

D.M. NAPLEKOV,<sup>1</sup> V.V. YANOVSKY<sup>1,2</sup><sup>1</sup> Institute for Single Crystals, Nat. Acad. of Sci. of Ukraine  
(60, Nauky Ave., Kharkiv 61001, Ukraine; e-mail: napdmitry@gmail.com)<sup>2</sup> V.N. Karazin Kharkiv National University  
(4, Svobody Sq., Kharkiv 61022, Ukraine)

## INHOMOGENEITY OF THE IDEAL GAS OF A FINITE NUMBER OF PARTICLES WITH ANGULAR MOMENTUM CONSERVATION

UDC 536

We continue to study various aspects of the behavior of a classical ideal gas in a stationary axisymmetric container. The symmetry of the vessel leads to the conservation of the gas's angular momentum and, hence, the state of gas rotation. We consider the case of a nonrotating two-dimensional gas of a finite number of colliding particles. In this case, the gas statistical distributions differ from the classical ones found in the nineteenth century. We will show that the filling of the axisymmetric vessel with a nonrotating gas is not uniform and provide the exact spatial distribution of gas particles. This previously unknown distribution depends on all the particle masses and is found explicitly. The absence of a rotation in gas layers is shown through the investigation of the distributions of the tangential components of particle momenta. We also show that, for any number of particles in a container, the behavior of a massive enough particle may be unusual. The analytic results are confirmed by simple numerical experiments.

*Key words:* ideal gas, finite number of particles, statistical distribution, angular momentum, law of conservation, round vessel.

### 1. Introduction

An ideal gas of colliding particles inside a stationary vessel is a classical nonlinear model system. Usually, the limiting case of an infinitely large number of particles  $N \rightarrow \infty$  and an infinitely large vessel volume  $V \rightarrow \infty$  with the finite concentration of particles  $n = N/V$  is considered. For the specific insulated vessel with invariable shape, the gas's total energy is considered to be the only conserved quantity. The

momentum and angular momentum are generally not conserved upon collisions of the gas particles with the walls of the container. A number of classical results [1–5] are related to this case, such as the Boltzmann energy distribution  $p(E) \sim e^{-\frac{E}{kT}}$ , the Maxwell distribution of particle velocities, *etc.* A theorem about the uniform distribution of the energy over the degrees of freedom [6, 7] was proved under some assumptions. The exact limits of its applicability are still being debated [8, 9]. This case is the most deeply studied, but still there are new interesting results related to it [10, 11].

There are several factors that can lead to the establishment of distributions that differ from the standard ideal gas distributions. For example, the gas may have other conserved quantities, not only the energy. The distribution for the general case, when

Citation: Naplekov D.M., Yanovsky V.V. Inhomogeneity of the ideal gas of a finite number of particles with angular momentum conservation. *Ukr. J. Phys.* **69**, No. 1, 26 (2024). <https://doi.org/10.15407/ujpe69.1.26>.

Цитування: Наплеков Д.М., Яновський В.В. Некласичні розподіли ідеального газу скінченної кількості частинок із збереженням моменту імпульсу. *Укр. фіз. журн.* **69**, № 1, 26 (2024).

the total energy, momentum, and angular momentum of particles are conserved upon all collisions, was proposed by Maxwell in [12]. In the case of gas rotation, this distribution contains coordinate-dependent expressions added to the potential energy in order to account for the effect of centrifugal forces. In the general case, the logarithm of the distribution function is proportional not only to the energy, but to the linear combination of all additive conserved quantities [13]. A gas with an infinite number of degrees of freedom in the case of conservation of the angular momentum, as well as its generalizations to the relativistic and quantum cases, was considered in papers [14–16]. The need to consider the conservation of angular momentum may arise in a variety of areas from giant rotating molecular clouds in astronomy [17] to rotation and vortices in quantum gases [18], which play an important role in macroscopic quantum phenomena.

When an ideal gas is placed in a vessel, it is usually assumed that its statistical distributions are independent of the vessel's shape. However, in containers with axial symmetry, a stationary circular gas flow [19, 20] is possible. This is a consequence of the fact that, due to the boundary symmetry, the conservation of angular momentum is not violated upon collisions of the particles with the vessel walls. The difference between the round vessel and all the others for the gas of noncolliding particles was noticed by Poincaré [21]. Such a gas does not evenly fill the round vessel. In the general case, the shape of the vessel can significantly affect the equation of state of the gas of noncolliding particles [22].

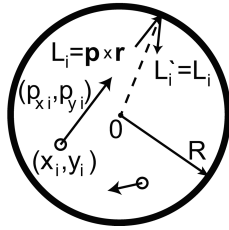
Another factor affecting the gas distributions is the number of gas particles and, accordingly, the system's total number of degrees of freedom (DoF number). In the usual limiting case of an infinite number of degrees of freedom, the total energy of the system is infinitely large, and there is a nonzero probability for a particle or some subsystem to have any arbitrarily large energy. An essentially different possible case is an ideal gas of a finite number of particles that has a finite DoF number [23, 24]. In this case, the energy of an entire system is finite, and a particle or a subsystem cannot have its energy higher than the total system energy. Therefore, their velocity and energy distributions proceed only to some finite value, and then they are exactly equal to zero. For a two-dimensional gas of a finite number of particles, Boltzmann, in his clas-

sical paper [2], obtained the particle energy distribution  $p^{(N)}(E) = (N-1) \frac{(E_{\text{tot}}-E)^{N-2}}{E_{\text{tot}}^{N-1}}$  for  $E \leq E_{\text{tot}}$  and  $p^{(N)}(E) = 0$  for  $E > E_{\text{tot}}$ , where  $N$  is the number of particles in the vessel, and  $E_{\text{tot}}$  is their total energy. This distribution does not depend on the masses or sizes of particles. All particles have the same distribution and the same average energy. By passing to the limit  $N \rightarrow \infty$  and  $E_{\text{tot}} \rightarrow \infty$  at  $E_{\text{tot}}/N = \text{const}$ , this distribution transfers into the Boltzmann distribution  $p_{\text{Bol}}(E) = \beta e^{-\beta E}$  for an infinite number of particles. During this limit transfer, the temperature appears as the value of the ratio  $E_{\text{tot}}/N = \frac{1}{\beta} = kT$ . It is worth to note that, although the concept of temperature is old and well-established, it continues to be of constant interest. Different ways of introducing the temperature and new related questions can be found in the review [25].

The interest in issues related to the finiteness of the number of degrees of freedom is associated with an increase in the interest in objects of small or nanoscale size. In particular, biological machines, such as monomolecular motors [26, 27], whose operating principles are currently not fully understood. These individual molecules are able to efficiently produce mechanical work, acting at the thermal energy level. The effect of internal degrees of freedom on the transport properties of molecules is also being actively studied [28, 29]. For example, the influence of the rotational degrees of freedom of  $C_{60}$  molecules during their stochastic motion over the surface of graphene is discussed in paper [28]. Of course, these examples consider systems with a finite number of degrees of freedom in contact with the medium. However, for their understanding, and not only for them, simple model cases which determine the basic effects and the main distributions are important. The new distribution of the energy in such a case was considered in our paper [20]. Now, we continue to study it, demonstrating other ideal gas distributions, and the key feature is the dependence on the masses of particles. Despite the fact that a usual nonrotating ideal gas in a stationary container is considered, these distributions are new and differ from the well-known classical results.

## 2. Gas in a Round Vessel

Let us consider the two-dimensional motion of a finite number  $N$  of colliding particles placed in a station-



**Fig. 1.** A stationary round vessel of radius  $R$  contains  $N$  particles with masses  $m_i$  and radii  $r_i$ . The angular momentum of a particle  $L_i$  remains unchanged after the reflection at any point of the vessel's boundary  $L'_i = L_i$ , due to its symmetry. Therefore, the total angular momentum of the gas  $L_{tot} = \sum_{i=1}^N (p_{yi}x_i - p_{xi}y_i)$  is the integral of motion, whose presence distinguishes the round (axisymmetric) containers

any circular container of radius  $R$ . All particles will be of a round shape with radii  $r_i$  and masses  $m_i$ , generally different. The motion of particles between collisions will be rectilinear and uniform, and all collisions of particles between themselves and with the vessel walls are absolutely elastic. Thus, we consider the classical model of a gas of absolutely rigid disks that do not interact at a distance, but collide with each other. The general view of this system is shown in Fig. 1. Both the case of negligibly small particles, corresponding to an ordinary ideal gas, and some deviations from it, associated with the finiteness of particle sizes, will be considered. The size of the vessel  $R$  will be finite since the concentration of particles should be finite. In a vessel of infinite size, several particles will forever scatter after a finite number of collisions.

In elastic collisions of particles with the walls of a stationary container, the energy of the particle after a reflection is equal to its energy before the collision, but the momentum of the particle changes at the reflection. The angular momentum of a particle is also not conserved in the general case, but the round vessel is special. The round boundary does not violate the invariance of the system under the rotation transformation, which is the origin of the angular momentum conservation. At each of its points, the circular boundary is locally perpendicular to the direction to the center of the vessel. For this reason, not only the momentum modulus, but also its shoulder do not change upon a reflection (see Fig. 1). Consequently, the particle's angular momentum  $L'_i$  remains equal to its initial angular momentum  $L_i$  after the reflection at any boundary point. When particles collide with each

other, the angular momentum is also conserved. As a result, the quantity  $L_{tot} = \sum_{i=1}^N (p_{yi}x_i - p_{xi}y_i)$  remains constant during the evolution, which means the conservation of the initial state of gas rotation. This distinguishes a round vessel (axisymmetric vessels in the 3D case) from all other possible vessels.

Further, we will consider the statistical behavior of the ideal gas in such a vessel. In order to unambiguously and repeatably determine the gas distributions, it is necessary to account for all the parameters on which they depend. In addition to the system parameters such as the particle masses, the gas distributions potentially depend on the values of all valid integrals of motion. These values are fixed, when the initial data are chosen. If, when choosing the initial data, only the total gas energy is taken into account, then the remaining integrals of motion will receive some random values. In particular, the gas in a round vessel will gain some random angular momentum. But the state of gas rotation also affects the gas distributions. Therefore, when choosing the initial data, the total gas angular momentum  $L_{tot}$  must be predefined. Here, we will consider a nonrotating gas, by choosing  $L_{tot} = 0$ . Despite the absence of a circular gas flow, the established gas distributions will still be different from those in other vessels.

### 3. Theoretical Consideration

Now, we will describe the theoretical approach used for the derivation of the required statistical distributions. We considered the system's phase space  $\Lambda = (x_1, \dots, x_N, y_1, \dots, y_N, p_{x1}, \dots, p_{xN}, p_{y1}, \dots, p_{yN})$ , with the phase variables being the coordinates and momentum components of all gas particles. The current state of the system is represented by a point in this space. During the evolution, this point fills some surface in the phase space, which is called invariant. The representing point does not fill all the phase space, because the phase variables are bound by the laws of conservation.

The general idea of our theoretical derivation of the gas distributions is straightforward. We calculate the filling density of the invariant surface, recalculate it to another probability density that can be integrated over the phase variables, and then do the integration to obtain the distributions of interest. Since the calculations are technically extremely cumbersome, we will present the results of the key derivation steps, omitting the details of the intermediate calculations.

For an insulated ideal gas of identical particles (if the energy is the only conserved quantity), the filling density of a constant energy surface is known to be uniform. In a more general case of different-mass particles, the filling density is also uniform with respect to the special measure. This measure is called gradient or ergodic and defines the hypervolume of the elementary surface part as  $d\Omega = \frac{d\Sigma}{|\text{grad } E|}$ , where  $d\Sigma$  is the element's hypervolume according to the usual Euclidean measure. For the system under consideration. The invariant surface is not the surface of constant energy, but its intersection with the surface of constant angular momentum. Its filling density can be obtained in a similar way to the derivation of the gradient measure, as follows:

$$d\rho_\Omega = \frac{\text{const } d\Sigma}{\sqrt{|\text{grad } E|^2 |\text{grad } L|^2 - (\text{grad } E \cdot \text{grad } L)^2}}. \quad (1)$$

This is the probability of finding a system in an elementary hypervolume  $d\Sigma$  (Euclidean) of a curvilinear  $2DN - 2$  - dimensional hypersurface. To obtain the required gas distributions, it must be integrated, which can be done in different ways. We represented the entire phase space as the direct product of two spaces  $\Lambda = \Lambda_1 \times \Lambda_2$ , where  $\Lambda_1 = (p_{xN}, p_{yN})$  and  $\Lambda_2 = (x_1, \dots, x_N, y_1, \dots, y_N, p_{x1} \dots p_{xN-1}, p_{y1}, \dots, p_{yN-1})$ . The equations of the invariant surface can be written as  $p_{xN} = f_1(x_1, \dots, p_{yN-1})$ ,  $p_{yN} = f_2(x_1, \dots, p_{yN-1})$ , thus expressing the momentum components of the last particle from the laws of conservation.

In principle, the invariant surface can be orthogonally projected onto the space  $\Lambda_2 = (x_1, \dots, p_{yN-1})$ , whose the dimension is equal to the dimension of the invariant surface. The corresponding projection filling density  $d\rho_{4N-2} = P(x_1, \dots, p_{yN-1}) dx_1, \dots, dp_{yN-1}$  can be further integrated directly over the phase variables. To calculate this probability density, we calculate how the elementary hypervolume of the invariant surface  $d\Sigma$  is related to the corresponding hypervolume of its projection onto the space  $\Lambda_2$ . Each of the set of  $4N$ -dimensional vectors  $\{dx_1, 0, \dots, 0\}, \dots, \{0, \dots, 0, dp_{yN-1}, 0\}$  that forms a  $\Lambda_2$  elementary hypervolume  $dx_1 \dots dp_{yN-1}$  is a projection of the corresponding  $4N$  vector lying on the invariant hypersurface  $\mathbf{v}_1 = \{dx_1, 0, \dots, 0, \frac{df_1}{dx_1} dx_1, 0, \dots, \frac{df_2}{dx_1} dx_1\}$ , ...,  $\mathbf{v}_{4N-2} = \{0, \dots, \frac{df_1}{dp_{yN-1}} dp_{yN-1}, 0, \dots, dp_{yN-1}, \frac{df_2}{dp_{yN-1}} dp_{yN-1}\}$ . The volume of an elementa-

ry parallelepiped spanned by the vectors  $\mathbf{v}_1 \dots \mathbf{v}_{4N-2}$  can be calculated as their vector product by adding, to them, one more vector  $\text{grad } E$  normal to all the others. We get

$$P(x_1, \dots, p_{yN-1}) = \frac{|\mathbf{v}_1 \times \dots \times \mathbf{v}_{4N-2} \times \text{grad } E|}{\text{const } |\text{grad } E|} \times \frac{1}{\sqrt{|\text{grad } E|^2 |\text{grad } L|^2 - (\text{grad } E \cdot \text{grad } L)^2}}. \quad (2)$$

This is a general expression for the probability density that the coordinates of gas particles will be  $x_1 \dots x_N, y_1, \dots, y_N$ , and the components of the momenta of particles will be  $p_{x1} \dots p_{xN-1}, p_{y1} \dots p_{yN-1}$ . The last two components,  $p_{xN}$  and  $p_{yN}$ , are determined by the laws of conservation. Let us substitute the explicit expressions for the energy and angular momentum into this general formula. After cumbersome calculations, we have obtained the following explicit form for this probability density:

$$P(x_1, \dots, p_{yN-1}) = \frac{\text{const}}{\sqrt{m_N (x_N^2 + y_N^2) \left( 2E_{\text{tot}} - \sum_{i=1}^{N-1} \frac{p_{xi}^2 + p_{yi}^2}{m_i} \right) - \left( \sum_{i=1}^{N-1} (p_{yi} x_i - p_{xi} y_i) \right)^2}}. \quad (3)$$

Further, we will integrate this expression over the phase variables within the appropriate limits to obtain the desired coordinate and momentum distributions. All of the integration limits will be finite, since both the gas energy and the vessel size are finite. The integration limits also account for the conservation of both integrals of motion, in particular, for the fact that a particle with mass  $m_1$  and energy  $E$  cannot be found at any point inside the vessel. It can only be located inside the strip of width

$$2\sqrt{\frac{(E_{\text{tot}} - E) \left( \sum_{i=2}^N m_i (x_i^2 + y_i^2) \right)}{m_1 E}},$$

oriented in the direction of the particle's momentum. Otherwise, the remaining energy will not be enough for other particles to compensate for the angular momentum of this particle.

#### 4. Gas Distributions in a Round Vessel

Now, we will consider the distributions for an ideal gas of a finite number of particles in a round ves-

sel. First, we consider the spatial density of the vessel filling with the gas. Since the gas under consideration consists of different particles, every single particle possesses its own probability density for its location at a distance  $r$  from the center of the vessel. To find this probability density for a particle with mass  $m_1$  (any particle may be named the first one), we have to integrate distribution (3) over all the components of momenta and the coordinates of all particles, but the first one. After the integration over the components of momenta, we have obtained:

$$p(r) = \int_{R_2=0}^R \dots \int_{R_N=0}^R \frac{\text{const} \prod_{i=2}^N R_i}{\sqrt{m_1 r^2 + J(R_2, \dots, R_N)}} dR_2 \dots dR_N. \quad (4)$$

Here,  $J(R_2, \dots, R_N) = \sum_{i=2}^N m_i R_i^2$  is the moment of inertia of other particles, and  $R_i = \sqrt{x_i^2 + y_i^2}$  is the distance to the center of the vessel;  $p(r)$  is the probability density to find a particle  $m_1$  in the vessel's elementary volume  $dx dy$  at a distance  $r$  from the vessel center. After the further integration over the particle positions, we have explicitly obtained this probability density as

$$p(r) = \text{const} \sum_{i=1}^{2^{N-1}} (-1)^{i+N} (m_1 r^2 + J_i)^{N-\frac{3}{2}}, \quad (5)$$

where  $J_i$  are all possible combinations of terms  $m_i R_i^2$  in the order of the growing number of such terms, starting from the empty one. Let us write out the first several distributions explicitly:

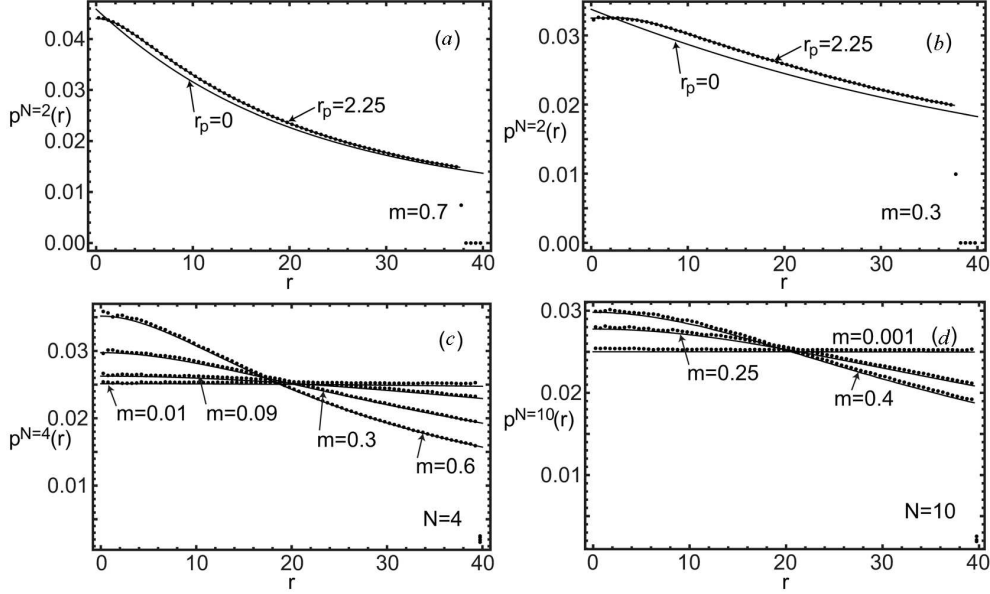
$$\begin{aligned} p^{\{N=2\}}(r) &= \text{const} [-(m_1 r^2)^{\frac{1}{2}} + (m_1 r^2 + m_2 R^2)^{\frac{1}{2}}]; \\ p^{\{N=3\}}(r) &= \text{const} [(m_1 r^2)^{\frac{3}{2}} - (m_1 r^2 + m_2 R^2)^{\frac{3}{2}} - \\ &\quad - (m_1 r^2 + m_3 R^2)^{\frac{3}{2}} + (m_1 r^2 + m_2 R^2 + m_3 R^2)^{\frac{3}{2}}]; \\ p^{\{N=4\}}(r) &= \text{const} [-(m_1 r^2)^{\frac{5}{2}} + (m_1 r^2 + m_2 R^2)^{\frac{5}{2}} + \\ &\quad + (m_1 r^2 + m_3 R^2)^{\frac{5}{2}} + (m_1 r^2 + m_4 R^2)^{\frac{5}{2}} - \\ &\quad - (m_1 r^2 + m_2 R^2 + m_3 R^2)^{\frac{5}{2}} - \\ &\quad - (m_1 r^2 + m_2 R^2 + m_4 R^2)^{\frac{5}{2}} - \\ &\quad - (m_1 r^2 + m_3 R^2 + m_4 R^2)^{\frac{5}{2}} + \\ &\quad + (m_1 r^2 + m_2 R^2 + m_3 R^2 + m_4 R^2)^{\frac{5}{2}}]. \end{aligned} \quad (6)$$

The plots of the spatial density distribution (5) and their comparison with the results of the numerical simulation of the particle motion are shown in Fig. 2. The simulation results are shown by dots, while continuous curves show theoretical distributions. It is evident that they are in good agreement. Thus, the spatial distribution of gas particles in a round vessel is found to be uneven. The most probable location of a particle is near the center of the vessel. The heavier the particle, the more uneven its distribution over the vessel's volume. In the case of the gas of particles with the same mass, its spatial distribution remains nonuniform. With the mass share of a particle tending to zero, its spatial distribution tends to be even. This can be explained theoretically, since  $p(r)$  in distribution (5) actually depends on  $m_1 r^2$ , and, with  $m_1$  being set to zero, the dependence on  $r$  disappears. But, for a nonzero-mass particle, its exact spatial distribution is uneven and depends on the masses of all gas particles.

The slight difference between simulation and theoretical results in Fig. 2 is due to the finiteness of a particle sizes. This difference is clearly visible in the case of two enlarged particles in Fig. 2, *a, b*. The gas of particles in a simulation is noideal due to their finite sizes, while the ideal gas of particles of negligible sizes was theoretically considered. But, such a nonideal gas can also be considered theoretically in a similar way. In order to account for the particle sizes, it is only necessary to change the area of integration in Eq. (4). All phase space regions corresponding to the intersection of particles must be excluded. The exact analytic description of such regions is complicated. In the simplest case of two particles in a vessel, for such spatial distribution corrected for the particle size  $r_p$ , we have obtained:

$$\begin{aligned} p_{r_p}^{\{N=2\}}(r) &= \text{const} \left( \int_{R_2=0}^{R-r_p} \frac{2\pi R_2 dR_2}{\sqrt{m_1 r^2 + m_2 R_2^2}} - \right. \\ &\quad \left. - \int_{y_2=r-2r_p}^{\min[r+2r_p, R-r_p]} \int_{x_2=-\sqrt{4r_p^2-(y_2-r)^2}}^{\sqrt{4r_p^2-(y_2-r)^2}} \frac{dx_2 dy_2}{\sqrt{m_1 r^2 + m_2(x_2^2 + y_2^2)}} \right). \end{aligned} \quad (7)$$

The first term repeats the all-area integration, and the second term corrects it for the excluded region. The limits of integration in the second term are



**Fig. 2.** The probability density distributions to find a particle with mass  $m$  at a distance  $r$  from the center of the round vessel of radius  $R = 40$ . Two particles of radius  $r_p = 2.25$  with masses (a, b)  $m_1 = 0.7$  (a) and  $m_2 = 0.3$  in the vessel (b). Dots show the results of the numerical simulation of the particle motion. Continuous curves show distributions (4) (no particle size account  $r_p = 0$ ) and Eq. (7). Four particles with masses  $m_i \in \{0.01, 0.09, 0.3, 0.6\}$  and size  $r_p = 0.45$  (c). Ten particles with masses  $m_i \in \{0.001, 0.004, 0.01, 0.015, 0.03, 0.06, 0.09, 0.14, 0.25, 0.4\}$  and size  $r_p = 0.45$  (d). It is seen that the smaller the particle mass share, the more uniformly it is distributed over the volume of the vessel

a bit simplified, which makes this expression not absolutely accurate. But, it is accurate enough to well agree with the results of a numerical simulation (see Fig. 2, a, b). The distributions for three or more finite-size particles can be obtained in a similar way, with the same difficulty of a cumbersome mathematical description of the excluded regions.

Thus, the obtained distributions show that the filling of a round vessel with a gas is not uniform. The probability of finding a particle in a unit volume depends on all the particles masses and decreases with the distance from the center of the vessel. For particles with almost zero mass share, this effect is minimal. With an increase in the number of particles in the vessel, the mass share of each of them decreases, tending to zero in the limit  $N \rightarrow \infty$ . Accordingly, if there are no supermassive particles, and if the gas's angular momentum is zero, then, with an increase in the number of particles, the gas will approach the even filling of the round vessel.

Let us now consider the momentum distributions of particles of the ideal gas in a round vessel. As with the spatial distributions, the momentum distributions of particles with different masses are different. The

momentum distribution appears to vary through the vessel depending on the location of a particle. For this reason, we will consider the distribution for a single particle  $m_1$  located at some distance  $r$  from the center of the vessel. The momentum of the particle can be decomposed into the radial and tangential components. The tangential component is of the greatest interest, since it allows one to judge the state of rotation of the gas layer at a given distance from the center of the vessel. To find the distribution of this component, we calculated the distribution of the momentum component  $p_{1x}$  of the particle  $m_1$  at the point  $x_1 = 0, y_1 = r$ , integrating distribution (3) over all the other variables. This distribution is also a distribution of the tangential momentum component at the given point. All other points at the same distance  $r$  will share the same distribution due to the system's symmetry. In this way, for the tangential component of the momentum of a particle  $m_1$  located at a distance  $r$ , we have obtained:

$$p(r, p_\tau) = A \int_{R_2=R_{\text{lim } 2}}^R \dots \int_{R_N=R_{\text{lim } N}}^R dR_2 \dots dR_N \times$$

$$\times \frac{((2E_{\text{tot}}m_1 - p_\tau^2)J(R_2, \dots, R_N) - m_1 p_\tau^2 r^2)^{N-2}}{J(R_2, \dots, R_N)^{N-3/2}} \prod_{n=2}^N R_n, \quad (8)$$

where  $A$  is the normalization constant, and the integration limits are:

$$R_{\text{lim } k} = \begin{cases} \sqrt{\frac{f(r, p_\tau, k)}{m_k}}, & f(r, p_\tau, k) \geq 0, \\ 0, & f(r, p_\tau, k) < 0 \end{cases} \quad (9)$$

and  $f(r, p_\tau, k)$  is:

$$f(r, p_\tau, k) = \frac{m_1 p_\tau^2 r^2}{2E_{\text{tot}}m_1 - p_\tau^2} - \sum_{i=2}^{k-1} m_i R_i^2 - \sum_{j=k+1}^N m_j R_j^2. \quad (10)$$

Due to the structure of the limits of integration, the resulting function consists of a number of branches corresponding to the fulfillment of the conditions within the limits of integration. Its explicit form in the general case is complicated.

The range of possible values of the particle's tangential momentum component  $p_\tau$  is limited by:

$$p_\tau^2 \leq 2E_{\text{tot}} m_1 \frac{\sum_{i=2}^N m_i R^2}{m_1 r^2 + \sum_{i=2}^N m_i R^2}. \quad (11)$$

It depends not only on the total energy  $E_{\text{tot}}$  and particle mass  $m_1$ , but it also decreases with the distance  $r$  from the center of the vessel. The comparison of distribution (8) with the results of the numerical simulation of the particle motion is shown at Fig. 3. The theoretical distribution (8) is in good agreement with the simulation results. It is also seen that all the distributions of the tangential momentum component for all particles are symmetric. A particle with any mass and at any place inside the vessel moves clockwise or counterclockwise with equal probability. This immediately follows from the probability density distribution (8), since it depends on the  $p_\tau^2$ . Hence, the probabilities for  $p_\tau$  and  $-p_\tau$  are always equal. Figures 3, *a-e* show how the three and ten particle distributions change with the distance from the center of the vessel. Figure 3, *f* shows separately the distribution of a heavy particle at different distances. In all cases, the tangential momentum distributions became narrower with the distance. This

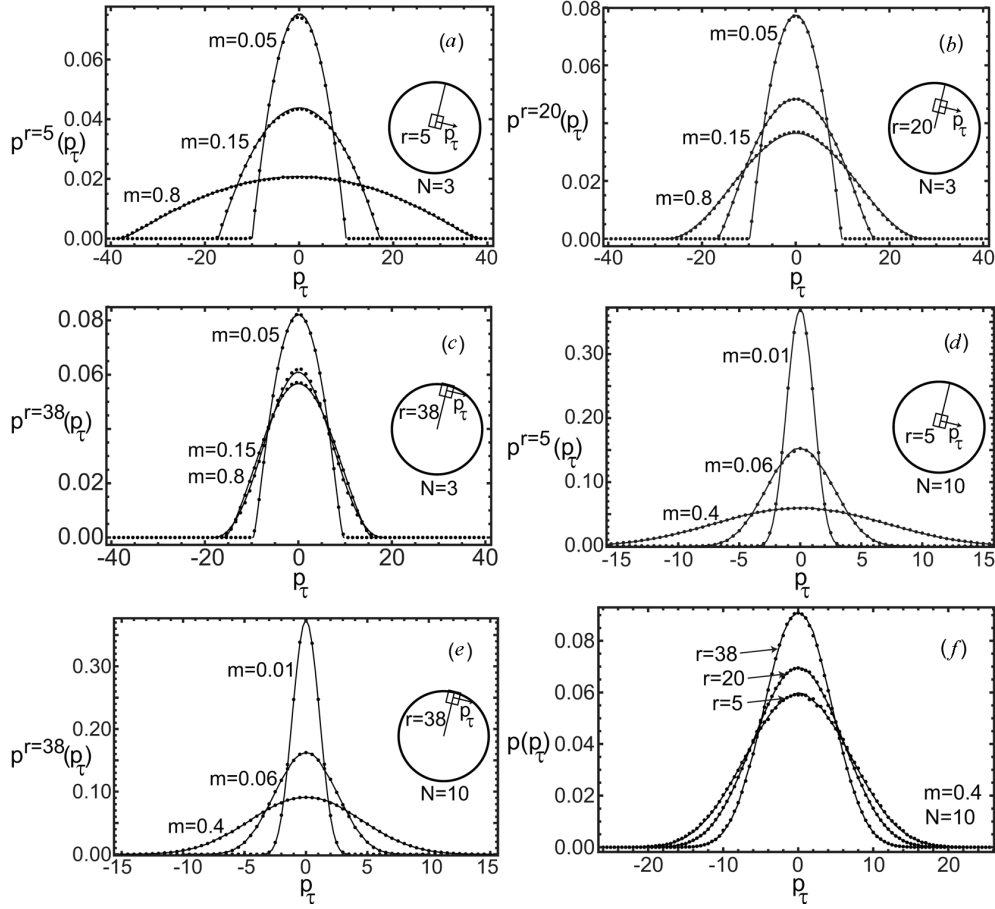
effect is more pronounced for heavy particles and minimal for particles with lower masses.

Thus, there is no preferred direction of motion for each individual gas particle at any place inside the round vessel. The zero total angular momentum of the gas corresponds to the total absence of the gas's rotation. Nevertheless, the distribution of the tangential momentum component depends on the position of the particle, unlike the other vessels. The further the particle is from the center of the vessel, the narrower the range of possible values of its tangential momentum. This effect is most pronounced for massive particles. The closer such a particle is to the boundary, the smaller its maximum possible tangential momentum. In other words, a heavy particle will never move along the round boundary at a high speed. Although such motion is allowed by the law of energy conservation, it is forbidden for massive particles by the law of conservation of angular momentum. For particles with a mass fraction close to zero, this effect is practically absent. They have almost identical distributions throughout the vessel.

The energy distributions and mean energies of ideal gas particles in a round vessel were considered in our paper [20]. Here, we will consider, in more details, how the particle energy distributions change with the growth of the number of particles in the vessel. For a particle of mass  $m_1$ , we have the previously obtained energy distribution:

$$P_{m_1}^{\{N\}}(E) = A \int_{\Lambda} \int dy_1^* dR_2 \dots dR_N \sqrt{R^2 - y_1^{*2}} \times \frac{((E_{\text{tot}} - E)J(R_2, \dots, R_N) - Em_1 y_1^{*2})^{N-\frac{5}{2}}}{J(R_2, \dots, R_N)^{N-2}} \prod_{n=2}^N R_n. \quad (12)$$

This energy distribution differs from the corresponding Boltzmann distribution  $p_{\text{Bol}}^{\{N\}}(E) = (N - 1) \frac{(E_{\text{tot}} - E)^{N-2}}{E_{\text{tot}}^{N-1}}$  at  $E \leq E_{\text{tot}}$ , and  $p_{\text{Bol}}^{\{N\}}(E) = 0$  at  $E > E_{\text{tot}}$ , where  $N$  is the number of particles, and  $E_{\text{tot}}$  is their total energy. The Boltzmann distribution does not depend on particle masses. Distribution (12) depends on all the particle masses and corresponds to the uneven mean energies of particles. Most essentially, the energy distribution of a particle depends on the mass share of this particle. If the mass of a particle  $m_1$  allows the term  $Em_1 y_1^{*2}$  to be neglected



**Fig. 3.** Distributions of the tangential component  $p_\tau$  of the momentum of a particle located at a distance  $r = (5, 20, 38)$  from the center of a round vessel of radius  $R = 40$ . The continuous curves show the theoretical distribution (8), dots show the simulation results. The case of three particles with masses  $m_i \in \{0.05, 0.15, 0.8\}$ , launched into the vessel (a–c). Ten particles with masses  $m_i \in \{0.001, 0.004, 0.01, 0.015, 0.03, 0.06, 0.09, 0.14, 0.25, 0.4\}$  in the vessel. All distributions are symmetric, showing the absence of a rotation in the gas layers (d–f). The change of the distribution of a massive particle with the distance from the center of the vessel (f)

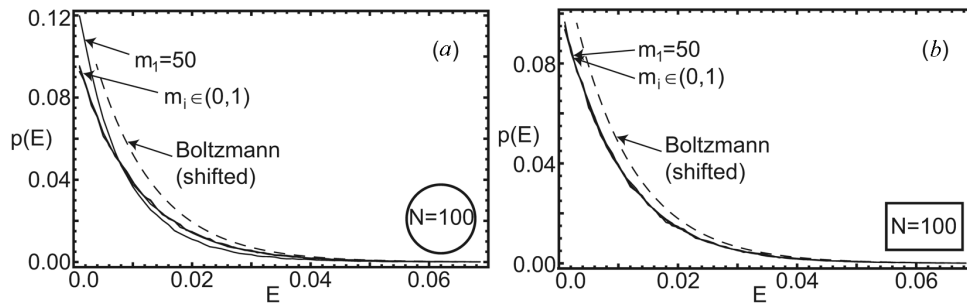
compared to  $(E_{\text{tot}} - E)J(R_2, \dots, R_N)$ , the limit of distribution (12) coincides with the limit of the Boltzmann distribution at  $N \rightarrow \infty$ . This will be the case where the number of particles  $N$  is large, and the particle  $m_1$  is not massive, so that its mass share can be considered close to zero. But if the particle is heavy enough, it is unclear from Eq. (12) what will be the result of its integration.

To account for the case of a gas with a massive particle, we have launched  $N = 100$  particles in the vessel, all but one with a random absolute mass within the range  $m_i \in (0, 0.01)$ ,  $i = 2, \dots, N$ , and one heavy particle with an absolute mass  $m_1 = 50$ . Thus, the mass of the first heavy particle is approximately equal

to the total mass of all the other particles. The size of this particle  $r_1 = 5$  was also greater than the size of other particles  $r_i = 1$ . For comparison, the same system of particles was launched into a rectangular vessel.

The experimentally obtained energy distributions for  $N = 100$  particles are shown in Fig. 4. The energy distributions of all particles in the rectangular vessel, including the massive one, completely coincided with the corresponding Boltzmann distribution (see Fig. 4, b). In the round vessel, the distributions of all particles, except for the heavy one, also practically coincide with the Boltzmann distribution, despite the difference in masses of these particles. At the





**Fig. 4.** Distributions of the particle energy in round and rectangular vessels with  $N = 100$  particles. The masses of all, but one, particles were random in the interval  $m_i \in (0, 0.01)$ , their size was  $r_i = 1$ ,  $i = 2, \dots, N$ . One more particle had a mass  $m_1 = 0.5$ , approximately equal to the total mass of all the other particles. The radius of this massive particle was  $r_1 = 5$ . The distribution of the energy of such a massive particle in a round vessel is different from the corresponding Boltzmann distribution (shown with a shifted dotted line), while the distributions of all the other particles practically coincide with it

same time, it is clearly visible that the distribution of the energy of a heavy particle in a round vessel is still different from the Boltzmann distribution. This result confirms the fact that the behavior of a particle depends on its mass share for any number of gas particles. If all particles are of comparable masses, then, with an increase in their number, the mass shares of all particles will become practically equal to zero. As a result, particles with equal mass shares have equal energy distributions and, hence, equal average energies. They will also fill the round vessel evenly. But, the behavior of a particle, sufficiently massive to have a nonzero mass share, will still be different even with a large number of particles in the vessel.

Thus, as the number of particles increases, the behavior of the ideal gas in a round vessel generally ceases to differ from its behavior in other vessels (only in the case of nonrotating gas  $L_{\text{tot}} = 0$ ). Particles tend to fill the vessel evenly, their momentum component distributions cease to depend on their location, and their energy distributions tend to the classical Boltzmann distribution. However, the behavior of a heavy and possibly large Brownian particle in a round vessel will still be unusual. The average energy of such a particle will be below the equipartition level, and its location will most probably be at the center of the vessel.

### 5. Exchange of Energy between Particles

Let us now consider, in more details, the energy exchange between particles whose average energies are at unequal levels. When the equilibrium is established, the long-time average energy of a particle does not change in time. Therefore, the amount of

the energy received by a particle in collisions with all the other particles must, on average, be equal to the amount lost by each single particle. Usually, such a balance is achieved with the mean energies of all particles being equal. But, in a round vessel, the mean energies of particles are generally different. They are also spatially distributed unevenly throughout the vessel. Therefore, it is interesting to find out how the energy is exchanged during particle collisions in a round vessel.

At each collision of two particles, some energy  $\Delta E$  is transferred from one particle to another one. From a theoretical point of view, this energy exchange is related to the subset of the invariant surface corresponding to the tangency of two particles (finite particle sizes are required). Its theoretical consideration is complicated; so, we will consider the distributions of the transferred energy  $\Delta E$  numerically. Let, for example, three particles with masses ( $m_i$ : 0.5, 0.35, 0.15) be launched into a round vessel. The distributions of the energy transferred in collisions of the first particle with the second and third ones are shown in Fig. 5. Each of these distributions is symmetric, which means the probability of receiving some energy in a collision is equal to the probability of giving that energy away. This also holds true for any pair of particles in a gas of a larger number of particles. Thus, there is a detailed equilibrium in the sense that what energy a particle receives on average from any other particle, it gives back to it. At the same time, the average energies of the gas particles may be significantly different.

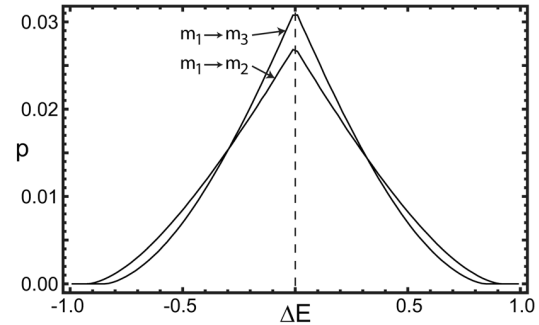
To explain how this happens, we note that if any of the particles has some angular momentum  $L$ , then the

remaining particles, in the case of a nonrotating gas, must have a  $-L$  total angular momentum. Hence, each of the particles moves against some counterflow, since the gas of the remaining particles rotates in the opposite direction with respect to the selected particle. This leads to an increase in the share of frontal collisions for every particle. It leads to a change in the statistical relationship between the energy transferred in collisions and the energies of colliding particles. Due to a different distribution of collision angles, in a round vessel, the balance of energy exchange is achieved with the mean particle energies being different. In this way, it is explained on a microscopical level how the angular momentum conservation leads to the violation of the energy equipartition.

## 6. Discussion

Usually, it is considered that the behavior of an ideal gas in the vessel does not depend on its shape. The coordinates and momentum components of all gas particles are considered to be possibly constrained only by the law of energy conservation. In this paper, we continue to study the special case of an ideal gas of particles, whose number is finite, with an additional quantity being conserved. The conservation of the angular momentum in a circular (axisymmetric) vessels leads to the gas distributions being different from the classical ideal gas distributions. These new distributions can be easily achieved in simple numerical experiments.

Thus, the existence of an additional conserved quantity may lead to a radical change in the behavior of a system, especially with a finite DoF number. It is obvious in the case of a gas with the angular momentum conservation, since it means the conservation of the state of gas rotation. Regardless of the number of particles, once the gas inside an axisymmetric vessel is rotated, it will never stop rotating. In other vessels, such a stationary circular gas flow is impossible. Even if the angular momentum is zero, the statistical gas distributions are still unusual. The spatial distribution of particles is uneven, the distributions of momentum components depend on the particle location, and the mean energies of different mass particles are different. For the same reason, for possible additional conserved quantities, deviations from the classical statistical distributions are possible in any



**Fig. 5.** Exchange of the energy between three particles with masses ( $m_i$ : 0.15, 0.35, 0.5). Shown are the distributions of the energy  $\Delta E$  transferred during collisions of the first particle  $m_1 = 0.15$  with the second and third particles. The probabilities of receiving and losing some energy  $\Delta E$  appear to be equal. The mean energies of the particles were ( $\langle E_i \rangle$ ): 0.364, 0.328, 0.308)

first-principles simulation. Such simulations are held in biophysics, physical chemistry, and many other fields.

## 7. Results

In this paper, the new statistical distributions are obtained for a nonrotating ideal gas of a finite number of particles placed inside a stationary round container. The spatial distribution of gas particles is found explicitly as Eq. (5). This distribution depends on all the masses of gas particles and corresponds to the uneven filling of the vessel with gas. The probability of finding a particle in a unit volume inside the vessel decreases with the distance from its center. With an increase in the number of particles, the vessel filling tends to be even, provided that the mass shares of all particles tend to be zero.

The distribution of the tangential momentum component of a gas particle is found in the form of a definite integral, Eq. (8). This exact distribution depends on all masses and on the position of the particle. It is always symmetric, which corresponds to the total absence of a gas rotation. For particles with a mass share close to zero, the spatial dependence of this momentum distribution practically disappears. Their energy distributions tend to follow the Boltzmann one, while particles with nonzero mass will have a significantly different energy distribution.

Thus, the exact ideal gas distributions in a round vessel differs from the known classical distributions. They depend on all the masses of the gas parti-

cles. With an increase in the number of particles, the behavior of a gas in a round vessel approaches that in other vessels, but only in the case of a nonrotating gas of particles with comparable masses.

1. J.W. Gibbs. *Elementary Principles in Statistical Mechanics* (Dover, 2015) [ISBN: 978-0486789958].
2. S.G. Brush. *The Kinetic Theory of Gases, an Anthology of Classic Papers with Historical Commentary* (Imperial College Press, 2003) [ISBN: 978-1783261055].
3. R. Kubo, H. Ichimura, T. Usui, N. Hashitsume. *Statistical Mechanics* (North-Holland, 1990) [ISBN: 978-0444871039].
4. J.S. Rowlinson. The Maxwell-Boltzmann distribution. *Mol. Phys.* **103**, 2821 (2005).
5. A.I. Khinchin. *Mathematical Foundations of Statistical Mechanics* (Dover, 1949) [ISBN: 978-0486601472].
6. J.C. Maxwell. *The Scientific Papers of James Clerk Maxwell* (Dover, 2013) [ISBN: 978-0486781662].
7. R.C. Tolman. A general theory of energy partition with applications to quantum theory. *Phys. Rev.* **11**, 261 (1918).
8. G. Magnano, B. Valesia. On the generalised equipartition law. *Ann. of Phys.* **427**, 168416 (2021).
9. A. Haro, R. Llave. New mechanisms for lack of equipartition of energy. *Phys. Rev. Lett.* **85**, 1859 (2000).
10. C. Jarzynski. Nonequilibrium equality for free energy differences. *Phys. Rev. Lett.* **78** (14), 2690 (1997).
11. M. Esposito, C. Van den Broeck. Three detailed fluctuation theorems. *Phys. Rev. Lett.* **104** (9), 090601 (2010).
12. J.C. Maxwell. A treatise on the kinetic theory of gases. *Nature* **16**, 242 (1877).
13. L.D. Landau, E.M. Lifshitz. *Statistical Physics. Vol. 5* (Elsevier Science, 2013) [ISBN: 978-0080570464].
14. F. Becattinia, L. Ferroni. The microcanonical ensemble of the ideal relativistic quantum gas with angular momentum conservation. *Eur. Phys. J. C* **52**, 597 (2007).
15. T.K. Nakamura. Relativistic statistical mechanics with angular momentum. *Prog. Theor. Phys.* **127**, 153 (2012).
16. I.M. Dubrovskii. The role of angular momentum conservation law in statistical mechanics. *Cond. Matt. Phys.* **11**, 585 (2008).
17. N. Imara, L. Blitz. Angular momentum in giant molecular clouds. I. The milky way. *ApJ* **732**, 78 (2011).
18. F. Chevy, K.W. Madison, J. Dalibard. Measurement of the angular momentum of a rotating Bose-Einstein condensate. *Phys. Rev. Lett.* **85**, 2223 (2000).
19. S. Chapman, T.G. Cowling, D. Burnett, C. Cercignani. *The Mathematical Theory of Non-uniform Gases: An Account of the Kinetic Theory of Viscosity, Thermal Conduction and Diffusion in Gases* (Cambridge University Press, 1990) [ISBN: 978-0521408448].
20. D.M. Naplekov, V.V. Yanovsky. Distribution of energy in the ideal gas that lacks equipartition. *Sci. Rep.* **13**, 3427 (2023).
21. H. Poincare. *Calcul des Probabilites* (Gauthier-Villars, 1912) [ISBN: 978-1114755871].
22. D.M. Naplekov, V.P. Semynozhenko, V.V. Yanovsky. Equation of state of an ideal gas with nonergodic behavior in two connected vessels. *Phys. Rev. E* **89**, 012920 (2014).
23. B.V. Chirikov, F.M. Izrailev, V.A. Tayursky. Numerical experiments on the statistical behaviour of dynamical systems with a few degrees of freedom. *Comp. Phys. Comm.* **5**, 116 (1973).
24. C.C. Zhou, Y.Z. Chen, W.S. Dai. Unified framework for generalized statistics: Canonical partition function, maximum occupation number, and permutation phase of wave function. *J. Stat. Phys.* **186**, 19 (2022).
25. A. Puglisi, A. Sarracino, A. Vulpiani. Temperature in and out of equilibrium: A review of concepts, tools and attempts. *Physics Reports* **709**, 1 (2017).
26. Y. Taniguchi, P. Karagiannis, M. Nishiyama, Y. Ishii, T. Yanagida. Single molecule thermodynamics in biological motors. *BioSystems* **88**, 283 (2007).
27. S. Toyabe, E. Muneyuki. Experimental thermodynamics of single molecular motor. *Biophysics* **9**, 91 (2013).
28. M. Jafary-Zadeh, C.D. Reddy, Y.W. Zhang. Effect of rotational degrees of freedom on molecular mobility. *J. Phys. Chem. C* **117**, 6800 (2013).
29. A.S. de Wijn. Internal degrees of freedom and transport of benzene on graphite. *Phys. Rev. E* **84**, 011610 (2011).

Received 11.09.23

Д. Наплеков, В. Яновський

#### НЕКЛАСИЧНІ РОЗПОДІЛИ ІДЕАЛЬНОГО ГАЗУ СКІНЧЕННОЇ КІЛЬКОСТІ ЧАСТИНОК ІЗ ЗБЕРЕЖЕННЯМ МОМЕНТУ ІМПУЛЬСУ

У цій статті ми продовжуємо вивчати різні аспекти поведінки класичного ідеального газу в стаціонарному осесиметричному контейнері. Симетрія контейнера приводить до збереження моменту імпульсу газу, а отже, стану його обертання. Ми розглядаємо випадок двовимірного газу з нульовим моментом імпульсу зі скінченною кількістю частинок. У цьому випадку статистичні розподіли газу відрізняються від класичних, знайдених у XIX сторіччі. У роботі показано, що заповнення осесиметричного контейнера таким газом не є рівномірним, і отримано у явному вигляді точний просторовий розподіл частинок газу. Цей раніше невідомий розподіл залежить від усіх мас частинок. Відсутність обертання шарів газу показано шляхом дослідження розподілу тангенціальних компонент імпульсів частинок. Також показано, що для будь-якої кількості частинок у контейнері поведінка досить масивної частинки може бути незвичною. Отримані аналітичні результати підтверджено простими чисельними експериментами.

*Ключові слова:* ідеальний газ, скінченна кількість частинок, статистичний розподіл, кутовий момент імпульсу, закон збереження, круглий контейнер.