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Transport coefficients for dense gases

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A scheme is proposed for calculating the coefficient of self-diffusion in a dense gas of rigid spheres. The method proceeds by deriving and solving a closed equation for the velocity distribution function f associated with a single sphere which has specified **initial** position and velocity in a system in which the other particles have initial distributions of equilibrium [5].

At low densities f satisfies a linearized form of Boltzmann's transport equation. It is shown how generalizations of Boltzmann's equation can be obtained which are suitable for describing a gas at any given density. In the derivation of these equations one approximates the many-body dynamical problem by treating the dynamics of a few particles exactly and by also including certain many-body dynamical events. By this approach one can obtain expressions suitable for calculating the coefficient of self-diffusion and at the same time avoid the divergence problem [4] which arises when the gas is analyzed in terms of contributions from finite numbers of isolated particles.

A generalization of Boltzmann's equation is considered which applies to gases dense enough for configurations of three particles in close proximity to be significant. This equation differs from the equation derived by Choh and Uhlenbeck [3] for describing such systems in that it accounts for certain many-body dynamical events as well as three-body

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collision sequences.

The coefficient of self-diffusion D , as usually defined, is equal to the integral over time of the velocity autocorrelation function which can be calculated from the velocity distribution function f . It is shown how D is obtained from the closed equations for f . Evaluation of D from generalizations of Boltzmann's equation requires detailed numerical analysis.

Thus in order to make a quantitative test of the proposed scheme we consider a one dimensional gas of impenetrable point particles. It is shown that the velocity distribution function and the coefficient of self-diffusion can be determined exactly for this model. A closed equation for f is derived which takes into account three-body dynamics as well as certain many-body events. The latter collision sequences must be included to avoid divergences which also arise in the one dimensional model. The coefficient of self-diffusion as calculated from this equation is found to be very close to the exact value.

A discussion is also presented of an appropriate definition of the coefficient of self-diffusion for dense systems. A modified definition is proposed which takes into account the observed correlations between the velocity of the diffusing particle and other particles of the gas.

Part of the material presented in this thesis can be found in papers by Green, Hoffman, and the author [*1*, *2*].

References

[*1*] G.R. Anstis, "Generalizations of Boltzmann's equation", *Austral. J. Phys.* 27 (1974), 773-786.

[*2*] G.R. Anstis, H.S. Green and D.K. Hoffman, "Kinetic theory of a one-dimensional model", *J. Mathematical Phys.* 14 (1973), 1437-1443.

[3] S.T. Choh, "The kinetic theory of phenomena in dense gases", (Doctoral dissertation, University of Michigan, 1958); also issued as US Government Technical Report PB138 502 by S.T. Choh and G.E. Uhlenbeck. In either form it has been found inaccessible; see S.G. Brush, *Kinetic theory*, Volume 3, pp. 73-74, footnote 57, and p. 82 (Pergamon Press, Oxford, New York, Toronto, Sydney, Braunschweig, 1972) from which it is quoted.

[4] M.H. Ernst, L.K. Haines, J.R. Dorfman, "Theory of transport coefficients for moderately dense gases", *Rev. Modern Phys.* 41 (1969), 296-316.

[5] H.S. Green, "Theories of transport in fluids", *J. Mathematical Phys.* 2 (1961), 344-348.