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Ideal gas in the round vessel: different behaviour

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We consider classical ideal gas of a finite number of colliding particles in a stationary vessel. A special case of the round vessel is considered and, for comparison, the results for the rectangular vessel are provided. It is proved that the distributions of energy and velocity of gas particles differ from similar distributions in a rectangular vessel. The paper investigates the case when a finite number of particles in a round vessel has zero total angular momentum. It is shown that these distributions in a round vessel depend on the particle masses and differ from the known classical distributions. As the number of particles increases, the distributions tend to the Boltzmann distribution. Finiteness of the number of particles or degrees of freedom is important for understanding the properties of nanosystems.
Keywords: gas of colliding particles, round vessel, finite number particles, additional law of conservation, distributions.

Ідеальний газ у круглій ємності: відмінності поведінки. ***Д.М.Напльоков, В.В.Яновський.***
Розглянуто класичний ідеальний газ кінцевої кількості частинок у нерухомій ємності. Досліджено особливий випадок ємності круглої форми і для порівняння наводяться результати для ємності прямокутної форми. Доведено, що розподіли енергії та швидкості частинок газу у ємності круглої форми відрізняються від аналогічних розподілів у прямокутній ємності. Головна увага приділена випадку, коли кінцева кількість частинок у круглій посудині має нульовий загальний момент імпульсу. Доведено, що ці розподіли в круглій посудині залежать від мас частинок і відрізняються від відомих класичних розподілів. Зі збільшенням числа частинок ці розподіли наближаються до розподілу Больцмана. Розгляд кінцевої кількості частинок або ступенів свободи важливий для розуміння властивостей наносистем.

1. Introduction

The ideal gas of colliding particles in a stationary vessel is a classical model system. The behavior of strong chaotic systems is widely studied on its example. As a rule, one considers the limiting case of an infinitely large number of gas particles $N \to \infty$ and an infinitely large volume of the vessel $V \to \infty$, such that the concentration of particles $n = N/V$ remains finite. The vessel may be either insulated or in contact with a thermostat. In the case of an insulated vessel, the only conserved quantity is the total energy of the system. The momentum and angular momentum of the gas particles are not conserved upon collisions with the vessel walls. A number of classical results [1, 2, 3, 4] are related to this case, such as the Maxwell distribution of particles velocities $p(v) \sim v^2 \exp(-\frac{mv^2}{2kT})$, the Boltzmann or the Gibbs distributions $p(E) \sim \exp(-\frac{E}{kT})$, etc. A theorem about the uniform distribution of the energy over the degrees of freedom [5, 6] is proved. This case is the most deeply studied, but still there are new interesting results related to it, such as the Jarzynski relations [7], fluctuation theorems [8], etc.

There are several factors that may 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 its energy. The distribution for the general case, when the total energy, momentum, and angular momentum of particles have been conserved during all collisions, was proposed by Maxwell in [9]. 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 [10]. A gas with an infinite number of degrees of freedom in the case of conservation of angular momentum, as well as its generalizations to the relativistic and quantum cases, was considered in papers [11, 12, 13, 14]. The need to take into account the conservation of angular momentum may arise in a variety of areas, from giant rotating molecular clouds in astronomy [15], to rotation and vortices in quantum gases [16], which play an important role in macroscopic quantum phenomena.

When an ideal gas is placed in a vessel, it is usually assumed that the established statistical distributions will not depend on the vessel shape. However, in vessels with axial symmetry, a stationary circular gas flow [17] is possible. This is a consequence of the fact that, due to the boundary symmetry, the conservation of angular momentum is not violated. The presence or absence of conservation of gas angular momentum affects the gas statistical behavior and is related to the shape of the vessel. The difference between the round vessel and all the others was noticed by Poincare [18] for the gas of non-colliding particles. The gas of non-colliding particles does not evenly fill the round vessel. In the general case, the shape of the vessel can significantly affect the equation of state of such a gas [19]. For a gas of colliding particles, as shown in particular in this paper, the shape of the vessel boundary can also play an important role.

Another factor affecting gas distributions is the number of particles inside the vessel and, accordingly, the number of degrees of freedom. 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 non-zero probability for a particle or some subsystem to have an arbitrarily large energy. An essentially different possible case is an ideal gas consisting of a finite number of particles with a finite number of degrees of freedom [20, 21]. In this case, the energy of an entire system is finite, and a particle or 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. In particular, for a two-dimensional gas of a finite number of particles, Boltzmann in his classical paper [22] obtained the particles energy distribution $p^{(N)}(E) = (N-1)\frac{(E_{tot}-E)^{N-2}}{E_{tot}^{N-1}}$ for $E \leq E_{tot}$ and $p^{(N)}(E) = 0$ for $E > E_{tot}$, where N is the number of particles in the vessel, E_{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. This distribution also does not contain temperature, only the total energy of the system. It is interesting to note that although the concept of temperature is old and well-established, it continues to be of constant interest. Different ways of introducing temperature and new related questions can be found in the review [23]. These questions arise, for example, in connection with the experimental observation of negative temperatures, "fluctuations" of temperature in nanoscale systems, etc. Interest in issues related to the finiteness of the number of degrees of freedom and the finiteness of the system dimensions is associated with an increase in interest in objects of small or nano sizes.

In this paper, we consider the case when simultaneously takes place both the finiteness of the number of particles and the conservation of the gas angular momentum, fixed at zero value. The properties of such a system were studied mainly via numerical simulation, their analytical description is currently an open question. The paper shows that a new class of energy and momentum distributions is realized in such a gas, despite the fact that it is a usual non-rotating ideal gas in the stationary vessel.

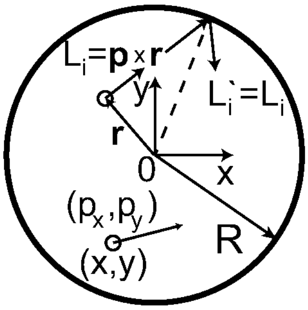

Fig. 1. A stationary round vessel of radius R contains n particles with masses m_i and radii r_i. Due to the vessel symmetry, the reflection of a particle from the vessels boundary does not change the value of its current angular momentum $L_i' = L_i$. The total angular momentum of the gas $L = \sum_{i=1}^{n}(p_{yi}x_i - p_{xi}y_i)$ in this case appears to be the additional integral of motion, unlike the other vessels.

2. Round vessel, angular momentum conservation.

Let's consider the motion of a finite number n of colliding particles in a stationary round vessel of radius R. We will consider the case of two-dimensional motion on a plane. Let all particles be of round shape with radii r_i and masses m_i, generally different. Their motion between collisions will be rectilinear, all collisions of particles between themselves and with the vessel boundary will be absolutely elastic. The general view of the considered system is shown in Fig.1.

The energy of the particle after elastic reflection from the stationary boundary is equal to its energy before the collision, but the momentum of the particle changes upon reflection. The angular momentum of the particle is also generally not conserved, but the round form of the boundary is a special case. The angular momentum of a particle L_i' after reflection from any point of the boundary remains equal to its initial angular momentum L_i (see Fig.1). In the collisions of particles, angular momentum is also conserved. As a result, the quantity $L = \sum_{i=1}^{n}(p_{yi}x_i - p_{xi}y_i)$ is being conserved during the motion of particles in the round vessel. This distinguishes a round-shaped vessel (axisymmetric vessels in the three-dimensional case) from all other possible vessels.

Further in the paper, the differences in the behavior of the ideal gas in such a vessel are studied. In order to unambiguously and repeatably determine or predict the gas parameters, for example, the energy distribution of some particle, it is necessary to take into account all that it depends on. In other vessels, it is sufficient to know the total gas energy and the number of particles in the vessel with their number of degrees of freedom. In a round vessel, knowledge of all system parameters and of total gas energy, as will be shown below, is not sufficient. The state of gas rotation will also affect the gas properties. Therefore, we will first discuss the necessity of taking into account all the integrals of motion when choosing the initial data of gas particles.

Potentially, the energy of a particle can depend on all the values of integrals of motion available for the system. These values are fixed when the initial data is chosen. If, when choosing the initial data, only the total energy of the gas is taken into account, then the remaining integrals of motion will receive some random values. In particular, a gas of particles in a round vessel will gain some random angular momentum. An interesting question is whether there are other global or local integrals of motion and whether it is possible to determine the presence of integrals of motion affecting the particle energy without knowing in advance about their existence.

Let's consider the time-averaged energy of some selected gas particle $< E(t_1) >= \frac{1}{t_1}\int_{t=0}^{t_1} E(t)dt$. The time t_1 will be finite since it is impossible to take an infinitely long time in the numerical calculation. The values of $< E(t_1) >$ for different initial data will differ due to two factors: the finiteness of the time t_1 and, possibly, the dependence of $< E >$ on the integrals of motion. By repeatedly randomly choosing initial data, one can construct the distribution $< E(t_1) >$ for the chosen particle and time t_1. As the time t_1 increases, the scattering associated with the finiteness of this time will decrease to zero. And the distribution will either turn into one definite value $< E >$, or some distribution will remain, showing the presence of factors not taken into account.

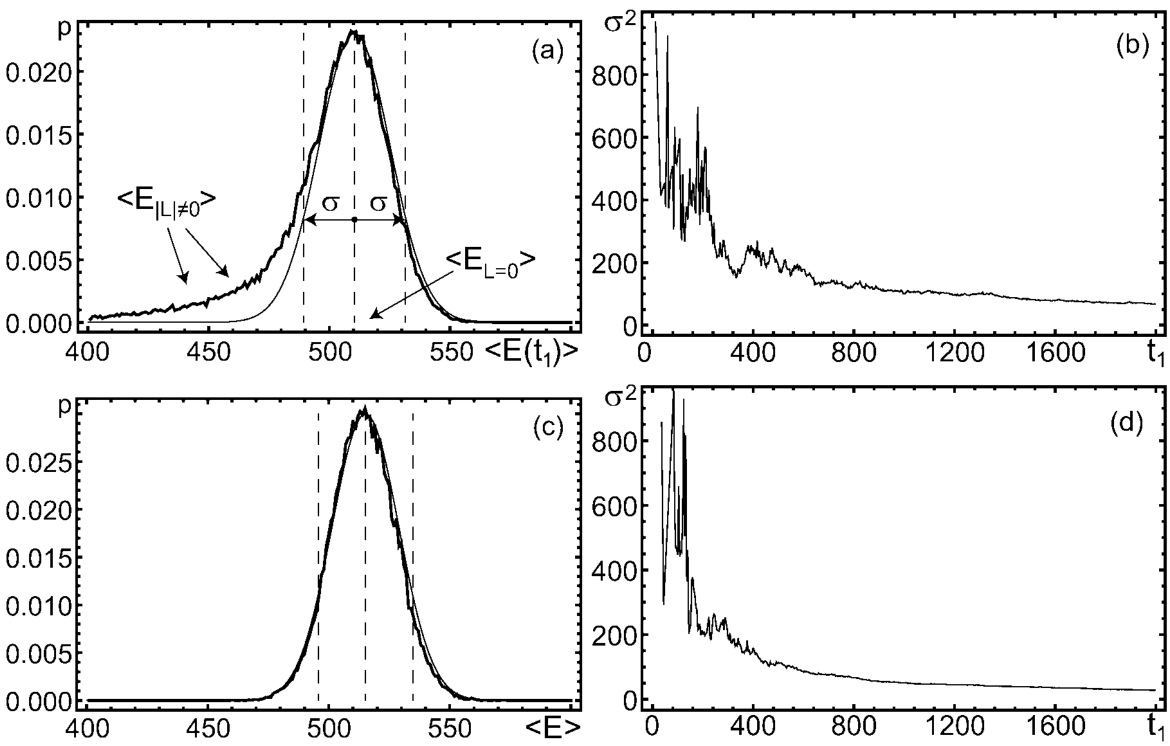

Fig. 2. Four particles are repeatedly launched into a round vessel with different initial conditions. The time-averaged energy of one of the particles is calculated each time. All parameters of the system are fixed, only the initial data changes. (a,c) The distribution of the averaged over a finite time $t_1 = 150$ energy of a particle with the mass $m_1 = 0.176$. During the choice of particles initial data (a) only the total energy was fixed, the asymmetry of the distribution is visible. This indicates the presence of an unaccounted integral of motion. (c) Both the energy and the angular momentum of particles are accounted for; the distribution is symmetrical. (b,d) The dependence of the dispersion σ^2 on time t_1 for corresponding average energy distributions. The dispersion is smaller for distributions with an angular momentum account. The masses of the remaining particles are $m_2 = 0.059$, $m_3 = 0.235$ and $m_4 = 0.53$. The size of all particles is $r_i = 1$, the vessel radius is $R = 40$.

Examples of the constructed $< E(t_1) >$ distributions for a vessel with four different particles are shown in Fig.2(a,c). In the first case, only the total energy of the system was fixed when choosing the initial data. It can be seen that in this case, the distribution is asymmetrical and does not coincide with the normal distribution. This asymmetry is a consequence of the fact that the angular momentum of the gas was not taken into account when choosing the initial data, and the established average energy depends on its value. Different initial data correspond to different L values, each of which corresponds to its own $< E >$ at $t_1 \to \infty$. The dependence of $< E >$ on L also takes place in the case of an infinitely large number of particles. According to Maxwell's paper [9], the particle energy E in the distribution $e^{-\beta E}$ is replaced by $E + w(p_x y - p_y x)$, and w is interpreted as the angular frequency of gas rotation. After appropriate averaging, taking into account the inhomogeneous distribution of particles over the vessel, the average particle energy remains dependent on w, i.e., the state of gas rotation. The case of a finite number of particles considered in this paper turns to that considered by Maxwell in the limit $N \to \infty$. Therefore, it is natural that for a finite number of particles, the energy depends on the state of gas rotation. Therefore, as time t_1 increases, the width of the average energy distribution will not decrease to zero, and instead of one certain value $< E >$, some distribution will remain. In the case shown in Fig.2(c), all initial data corresponded not only to the same total gas energy, but also to a fixed total angular momentum $L = 0$. This distribution coincides well with the normal distribution, and the scattering of $< E >$ values can only be related to the finiteness of time t_1.

As time t_1 increases, the width of the distribution in the first case should tend to some finite value, and to zero in the second case. The constructed distributions in the region of their maximum were approximated by a normal distribution. The width of this distribution can be characterized by the value of the standard deviation σ or the dispersion σ^2. Figures Fig.2(b,d) show the dependence of dispersion on time t_1 for both considered cases. It can be seen that in the second case, a smaller value of the dispersion is established than in the first case. Of course, with the help of a numerical calculation, it is impossible to determine that for $t_1 = \infty$ the dispersion of the average energy distribution will decrease precisely to zero. However, after taking into account the total angular momentum of the particles when choosing the initial data, the distribution of average particle energy no longer definitely indicates the presence of any other unaccounted integrals of motion.

Thus, the difference between the case under consideration and those considered earlier is the presence of one additional integral of motion affecting the behavior of the gas. Furthermore, when choosing the initial data, the particles total angular momentum will be set to zero ($L = 0$). All particle energies will be normalized to the total energy $E_{tot} = 1$. This is sufficient to ensure that the gas distributions and established energies are independent of the initial data. Despite the absence of a circular gas flow, they will still differ from similar distributions in other vessels.

3. Energy and velocity distributions

Let us now consider the distributions of the particle energy E_i and the velocity projection V_{xi}, in the case of a finite number of gas particles. For particles in rectangular and other vessels, the distribution of energy was first obtained by Boltzmann as $p_{Bol}(E) = (n-1)\frac{(E_{tot}-E)^{n-2}}{E_{tot}^{n-1}}$. The probability of a particle having some energy does not depend on the mass of that particle. Now, let four particles of the same size but with different masses be launched into a round vessel. The numerically constructed distributions for these particles are shown in Fig.3. Since the energy of each particle cannot exceed the total energy of the system, all distributions are exactly zero for energies greater than $E_{tot} = 1$ and, accordingly, for velocities outside the range $V_{xi} \in (-\sqrt{\frac{2E_{tot}}{m_i}}, \sqrt{\frac{2E_{tot}}{m_i}})$. Since in the considered system the momentum of particles is not conserved, the distributions proceed up to these limiting values of energy and velocity. In the possible case of both energy and momentum conservation, the entire system energy could not pass to one particle. In such a case, other distributions would be established with other limiting values. As it follows from Fig.3(a), the energy distributions of particles of different masses do not coincide with one another and, thus, do not coincide with the classical Boltzmann distribution.

Let us consider in more detail how particles with different energy distributions stay in equilibrium in a round vessel. To do this, we have launched three groups of three identical particles into a round vessel. The particles of the first group have masses $m_{1,2,3} = 0.017$, the second group of particles $m_{4,5,6} = 0.090$ and the third group $m_{7,8,9} = 0.226$. The form of energy distributions for these particles is shown in Fig.4(a). It can be seen that with an increase in the number of particles in the vessel, the distributions of particles of different masses approach each other and approach the Boltzmann distribution. However, the difference is still much greater than the limitations associated with the accuracy of numerical calculation.

When two particles collide, a certain amount of energy is transferred from one particle to another. Let us now consider how this energy exchange occurs in collisions between particles from different groups. Figure4(b) shows the number of collisions during the evolution of the system, in which particles from different groups collided and energy transferred was within a certain range. It can be seen that each of these distributions is symmetrical, the maximum of the distributions coincides with a zero transferred energy. Thus, all groups of particles are in equilibrium with each other in the sense that how much energy one group receives from another, the same amount it returns to it.

The energy and momentum distributions of particles in the considered case can, in principle, be obtained analytically. One of the possible ways, in the most general terms, is to consider a new invariant surface in the phase space of the system, construct an analogue of the microcanonical distribution and integrate it to obtain all distributions of interest. However, the construction of such a theory that generalizes statistical physics to the case of a system with a finite number of degrees of freedom and with additional integrals of motion is a large-scale and currently unsolved problem. Nevertheless, we can give some par-

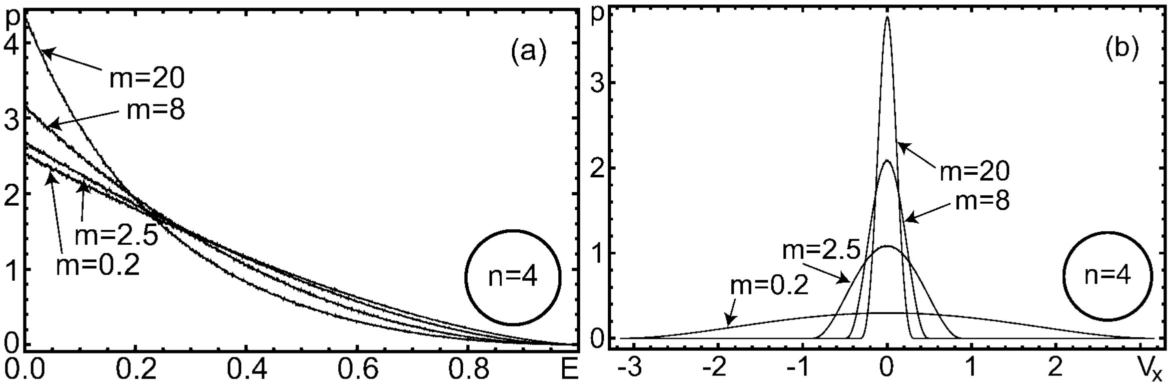

Fig. 3. Distributions of energy and velocity for four particles with masses $m_1 = 0.2$, $m_2 = 2.5$, $m_3 = 8.0$, and $m_4 = 20.0$. Particles are located in the round vessel $R = 40$ and have the same size $r_i = 1$. Their distributions are naturally truncated at $E_i = E_{tot} = 1$ and $V_{xi} = \pm\sqrt{2}E_{tot}m_i$, and then equal to zero. It is visible that the distribution of the particle's energy depends on its mass, in contrast to the identical, mass-independent distributions in a rectangular vessel.

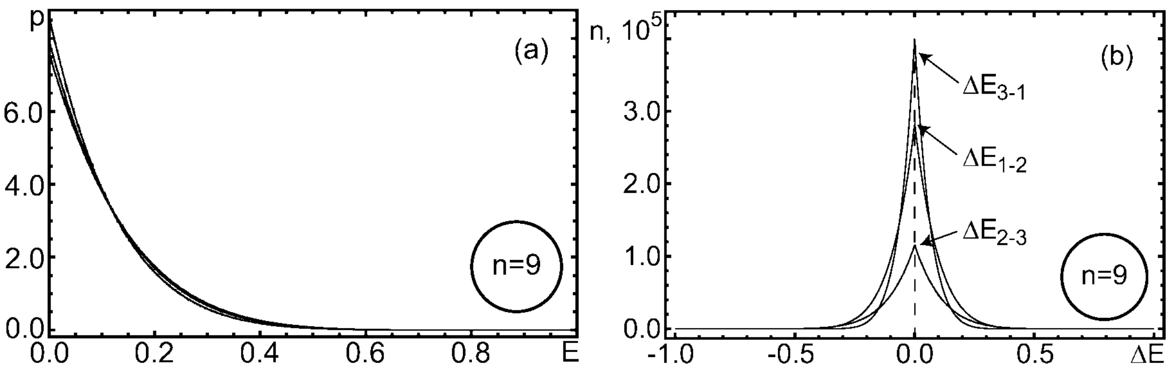

Fig. 4. Distributions for three groups of three identical particles launched into a round vessel of radius $R = 40$. Masses of particles $m_{1,2,3} = 0.017$, $m_{4,5,6} = 0.09$ and $m_{7,8,9} = 20.0$, the size of all particles is $r = 2.0$. (a) Particles energy distributions. In the case of nine particles, their distributions are not that different as in the case of four particles in the vessel. (b) Energy exchange between groups of particles. The distributions of the energy transferred during collisions of particles from different groups are shown. It can be seen that despite the different energy distributions, each group is in equilibrium with the other two groups.

ticular analytical results for the simplest cases, considered numerically in this paper. We present them below without derivation, as phenomenological expressions that well describe the experimental curves.

The curve of a momentum projection distribution in the case when there are three identical (with equal masses) particles with zero total angular momentum in a round vessel is analytically well described by the following definite integral:

$$P_{rnd}(p_{x_1}) = \int_{p_{y_1}=-\sqrt{p_{max}^2-p_{x_1}^2}}^{\sqrt{p_{max}^2-p_{x_1}^2}} \int_{y_2=-R}^{R} \int_{x_2=-\sqrt{R^2-y_2^2}}^{\sqrt{R^2-y_2^2}} \int_{y_3=-R}^{R} \int_{x_3=-\sqrt{R^2-y_3^2}}^{\sqrt{R^2-y_3^2}} \int_{y_1^*=\max(-y_{1lim},-R)}^{\min(y_{1lim},R)} \int_{x_1=-\sqrt{R^2-y_1^{*2}}}^{\sqrt{R^2-y_1^{*2}}} \int_{p_{x_2}=p_{x_2min}}^{p_{x_2max}} \int_{p_{x_3}=p_{x_3min}}^{p_{x_3max}} \frac{const}{\sqrt{F(\mathbf{p},\mathbf{r})}}\, dp_{y_1} dy_2 dx_2 dy_3 dx_3 dy_1^* dx_1 dp_{x_2} dp_{x_3} \quad (1)$$

where the function under integration:

$$F(\mathbf{p},\mathbf{r}) = (p_{max}^2 - p_{x_1}^2 - p_{x_2}^2 - p_{x_3}^2 - p_{y_1}^2)(x_2^2 + x_3^2) - (p_{x_2}y_2 + p_{x_3}y_3 + \sqrt{p_{x_1}^2 + p_{y_1}^2}\, y_1^*)^2$$

const is a dimensional normalization constant calculated from the condition

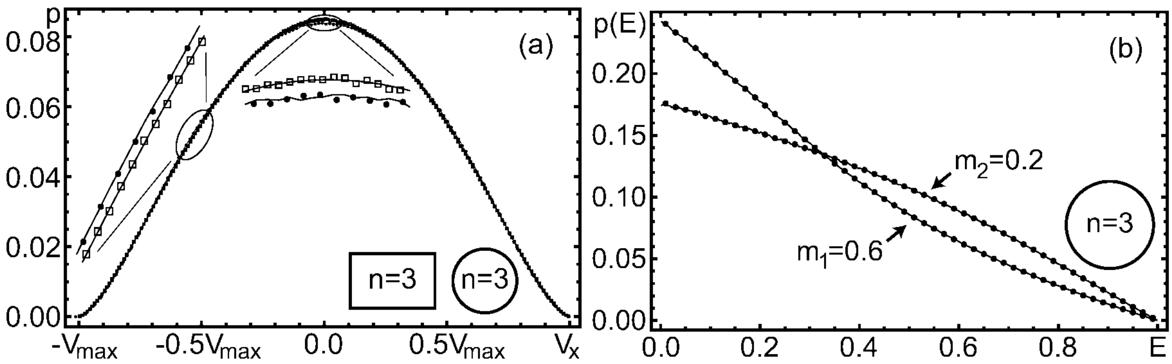

Fig. 5. (a) Distributions of the momentum projection for three identical particles in round and rectangular vessels. Circles and rectangles show the results of the simulation of particles motion in round and rectangular vessels, respectively. The continuous curves show the form of these distributions according to Eq.2 and Eq.1. It is visible that even in the case of equal average energies of particles, momentum distributions in round and rectangular vessels are noticeably different. (b) Distributions of energy in a round vessel, in the case of three particles, one of which has a mass $m_1 = 0.6$, and the other two have the same mass $m_2 = 0.2$. The continuous curves show the form of these distributions according to Eq.3 and Eq.4, the circles show the results of numerical simulation.

$$\int_{p_{x_1}=-p_{max}}^{p_{max}} P_{rnd}(p_{x_1}) dp_{x_1} = 1.$$

and the quantities within the limits of integration:

$$y_{1lim} = \frac{\sqrt{p_{max}^2-(p_{x_1}^2+p_{y_1}^2)}}{\sqrt{p_{x_1}^2+p_{y_1}^2}}\sqrt{x_2^2+y_2^2+x_3^2+y_3^2}$$

$$p_{x_2min} = \frac{-\sqrt{p_{x_1}^2+p_{y_1}^2}\,y_1^* y_2-\sqrt{(x_2^2+x_3^2+y_3^2)((p_{max}^2-p_{x_1}^2-p_{y_1}^2)(x_2^2+y_2^2+x_3^2+y_3^2)-(p_{x_1}^2+p_{y_1}^2)y_1^{*2})}}{x_2^2+y_2^2+x_3^2+y_3^2}$$

$$p_{x_2max} = \frac{-\sqrt{p_{x_1}^2+p_{y_1}^2}\,y_1^* y_2+\sqrt{(x_2^2+x_3^2+y_3^2)((p_{max}^2-p_{x_1}^2-p_{y_1}^2)(x_2^2+y_2^2+x_3^2+y_3^2)-(p_{x_1}^2+p_{y_1}^2)y_1^{*2})}}{x_2^2+y_2^2+x_3^2+y_3^2}$$

$$p_{x_3min} = \frac{-(\sqrt{p_{x_1}^2+p_{y_1}^2}\,y_1^*+p_{x_2}y_2)y_3-\sqrt{(x_2^2+x_3^2)((p_{max}^2-p_{x_1}^2-p_{y_1}^2-p_{x_2}^2)(x_2^2+x_3^2+y_3^2)-(\sqrt{p_{x_1}^2+p_{y_1}^2}\,y_1^*+p_{x_2}y_2)^2)}}{x_2^2+x_3^2+y_3^2}$$

$$p_{x_3max} = \frac{-(\sqrt{p_{x_1}^2+p_{y_1}^2}\,y_1^*+p_{x_2}y_2)y_3+\sqrt{(x_2^2+x_3^2)((p_{max}^2-p_{x_1}^2-p_{y_1}^2-p_{x_2}^2)(x_2^2+x_3^2+y_3^2)-(\sqrt{p_{x_1}^2+p_{y_1}^2}\,y_1^*+p_{x_2}y_2)^2)}}{x_2^2+x_3^2+y_3^2}$$

Here and below, when choosing the integration region, particle sizes were not taken into account. A similar distribution for three particles in a rectangular vessel has the form:

$$P_{rec}(p_x) = \frac{8(p_{max}^2 - p_x^2)^{3/2}}{3\pi p_{max}^4} \tag{2}$$

The graphs of these two distributions are nearly identical, as shown in Fig.5(a). However, these two analytical expressions do not exactly coincide with each other. The circles and rectangles in Fig.5(a) show the results of the numerical simulation of particles motion in the corresponding vessels. It can be seen that, within the accuracy of the calculation, the distributions obtained in the numerical experiment completely coincide with the corresponding analytical expressions. Thus, even if the particles in the round vessel are identical and their total angular momentum is zero, conservation of angular momentum still changes the shape of their distributions, albeit insignificantly.

Let us now consider the distributions of particle energy in the case when there is one particle with mass m_1 and two more particles with equal masses m_2 in a round vessel. The total angular momentum of these three particles is zero. The energy distribution of the first particle can be described by the following expression:

$$P_{rnd}(E_1) = \int_{y_2=-R}^{R}\int_{x_2=-\sqrt{R^2-y_2^2}}^{\sqrt{R^2-y_2^2}}\int_{y_3=-R}^{R}\int_{x_3=-\sqrt{R^2-y_3^2}}^{\sqrt{R^2-y_3^2}}\int_{y_1^*=\max(-y_{1lim},-R)}^{\min(y_{1lim},R)}\int_{x_1=-\sqrt{R^2-y_1^{*2}}}^{\sqrt{R^2-y_1^{*2}}} \int_{p_{x_2}=p_{x_2min}}^{p_{x_2max}}\int_{p_{x_3}=p_{x_3min}}^{p_{x_3max}} \frac{const}{\sqrt{F_1(E_1,\mathbf{p},\mathbf{r})}}\, dy_2 dx_2 dy_3 dx_3 dy_1^* dx_1 dp_{x_2} dp_{x_3} \tag{3}$$

where the integrated function:

$$F_1(E_1,\mathbf{p},\mathbf{r}) = (2(E_{tot}-E_1)m_2 - p_{x_2}^2 - p_{x_3}^2)(x_2^2+x_3^2) - (p_{x_2}y_2 + p_{x_3}y_3 + \sqrt{2E_1m_1}y_1^*)^2$$

and the quantities within the integration limits:

$$y_{1lim} = \sqrt{\frac{m_2}{m_1}}\sqrt{\frac{E_{tot}-E1}{E1}}\sqrt{x_2^2+y_2^2+x_3^2+y_3^2}$$

$$p_{x_2min} = \frac{-\sqrt{2E_1m_1}y_1^*y_2 - \sqrt{(x_2^2+x_3^2+y_3^2)(2m_2(E_{tot}-E_1)(x_2^2+y_2^2+x_3^2+y_3^2)-2E_1m_1y_1^{*2})}}{x_2^2+y_2^2+x_3^2+y_3^2}$$

$$p_{x_2max} = \frac{-\sqrt{2E_1m_1}y_1^*y_2 + \sqrt{(x_2^2+x_3^2+y_3^2)(2m_2(E_{tot}-E_1)(x_2^2+y_2^2+x_3^2+y_3^2)-2E_1m_1y_1^{*2})}}{x_2^2+y_2^2+x_3^2+y_3^2}$$

$$p_{x_3min} = \frac{-(\sqrt{2E_1m_1}y_1^*+p_{x_2}y_2)y_3 - \sqrt{(x_2^2+x_3^2)((2m_2(E_{tot}-E_1)-p_{x_2}^2)(x_2^2+x_3^2+y_3^2)-(\sqrt{2E_1m_1}y_1^*+p_{x_2}y_2)^2)}}{x_2^2+x_3^2+y_3^2}$$

$$p_{x_3max} = \frac{-(\sqrt{2E_1m_1}y_1^*+p_{x_2}y_2)y_3 + \sqrt{(x_2^2+x_3^2)((2m_2(E_{tot}-E_1)-p_{x_2}^2)(x_2^2+x_3^2+y_3^2)-(\sqrt{2E_1m_1}y_1^*+p_{x_2}y_2)^2)}}{x_2^2+x_3^2+y_3^2}$$

The energy distribution of the second particle:

$$P_{rnd}(E_2) = \int_{y_1=-R}^{R}\int_{x_1=-\sqrt{R^2-y_1^2}}^{\sqrt{R^2-y_1^2}}\int_{y_3=-R}^{R}\int_{x_3=-\sqrt{R^2-y_3^2}}^{\sqrt{R^2-y_3^2}}\int_{y_2^*=\max(-y_{2lim},-R)}^{\min(y_{2lim},R)}\int_{x_2=-\sqrt{R^2-y_2^{*2}}}^{\sqrt{R^2-y_2^{*2}}} \int_{p_{x_1}=p_{x_1min}}^{p_{x_1max}}\int_{p_{x_3}=p_{x_3min}}^{p_{x_3max}} \frac{const}{\sqrt{F_2(E_2,\mathbf{p},\mathbf{r})}}\, dy_1dx_1dy_3dx_3dy_2^*dx_2dp_{x_1}dp_{x_3} \quad (4)$$

where the integrated function:

$$F_2(E_2,\mathbf{p},\mathbf{r}) = (2(E_{tot}-E_2) - p_{x_1}^2/m_1 - p_{x_3}^2/m_2)(m_1x_1^2+m_2x_3^2) - (p_{x_1}y_1 + p_{x_3}y_3 + \sqrt{2E_2m_2}y_2^*)^2$$

and the quantities within the integration limits:

$$y_{2lim} = \sqrt{\frac{E_{tot}-E2}{E2}}\sqrt{\frac{m_1}{m_2}(x_1^2+y_1^2)+x_3^2+y_3^2}$$

$$p_{x_1min} = \frac{-m_1\sqrt{2E_2m_2}y_2^*y_1 - \sqrt{m_1(m_1x_1^2+m_2(x_3^2+y_3^2))(2(E_{tot}-E_2)(m_1(x_1^2+y_1^2)+m_2(x_3^2+y_3^2))-2E_2m_2y_2^{*2})}}{m_1(x_1^2+y_1^2)+m_2(x_3^2+y_3^2)}$$

$$p_{x_1max} = \frac{-m_1\sqrt{2E_2m_2}y_2^*y_1 + \sqrt{m_1(m_1x_1^2+m_2(x_3^2+y_3^2))(2(E_{tot}-E_2)(m_1(x_1^2+y_1^2)+m_2(x_3^2+y_3^2))-2E_2m_2y_2^{*2})}}{m_1(x_1^2+y_1^2)+m_2(x_3^2+y_3^2)}$$

$$p_{x_3min} = \frac{-m_2(\sqrt{2E_2m_2}y_2^*+p_{x_1}y_1)y_3 - \sqrt{\frac{m_2}{m_1}(m_1x_1^2+m_2x_3^2)((2m_1(E_{tot}-E_2)-p_{x_1}^2)(m_1x_1^2+m_2(x_3^2+y_3^2))-m_1(\sqrt{2E_2m_2}y_2^*+p_{x_1}y_1)^2)}}{m_1x_1^2+m_2(x_3^2+y_3^2)}$$

$$p_{x_3max} = \frac{-m_2(\sqrt{2E_2m_2}y_2^*+p_{x_1}y_1)y_3 + \sqrt{\frac{m_2}{m_1}(m_1x_1^2+m_2x_3^2)((2m_1(E_{tot}-E_2)-p_{x_1}^2)(m_1x_1^2+m_2(x_3^2+y_3^2))-m_1(\sqrt{2E_2m_2}y_2^*+p_{x_1}y_1)^2)}}{m_1x_1^2+m_2(x_3^2+y_3^2)}$$

These two distributions are shown in Fig.5(b) as continuous curves. The circles show the distributions obtained by the numerical simulation of particles motion. It is visible that the provided analytical expressions well coincide with the distributions observed in the numerical experiment. These distributions are qualitatively different from the corresponding Boltzmann three-particle distribution. The energy distribution for two lighter particles turns out to be convex, i.e., it has a negative second derivative. The distribution for a heavier particle has a slight inflection in the initial part of the distribution. Thus, the considered distributions qualitatively depend on the masses of the particles. In principle, they also depend on the particles sizes, but the associated amendments are usually negligible.

As a result, the energy and momentum distributions of particles in a round vessel depend significantly on the masses of these particles and may differ significantly from the classical Boltzmann distributions established in vessels of other forms. The fewer particles in a round vessel and the greater the spread of their masses, the more significant this difference will be. For particles of the same mass or for a sufficiently large number of particles of comparable masses, the difference from classical distributions is minimal.

4. Results.

Usually, when an ordinary ideal gas is considered, it is assumed that the shape of a vessel with gas does not affect its properties. In this paper, we study a special case when the choice of the symmetric vessel boundary leads to unusual distributions of energy and momentum of gas particles. The mechanism of vessels form influence on the gas statistical distributions is its connection with the laws of conservation. The reflection of particles from a circular boundary, due to its symmetry, does not violate the law of conservation of angular momentum, which means the conservation of an initial state of gas rotation. In this paper, we considered a gas with a small number of particles and with zero total angular momentum $L = 0$. It was shown that the presence of an additional law of conservation still leads to the different gas behavior.

The steady average energy of a particle means that the average energies received and lost in collisions are equal. In other vessels, this balance is achieved when the energy distributions of all gas particles are equal. In the round vessel, gas of a small number of different particles is found to be in such state of equilibrium when the particles have different energy distributions. This difference is easily determined via numerical simulation of particles motion.

The energy and momentum distributions of particles in the round vessel can differ significantly from the corresponding classical Boltzmann distributions. There is currently no theoretical description that gives a general analytical form of these distributions (for a finite number of particles). In this paper, some particular analytical results are presented for the case of three particles in a round vessel, but mainly this system was considered numerically. The constructed distribution functions for a finite number of particles are concentrated over a finite region, outside of which they are equal to zero. The forms of these distributions depend on the masses of gas particles. The smaller is the number of particles in the vessel, and the greater the spread of their masses, the more significantly the obtained distributions differ from the corresponding Boltzmann distributions.

References

1. Gibbs J W 2014 *Elementary principles in statistical mechanics* (New-York:Dover), 2014.
2. Boltzmann L 1912 *Vorlesungen uber Gastheorie* (Leipzig: Ambrosius Barth)
3. Rowlinson J S 2005 The Maxwell-Boltzmann distribution *Molecular Physics*, **103** 2821-2828
4. Hincin A Y 1943 *Mathematical justification of statistical mechanics* (M.-L.: Gostechizdat)
5. Maxwell J C 2003 Illustrations of the Dynamical Theory of Gases *The Scientific Papers of James Clerk Maxwell* (New-York: Dover)
6. Boltzmann L 1876 Uber die Natur der Gasmolekule *Wiener Berichte* **74** 553-560
7. Jarzynski C 1997 Nonequilibrium Equality for Free Energy Differences *Phys. Rev. Lett.* **78** 2690
8. Esposito M and Van den Broeck C 2010 Three Detailed Fluctuation Theorems *Phys. rev. lett.* **104** 090601
9. Maxwell J C 1877 The kinetic theory of gases *Nature* **16** 242
10. Landau L D and Lifshitz E M 2013 *Statistical Physics: Volume 5* (?? : Elsevier Science),
11. Becattinia F and Ferroni L 2007 The microcanonical ensemble of the ideal relativistic quantum gas with angular momentum conservation *Eur. Phys. J. C* **52** 597-615
12. Nakamura T K 2012 Relativistic Statistical Mechanics with Angular Momentum *Prog. Theor. Phys.* **127** 153
13. Thomas M W and Snider R F 1970 Boltzmann Equation and Angular Momentum Conservation *J. of Stat. Phys.* **2** 61
14. Dubrovskii I M 2008 The role of angular momentum conservation law in statistical mechanics *Cond. Matt. Phys.* **11** 585-596
15. Imara N and Blitz L 2011 Angular momentum in giant molecular clouds. I. The milky way *The Astrophysical Journal*, **732** 78
16. Chevy F, Madison K W and Dalibard J. 2000 Measurement of the Angular Momentum of a Rotating Bose-Einstein Condensate *Phys. Rev. Lett.* **85** 2223
17. Chapman S, Cowling T G, Burnett D and Cercignani C 1990 *The Mathematical Theory of Non-uniform Gases: An Account of the Kinetic Theory of Viscosity, Thermal Conduction and Diffusion in Gases* (Cambridge:Cambridge University Press)
18. Poincare H 1912 *Calcul des probabilites* (Paris:Gauthier-Villars)

19. Naplekov D M, Semynozhenko V P and Yanovsky V V 2014 Equation of state of an ideal gas with nonergodic behavior in two connected vessels, *Phys. Rev. E* **89** 012920
20. Chirikov B V, Izrailev F M and Tayursky V A 1973 Numerical experiments on the statistical behaviour of dynamical systems with a few degrees of freedom *Comp. Phys. Comm.* **5** 11-16
21. Kozlov V V 2002 On justification of Gibbs distribution *Regular And Chaotic Dynamics* **7** 1-10
22. Brush S G 2003 *The Kinetic Theory of Gases, an Anthology of Classic Papers with Historical Commentary* (London:Imperial College Press)
23. Puglisi A *et al* 2017 Temperature in and out of equilibrium: A review of concepts, tools and attempts *Physics Reports* **709** 1-60