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## LETTER TO THE EDITOR

## A new derivation of the Boltzmann transport equation

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Abstract. A new way of deducing the Boltzmann transport equation from the Liouville equation is presented. The major advantage of the new method is that it provides for generalization by means of less restrictive assumptions.

Many authors have described methods of deducing the Boltzmann transport equation from the Liouville equation (these include Kirkwood 1946, Bogoliubov 1946, Born and Green 1949, Hollinger and Curtiss 1960, Hoffman and Green 1965). We present a new way which has the following advantages:

(i) The basic statistical assumption is made explicitly, on the distribution function  $\rho(\mathbf{r}_1, \mathbf{p}_1, \dots, \mathbf{r}_N, \mathbf{p}_N, t)$  in the Liouville equation, rather than implicitly.

(ii) The origin of the time irreversibility is obvious.

(iii) The theory provides for generalization by means of less restrictive assumptions. This is the most important feature.

We start by assuming an initial state of the ensemble, at time t = 0, without statistical correlations:

$$\rho(\mathbf{r}_1, \mathbf{p}_1, \mathbf{r}_2, \mathbf{p}_2, \dots, \mathbf{r}_N, \mathbf{p}_N, t = 0) = \frac{N!}{V^N} g_0(\mathbf{r}_1, \mathbf{p}_1) g_0(\mathbf{r}_2, \mathbf{p}_2) \dots g_0(\mathbf{r}_N, \mathbf{p}_N)$$
(1)

where  $g_0(\mathbf{r}, \mathbf{p})$  is an arbitrary function normalized by

$$\int g_0(\boldsymbol{r}, \boldsymbol{p}) \mathrm{d}^3 \boldsymbol{r} \, \mathrm{d}^3 \boldsymbol{p} = V, \tag{2}$$

where V is the volume of the container. The time development of  $\rho$  is governed by the Liouville equation

$$\frac{\partial \rho}{\partial t} = [\rho, H_N] \tag{3}$$

where the bracket is a Poisson bracket, and  $H_N$  is the N-particle hamiltonian.

Let  $\Delta t$  be a time interval which is (a) appreciably longer than the duration of one collision, and (b) much shorter than the mean free time between collisions, with  $\rho$  at t = 0 given by (1);  $\rho$  at time  $t = \Delta t$  is not of the form

$$\frac{N!}{V^N}g(\boldsymbol{r}_1, \boldsymbol{p}_1, \Delta t)g(\boldsymbol{r}_2, \boldsymbol{p}_2, \Delta t) \dots g(\boldsymbol{r}_N, \boldsymbol{p}_N, \Delta t)$$
(4)

no matter what we choose to be the function  $g(r, p, \Delta t)$ .

However, we now ask: How should  $g(\mathbf{r}, \mathbf{p}, \Delta t)$  be chosen so that (4) represents the best approximation to the true distribution function  $\rho$  at time  $t = \Delta t$ ? This becomes a sensible question as soon as we decide what we mean by 'best.'

Our criterion of 'best' is: For all physical quantities Q which are sums of quantities depending upon the coordinates of each particle separately, ie, for all Q of form

$$Q = \sum_{i=1}^{N} q(\boldsymbol{r}_i, \boldsymbol{p}_i), \tag{5}$$

the expectation value of Q,

$$\langle Q \rangle = \int Q \rho \, \mathrm{d}^N \tau,$$
 (6)

should be the same for the exact  $\rho$  at time  $t = \Delta t$ , as for the approximate  $\rho$  of form (4).

Without going into details (which will appear in a separate publication) it follows that the 'best' g is given by

$$g(\mathbf{r}_1, \mathbf{p}_1, \Delta t) = V \frac{\int \rho \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_3 \dots \, \mathrm{d}\tau_N}{\int \rho \, \mathrm{d}^N \tau}$$
(7)

where  $\rho$  is the exact distribution at time  $\Delta t$ .

By making approximations suitable to a dilute gas in the evaluation of (7), it is possible to deduce a value for the change

$$\Delta g = g(\mathbf{r}, \mathbf{p}, \Delta t) - g_0(\mathbf{r}, \mathbf{p}). \tag{8}$$

The approximation allows evaluation of the integral (7) over configurations in which either (a) particle 1 suffers no collision in time  $\Delta t$ , or (b) particle 2 suffers one binary collision in time  $\Delta t$ , but excludes configurations leading to ternary or even higher-order collisions in that time. If f is then defined by

$$f(\mathbf{r}, \mathbf{p}, \Delta t) = \frac{N}{V} g(\mathbf{r}, \mathbf{p}, \Delta t)$$
(9)

and we approximate:

$$\frac{\partial f}{\partial t} \simeq \frac{N}{V} \frac{\Delta g}{\Delta t} \tag{10}$$

then the result is the Boltzmann equation in its usual form.

The origin of irreversibility is clear from this derivation. The replacement of the exact N-particle distribution function  $\rho$  by the approximate form (4) clearly throws away information about the state of the ensemble at time  $t = \Delta t$ , information which is essential to the recovery of the exact initial state.

The major advantage of this new derivation is that the basic idea is not restricted to the ansatz (4), but can be used with a more general ansatz, for example, one which includes pair correlation functions  $h(r_1, p_1, r_2, p_2, t)$  explicitly. This then allows derivation of equations more general, and more accurate, than the Boltzmann equation. The detailed calculations are not simple, and the results are not such as one would be likely to obtain by purely intuitive arguments similar to those of Boltzmann. These results will be reported later.

## References

Bogoliubov J 1946 J. Phys. (USSR) 10 256 Born M and Green H S 1949 A General Kinetic Theory of Liquids (New York: Cambridge University Press) Hoffman D K and Green H S 1965 J. Chem. Phys. 43 4007 Hollinger H G and Curtiss C F 1960 J. Chem. Phys. 33 1386 Kirkwood J G 1946 J. Chem. Phys. 14 180