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MICROSCOPIC SOLUTIONS OF THE BOLTZMANN-ENSKOG EQUATION IN THE KINETIC THEORY OF HARD SPHERES

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As is well known the Vlasov equation has microscopic solutions corresponding to the exact solutions of the equations of classical mechanics*.

We shall consider now, also in the scheme of classical mechanics a dynamical system of N identical hard spheres, with diameter a and mass m, moving in a macroscopic volume V.

The purpose of this paper is to demonstrate that the Boltzmann-Enskog equation, which always was considered as a low density approximation possesses also microscopic solutions, corresponding to the exact movement of particles.

Let us denote by $\vec{q}_j(t), \vec{w}_j(t)$ - the positions and velocities of the centers of our spheres at the time t. Evidently they are functions of t depending also on their initial values for $t = 0$.

Denote by Γ:

$$\Gamma = (\vec{q}_1^{(0)}, \vec{w}_1^{(0)}, \ldots \vec{q}_N^{(0)}, \vec{w}_N^{(0)})$$

the set of these initial values, which we shall consider as a point in $6N$ -dimensional phase space.

Of course, we restrict the relevant domain of this phase space by the conditions:

$$|\vec{q}_{j_1} - \vec{q}_{j_2}| \geqq a, \qquad \text{for any } j_1 \neq j_2 \tag{1}$$

thus excluding the unphysical overlapping configurations of our spheres.

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*This important remark was first published by A.A.Vlasov himself in the monography /1/ (1950).

We may write:

$$\vec{q}_j(t) = \vec{q}_j(t;\Gamma); \quad \vec{w}_j(t) = \vec{w}_j(t,\Gamma); \qquad j = 1,\dots N. \tag{2}$$

Consider now arbitrary dynamical variables of additive and binary type:

$$\mathcal{A}(t) = \sum_{(1\leqq j\leqq N)} A(\vec{q}_j(t), \vec{w}_j(t))$$
$$\mathcal{B}(t) = \sum_{(1\leqq j_1<j_2\leqq N)} B(\vec{q}_{j_1}(t), \vec{w}_{j_1}(t); \vec{q}_{j_2}(t), \vec{w}_{j_2}(t)). \tag{3}$$

Here $A(\vec{q},\vec{w})$ is an arbitrary function of $\vec{q}$, $\vec{w}$, and $B(\vec{q},\vec{w};\vec{q}\,',\vec{w}\,')$ is an arbitrary symmetric function of $(\vec{q},\vec{w})$, $(\vec{q}\,',\vec{w}\,')$:

$$B(\vec{q},\vec{w},\vec{q}\,',\vec{w}\,') = B(\vec{q}\,',\vec{w}\,';\vec{q},\vec{w}) . \tag{4}$$

Because of (2) the expressions (3) are also functions of Γ, so more explicitly we may write:

$$\mathcal{A}(t) = \mathcal{A}(t;\Gamma); \mathcal{B}(t) = \mathcal{B}(t;\Gamma).$$

We introduce now, in the phase space of points Γ, a probability distribution function $D(\Gamma)$

$$\int D(\Gamma)\, d\Gamma = 1,$$

which is sufficiently regular in the relevant domain (1) and equal to zero outside of it (i.e., for overlapping configurations).

Then the average values of dynamical variables (3) may be defined as:

$$<\sum_{(1\leqq j\leqq N)} A(\vec{q}_j(t), \vec{w}_j(t))> = \int \mathcal{A}(t,\Gamma)\, D(\Gamma)\, d\Gamma$$
$$<\sum_{(1\leqq j_1<j_2\leqq N)} B(\vec{q}_{j_1}(t), \vec{w}_{j_1}(t); \vec{q}_{j_2}(t) \vec{w}_{j_2}(t)> = \int \mathcal{B}(t,\Gamma)\, D(\Gamma) d\Gamma. \tag{5}$$

On the other hand we have identically:

$$\sum_{(1\leqq j\leqq N)} A(\vec{q}_j(t), \vec{w}_j(t)) =$$
$$\int A(\vec{r},\vec{v}) \sum_{(1\leqq j\leqq N)} \delta(\vec{r}-\vec{q}_j(t))\, \delta(\vec{v}-\vec{w}_j(t))\, d\vec{r}\, d\vec{v}, \tag{6}$$

and because of the symmetry condition (4)

$$\sum_{(1\leqq j_1<j_2\leqq N)} B(j_1;j_2) = \frac{1}{2} \sum_{\substack{1\leqq j_1\leqq N\\ 1\leqq j_2\leqq N\\ j_1\neq j_2}} B(j_1;j_2) =$$
$$= \frac{1}{2} \sum_{\substack{1\leqq j_1\leqq N\\ 1\leqq j_2\leqq N}} B(j_1;j_2) - \frac{1}{2} \sum_{(1\leqq j_1\leqq N)} B(j_1;j_1),$$

or, more explicitly:

$$\sum_{(1\leqq j_1<j_2\leqq N)} B(\vec{q}_{j_1}(t), \vec{w}_{j_1}(t); \vec{q}_{j_2}(t), \vec{w}_{j_2}(t)) =$$
$$= \frac{1}{2} \sum_{\substack{1\leqq j_1\leqq N\\ 1\leqq j_2\leqq N}} B(\vec{q}_{j_1}(t), \vec{w}_{j_1}(t); \vec{q}_{j_2}(t), \vec{w}_{j_2}(t)) -$$
$$- \frac{1}{2} \sum_{(1\leqq j_1\leqq N)} B(\vec{q}_{j_1}(t), \vec{w}_{j_1}(t); \vec{q}_{j_1}(t), \vec{w}_{j_1}(t)) =$$
$$= \frac{1}{2} \int B(\vec{r}_1,\vec{v}_1;\vec{r}_2,\vec{v}_2) \{ \sum_{(1\leqq j_1\leqq N)} \delta(\vec{r}_1-\vec{q}_{j_1}(t))\delta(\vec{v}_1-\vec{w}_{j_1}(t))\times$$

$$\times \sum_{(1\leq j_2 \leq N)} \delta(\vec r_2-\vec q_{j_2}(t))\,\delta(\vec v_2-\vec w_{j_2}(t)) - \delta(\vec r_1-\vec r_2)\,\delta(\vec v_1-\vec v_2)\times$$

$$\times \sum_{(1\leq j_1\leq N)} \delta(\vec r_1-\vec q_{j_1}(t))\,\delta(\vec v_1-\vec w_{j_1}(t))\,\}\,d\vec r_1 d\vec v_1 d\vec r_2 d\vec v_2 . \tag{7}$$

It is convenient to introduce the function:

$$f(t,\vec r,\vec v;\Gamma) = n^{-1}\sum_{(1\leq j\leq N)} \delta(\vec r-\vec q_j(t))\,\delta(\vec v-\vec w_j(t)) , \tag{8}$$

where

$$n = \frac{N}{V}$$

is the particle density.

With the help of this function (8) the identities (6), (7) may be rewritten as:

$$\mathfrak{A}(t;\Gamma) = n\int A(\vec r,\vec v)\,f(t,\vec r,\vec v;\Gamma)\,d\vec r\,d\vec v$$

$$\mathfrak{B}(t,\Gamma) =$$

$$= \frac{1}{2}\int B(\vec r_1,\vec v_1;\vec r_2,\vec v_2)\{n^2 f(t,\vec r_1,\vec v_1;\Gamma)f(t,\vec r_2,\vec v_2;\Gamma) -$$

$$-\delta(\vec r_1-\vec r_2)\,\delta(\vec v_1-\vec v_2)\,n f(t,\vec r_1,\vec v_1;\Gamma)\}\,d\vec r_1\,d\vec v_1\,d\vec r_2\,d\vec v_2$$

and hence:

$$<\sum_{(1\leq j\leq N)} A(\vec q_j(t),\vec w_j(t))> = n\int A(\vec r,\vec v)\,f(t,\vec r,\vec v;\Gamma)D(\Gamma)\,d\vec r\,d\vec v\,d\Gamma$$

$$<\sum_{(1\leq j_1\leq j_2\leq N)} B(\vec q_{j_1}(t),\vec w_{j_1}(t);\vec q_{j_2}(t),\vec w_{j_2}(t))> =$$

$$= \frac{1}{2}\int B(\vec r_1,\vec v_1;\vec r_2,\vec v_2)\times\{n^2 f(t,\vec r_1,\vec v_1;\Gamma)\,f(t,\vec r_2,\vec v_2;\Gamma) - \tag{9}$$

$$-\delta(\vec r_1-\vec r_2)\,\delta(\vec v_1-\vec v_2)\,n f(t,\vec r_1,\vec v_1;\Gamma)\}D(\Gamma)\,d\vec r_1\,d\vec v_1\,d\vec r_2\,d\vec v_2\,d\Gamma .$$

Consider now, on the other hand, the usual reduced one-particle and two-particle distribution functions:

$$F_1(t,\vec r,\vec v);\quad F_2(t,\vec r_1,\vec v_1;\vec r_2,\vec v_2) .$$

In virtue of their definition, we have:

$$<\sum_{(1\leq j\leq N)} A(\vec q_j(t),\vec w_j(t))> = n\int A(\vec r,\vec v)\,F_1(t,\vec r,\vec v)\,d\vec r\,d\vec v$$

$$<\sum_{(1\leq j_1\leq j_2\leq N)} B(\vec q_{j_1}(t),\vec w_{j_1}(t);\vec q_{j_2}(t),\vec w_{j_2}(t))> =$$

$$= \frac{n^2}{2}\int B(\vec r_1,\vec v_1;\vec r_2,\vec v_2)\,F_2(t,\vec r_1,\vec v_1,\vec r_2,\vec v_2)\,d\vec r_1\,d\vec v_1\,d\vec r_2\,d\vec v_2 .$$

By comparing these formulae with (9) we get:

$$F_1(t,\vec r,\vec v) = \int f(t,\vec r,\vec v;\Gamma)\,D(\Gamma)\,d\Gamma$$

$$F_2(t,\vec r_1,\vec v_1;\vec r_2,\vec v_2) =$$

$$= \int\{f(t,\vec r_1,\vec v_1;\Gamma)f(t,\vec r_2,\vec v_2;\Gamma) - \tag{10}$$

$$-n^{-1}\,\delta(\vec r_1-\vec r_2)\,\delta(\vec v_1-\vec v_2)\,f(t,\vec r_1,\vec v_1;\Gamma\}D(\Gamma)\,d\Gamma$$

and, in particular:

$$F_2(t,\vec r_1,\vec v_1;\vec r_2,\vec v_2) = \int f(t,\vec r_1,\vec v_1;\Gamma)\,f(t,\vec r_2,\vec v_2;\Gamma)D(\Gamma)\,d\Gamma ;$$

for $\tag{11}$

$$r_1 \neq r_2 .$$

We shall utilise now the hierarchy for the reduced distribution functions, which was established also in the kinetic theory of hard spheres/2/. We need here only the first equation of this hierarchy, which will be written in the form:

$$\frac{\partial F_1(t,\vec{r}_1,\vec{v}_1)}{\partial t} + v_1 \cdot \frac{\partial}{\partial \vec{r}_1} F_1(t,\vec{r}_1,\vec{v}_1) -$$

$$- n a^2 \int_{(\vec{v}_{21}\vec{\sigma})\geqq 0} (\vec{v}_{2,1}\vec{\sigma})\{F_2(t,\vec{r}_1,\vec{v}_1^*;\vec{r}_1+a\vec{\sigma},\vec{v}_2^*) - \tag{12}$$

$$- F_2(t,\vec{r}_1,\vec{v}_1;\vec{r}_1 - a\vec{\sigma},\vec{v}_2)\}\, d\vec{\sigma}\, d\vec{v}_2 = 0,$$

where

$$\vec{v}_{2,1} = \vec{v}_2 - \vec{v}_1;\ \vec{v}_1^* = \vec{v}_1 + \vec{\sigma}(\vec{v}_{2,1}\cdot\vec{\sigma});\ \vec{v}_2 = \vec{v}_2 - \vec{\sigma}(\vec{v}_{2,1}\cdot\vec{\sigma}), \tag{13}$$

$\vec{\sigma}$ is a unit vector and $\vec{\sigma}$ integration is an angular integration over the 3-dimensional unit sphere.

In (12) $a\vec{\sigma}$ is being understood as $(a+0)\vec{\sigma}$. We thus denote by

$$F_2(t,\vec{r}_1,\vec{v};\vec{r}_1 \pm a\vec{\sigma},\vec{v}')$$

the corresponding limits

$$\lim_{\substack{\epsilon > 0\\ \epsilon\to 0}} F_2(t,\vec{r}_1,\vec{v};\vec{r}_1 \pm (a+\epsilon)\vec{\sigma},v').$$

The values of $F_2(t,\vec{r}_1,\vec{v},\vec{r}_2,v')$ on the surface $|\vec{r}_1-\vec{r}_2|=a$ are always taken here from the outside region $|\vec{r}_1-\vec{r}_2|>a$. In the inside region $|\vec{r}_1-\vec{r}_2|<a$, F is zero.

The substitution of the expressions (10), (11) into (12) yields:

$$\int E(t,\vec{r}_1,\vec{v}_1;\Gamma)D(\Gamma)\,d\Gamma = 0, \tag{14}$$

where

$$E(t,\vec{r}_1,\vec{v}_1;\Gamma) = \frac{\partial f(t,\vec{r}_1,\vec{v}_1;\Gamma)}{\partial t} + \vec{v}_1\cdot\frac{\partial}{\partial\vec{r}_1} f(t,\vec{r}_1,\vec{v}_1;\Gamma) -$$

$$-na^2 \int_{(v_{2,1}\cdot\sigma)\geqq 0} (\vec{v}_{2,1}\cdot\vec{\sigma})\{f(t,\vec{r}_1,\vec{v}_1^*;\Gamma)\, f(t,\vec{r}_1+a\vec{\sigma},\vec{v}_2^*;\Gamma) - \tag{15}$$

$$- f(t,\vec{r}_1,\vec{v}_1;\Gamma)\, f(t,\vec{r}_1 - a\vec{\sigma},\vec{v}_2);\Gamma)\}\, d\vec{\sigma}\, d v_2 .$$

Since the function $D(\Gamma)$ is arbitrary in the physical region (1) of the phase space it follows from (15) that in this region:

$$E(t,\vec{r}_1,\vec{v}_1;\Gamma) = 0. \tag{16}$$

We thus see that the nonlinear Boltzmann-Enskog equation:

$$\frac{\partial f(t,\vec{r}_1,\vec{v}_1)}{\partial t} + \vec{v}_1\cdot\frac{\partial}{\partial r_1} f(t,\vec{r}_1,\vec{v}_1) =$$

$$= na^2 \int_{(v_{2,1}\cdot\sigma)\geqq 0} (\vec{v}_{2,1}\cdot\vec{\sigma})\{f(t,\vec{r}_1,\vec{v}_1^*)\, f(t,\vec{r}_1+a\vec{\sigma},\vec{v}_2^*) - \tag{17}$$

$$- f(t,\vec{r}_1,\vec{v}_1)\, f(t,\vec{r} - a\vec{\sigma},\vec{v}_2)\}\, d\vec{\sigma}\, d\vec{v}_2,$$

has not only usually considered solutions, corresponding to the elementary low-density approximation, but possesses also the "mircoscopic solutions" of the type (8):

$$f = f(t,\vec{r},\vec{v};\Gamma) \tag{18}$$

corresponding to the exact dynamics of our hard sphere system.

This fact exhibits that the B.E. equation may serve as a source * for obtaining higher approximations.

As an illustration of such a possibility we may also quote here the paper [4] by J.T.Ubbink and E.H. Hauge, where they started from the nonlinear Boltzmann equation and succeeded in obtaining correct long time behaviour of the correlation functions for the low-density case ** .

In conclusion let us remark that our treatment can be extended also to the situation where in addition to a hard core interaction (that of hard spheres) we have also "normal" binary interactions, described by a smooth function $\Phi_0(r)$ defined for $r \geq a$ and which we formally continue for $r < a$ by putting

$$\Phi_0'(r) = 0 \qquad \text{for} \qquad r < a . \tag{19}$$

Such a case was considered by Ernst, Dorfman, Hoegy and van Leeuwen [2] for the construction of pseudo-Liowille operators.

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* It is easy to see that the whole hierarchy equations for the reduced distribution functions may be obtained directly from (17), starting with the solutions (18). We need only to express $\frac{d}{dt} < f(1;\Gamma) \dots f(s;\Gamma) >$ by means of (17) in terms of $<f(1,\Gamma) \dots f(s;\Gamma)>, <f(1,\Gamma) \dots f(s+1;\Gamma)>$ and to notice that F_s is a linear form of $<f(1,\Gamma) \dots f(j;\Gamma)> (j \leq s)$ and vice versa. We may also remark that these relations between F_s and averaged products of $f(j;\Gamma)$ are in close analogy with the relations between

$<\psi^+(\vec{r}_1) \dots \psi^+(\vec{r}_s)\psi(\vec{r}_s) \dots \psi(r_1)>$ and $<\psi^+(\vec{r}_1)\psi(\vec{r}_1') \dots \psi^+(\vec{r}_j)\psi(\vec{r}_j')>$

in the second quantisation method [3] in quantum statistics.

** Note that in this case the terms $\pm a\vec{\sigma}$ in (17) which distinguish the B.E. equation from the ordinary B. equation are not too relevant, when dealing with the first approximations.

In this situation we need only to supply the left-hand side of the equation (12) with the term:

$$-\frac{1}{m}\int \frac{\partial \Phi_0(\vec{r}_1 - \vec{r}_2)}{\partial \vec{r}_1} \cdot \frac{\partial}{\partial \vec{v}_1} F_2(t, \vec{r}_1, \vec{v}_1; \vec{r}_2, \vec{v}_2)\, d\vec{r}_2\, d\vec{v}_2 \tag{20}$$

Then by literally repeating our reasonning we find that the generalized Boltzmann-Enskog equation, supplied with the "Vlasov term":

$$\frac{\partial f(t, \vec{r}_1, \vec{v}_1)}{\partial t} + \vec{v}_1 \cdot \frac{\partial}{\partial \vec{r}_1} f(t, \vec{r}_1; \vec{v}_1) =$$

$$= n a^2 \int_{(\vec{v}_{2,1} \cdot \vec{\sigma}) \geq 0} (\vec{v}_{2,1} \cdot \vec{\sigma}) \{ f(t, \vec{r}_1, \vec{v}_1^*) f(t, \vec{r}_1 + a\vec{\sigma}, \vec{v}_2^*) -$$

$$- f(t, \vec{r}_1, \vec{v}_1) f(t, \vec{r}_1 - a\vec{\sigma}, \vec{v}_2) \}\, d\vec{\sigma}\, d\vec{v}_2 + \tag{21}$$

$$+ n/m \int \frac{\partial \Phi_0(\vec{r}_1 - \vec{r}_2)}{\partial \vec{r}_1} \rho(t, \vec{r}_2)\, d\vec{r}_2 \cdot \frac{\partial}{\partial \vec{v}_1} f(t, \vec{r}_1, \vec{v}_1)$$

where

$$\rho(t, \vec{r}_2) = \int f(t, \vec{r}_2, \vec{v}_2)\, d\vec{v}_2 ,$$

also possesses microscopic solutions of the form (8), (18), corresponding to the exact movement of particles in the considered dynamical system.

Therefore the equation (21) can provide a basis for obtaining higher approximations.

By substituting the microscopic solutions in this equation the whole system of equations for $F_1, F_2, \dots F_s, \dots$ may easily be obtained.

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