_0, 0)$. As an object moving with an initial velocity $v_{a,0} = 300$ m/s towards the fullerene molecule, we take: a carbon (12 Da), xenon (131 Da) atoms and carbon structures with a molecular mass of 720 Da, which we denote like C, Xe and A$_{60}$ respectively. In order to simplify the analysis of the calculation results, we exclude from consideration the interaction with individual atoms of the carbon structures A$_{60}$. We suppose that the effect of fullerene on C, Xe and A$_{60}$ is determined only by the equation of motion of the center of mass similar to (2). Accordingly, the rotational component of the movement for C, Xe, A$_{60}$ will not be taken into account in the calculations.

Figure 3 shows the path of movement of A$_{60}$ (curve 1) and C$_{60}$ (curve 2) in the 0xy plane. At the initial moment of time, A$_{60}$ is at the point (−2, 0.4, 0), C$_{60}$ is (0, 0, 0). Figure 3 shows that A$_{60}$ deviates from its original direction of motion when approaching a fairly close distance to fullerene (curve 1), and continues to move at a certain angle to the 0x axis. The fullerene molecule also moves from its initial position. Figure 4 illustrates the effect of the mass of a moving particle on the precession motion of a rotating fullerene. The dashed curve corresponds to C, the solid curve corresponds to Xe, and the dashed curve to A$_{60}$. It is seen that with an increase in molecular weight (from C to A$_{60}$), the amplitude, number, and duration of oscillations of the magnitude of the component of the angular velocity $q$ increase. In this case, the precessional movement of C$_{60}$ begins at later times. It is worth noting that the components of the angular velocity $p$ and $r$ also change in the considered time interval.

![Figure 3. The trajectory of the particle (curve 1) and fullerene C$_{60}$ (curve 2)](image)

![Figure 4. Projection of the angular velocity on the C$_{60}$ axis](image)

Consider the C$_{60}$-A$_{60}$ system in the time range from 0.0036 to 0.004 ns, during which, according to Figure 4, the precession movement of C$_{60}$ is observed. Figure 5 shows the time dependence of the magnitude of the displacement of fullerene relative to the initial position, determined by the formula

$$
\Delta s = \left( x^2 + y^2 + z^2 \right)^{0.5}.
$$
The angular velocities \( \omega_0 = 0, 10^2, 10^3, 10^4 \) rad/ns correspond to curves 1, 2, 3, 4 respectively. It is seen that the smallest deviation was obtained for \( \omega_0 = 10^2 \) rad/ns, the largest deviation is for \( \omega_0 = 0 \) and \( 10^4 \) rad/s.

**Figure 5.** Time dependence of the deviation of the center of mass of the \( C_{60} \) molecule

Let \( \Delta s_0 \) be the deviation of the fullerene \( C_{60} \) from its initial position at \( \omega_0 = 0 \) rad/ns (\( \Delta s_0 = 6.4 \cdot 10^{-2} \) nm), \( \Delta s_\omega \) be the deviation at some value of \( \omega_0 \) that is non-zero. We introduce the quantity \( \varepsilon \) in the following form

\[
\varepsilon = \frac{\Delta s_\omega - \Delta s_0}{\Delta s_0} \times 100\%.
\]

Table 1 presents the results illustrating the influence of angular velocities and the orientation of the axis of rotation on the displacement \( \Delta s \) at time 0.004 ns relative to its position at time \( t = 0 \) s. Negative values of \( \varepsilon \) characterize lower values than at \( \omega_0 = 0 \) rad/ns, positive values indicate large values. From Table 1, it can be seen that the smallest \( \varepsilon \) was obtained at angular rotational speeds \( \omega_0 = 10^2 \) rad/ns and an axis of rotation \( C_{60} \) directed along the axis 0y.

**Table 1.** Effect of angular velocity and orientations of the rotation axis on the value of \( \varepsilon \).

| \((\rho_0, q_0, r_0)\) | \(\omega_0\), rad/ns | \(10^2\) | \(10^3\) | \(10^4\) |
|-----------------|-----------------|-----|-----|-----|
| \((\omega_0, 0, 0)\) | -3.8% | 2.7% | 2.2% |
| \((0, \omega_0, 0)\) | -7.9% | 1.2% | -4.0% |
| \((0, 0, \omega_0)\) | 5.4% | 3.4% | 2.0% |

**4. Summary**

As a result of numerical experiments, a manifestation of gyroscopic effects was discovered. It was found that the displacement of fullerene from its initial position depends on the choice of the initial angular velocity and the orientation of the rotation axis. Depending on the angle formed by the vectors of the angular velocity of rotation of the fullerene and the velocity of the incident particle, an increase or decrease in the deflection of the rotating fullerene was observed compared with the case of no rotation.

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**References**

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