

# Approach to Translational Equilibrium in a Rigid Sphere Gas

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## Approach to Translational Equilibrium in a Rigid Sphere Gas

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(Received 10 May 1963)

It is usually assumed that the translational degree of freedom in a gas reaches equilibrium in a time of the order of the mean collision time. Some confirmation of this has been supplied by Alder and Wainwright<sup>1</sup> who used their "molecular dynamic" method to determine the rate of approach to Maxwellian equilibrium of a set of molecules which all start with the same speed. This method effectively solves the simultaneous equations of all the molecules in a closed container and is valid for dense gases. However, it makes great demands on computer time and storage capacity, and Alder and Wainwright were limited to 100 molecules which was an insufficient number to enable information to be gained on the rate of approach to equilibrium in the higher speed ranges of the distribution. The present note reports on an investigation of this problem using a Monte Carlo type method which is valid for gases at normal and low densities, and is sufficiently economical in its computing requirements to enable information to be obtained on the velocity dependence of the rate of approach to equilibrium.

In the present method, only the speeds of the molecules are stored and, initially, these are all equal to a speed which corresponds to the root mean square speed. Two molecules are chosen at random and a random direction is assigned to one relative to the other. The relative velocity between them is then calculated and, since the gas is assumed to be at a constant density, this pair of molecules is assigned a probability of collision which is proportional only to the magnitude of the relative velocity. For the molecules that do collide, the direction of relative motion after impact is chosen at random and the new molecular speeds are calculated and stored in place of the previous values.

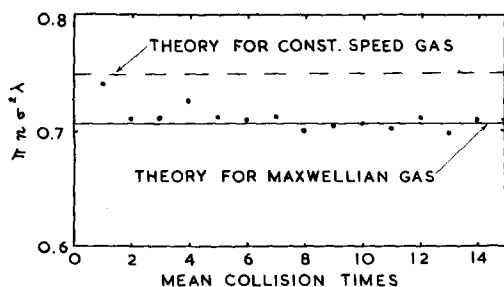


FIG. 1. Behavior of mean free path.

Using the Silliac digital computer in the University of Sydney, more than 30 000 collisions were computed per hour of computing time. The results quoted below are based on the mean of ten runs each involving 500 molecules. As a check on the accuracy of the Monte Carlo-type approach, the mean free path and the collision frequency were calculated by assigning the appropriate time interval to each collision. Figure 1 shows the behavior of the mean free path  $\lambda$  with the mean collision time (i.e. the time in which each molecule suffers an average of one collision). The six percent change in the mean free path from the Clausius value<sup>2</sup> for a constant-speed gas to the value for a Maxwellian gas is discernable. The collision frequency was also in excellent agreement with the theoretical value.

It was found that the general features of the Maxwellian distribution were established after about four collisions. For instance, Fig. 2 shows the fraction  $f$  of molecules with speeds between 0.9 and 1.1 times the root mean square speed  $v_r$ . This fraction is initially unity and, after collisions have started, it tends rapidly to its Maxwellian value of 0.1838. The lower speed ranges were filled from zero

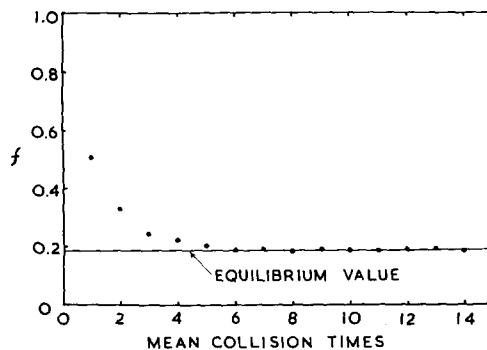


FIG. 2. Fraction of molecules in range 0.9 to 1.1  $v_r$ .

in similar times. However, in the very high speed ranges, a progressively larger number of collisions were required before the number of molecules in the range reached the equilibrium value. Figure 3 shows the ratio of the actual to theoretical number in various ranges as a function of time. Because of the smaller samples which are involved in the higher speed ranges, the scatter of the points becomes progressively greater. However, it is clear that it requires at least ten to fifteen collisions before the fraction of molecules with speeds of the order of twice the root mean square speed reaches its equilibrium value.

Some information on the velocity dependence of the rate of approach to equilibrium was given by Alder and Wainwright<sup>1</sup> from a numerical solution of the Boltzmann equation for the decay of a

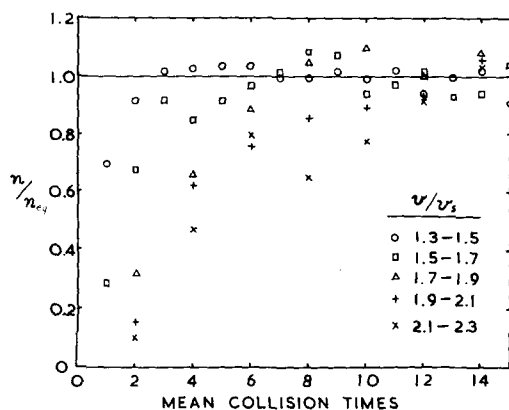


FIG. 3. Approach to equilibrium in higher speed ranges.

highly peaked velocity distribution function. Their results indicate that the population of molecules with a speed of 1.8 times the root mean square speed (the highest speed for which they present results) reaches about one third of the equilibrium value after two mean collision times, and about two thirds of the equilibrium value after four mean collision times. These values are in agreement with the results shown in Fig. 3.

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<sup>1</sup> B. J. Alder and T. Wainwright, *Proceedings of the International Symposium on Transport Processes in Statistical Mechanics* (Interscience Publishers, Inc., New York, 1958), p. 97.

<sup>2</sup> E. H. Kennard, *Kinetic Theory of Gases* (McGraw-Hill Book Company, Inc., New York, 1938).

## Wiener-Hermite Functional Expansion in Turbulence with the Burgers Model

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OUR ultimate aim is to exploit the nearness to Gaussianity of velocity probability distributions in turbulence, by expanding the velocity field function about the Gaussian approximation. Many of the mathematical manifestations of our method are so new, however, that it is hard to obtain physical insight into them. Hence, we have undertaken a preliminary, pilot study of a simplified nature, which uses instead of the Navier-Stokes or

magnetohydrodynamic equations, the Burgers one-dimensional model equation:<sup>1</sup>

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = 0. \quad (1)$$

The expansion is in terms of Wiener-Hermite functionals:<sup>2,3,4</sup>

$$u(x, t) = \int K^{(1)}(x - x_1) H^{(1)}(x_1) dx_1 \\ + \iint K^{(2)}(x - x_1, x - x_2) H^{(2)}(x_1, x_2) \\ \cdot dx_1 dx_2 + \dots \quad (2)$$

The  $K^{(i)}$ , which are implicitly functions of time ( $t$ ), are ordinary (nonrandom) functions. Integrations are over  $(-\infty, \infty)$ . The  $H^{(i)}$  are the Wiener-Hermite functionals as defined in reference 4. They are random functions, whose salient properties are (a) their mutual statistical orthogonality, expressed by such relations as

$$\langle H^{(i)} H^{(j)} \rangle = 0 \quad \text{if } i \neq j,$$

$$\langle H^{(1)}(x_1) H^{(1)}(x_2) \rangle = \delta(x_1 - x_2), \quad \text{etc.};$$

(b)  $H^{(1)}$  is the "ideal random function",<sup>4,5</sup> or derivative of the Wiener function,<sup>6,7</sup> whence the first term of (2) is a Gaussian function, and the later terms are in some sense successively higher corrections to Gaussianity.

Alternatively stated, the quantity  $H^{(1)}(x_1)$  is a set of functions with the property that the values at a single point  $x_1$  are uniformly distributed and the values are uncorrelated from point to point in  $x_1$ . The higher-order functionals  $H^{(2)}$ , etc., are linear combinations of powers of  $H^{(1)}$  with delta functions, chosen in such a way that they are mutually statistically orthogonal. The kernels in (2) are simply related to such familiar physical quantities as correlations and energy spectrum functions. For instance, the usual energy spectrum function is easily seen from the above definitions to be given by

$$E(\kappa) = (2\pi)^{-1} |K^{(1)}(\kappa)|^2 + 2(2\pi)^{-2}$$

$$\cdot \int |K^{(2)}(\kappa_1, \kappa - \kappa_1)|^2 d\kappa_1 + O[K^{(3)2}],$$

where  $K^{(i)}(\kappa)$  is the Fourier transform of  $K^{(i)}(x)$ , etc. {see (3) below}. The expansion (2) is rigorously convergent for a broad class of random functions. It should also be noted that (2) is an expansion of the random function, not of its probability distribution, and is therefore not equivalent (for example) to the Gram-Charlier series of the probability distribution