International Journal of Pure and Applied Mathematics
Volume 119 No. 4 2018, 717-726
ISSN: 1311-8080 (printed version); ISSN: 1314-3395 (on-line version)
url: http://www.ijpam.eu
doi: 10.12732/ijpam.v119i4.13

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MATHEMATICAL DESCRIPTION OF THE EQUILIBRIUM STATE OF SYMMETRIC PARTICLE SYSTEMS

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Abstract: One-dimensional symmetric system of particles (hard spheres) is considered in this paper. In equilibrium state of this system, the limit distribution of the configuration Gibbs distribution in the Boltzmann-Grad limit ($d \to 0$, n is fixed) is uniform (the speed distribution is the Maxwell one and is unchanged).

AMS Subject Classification: 35Q82
Key Words: BBGKY hierarchy of equations, Maxwell speed distribution, symmetric particle system, equilibrium state

1. Introduction

The mathematical basis of the description of the evolution of dynamical systems of particles (hard spheres) is the BBGKY hierarchy of equations [1, 2, 3, 4]. However, in some cases, simpler approaches can be applied. In particular, these approaches are applied to one-dimensional system of hard spheres.

The main feature of such a system is that there are no changes of speeds of colliding particles, there is exchange of speeds. Thus, there is no change in the speed distribution function. This function is specified by an initial distribution

Received: February 22, 2018
Revised: Jule 30, 2018
Published: August 10, 2018

which can be arbitrary. For example, as the initial distribution, we choose the Maxwell speed distribution:

$$\varphi(v) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{v^2}{2\sigma^2}},$$

where $\sigma = \sqrt{\frac{kT}{m}}$ is a root-mean-square speed.

2. Formulation of the Problem

Consider one-dimensional symmetric system of N identical particles (hard spheres) with the mass $m = 1$ and the diameter $2d > 0$ moving along the segment of the straight line with a length of L. Each particle is characterized by the coordinate of the centre q_i of the sphere and by its momentum p_i, i.e. $(q_i,\, p_i) = x_i$.

By the Gibbs hypothesis, the equilibrium state is described by the distribution function that has the form

$$f(x_1, \ldots, x_N) = \Xi^{-1} e^{-\beta H_N^L}$$

where β is inversely proportional to the temperature T, the statistical sum

$$\Xi = \int\limits_{(L\times R^1)^N} dx_1 \ldots dx_N e^{-\beta H_N^L},$$

the Hamiltonian

$$H_N^L = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N-1} \Phi(|q_i - q_{i+1}|) + \sum_{i=1}^{N} u^L(q_i),$$

the pair hard-core interaction potential

$$\Phi(|q|) = \begin{cases} +\infty, & |q_i - q_{i+1}| \le 2d, \\ 0, & |q_i - q_{i+1}| > 2d, \end{cases}$$

the set of forbidden configurations

$$W_N = \{(q_1, \ldots, q_N) \in L: \ |q_i - q_{i+1}| \le 2d \text{ at least for a single pair}$$

$$(q_i,\ q_{i+1}),\ i = \overline{1,\ N-1}\},$$

the set of permissible configurations

$$L \setminus W_N = \{(q_1, \ldots, q_N) \in L : \ |q_i - q_{i+1}| > 2d, \ i = \overline{1, \ N-1}\},$$

the holding potential

$$u^L(q) = \begin{cases} +\infty, & q < d, \ q > L - d, \\ 0, & d < q < L - d. \end{cases}$$

For this system, we assume that

- initial speeds v_i and coordinates q_i of particles are independent random variables;
- speed distributions are not degenerate;
- the mathematical expectation $\bar{v}_i = 0$ and the function $\varphi(v_i)$ is even.

Nearest neighbours interaction is typical for this system. However, collisions lead to the exchange of speeds (particles as though pass through each other), which actually eliminates mixing of speeds. Thus, the speed distribution function is unchanged.

Let the particles be located in the interval $\left[-\frac{L}{2}, \ \frac{L}{2}\right]$ at the initial moment of time. Assuming that $L \to \infty$, we neglect the influence of the boundaries on the particles motion. In this case, the distribution function of the system state at arbitrary moment of time t can unambiguously be expressed in terms of the distribution function at $t = 0$:

$$D(q_1, v_1; q_2, v_2; \ldots; t) = D_0(q_1 - v_1 t, v_1; q_2 - v_2 t, v_2; \ldots)$$

where $(q_i - v_i t, \ v_i)$ is the system state at $t = 0$, $(q_i, \ v_i)$ is the system state at arbitrary moment of time t. This relation underlines the fact that this one-dimensional symmetric system can be considered as the system of non-interacting particles.

Thus, the system can be described by considering the motion of each particle independently from each other.

We assume that sizes of particles tend to zero because

- we can consider particle sizes in the initial distribution function D_0 (the presence of forbidden configurations),
- the coordinates of centres can be redetermined to consider sizes of particles.

The concentration can be considered a small fixed value and the average distance $\frac{1}{n}$ between particles can be considered significantly larger than sizes of particles, i.e. $\frac{1}{n} \gg 2d$.

3. Equilibrium State of Symmetric Systems of Particles (Hard Spheres) in the Boltzmann-Grad Limit

The following theorem is true.

Theorem 1. *The limit distribution of the configuration Gibbs distribution in the Boltzmann-Grad limit ($d \to 0$, n is fixed) which describes equilibrium state of one-dimensional symmetric system of particles (hard spheres) is uniform (the speed distribution is the Maxwell one and is unchanged).*

Proof. Let, at the initial moment of time, the zero particle be at the point with the coordinate $q_0^{(0)} = 0$ and has the speed v_0. We find the distribution function of the coordinate of its first collision. First, we find the probability that any other particle (let us denote it by number one) has no collisions with the zero particle in the time interval $[0, t_1]$. Let this particle have the coordinate $q_1^{(0)}$ and the speed v_1 for $t = 0$. There being nearest neighbours interaction, particles exchanging momenta as though pass through each other. Then in order to calculate the time of the collision of the chosen particle (the zero particle), the collisions of other particles with each other should not be considered, that is to say the collision of the zero particle with any other. Let us prove this statement graphically.

Graphs of laws of motion of several particles are shown in Figure 1.

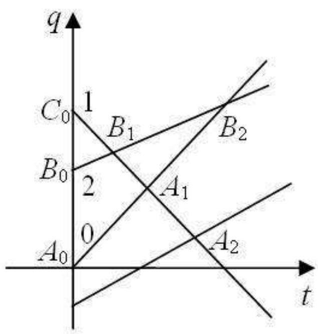

Figure 1

The true motion of the zero particle is $A_0A_1A_2$, of the first particle $C_0B_1B_2$, of the second particle $B_0B_1A_1B_2$. However, the first collision of the zero particle at the point A_1 (with the second one) can be found as the collision with the particle moving along the straight line $C_0A_1A_2$.

Let us write laws of motion of the zero and first particles:

$$q_0 = v_0 t, \quad q_1 = q_1^{(0)} + v_1 t.$$

Time of their collision is $t = \frac{q_1^{(0)}}{v_0 - v_1}$. For the particles to be collided in the time interval $[0,\, t_1]$, the condition $0 < \frac{q_1^{(0)}}{v_0 - v_1} < t_1$ must be fulfilled or

$$\begin{cases} q_1^{(0)} > 0, \\ q_1^{(0)} < (v_0 - v_1)t_1, \quad v_0 > v_1; \end{cases}$$

$$\begin{cases} q_1^{(0)} < 0, \\ q_1^{(0)} > (v_0 - v_1)t_1, \quad v_0 < v_1. \end{cases}$$

These inequalities determine the region of initial conditions for the first particle under which the collision will occur in the time interval $[0,\, t_1]$. This region is shown in Figure 2.

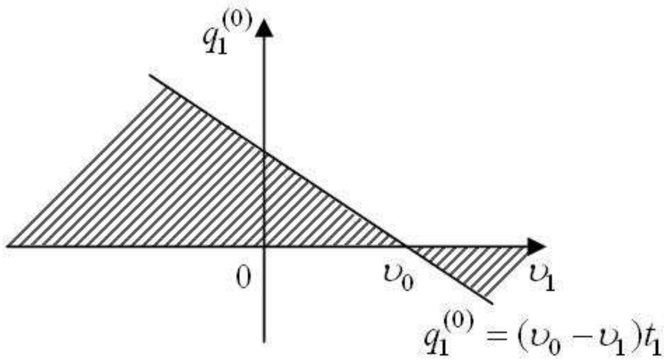

Figure 2

Therefore, the probability of collision of the zero particle with the first one for time t_1 $P_1(v_0, t_1)$ is determined as follows:

$$P_1(v_0, t_1) = \int\limits_{-\infty}^{v_0} dv_1 \int\limits_{0}^{(v_0-v_1)t_1} f_1(v_1, q_1)dq_1 + \int\limits_{v_0}^{\infty} dv_1 \int\limits_{(v_0-v_1)t_1}^{0} f_1(v_1, q_1)dq_1,$$

where f_1 is one-particle distribution function of initial coordinates of the first particle.

Assume that this function is the product $f_{1v_1}(v_1)f_{1q_1}(q_1)$ and $f_{1q_1}(q_1) = \text{const} = \frac{1}{L}$. Then

$$\begin{aligned} P_1(v_0, t_1) &= \int_{-\infty}^{v_0} f_{1v_1}(v_1)\frac{v_0 - v_1}{L} t_1\, dv_1 + \int_{v_0}^{\infty} f_{1v_1}(v_1)\frac{v_1 - v_0}{L} t_1\, dv_1 \\ &= \int_{-\infty}^{\infty} f_{1v_1}(v_1)\frac{|v_0 - v_1|}{L} t_1\, dv_1 = \frac{u(v_0)}{L} t_1, \end{aligned}$$

where $u(v_0) = \int_{-\infty}^{\infty} f_{1v_1}(v_1)|v_0 - v_1|\, dv_1$ is the average relative speed of the first particle provided that the zero particle has the speed v_0.

Obviously, the probability that a collision of the zero particle with the first one will occur in a small time interval dt_1 has the form

$$P_1(v_0, dt_1) = \psi_1(v_0, t_1)\, dt_1 = \frac{\partial P_1(v_0, t_1)}{\partial t_1} dt_1 = \frac{u(v_0)}{L} dt_1$$

where $\psi_1(v_0, t_1)$ is a distribution function of the time of the first collision of the zero particle with the first one.

Hence, the probability of lacking collision is equal to $\mathcal{Q}_1(v_0, dt_1) = 1 - \frac{u(v_0)}{L}\, dt_1$. If there are $N + 1$ particles in the system, then the probability of lacking collisions of the zero particle with another N particles is equal to

$$\begin{aligned} \mathcal{Q}_N(v_0, dt_1) &= \left(1 - \frac{u(v_0)}{L} dt_1\right)^N \\ &\approx 1 - N\frac{u(v_0)}{L} dt_1 = 1 - nu(v_0)\, dt_1 \text{ as } dt_1 \to 0. \end{aligned}$$

Let us find the distribution function of the time of the first collision of the zero particle with N particles.

Indeed, the probability of lacking of collisions of the zero particle with N particles $\mathcal{Q}_N(v_0, t_1)$ for time t_1 satisfies the equation

$$\mathcal{Q}_N(v_0, t_1 + dt_1) = \mathcal{Q}_N(v_0, t_1)\mathcal{Q}_N(v_0, dt_1)$$

or

$$\mathcal{Q}_N(v_0, t_1 + dt_1) = \mathcal{Q}_N(v_0, t_1)(1 - nu(v_0)\, dt_1),$$

which solution has the form $\mathcal{Q}_N(v_0, t_1) = e^{-nu(v_0)t_1}$. Therefore, the distribution function of the time of the first collision of the zero particle with N particles has the form

$$\psi_N(v_0, t_1) = -\frac{\partial \mathcal{Q}_N(v_0, t_1)}{\partial t_1} = nu(v_0)e^{-nu(v_0)t_1}.$$

From $\varphi_N(q, v_0)\, dq = \psi_N(v_0, t_1)\, dt_1$ and $q = v_0 t_1$, we find the distribution function of the coordinates of the first collision of the zero particle with any other:

$$\varphi_N(q, v_0) = \frac{nu(v_0)}{|v_0|} e^{-\frac{nu(v_0)}{|v_0|}|q|}.$$

Otherwise, this function can be explained as follows: $\varphi_N(q, v_0)$ is the distribution function of the displacement of the particle between two collisions provided that this particle had the speed v_0 in this interval. Note, that for $v_0 = 0$, $\varphi_N(q, v_0) = \delta(0)$ we obtain a trivial case: the collision will occur at the point $q = 0$. For the unconditional distribution function $\bar{\varphi}_N(q, v_0)$ of the displacement of the particle to be found, we should average the obtained function by v_0, i.e.:

$$\bar{\varphi}_N(q, v_0) = \int\limits_{-\infty}^{\infty} \varphi_N(q, v_0) f(v_0)\, dv_0 = \int\limits_{0}^{\infty} \frac{nu(v_0)}{|v_0|} e^{-\frac{nu(v_0)}{|v_0|}|q|} f(v_0)\, dv_0.$$

Then we find the expression for the distribution function of the displacement after k collisions. For this, we make use of a technique of characteristic functions. The characteristic function of one displacement has the form:

$$\begin{aligned}
\chi_q(z) &= \int\limits_{-\infty}^{\infty} \bar{\varphi}_N(q, v_0) e^{i|q|z}\, dq \\
&= \int\limits_{0}^{\infty} f(v_0) \frac{nu(v_0)}{|v_0|} \int\limits_{-\infty}^{\infty} e^{-\frac{nu(v_0)}{|v_0|}|q|} e^{i|q|z}\, dq dv_0 \\
&= \int\limits_{0}^{\infty} f(v_0) \left(\frac{nu(v_0)}{v_0}\right)^2 2 \frac{1}{z^2 + \left(\frac{nu(v_0)}{v_0}\right)^2}\, dv_0.
\end{aligned}$$

Since the characteristic function of the sum of random variables is equal to the product of characteristic functions-summands, the displacement for k steps

$Q_k = \sum\limits_{i=1}^{k} q_i$ satisfies the distribution with the characteristic function

$$\chi_{Q_k}(z) = \prod_{i=1}^{k} \chi_{q_i}(z) = \prod_{i=1}^{k} \int\limits_{0}^{\infty} f(v_{0i}) \left(\frac{nu_i}{v_{0i}}\right)^2 2\frac{1}{z^2 + \left(\frac{nu_i}{v_{0i}}\right)^2} dv_{0i},$$

where v_{0i} is the speed before the i-th collision, $u_i = u(v_{0i})$.

By reduction formula, we obtain

$$\varphi_N(Q_k) = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} \chi_{Q_k}(z) e^{-iQ_k z} dz = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} \prod_{i=1}^{k} \chi_{q_i}(z) e^{-iQ_k z} dz$$

$$= \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} dz \prod_{i=1}^{k} \int\limits_{0}^{\infty} f(v_{0i}) \left(\frac{nu_i}{v_{0i}}\right)^2 2\frac{1}{z^2 + \left(\frac{nu_i}{v_{0i}}\right)^2} e^{-iQ_k z} dv_{0i}.$$

Since there are factors $\frac{1}{z^2+\left(\frac{nu_i}{v_{0i}}\right)^2}$ that have Gaussian form and depend on z, and acquire the maximum for $z = 0$, and their product tends to δ-function (from $\delta(0)$), then $\varphi_N(Q_k) \to$ const. In other words, the distribution of the coordinate of the particle located at the point $q = 0$ tends to uniform one, what confirms hypothesis about uniformity of the distribution function of coordinates that describes eqiulibrium state.

The conclusion is almost independent of the choice of the speed distribution function $f(v)$ excluding a trivial case, for example all $v_i = v_0$ when there are no collisions (then $u = 0$).

Let us calculate the statistical sum for the Gibbs distribution function:

$$\Xi = \Xi_p \Xi_q = \int\limits_{-\infty}^{\infty} dp_1 \dots dp_N e^{-\beta \sum\limits_{i=1}^{N} \frac{p_i^2}{2}} \int\limits_{d}^{L-d} dq_1 \dots dq_N$$

$$= \int\limits_{-\infty}^{\infty} dp_1\, e^{-\frac{p_1^2}{2kT}} \int\limits_{-\infty}^{\infty} dp_2\, e^{-\frac{p_2^2}{2kT}} \dots \int\limits_{-\infty}^{\infty} dp_N\, e^{-\frac{p_N^2}{2kT}}$$

$$\times N! \int\limits_{d}^{L-2d(N-1)-d} dq_1 \int\limits_{q_1+2d}^{L-2d(N-2)-d} dq_2 \dots \int\limits_{q_{N-2}+2d}^{L-3d} dq_{N-1} \int\limits_{q_{N-1}+2d}^{L-d} dq_N$$

$$= (2\pi kT)^{\frac{N}{2}} N! \int\limits_{d}^{L-2d(N-1)-d} dq_1 \int\limits_{q_1+2d}^{L-2d(N-2)-d} dq_2 \ldots$$

$$\times \int\limits_{q_{N-2}+2d}^{L-3d} dq_{N-1}(L-3d-q_{N-1}) = (2\pi kT)^{\frac{N}{2}} N! \int\limits_{d}^{L-2d(N-1)-d} dq_1$$

$$\times \int\limits_{q_1+2d}^{L-2d(N-2)-d} dq_2 \ldots \int\limits_{q_{N-3}+2d}^{L-5d} dq_{N-2} \frac{(L-5d-q_{N-2})^2}{2}$$

$$= (2\pi kT)^{\frac{N}{2}} N! \int\limits_{d}^{L-2d(N-1)-d} dq_1 \int\limits_{q_1+2d}^{L-2d(N-2)-d} dq_2 \ldots$$

$$\times \int\limits_{q_{N-4}+2d}^{L-7d} dq_{N-3} \frac{(L-7d-q_{N-3})^3}{2 \cdot 3} = (2\pi kT)^{\frac{N}{2}} N! \frac{(L-(2N+1)d)^N}{N!}$$

$$= (2\pi kT)^{\frac{N}{2}} (L-(2N+1)d)^N.$$

Since $L \gg (2N+1)d$, then $\Xi \approx (2\pi\sigma^2)^{\frac{N}{2}} L^N$.

Therefore, for the Maxwell speed distribution, the limit distribution of the configuration Gibbs distribution in the Boltzmann-Grad limit is the uniform distribution, what was required to prove. □

4. Conclusions

We proved that in equilibrium state of one-dimensional symmetric system of particles (hard spheres), the limit distribution of the configuration Gibbs distribution in the Boltzmann-Grad limit ($d \to 0$, n is fixed) is uniform (the speed distribution is the Maxwell one and is unchanged).

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