THE EVOLUTION EQUATION FOR THE MICROSCOPIC PHASE DENSITY OF INELASTICALLY COLLIDING PARTICLES

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A dynamical system of spherical particles is studied on the basis of a model mechanism for the momentum and angular momentum exchange. In the model of absolutely hard balls with rough surfaces, a mechanism for the momentum and angular momentum exchange under collisions is proposed. For this model, the equation of evolution for the delta-function microscopic density in the nine-dimensional phase space is obtained. In case of the system bounded by an inelastic wall, the obtained equation is modified taking into account the boundary conditions.

1. Introduction

A large number of works is devoted to the study of the kinetics of classical model systems with the purpose to achieve a better understanding of the behavior of dissipative systems (see, e.g., works [1] and [2]). The aim of this work is the construction of an evolution equation for the microscopic phase density of a model dynamical system taking the boundary conditions into account. The evolution equation for the microscopic density can be used for the construction of approximate equations for the averaged microscopic density. These approximate equations for the macroscopic distribution (the averaged microscopic density) can be used to study the kinetics and hydrodynamics of a respective statistical system taking into account the interaction with a plane surface.

In the works by Bogolyubov [3] and [4], an evolution equation for the microscopic phase density was built for a system of identical hard spherical particles with zero intrinsic angular momentum. It is shown that the evolution equation for the microscopic density in the phase space of coordinates and velocities can be presented in the form of the Boltzmann–Enskog equation.

The main feature of the dynamical system under study is the presence of inelastic collisions between particles. We define the collisions with the exchange of momenta and intrinsic angular momenta between the particles under inelastic collisions.In the present work, we consider the case of hard particles: the modulus in torsion and the modulus in tension are infinitely large (the shear deformation and the torsional strain are absent).

The formulation of the microscopic equation for inelastically colliding particles is sufficiently new, though the kinetic theory was considered in the literature (see, e.g., [5], where the microscopic equations are deduced without taking binary correlations into account).

We generalize the Bogolyubov's technique in order to consider a more complicated dynamical system with the established physical mechanism for the momentum and angular momentum exchanges.

2. The Equation for a State Function

Consider the dynamical system with a fixed number of particles. First, we examine a classical system of two identical hard spherical bodies (particles) with nonzero intrinsic angular momentum. The following collection of symbols is used: $\boldsymbol{q}_i = \boldsymbol{q}_i(t)$ is the center-of-mass position of the i-th particle, $\boldsymbol{p}_i = \boldsymbol{p}_i(t)$ is the center-of-mass momentum of the i-th particle, $\boldsymbol{M}_i = \boldsymbol{M}_i(t)$ is the angular momentum of the spherical particle i relative to its center of mass (we define it as the own or intrinsic angular momentum), $\theta()$ is the threshold function (the theta function), a is the particle's diameter, J is the particle's moment of inertia, and m is the particle's mass, and $\boldsymbol{q}_i$, $\boldsymbol{p}_i$, and $\boldsymbol{M}_i$ are three-dimensional vectors. Since the particles are spherically symmetric, the state of the system including N particles is determined by the $9N$-dimensional state vector $\boldsymbol{X}(t)$:

$$\boldsymbol{X}_N(t) = \big(\boldsymbol{q}_i(t), \boldsymbol{p}_i(t), \boldsymbol{M}_i(t); \boldsymbol{q}_2(t), \boldsymbol{p}_2(t),$$

$$\boldsymbol{M}_2(t); ...; \boldsymbol{q}_N(t), \boldsymbol{p}_N(t), \boldsymbol{M}_N(t)\big).$$

2.1. The system of two identical hard spherical bodies with a nonzero intrinsic angular momentum

We modify the Bogolyubov's technique for the construction of the evolution equation for a state function in the case of inelastically colliding particles.

For the state function of two hard particles $F(\boldsymbol{X}_2(t)) = F(\boldsymbol{q}_1(t), \boldsymbol{p}_1(t), \boldsymbol{M}_1(t); \boldsymbol{q}_2(t), \boldsymbol{p}_2(t), \boldsymbol{M}_2(t))$, we will construct its time derivative

$$\frac{\partial}{\partial t} F(\boldsymbol{X}_2(t)).$$

To this end, we examine the differential of the state function in an infinitesimal interval

$$\Delta F = F\left(\boldsymbol{X}_2(t+\Delta t)\right) - F\left(\boldsymbol{X}_2(t)\right) . \tag{1}$$

If the motion of the particle's center of mass is rectilinear and uniform during Δt (the free movement), we get

$$\boldsymbol{q}_i(t+\Delta t) = \boldsymbol{q}_i(t) + \frac{\boldsymbol{p}_i(t)}{m}\Delta t, \qquad \boldsymbol{p}_i(t+\Delta t) = \boldsymbol{p}_i(t),$$

$$\boldsymbol{M}_i(t+\Delta t) = \boldsymbol{M}_i(t). \tag{2}$$

In the general case, differential (1) can be presented as

$$\Delta F = \Delta_P + \Delta_M + \Delta_q,$$

where

$$\Delta_p = F\big(\boldsymbol{q}_1(t+\Delta t), \boldsymbol{p}_1(t+\Delta t), \boldsymbol{M}_1\big(t+$$

$$+\Delta t\big); \boldsymbol{q}_2(t+\Delta t), \boldsymbol{p}_2(t+\Delta t), \boldsymbol{M}_2(t+\Delta t)\big) -$$

$$-F\big(\boldsymbol{q}_1(t+\Delta t), \boldsymbol{p}_1(t), \boldsymbol{M}_1\big(t+$$

$$+\Delta t\big); \boldsymbol{q}_2(t+\Delta t), \boldsymbol{p}_2(t), \boldsymbol{M}_2(t+\Delta t)\big),$$

$$\Delta_M = F\big(\boldsymbol{q}_1(t+\Delta t), \boldsymbol{p}_1(t), \boldsymbol{M}_1\big(t+$$

$$+\Delta t\big); \boldsymbol{q}_2(t+\Delta t), \boldsymbol{p}_2(t), \boldsymbol{M}_2(t+\Delta t)\big) -$$

$$-F\big(\boldsymbol{q}_1(t+\Delta t), \boldsymbol{p}_1(t), \boldsymbol{M}_1(t); \boldsymbol{q}_2\big(t+$$

$$+\Delta t\big), \boldsymbol{p}_2(t), \boldsymbol{M}_2(t)\big);$$

$$\Delta_q = F\big(\boldsymbol{q}_1(t+\Delta t), \boldsymbol{p}_1(t), \boldsymbol{M}_1(t); \boldsymbol{q}_2\big(t+$$

$$+\Delta t\big), \boldsymbol{p}_2(t), \boldsymbol{M}_2(t)\big) -$$

$$-F\big(\boldsymbol{q}_1(t), \boldsymbol{p}_1(t), \boldsymbol{M}_1(t); \boldsymbol{q}_2(t), \boldsymbol{p}_2(t), \boldsymbol{M}_2(t)\big).$$

We note that Δ_P and Δ_M are nonzero only in case of the occurrence of a collision in the time interval Δt. For hard particles, the interaction time is negligibly small. For the occurrence of a collision in this infinitesimal time interval Δt, we can write down

$$|\boldsymbol{q}_2(t) - \boldsymbol{q}_1(t)| \geq a$$

and

$$|\boldsymbol{q}_2(t+\Delta t) - \boldsymbol{q}_1(t+\Delta t)| < a, \quad \Delta t \to 0$$

or, if the particles go freely to the collision instant,

$$|\boldsymbol{q}_2(t) - \boldsymbol{q}_1(t)| \geq a$$

and

$$|\boldsymbol{q}_2(t) - \boldsymbol{q}_1(t) + \frac{\boldsymbol{p}_2(t) - \boldsymbol{p}_1(t)}{m}\Delta t| < a, \quad \Delta t \to 0. \tag{3}$$

For brevity, we set

$$\boldsymbol{q}_2(t) - \boldsymbol{q}_d(t) = \boldsymbol{r}, \qquad |\boldsymbol{q}_2(t) - \boldsymbol{q}_1(t)| = r,$$

$$\frac{\boldsymbol{q}_2(t) - \boldsymbol{q}_1(t)}{|\boldsymbol{q}_2(t) - \boldsymbol{q}_1(t)|} = \boldsymbol{e}, \quad \frac{\boldsymbol{p}_2(t) - \boldsymbol{p}_1(t)}{m} = \boldsymbol{v}.$$

Then the expression $\theta(-\boldsymbol{ev})\big\{\theta(r-a) - \theta(r-a+ +(\boldsymbol{ev})\Delta t)\big\}$ equals unity in area (3). Otherwise, it equals zero.

Using the one-dimensional δ-function $\delta(x)$ localized in the interval $(0, +\infty)$ (see [4]), we can present the $\Delta_P + \Delta_M$ as

$$\Delta_p + \Delta_M = \Delta t |\boldsymbol{ev}| \theta(-\boldsymbol{ev}) \delta(r-a) \times$$

$$\times \big\{F(\boldsymbol{q}_1, \boldsymbol{p}_1^*, \boldsymbol{M}_1^*; \boldsymbol{q}_2, \boldsymbol{p}_2^*, \boldsymbol{M}_2^*) -$$

$$-F(\boldsymbol{q}_1, \boldsymbol{p}_1, \boldsymbol{M}_1; \boldsymbol{q}_2, \boldsymbol{p}_2, \boldsymbol{M}_2)\big\}, \tag{4}$$

where $\boldsymbol{p}_1^*$ and $\boldsymbol{p}_2^*$, $\boldsymbol{M}_1^*$ and $\boldsymbol{M}_2^*$ are the momenta and the angular momenta of particles 1 and 2 after the collision, respectively. For the infinitesimal Δt, the positions of particles $\boldsymbol{q}_i(t+\Delta t) = \boldsymbol{q}_i(t) + \frac{\boldsymbol{p}_i}{m}\Delta t$ are closely approximated to the initial values $\boldsymbol{q}_i$, $i = 1, 2$.

The dynamical system is determinate, which allows us to define the $(\boldsymbol{q}_1^*, \boldsymbol{p}_1^*, \boldsymbol{M}_1^*; \boldsymbol{q}_2^*, \boldsymbol{p}_2^*, \boldsymbol{M}_2^*)$ as the functions of the initial state $(\boldsymbol{q}_1, \boldsymbol{p}_1, \boldsymbol{M}_1; \boldsymbol{q}_2, \boldsymbol{p}_2, \boldsymbol{M}_2)$ of the system. We introduce the scattering operator $\hat{S}$ which transforms the initial state of the particles into the final state due to the inelastic collision:

$$\boldsymbol{X}_2^*(t) = \hat{S}(\boldsymbol{X}_2(t)) \cdot \boldsymbol{X}_2(t), \tag{5}$$

where $\boldsymbol{q}_i^* = \boldsymbol{q}_i(t)$, $i = 1, 2$, in the zero-order approximation in Δt. We make change of the variables as

$$(\boldsymbol{q}_1, \boldsymbol{p}_1, \boldsymbol{M}_1; \boldsymbol{q}_2, \boldsymbol{p}_2, \boldsymbol{M}_2) \to$$

$$\to (\boldsymbol{q}_1, \boldsymbol{p}_1, \boldsymbol{M}_1, \boldsymbol{e}, |\boldsymbol{q}_1 - \boldsymbol{q}_2|, \boldsymbol{p}_2, \boldsymbol{M}_2).$$

Here,

$$\boldsymbol{e} = \frac{\boldsymbol{q}_1 - \boldsymbol{q}_2}{|\boldsymbol{q}_1 - \boldsymbol{q}_2|}.$$

Then the coefficient of Δt in (4) is a function of the unit vector $\boldsymbol{e}$,

$$\delta(r-a) f\left(\frac{\boldsymbol{r}}{r}\right) = \delta(r-a) f(\boldsymbol{e}),$$

and depends on $\boldsymbol{q}_1$, $|\boldsymbol{q}_1 - \boldsymbol{q}_2|$, $\boldsymbol{p}_1$, $\boldsymbol{p}_2$, $\boldsymbol{M}_1$, $\boldsymbol{M}_2$, t as well.

We use the relation

$$\delta(r-a) f\left(\frac{\boldsymbol{r}}{r}\right) = \int \delta(\boldsymbol{r} - \boldsymbol{R}) \delta(R-a) f\left(\frac{\boldsymbol{R}}{R}\right) d\boldsymbol{R}.$$

Let us introduce the unit vector $\boldsymbol{\sigma}$ which is parallel to $\boldsymbol{R}$: $\boldsymbol{R} = R\boldsymbol{\sigma}$, $d\boldsymbol{R} = R^2 dR d\boldsymbol{\sigma}$, where $d\boldsymbol{\sigma}$ is the infinitesimal element of a spatial angle. Thus, we have

$$\delta(r-a) f(\boldsymbol{e}) = \int \delta(\boldsymbol{r} - R\boldsymbol{\sigma}) \delta(R-a) f(\boldsymbol{\sigma}) R^2 dR d\boldsymbol{\sigma} =$$

$$= a^2 \int \delta(\boldsymbol{r} - a\boldsymbol{\sigma}) f(\boldsymbol{\sigma}) d\boldsymbol{\sigma}.$$

We now use (5) for the definition of the operator $\hat{B}_{1,2}$:

$$\hat{B}_{1,2} F(\boldsymbol{X}_2) = F\left(\hat{S}\left(\boldsymbol{X}_2\right)\right) = F(\boldsymbol{X}_2^*(\boldsymbol{X}_2)) =$$

$$= F(\boldsymbol{X}_2^*(\boldsymbol{q}_1, |\boldsymbol{q}_1 - \boldsymbol{q}_2|, \boldsymbol{p}_1, \boldsymbol{p}_2, \boldsymbol{M}_1, \boldsymbol{M}_2, \boldsymbol{\sigma})).$$

Thus, $\Delta_P + \Delta_M$ in (4) can be presented as

$$\frac{\Delta t}{m} a^2 \int \theta((\boldsymbol{p}_1 - \boldsymbol{p}_2)\boldsymbol{\sigma}) |(\boldsymbol{p}_1 -$$

$$-\boldsymbol{p}_2)\sigma| \delta(\boldsymbol{q}_2 - \boldsymbol{q}_1 - a\boldsymbol{\sigma}) \left\{\hat{B}_{1,2}(\boldsymbol{\sigma}) - 1\right\} F(\boldsymbol{X}_2) d\boldsymbol{\sigma}.$$

Δ_q can be presented in the form

$$\Delta_q = \sum_{i=1,2} \frac{\boldsymbol{p}_i}{m} \frac{\partial}{\partial \boldsymbol{q}_i} F(\boldsymbol{X}_2) \Delta t,$$

where $\boldsymbol{p}_i \frac{\partial}{\partial \boldsymbol{q}_i}$ denotes the scalar product of the vector $\boldsymbol{p}_i$ and the nabla operator.

Hence, we have

$$\frac{\partial}{\partial t} F(\boldsymbol{X}_2) = \sum_{i=1,2} \frac{\boldsymbol{p}_i}{m} \frac{\partial}{\partial \boldsymbol{q}_i} F(\boldsymbol{X}_2) + T_{1,2} \cdot F(\boldsymbol{X}_2), \tag{6}$$

where

$$T_{1,2} F(\boldsymbol{X}_2) = \frac{a^2}{m} \int \theta\left((\boldsymbol{p}_1 - \boldsymbol{p}_2)\boldsymbol{\sigma}\right) |(\boldsymbol{p}_1 - \boldsymbol{p}_2)\boldsymbol{\sigma}| \times$$

$$\times \delta(\boldsymbol{q}_2 - \boldsymbol{q}_1 - a\boldsymbol{\sigma}) \left\{\hat{B}_{1,2}(\boldsymbol{\sigma}) - 1\right\} F(\boldsymbol{X}_2) d\boldsymbol{\sigma}.$$

Note that there is an arbitrary operator $\hat{S}$ (for an arbitrary dynamical system) in $T_{1,2}$. Therefore, Eq. (10) can be used to describe the systems with energy dissipation.

Let us introduce the operator P interchanging the order of indices:

$$P \cdot T_{1,2} = T_{2,1}.$$

If the state function is symmetric relatively a permutation of indices, we can replace $\boldsymbol{\sigma}$ by $-\boldsymbol{\sigma}$ and permutate the phase coordinates in $T_{2,1} \cdot F(\boldsymbol{q}_2, \boldsymbol{q}_2, \boldsymbol{p}_2, \boldsymbol{M}_2; \boldsymbol{q}_1, \boldsymbol{p}_1, \boldsymbol{M}_1)$. In this case,

$$\hat{B}_{2,1}(-\boldsymbol{\sigma}) \cdot F(\boldsymbol{q}_2, \boldsymbol{p}_2, \boldsymbol{M}_2; \boldsymbol{q}_1, \boldsymbol{p}_1, \boldsymbol{M}_1) =$$

$$= \hat{B}_{1,2}(\boldsymbol{\sigma}) \cdot F(\boldsymbol{q}_1, \boldsymbol{p}_1, \boldsymbol{M}_1; \boldsymbol{q}_2, \boldsymbol{p}_2, \boldsymbol{M}_2).$$

For the asymmetric state function, we have

$$(P \cdot T_{1,2}) = T_{1,2} \quad \text{and} \quad \hat{B}_{2,1}(-\boldsymbol{\sigma}) = \hat{B}_{1,2}(\boldsymbol{\sigma}).$$

Hence, using the obtained equation, we can describe the dissipative scattering of particles.

2.2. *The system of* N *particles*

Consider N identical particles and denote their positions, momenta, and own angular momenta by $\boldsymbol{q}_1, ..., \boldsymbol{q}_N$, $\boldsymbol{p}_1, ..., \boldsymbol{p}_N$, and $\boldsymbol{M}_1, ..., \boldsymbol{M}_N$, respectively.

The average density of particles is small, the time of the interaction between particles is negligibly small in the accepted scheme of classical mechanics, and the simultaneous interaction between three, four, and more particles may be disregarded.

We consider some function of a dynamical state

$$F(t) = F(X_N(t)) =$$

$$= F(\boldsymbol{q}_1, \boldsymbol{p}_1, \boldsymbol{M}_1; \ldots; \boldsymbol{q}_j, \boldsymbol{p}_j, \boldsymbol{M}_j; \ldots; \boldsymbol{q}_N, \boldsymbol{p}_N, \boldsymbol{M}_N),$$

where $\boldsymbol{q}_j = \boldsymbol{q}_j(t, \boldsymbol{X}_N(t_0))$, $\quad \boldsymbol{p}_j = \boldsymbol{p}_j(t, \boldsymbol{X}_N(t_0))$, $\boldsymbol{M}_j = \boldsymbol{M}_j(t, \boldsymbol{X}_N(t_0))$.

For the initial state, the physical condition of impenetrability looks like

$$|\boldsymbol{q}_k(t_0) - \boldsymbol{q}_l(t_0)| \geq a, \quad \text{коли} \quad k \neq l.$$

The particles go freely up to the first instant, until two of them fulfill the condition $|\boldsymbol{q}_k(t) - \boldsymbol{q}_l(t)| = a$. Then they collide according to rule (5). Then the particles go on up to the instant of the next collision which is performed by the same rule, and so on. Thus, taking into account Eq. (6), we have

$$\frac{\partial}{\partial t} F(t) = \sum_{1 \leq j \leq N} \frac{\boldsymbol{p}_j}{m} \frac{\partial}{\partial \boldsymbol{q}_j} F(t) + \sum_{\alpha} T_\alpha F(t). \tag{7}$$

Here, $\sum\limits_{\alpha}$ denotes the summation over all pairs of particles. We take into account every pair only once. We use Eq. (7) in a particular case of the function $F(\boldsymbol{X}_N(t))$:

$$f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) =$$

$$= \delta(\boldsymbol{q} - \boldsymbol{q}_j(t)) \delta(\boldsymbol{p} - \boldsymbol{p}_j(t)) \delta(\boldsymbol{M} - \boldsymbol{M}_j(t)), \tag{8}$$

which is the distribution function for the j-th particle in the phase space $(\boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M})$. Every delta function is three-dimensional.

The collision is instantaneous. Then there exists such time interval from t to $t + \Delta t$, on which the j-th particle interacts only with one of $N - 1$ particles. Hence, in the time interval $\Delta t \to 0$, the distribution function (8) obeys the equation

$$\frac{\partial}{\partial t} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) =$$

$$= \frac{\boldsymbol{p}_j}{m} \frac{\partial}{\partial \boldsymbol{q}_j} \delta(\boldsymbol{q} - \boldsymbol{q}_j) \delta(\boldsymbol{p} - \boldsymbol{p}_j) \delta(\boldsymbol{M} - \boldsymbol{M}_j) +$$

$$+ \sum_{\substack{1 \leq k \leq N \\ k \neq j}} T_{j,k} \cdot f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}), \tag{9}$$

where

$$T_{j,k} f_j = \frac{a^2}{m} \int \theta(\boldsymbol{p}_{jk} \cdot \boldsymbol{\sigma}) |\boldsymbol{p}_{jk} \cdot \boldsymbol{\sigma}| \delta(\boldsymbol{q}_k - \boldsymbol{q}_j - a\boldsymbol{\sigma}) \times$$

$$\times \left\{ \hat{B}_{j,k} - 1 \right\} \delta(\boldsymbol{q} - \boldsymbol{q}_j) \delta(\boldsymbol{p} - \boldsymbol{p}_j) \delta(\boldsymbol{M} - \boldsymbol{M}_j) d\boldsymbol{\sigma},$$

and

$$\hat{B}_{j,k} \delta(\boldsymbol{q} - \boldsymbol{q}_j) \delta(\boldsymbol{p} - \boldsymbol{p}_j) \delta(\boldsymbol{M} - \boldsymbol{M}_j) =$$

$$= \delta(\boldsymbol{q} - \boldsymbol{q}_j) \delta(\boldsymbol{p} - \boldsymbol{p}_j^*) \delta(\boldsymbol{M} - \boldsymbol{M}_j^*), \quad \boldsymbol{p}_{j,k} = \boldsymbol{p}_j - \boldsymbol{p}_k.$$

Using the properties of $\delta-$functions, we get

$$\frac{\boldsymbol{p}_j}{m} \frac{\partial}{\partial \boldsymbol{q}_j} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) = -\frac{\boldsymbol{p}}{m} \frac{\partial}{\partial \boldsymbol{q}} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}),$$

and, hence,

$$\frac{\partial}{\partial t} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) = -\frac{\boldsymbol{p}}{m} \frac{\partial}{\partial \boldsymbol{q}} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) +$$

$$+ \sum_{\substack{1 \leq k \leq N \\ k \neq j}} T_{j,k} \cdot f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}). \tag{10}$$

For the microscopic density of N particles

$$f = \sum_j f_j = \sum_j \delta(\boldsymbol{q} - \boldsymbol{q}_j(t)) \delta(\boldsymbol{p} - \boldsymbol{p}_j(t)) \delta(\boldsymbol{M} - \boldsymbol{M}_j(t)), \tag{11}$$

we obtain the equation

$$\frac{\partial}{\partial t} f = -\frac{\boldsymbol{p}}{m} \frac{\partial}{\partial \boldsymbol{q}} f + \sum_{j,k; j \neq k} T_{j,k} \cdot f_j. \tag{12}$$

In the next section, we will consider the case of a linear operator $\hat{S}$ which possesses the reflection property, analyze the dynamics of the system, and deduce the evolution equation for the delta-function phase density of N particles.

3. The Microscopic Equation

If the linear operator $\hat{S}$ has the reflection property $\hat{S}^2(\boldsymbol{\sigma}) = E$, where E is the unit matrix, then we easily get

$$T_{j,\,k}\cdot f_j = \frac{a^2}{m}\int d\boldsymbol{q}^{'}d\boldsymbol{p}^{'}d\boldsymbol{M}^{'}d\boldsymbol{\sigma}\ \theta(\boldsymbol{p}_{j,k}\boldsymbol{\sigma})|\boldsymbol{p}_{j,k}\boldsymbol{\sigma}|\times$$

$$\times\{f_j(\boldsymbol{q},\boldsymbol{p}^*,\boldsymbol{M}^*,t)f_k(\boldsymbol{q}^{'},\boldsymbol{p}^{'*},\boldsymbol{M}^{'*},t)-$$

$$-f_j(\boldsymbol{q},\boldsymbol{p},\boldsymbol{M},t)f_k(\boldsymbol{q}^{'},\boldsymbol{p}^{'},\boldsymbol{M}^{'},t)\}, \qquad (13)$$

where $\boldsymbol{X}_2 = (\boldsymbol{q},\boldsymbol{p},\boldsymbol{M};\boldsymbol{q}^{'},\boldsymbol{p}^{'},\boldsymbol{M}^{'})$ and $\boldsymbol{X}_2(j,k) = (\boldsymbol{q}_j,\boldsymbol{p}_j,\boldsymbol{M}_j;\boldsymbol{q}_k,\boldsymbol{p}_k,\boldsymbol{M}_k)$.

In other words, the equality

$$\hat{B}_{j,k}\cdot f_j(t,\boldsymbol{X})f_k(t,\boldsymbol{X}^{'}) = f_j(t,\boldsymbol{X}^{'*})f_k(t,\boldsymbol{X}^{'*})$$

holds true, where $(\boldsymbol{X}^*;\boldsymbol{X}^{'*}) = \hat{S}(\boldsymbol{\sigma})\cdot((\boldsymbol{q},\boldsymbol{p},\boldsymbol{M}); (\boldsymbol{q}^{'},\boldsymbol{p}^{'},\boldsymbol{M}^{'}))$.

Now we transform the second term of Eq. (12) so that it becomes the equation for the delta-function microscopic density of N particles in the nine-dimensional phase space.

In view of (13) and after the obvious transformations, the collision integral looks like

$$T_{j,\,k}f_j(t,\boldsymbol{X}) = \frac{a^2}{m}\int \theta(\boldsymbol{p}_{jk}\cdot\boldsymbol{\sigma})|\boldsymbol{p}_{jk}\boldsymbol{\sigma}|\delta(\boldsymbol{q}_k-\boldsymbol{q}_j-a\boldsymbol{\sigma})\times$$

$$\times\left\{\hat{B}_{j,k}-1\right\}f_j(t,\boldsymbol{X})d\boldsymbol{\sigma} =$$

$$= \frac{a^2}{m}\int \theta(\boldsymbol{p}_{j,k}\cdot\boldsymbol{\sigma})|\boldsymbol{p}_{j,k}\boldsymbol{\sigma}|\delta(\boldsymbol{q}_k-\boldsymbol{q}_j-a\boldsymbol{\sigma})\times$$

$$\times\left\{f_j(t,\boldsymbol{X}^*)f_k(t,\boldsymbol{X}^{'*}) - f_j(t,\boldsymbol{X})f_k(t,\boldsymbol{X}^{'})\right\}\times$$

$$\times d\boldsymbol{q}^{'}d\boldsymbol{p}^{'}d\boldsymbol{M}^{'}d\boldsymbol{\sigma}, \qquad (14)$$

where the phases $(\boldsymbol{X}^*;\boldsymbol{X}^{'*}) = (\boldsymbol{q},\boldsymbol{p}^*,\boldsymbol{M}^*;\boldsymbol{q}^{'},\boldsymbol{M}^{'*},\boldsymbol{p}^{'*})$ are taken from work [6] in a particular case of the operator $\hat{S}$:

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

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

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

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

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

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

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

$$+\varkappa\boldsymbol{\sigma}((\boldsymbol{M}+\boldsymbol{M}^{'})\boldsymbol{\sigma})\Big\}. \qquad (15)$$

Here, $(\boldsymbol{\sigma}(\boldsymbol{M}+\boldsymbol{M}^{'}))$ is the scalar product of the unit vector $\boldsymbol{\sigma}$ and the vector $(\boldsymbol{M}+\boldsymbol{M}^{'})$; and $[\left(\boldsymbol{M}+\boldsymbol{M}^{'}\right)\times\boldsymbol{\sigma}]$ is the vector product. Here, we use the symbol $\varkappa = \dfrac{ma^2}{4J}$.

For this dynamical model, $(\boldsymbol{p}_j^*-\boldsymbol{p}_k^*)\boldsymbol{\sigma} = -(\boldsymbol{p}_j-\boldsymbol{p}_k)\boldsymbol{\sigma}$ (see Eq. (15)), and we make change of the variables $(\boldsymbol{p}_{j,k}\boldsymbol{\sigma}\to(\boldsymbol{p}-\boldsymbol{p}^{'})\boldsymbol{\sigma}$ in the collision integral. Also we can pass to the $\delta(\boldsymbol{q}^{'}-\boldsymbol{q}-a\boldsymbol{\sigma})$ instead of $\delta(\boldsymbol{q}_k-\boldsymbol{q}_j-a\boldsymbol{\sigma})$ in the collision integral by using the properties of the delta function. Then, using expression (14) for the collision integral in Eq. (10), after the integration with respect to $\boldsymbol{q}'$ and the summation over $j = 1,\ldots,N$ and $k = 1,\ldots,N$, we obtain the evolution equation for the microscopic density (11) as

$$\frac{\partial}{\partial t}f(t,\boldsymbol{q},\boldsymbol{p},\boldsymbol{M}) = -\frac{\boldsymbol{p}}{m}\frac{\partial}{\partial\boldsymbol{q}}f(t,\boldsymbol{q},\boldsymbol{p},\boldsymbol{M})+$$

$$+\frac{a^2}{m}\int d\boldsymbol{p}^{'}d\boldsymbol{M}^{'}d\boldsymbol{\sigma}\ \theta\left\{\left(\boldsymbol{p}^{'}-\boldsymbol{p}\right)\boldsymbol{\sigma}\right\}\left|\left(\boldsymbol{p}-\boldsymbol{p}^{'}\right)\boldsymbol{\sigma}\right|\times$$

$$\times\{f(t,\boldsymbol{q},\boldsymbol{p}^*,\boldsymbol{M}^*)f(t,\boldsymbol{q}+a\boldsymbol{\sigma},\boldsymbol{p}^{'*},\boldsymbol{M}^{'*})-$$

$$-f(t,\boldsymbol{q},\boldsymbol{p},\boldsymbol{M})f(t,\boldsymbol{q}-a\boldsymbol{\sigma},\boldsymbol{p}^{'},\boldsymbol{M}^{'})\}. \qquad (16)$$

Equation (16) has the form of the Boltzmann–Enskog equation, but it is written for the nine-dimensional phase space and describes the evolution of the microscopic density (11) for the given model (15). In a particular case of $k \to \infty$ and the zero rotation $M_j = 0$, we have a simple model of hard spherical particles with smooth surfaces (collisions are elastic). Thus, in the limit of elastic colliding hard spheres, we obtain the Boltzmann–Enskog equation.

4. The System Bounded by a Wall

We consider the case of a sufficiently rarefied gas of hard spherical particles which is in contact with a planar solid surface. In this case, a particle changes the normal component of its momentum after the collision with a wall to the opposite one: $\boldsymbol{n}\boldsymbol{p}_j = -\boldsymbol{n}\boldsymbol{p}_j^\star$, where $\boldsymbol{p}_j^\star$ is the momentum of the j-th particle after the collision with the wall, and the vector $\boldsymbol{n} = (0, 0, 1)$ is normal to the wall XOY.

The evolution equation for the microscopic density of the j-th particle can be complemented by a term which describes the interaction with the wall:

$$\frac{\partial}{\partial t} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) = -\frac{\boldsymbol{p}}{m}\frac{\partial}{\partial \boldsymbol{q}} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) +$$

$$+ \sum_{\substack{1 \le k \le N \\ k \ne j}} T_{j,k} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) + L_j \cdot f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}), \quad (17)$$

where $L_j \cdot f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M})$ is non-zero in the case of the interaction of the j-th particle with the wall in the interval Δt. The condition for a collision for the interval Δt is as follows:

$$\boldsymbol{q}_j \boldsymbol{n} - \frac{a}{2} \ge 0, \quad \left(\boldsymbol{q}_j + \frac{1}{m}\boldsymbol{p}_j \Delta t\right) \boldsymbol{n} - \frac{a}{2} < 0,$$

$$\Delta t \to 0. \quad (18)$$

Here, $\boldsymbol{q}_j(t)\boldsymbol{n}$ and $\boldsymbol{n}\boldsymbol{p}_j$ are the scalar products of the vectors $\boldsymbol{n}$ and $\boldsymbol{q}$, $\boldsymbol{p}$, respectively.

Then, for phases from area (18), the expression $\theta(-\boldsymbol{n}\boldsymbol{p}_j)\left\{\theta\left(\boldsymbol{q}_j\boldsymbol{n} - \frac{a}{2}\right) - \theta\left((\boldsymbol{q}_j + \frac{1}{m}\boldsymbol{p}_j\Delta t)\boldsymbol{n} - \frac{a}{2}\right)\right\}$ equals unity. Otherwise, it equals zero. Then $L_j \cdot f_j(t, \boldsymbol{X})$ can be presented as

$$L_j f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) = \frac{1}{m}\theta(-\boldsymbol{n}\boldsymbol{p}_j(t))\left|\boldsymbol{n}\boldsymbol{p}_j(t)\right| \times$$

$$\times \delta\left(\boldsymbol{q}_j(t)\boldsymbol{n} - \frac{a}{2}\right)\left\{\hat{l}_j(\boldsymbol{n}) - 1\right\} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}), \quad (19)$$

where the linear operator $\hat{l}_j(\boldsymbol{n})$ transforms the phase of the j-th particle before the collision with the wall into that after the the collision

$$\hat{l}_j(\boldsymbol{n}) f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) =$$

$$= \delta(\boldsymbol{q} - \boldsymbol{q}_j(t))\delta(\boldsymbol{p} - \boldsymbol{p}_j^\star(t))\delta(\boldsymbol{M} - \boldsymbol{M}_j^\star(t)).$$

We will discuss the linear operator $\hat{l}_j(\boldsymbol{n})$ such that its square is equal to unity: $\hat{l}_j(\boldsymbol{n})^2 = 1$. By taking into account the relation $\boldsymbol{n}\boldsymbol{p}_j = -\boldsymbol{n}\boldsymbol{p}_j^\star$ and by summing (19) over j, we get (for N particles)

$$\frac{1}{m}\sum_{1 \le j \le N} \theta(-\boldsymbol{n}\boldsymbol{p}_j(t))\left|\boldsymbol{n}\boldsymbol{p}_j(t)\right| \delta\left(\boldsymbol{q}_j(t)\boldsymbol{n} - \frac{a}{2}\right) \times$$

$$\times \left\{\hat{l}_j(\boldsymbol{n}) - 1\right\} f_j(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) = \frac{1}{m}|\boldsymbol{n}\boldsymbol{p}|\delta\left(\boldsymbol{q}\boldsymbol{n} - \frac{a}{2}\right) \times$$

$$\times \left\{\theta(\boldsymbol{n}\boldsymbol{p}) f(t, \boldsymbol{q}, \boldsymbol{p}^\star, \boldsymbol{M}^\star) - \theta(-\boldsymbol{n}\boldsymbol{p}) f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M})\right\}. \quad (20)$$

Finally, the summation of (17) over $j = 1, \ldots, N$ yields

$$\frac{\partial}{\partial t} f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) = -\frac{\boldsymbol{p}}{m}\frac{\partial}{\partial \boldsymbol{q}} f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) + \frac{a^2}{m} \times$$

$$\times \int d\boldsymbol{p}' d\boldsymbol{M}' d\boldsymbol{\sigma}\, \theta\left\{\left(\boldsymbol{p}' - \boldsymbol{p}\right)\boldsymbol{\sigma}\right\}\left|\left(\boldsymbol{p} - \boldsymbol{p}'\right)\boldsymbol{\sigma}\right| \times$$

$$\times \{f(t, \boldsymbol{q}, \boldsymbol{p}^*, \boldsymbol{M}^*) f(t, \boldsymbol{q} + a\boldsymbol{\sigma}, \boldsymbol{p}'^*, \boldsymbol{M}'^*) -$$

$$- f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) f(t, \boldsymbol{q} - a\boldsymbol{\sigma}, \boldsymbol{p}', \boldsymbol{M}')\} + \frac{1}{m}|\boldsymbol{n}\boldsymbol{p}| \times$$

$$\times \delta\left(\boldsymbol{q}\boldsymbol{n} - \frac{a}{2}\right)\{\theta(\boldsymbol{n}\boldsymbol{p}) f(t, \boldsymbol{q}, \boldsymbol{p}^\star, \boldsymbol{M}^\star) -$$

$$- \theta(-\boldsymbol{n}\boldsymbol{p}) f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M})\}. \quad (21)$$

As usual, the macroscopic equation can be defined without inclusion of boundary conditions into it. Let us consider the equation for the system including only one particle:

$$\frac{\partial}{\partial t} f(t, \boldsymbol{X}) = -\frac{\boldsymbol{p}}{m}\frac{\partial}{\partial \boldsymbol{q}} f(t, \boldsymbol{X}) + \frac{1}{m}|\boldsymbol{n}\boldsymbol{p}|\delta\left(\boldsymbol{q}\boldsymbol{n} - \frac{a}{2}\right) \times$$

$$\times \{\theta(\boldsymbol{np}) f(t,\, \boldsymbol{X}^\star) - \theta(-\boldsymbol{np}) f(t,\, \boldsymbol{X})\}\,.$$

Its solution can be presented as $f(\boldsymbol{X},t) = f_0(\boldsymbol{X} - \mathsf{X}(\boldsymbol{t}) + \mathsf{X}(\boldsymbol{0}))$, where $f_0(\boldsymbol{X})$ is the initial distribution; $\mathsf{X}(\boldsymbol{t}) = (\mathsf{q}(t), \mathsf{p}(t), \mathsf{M}(t))$ is the phase of the particle at the time moment t. To satisfy the equation, the phases $\boldsymbol{X}$ must be taken along a phase trajectory. Thus, the solution can be rated as a translation of the initial distribution along the phase trajectory in the course of time. In addition, the equation has a microscopic solution.

5. The Macroscopic Equation

When the number of particles under consideration is large, Eq. (21) can be averaged and written for the one-particle probability density, which is the microscopic density averaged over the statistical ensemble:

$$\langle f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M})\rangle =$$

$$= \int d\boldsymbol{X}_N D\left(\boldsymbol{X}_N(0)\right) f\left(\boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}, \boldsymbol{X}_N(\boldsymbol{X}_N(0), t)\right),$$

where $D\left(\boldsymbol{X}_N(0)\right)$ is the adjusted state distribution.

In the case of a chaotic initial state, we expect that the dynamics creates no correlations:

$$\langle f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M}) f(t, \boldsymbol{q}, \boldsymbol{p}', \boldsymbol{M}')\rangle =$$

$$= \langle f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M})\rangle \langle f(t, \boldsymbol{q}, \boldsymbol{p}', \boldsymbol{M}')\rangle.$$

Then we have the kinetic equation for the macroscopic density after the averaging:

$$\frac{\partial}{\partial t}\langle f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M})\rangle = -\frac{\boldsymbol{p}}{m}\frac{\partial}{\partial \boldsymbol{q}}\langle f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M})\rangle +$$

$$+\frac{a^2}{m}\int d\boldsymbol{p}^{'} d\boldsymbol{M}^{'} d\boldsymbol{\sigma}\, \theta\left\{\left(\boldsymbol{p}^{'} - \boldsymbol{p}\right)\boldsymbol{\sigma}\right\}\left|\left(\boldsymbol{p} - \boldsymbol{p}^{'}\right)\boldsymbol{\sigma}\right| \times$$

$$\times\big\{\langle f(t, \boldsymbol{q}, \boldsymbol{p}^*, \boldsymbol{M}^*)\rangle\langle f(t, \boldsymbol{q} + a\boldsymbol{\sigma}, \boldsymbol{p}^{'*}, \boldsymbol{M}^{'*})\rangle -$$

$$-\langle f(t, \boldsymbol{q}, \boldsymbol{p}, \boldsymbol{M})\rangle\langle f(t, \boldsymbol{q} - a\boldsymbol{\sigma}, \boldsymbol{p}^{'}, \boldsymbol{M}^{'})\rangle\big\} +$$

$$+\frac{1}{m}|\boldsymbol{np}|\delta\left(\boldsymbol{qn} - \frac{a}{2}\right)\{\theta(\boldsymbol{np})\langle f(t,\, \boldsymbol{q},\, \boldsymbol{p}^\star,\, \boldsymbol{M}^\star)\rangle -$$

$$-\theta(-\boldsymbol{np})\langle f(t,\, \boldsymbol{q},\, \boldsymbol{p},\, \boldsymbol{M})\rangle\big\}. \tag{22}$$

It is interesting that the equilibrium solution of the equation is proportional to the Maxwell distribution for phases which are far from the wall (surface). It has been shown that this kinetic equation (22) for the inelastically colliding particles with regard for boundary conditions has the microscopic solution which is presented in the form (11).

6. Conclusion

Thus, taking into account the operator of reflection of the state vector in inelastic collisions, it is proved that the evolution equation for the microscopic density in the nine-dimensional phase space can be presented in the form of the Boltzmann—Enskog equation. The equation obtained is modified for the case of the system bounded by a planar solid surface.

In the case of a large number of particles, the obtained result can be used for the investigation of statistical systems in any approximation. As an example with the use of the exact equation, we have built an approximation which describes the kinetics of the system near the equilibrium position.

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РІВНЯННЯ ЕВОЛЮЦІЇ МІКРОСКОПІЧНОЇ ФАЗОВОЇ ГУСТИНИ ДЛЯ СИСТЕМИ НЕПРУЖНО ВЗАЄМОДІЮЧИХ КУЛЬОК

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Р е з ю м е

Досліджено динамічну систему кульок з модельним механізмом обміну імпульсами та власними моментами імпульсу. Для моделі абсолютно твердих шорстких кульок запропоновано механізм обміну імпульсами та власними моментами імпульсу при зіткненні. Для цієї моделі динамічної системи рівняння еволюції мікроскопічної фазової густини у дев'ятивимірному фазовому просторі може бути представлене у формі рівняння Больцмана—Енскога. Отримане рівняння записане з урахуванням крайових умов у випадку пружної взаємодії з поверхнею.