# THE DYNAMIC SYMMETRY OF A MODEL SYSTEM OF TWO MOLECULES

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This work is devoted to the research of the dynamic symmetry for a model mechanical system of two identical spherical bodies relative to orthogonal transformations. The mechanical energy symmetry to the action of the reflection operator of a state vector is considered. For the model mechanism of the momentum and angular momentum exchange between the hard rough spheres, an explicit mathematical expression for the reflection operator is found.

## 1. Introduction

In this work, the attempt to find an effective method for the construction of the models of classical dynamic systems of two hard bodies is made. One of the methods, which is based on the dynamic symmetry of a physical system, consists in the use of the group theory (see, e.g., [1]). So, a certain class of model Hamiltonians keeps its form for the orthogonal and unitary groups of transformations of state vectors (see, e.g., [2]). In the presented work, starting from the principles of symmetry, we construct the equations which describes the connection between state vectors before and after the collision.

To describe a relation between the initial and final states of a classical system, we consider a symmetry of the total mechanical energy relative to linear transformations of the initial state vector. By a state vector of the system, we name the collection of coordinates, momenta, and own angular momenta of both bodies.

We have analyzed the properties of orthogonal transformations of twelve-dimensional state vectors (without taking the coordinates of the centers of masses into account), including the properties of the reflection operator.

As an example, the mechanisms of momentum and angular momentum exchanges between the rough hard particles are considered, and the opportunity of and the conditions for an application of the developed formalism to polyatomic molecules are discussed.

## 2. Orthogonal Transformation and Reflection Operator

Let us consider a transformation $\hat{S}$ in the twelve-dimensional linear phase space $\boldsymbol{X} = (\boldsymbol{P}, \boldsymbol{M}; \boldsymbol{P}', \boldsymbol{M}')$ which describes a change of the state vector under a collision of two identical bodies. For each body, the transformation $\hat{S}$ acts only on the momentum and angular momentum by virtue of the instantaneousness of the interaction and is defined by the condition of conservation of the state vector norm. In the matrix representation, we introduce the corresponding operator by the relation

$$\sum_j S_{ij}^T S_{jk} = \delta_{ik}, \tag{1}$$

where $S_{ij}^T = S_{ji}$. That is, we have a orthogonality condition for the transformation.

For orthogonal transformations, we have $\det S = \pm 1$ where the own values are $\pm 1$. Let's consider the case of a transformation with negative determinant: $\det S = -1$. This transformation can describes the irregular rotation of a vector (for example, the mirror reflection relative to some axis in the twelve-dimensional space). The operator $\hat{S}$ doesn't change the transformation axis direction. Let us write the equation for the eigenvectors:

$$\lambda \boldsymbol{X} = \hat{S} \cdot \boldsymbol{X}. \tag{2}$$

If the transformation has axis, then, for a vector lying on this axis, the own value will be 1.

For the mirror reflection operator, it is necessary that the squared operator will be equal to the identity one:

$$\hat{S}^2 = 1. \tag{3}$$

Hence, the own vector satisfying the equation $\boldsymbol{n} = \hat{S} \cdot \boldsymbol{n}$ sets an immovable axis. This axis can specify a hyperplane:

$$\boldsymbol{X} \cdot \boldsymbol{n} = 0.$$

The considered method looks like that described in [3] for the systems whose physical symmetry can be described by the groups of rotations $O_3$ and $SO_3$ and by the $SO_4$ group.

## 3. A Model Mechanism of the Exchange by Momentum and Angular Momentum upon a Collision of Two Spherically Symmetric Bodies

We will examine a specific realization of the reflection operator $\hat{S}$. To this end, we consider the behavior of two identical hard rough spheres, denoting their positions, momenta, and angular momenta by $(\boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}; \boldsymbol{q}', \boldsymbol{p}', \boldsymbol{M}')$, respectively. The particles moves freely if their phases are outside the area

$$|\boldsymbol{q}(t) - \boldsymbol{q}'(t)| \geq a \qquad \text{and}$$

$$|\boldsymbol{q}(t) - \boldsymbol{q}'(t) + \frac{\boldsymbol{p}'(t) - \boldsymbol{p}(t)}{m} \Delta t| < a, \;\; \Delta t \to 0, \tag{4}$$

where $a$ is the particle diameter, and $m$ is the particle mass. They collide according to the rule

$$\boldsymbol{X}^*(t) = \hat{S}(\boldsymbol{X}(t)) \cdot (\boldsymbol{X}(t)). \tag{5}$$

Here, $\hat{S}$ is real, and its action satisfies the following conditions in the phase space $\boldsymbol{X} = (\boldsymbol{p}, \boldsymbol{M}; \boldsymbol{p}^{'}, \boldsymbol{M}^{'})$:

1) The conservation of the total energy in the collision:

$$E^*{}_{\rm tr} + E'^*{}_{\rm tr} + E^*{}_{\rm rot} + E'^*{}_{\rm rot} =$$

$$= E_{\rm tr} + E'{}_{\rm tr} + E_{\rm rot} + E'{}_{\rm rot}, \tag{6}$$

where $E_{\rm tr}$, $E'{}_{\rm tr}$ and $E^*{}_{\rm tr}$, $E'^*{}_{\rm tr}$ are the initial and final translational energies of the first particle and the second one, respectively; $E_{\rm rot}$, $E'{}_{\rm rot}$ and $E^*{}_{\rm rot}$, $E'^*{}_{\rm rot}$ are the initial and final rotational energies of first particle and the second one, respectively. In terms of $(\boldsymbol{p}, \boldsymbol{M}; \boldsymbol{p}', \boldsymbol{M}')$, we can write down relation (6) as

$$\frac{1}{2m}\left(\boldsymbol{p}^{*2} + \boldsymbol{p}^{'*2}\right) + \frac{1}{2J}\left(\boldsymbol{M}^{*2} + \boldsymbol{M}^{'*2}\right) =$$

$$= \frac{1}{2m}\left(\boldsymbol{p}^{2} + \boldsymbol{p}^{'2}\right) + \frac{1}{2J}\left(\boldsymbol{M}^{2} + \boldsymbol{M}^{'2}\right), \tag{7}$$

where $J$ is the moment of inertia of the body.

2) The conservation of the total angular momentum for every particle in the c.m. system of two particles:

for the first body,

$$\frac{a}{2}\left[\boldsymbol{e} \times \frac{1}{2}(\boldsymbol{p}^* - \boldsymbol{p}^{'*})\right] + \boldsymbol{M}^* =$$

$$= \frac{a}{2}\left[\boldsymbol{e} \times \frac{1}{2}(\boldsymbol{p} - \boldsymbol{p}')\right] + \boldsymbol{M}, \tag{8}$$

for the second body,

$$\frac{a}{2}\left[\boldsymbol{e} \times \frac{1}{2}(\boldsymbol{p}^* - \boldsymbol{p}^{'*})\right] + \boldsymbol{M}^{'*} =$$

$$\frac{a}{2}\left[\boldsymbol{e} \times \frac{1}{2}(\boldsymbol{p} - \boldsymbol{p}')\right] + \boldsymbol{M}', \tag{9}$$

where $\left[\boldsymbol{e} \times \frac{1}{2}(\boldsymbol{p} - \boldsymbol{p}')\right]$ is the vector product of the vector $\boldsymbol{e}$ and the relative momentum $\frac{1}{2}(\boldsymbol{p} - \boldsymbol{p}')$; the three-dimensional vectors $\boldsymbol{p}, \boldsymbol{p}', \boldsymbol{p}^*, \boldsymbol{p}'^*$ are taken in the laboratory system, and each of the three-dimensional vectors $\boldsymbol{M}, \boldsymbol{M}', \boldsymbol{M}^*, \boldsymbol{M}'^*$ is taken in the c.m. system of the first particle and the second one, respectively (the own angular momenta); $\boldsymbol{e} = \dfrac{\boldsymbol{q}' - \boldsymbol{q}}{|\boldsymbol{q}' - \boldsymbol{q}|}$ is the unit vector aligned to the vector which joins the centers of two particles. Upon the collision, $|\boldsymbol{q}' - \boldsymbol{q}| = a$.

3) The conservation of the total momentum:

$$\boldsymbol{p}^* + \boldsymbol{p}'^* = \boldsymbol{p} + \boldsymbol{p}\prime. \tag{10}$$

4) For hard spheres, we set

a) the component of the vector of relative momentum $\frac{1}{2}(\boldsymbol{p} - \boldsymbol{p}')$ which is parallel to the vector $\boldsymbol{e}$ changes its sign on the opposite one after the collision:

$$(\boldsymbol{p}^* - \boldsymbol{p}^{'*})\boldsymbol{e} = -(\boldsymbol{p} - \boldsymbol{p}')\boldsymbol{e}; \tag{11}$$

b) the vector components $M_z$ and $M'_z$ which are parallel to $\boldsymbol{e}$ are invariable upon the collision:

$$M_z^* = M_z, \quad M_z'^* = M'_z, \quad \text{where axis} \quad 0z \parallel \boldsymbol{e}. \tag{12}$$

5) We assume that the operator $\hat{S}$ is a linear transformation in the real vector space $\boldsymbol{X}$:

$$\alpha\boldsymbol{X}_1^* + \beta\boldsymbol{X}_2^* = \hat{S}\cdot(\alpha\boldsymbol{X}_1 + \beta\boldsymbol{X}_2) =$$

$$\alpha\hat{S}\cdot\boldsymbol{X}_1 + \beta\hat{S}\cdot\boldsymbol{X}_2, \tag{13}$$

where $\alpha$, $\beta$ are real numbers.

In the new notation (calibration)

$$(\boldsymbol{p}, \boldsymbol{M}; \boldsymbol{p}', \boldsymbol{M}') \to \left(\frac{\boldsymbol{p}}{\sqrt{m}}, \frac{\boldsymbol{M}}{\sqrt{J}}; \frac{\boldsymbol{p}'}{\sqrt{m}}, \frac{\boldsymbol{M}'}{\sqrt{J}}\right), \tag{14}$$

the expressions satisfying conditions 1)—5) can look like

$$\boldsymbol{p}^* = \frac{1}{1+\varkappa}\Big\{\varkappa\boldsymbol{p} + \boldsymbol{p}' + \sqrt{\varkappa}[(\boldsymbol{M} + \boldsymbol{M}')\times\boldsymbol{\sigma}] -$$

$$-\varkappa\boldsymbol{\sigma}((\boldsymbol{p} - \boldsymbol{p}')\boldsymbol{\sigma})\Big\},$$

$$\boldsymbol{M}^* = \frac{1}{1+\varkappa}\Big\{\boldsymbol{M} - \varkappa\boldsymbol{M}' + \sqrt{\varkappa}[\boldsymbol{\sigma}\times(\boldsymbol{p} - \boldsymbol{p}')] +$$

$$+\varkappa\boldsymbol{\sigma}((\boldsymbol{M} + \boldsymbol{M}')\boldsymbol{\sigma})\Big\},$$

$$\boldsymbol{p}^{'*} = \frac{1}{1+\varkappa}\Big\{\varkappa\boldsymbol{p}' + \boldsymbol{p} - \sqrt{\varkappa}[(\boldsymbol{M} + \boldsymbol{M}')\times\boldsymbol{\sigma}] +$$

$$+\varkappa\boldsymbol{\sigma}((\boldsymbol{p} - \boldsymbol{p}')\boldsymbol{\sigma})\Big\},$$

$$\boldsymbol{M}^{'*} = \frac{1}{1+\varkappa}\Big\{\boldsymbol{M}' - \varkappa\boldsymbol{M} + \sqrt{\varkappa}[\boldsymbol{\sigma}\times(\boldsymbol{p} - \boldsymbol{p}')] +$$

$$+\varkappa\boldsymbol{\sigma}((\boldsymbol{M} + \boldsymbol{M}')\boldsymbol{\sigma})\Big\}, \tag{15}$$

where $\big(\boldsymbol{e}(\boldsymbol{M} + \boldsymbol{M}')\big)$ is the scalar product of the unit vector $\boldsymbol{e}$ by the three-dimensional vector $\big(\boldsymbol{M} + \boldsymbol{M}'\big)$. Here, we use the notation $\varkappa = \frac{ma^2}{4J}$.

Now we write down the operator $\hat{S}$ in the matrix form. For various bases of the space, in which $\boldsymbol{e}$ is not parallel to the $0Z$ axis, the matrices of a linear operator are similar matrices. Therefore, without loss of generality, we will examine the matrix in the coordinate system, in which the vector $\boldsymbol{e}$ is parallel to the $0Z$ axis. In this case, we have

$$(1+\varkappa)\cdot S(\boldsymbol{e}) = \begin{pmatrix}
\varkappa & 0 & 0 & 0 & \sqrt{\varkappa} & 0 & 1 & 0 & 0 & 0 & \sqrt{\varkappa} & 0 \\
0 & \varkappa & 0 & -\sqrt{\varkappa} & 0 & 0 & 0 & 1 & 0 & -\sqrt{\varkappa} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1+\varkappa & 0 & 0 & 0 \\
0 & -\sqrt{\varkappa} & 0 & 1 & 0 & 0 & 0 & \sqrt{\varkappa} & 0 & -\varkappa & 0 & 0 \\
\sqrt{\varkappa} & 0 & 0 & 0 & 1 & 0 & -\sqrt{\varkappa} & 0 & 0 & 0 & -\varkappa & 0 \\
0 & 0 & 0 & 0 & 0 & 1+\varkappa & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & -\sqrt{\varkappa} & 0 & \varkappa & 0 & 0 & 0 & -\sqrt{\varkappa} & 0 \\
0 & 1 & 0 & \sqrt{\varkappa} & 0 & 0 & 0 & \varkappa & 0 & \sqrt{\varkappa} & 0 & 0 \\
0 & 0 & 1+\varkappa & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\sqrt{\varkappa} & 0 & -\varkappa & 0 & 0 & 0 & \sqrt{\varkappa} & 0 & 1 & 0 & 0 \\
\sqrt{\varkappa} & 0 & 0 & 0 & -\varkappa & 0 & -\sqrt{\varkappa} & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1+\varkappa
\end{pmatrix}. \tag{16}$$

It is a symmetric matrix, and its determinant $\det S(\boldsymbol{e}) = -1$. Therefore, the squared transformation operator equals the identity operator.

We can say that matrix (16) is a representation of the operator of mirror hyperplane reflection. The hyperplane reflection corresponds to the following property of particle: the particle is hard, and this means that the torsion modulus and the tension modulus are infinitely large (the shear deformation and the torsional one are absent). It is the slipless collision. Moreover, the modulus of the state vector in new terms (14) $\left(\frac{\boldsymbol{p}}{\sqrt{m}}, \frac{\boldsymbol{M}}{\sqrt{J}}; \frac{\boldsymbol{p}'}{\sqrt{m}}, \frac{\boldsymbol{M}'}{\sqrt{J}}\right)$ is conserved upon the collision by the energy conservation law (the matrix determinant modulus is unity). We can say that the final state arises as a result of the mirror hyperplane reflection of the initial vector. The hyperplane is determined by the relative velocity of points of the contact of the particles. For example, we can see it clearly for some components of the state vector in Eq. (11). In the particular case of $\varkappa \to \infty$ and the zero rotation $\boldsymbol{M} = 0$, we have a simple model of elastic spherical particles.

If we neglect the attractive interaction between the polyatomic molecules, then they can be considered as hard bodies in a certain temperature range. To avoid the excitement of molecular vibrations, the average temperature of the system must be maintained in the appropriate range: for a wide class of molecules, the energy of molecular vibrations is higher than the energy of molecular rotations (see, e.g., [4]— [7]).

As for the nonspherical molecules, some results can be found in work [8] in the semiclassical approximation. But the expressions obtained there have a phenomenological character, and the results were derived without using the method described in the presented work.

## 4. Conclusion

The considered model of the dynamic system can be applied to the study of a low-density gas of non-polar polyatomic molecules in vacuum (see, e.g., work [9]).

Thus, we have analyzed the symmetry of the mechanical energy relative to the action of the reflection operator of a state vector. For the model mechanism of exchange by the momentum and angular momentum between two hard rough spheres, the explicit mathematical expression for the reflection operator is derived.

1. *Holod P.I., Klimyk A.U.* Mathematical Foundations of Symmetry Theory. — Kyiv: Naukova Dumka, 1992 (in Ukrainian).

2. *Kuznetsov G.I., Moskalyuk S.S.* The Graphic Theory of Representations of Orthogonal and Unitary Groups. — Kyiv: Naukova Dumka, 1992 (in Russian).

3. *Svidzyns'kyi A.* Mathematical Methods of Theoretical Physics. — Lutsk: Vezha, 2004 (in Ukrainian).

4. *Landau L.D., Lifshits E.M.* Statistical Physics. — Moscow: Fizmatlit, 2001 (in Russian).

5. *Biedenharn I.C., Louck J.D.* Angular Momentum in Quantum Physics. — Reading: Addison-Wesley, 1979.

6. *Herzberg G.* Molecular Spectra and Molecular Structure. — New York: van Nostrand, 1966.

7. *Nakamoto K.* Infrared Spectra and Coordination Compounds. — New York: Wiley, 1966.

8. *Singh S.N., Singh G.S., Kumar B.* // Physica A. — 1998. — **255**. — P. 293.

9. *Sizhuk A.S., Yezhov S.M.* // Ukr. J. Phys. — 2005. — **50**, N 10. — P. 1193—1201.

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ДИНАМІЧНА СИМЕТРІЯ МОДЕЛЬНОЇ СИСТЕМИ ДВОХ ТІЛ

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Р е з ю м е

Досліджено симетрію динаміки механічної модельної системи двох однакових тіл відносно ортогональних перетворень. Розглянуто симетрію механічної енергії системи щодо дії оператора відбиття на вектор стану двох тіл. Для модельного механізму обміну імпульсами та власними моментами імпульсу при зіткненні абсолютно твердих шорстких кульок знайдено явний вигляд оператора відбиття.