Self-diffusion in confined systems

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Diffusion in fluids is one of the widest studied process in the context of Statistical Mechanics. Starting from stochastic methods or by kinetic theory, how a particle diffuses is well understood, at least in the low-density limit.

When the system is confined over regions with a width of the order of the diameter of the particles, the situation is much more complex and there is no microscopic theory that allows us to understand diffusion as well as in the non-confined case. One of the simplest models to carry out the study is an ensemble of elastic hard particles confined by two fixed parallel walls separated a distance of the order of the particles' diameter. In fact, in the last years a kinetic theory for such a system has been formulated when the system is ultraconfined, i.e., the separation between the plates is smaller than twice the diameter of the particles, so that the particles can not jump over each other [1-3].

We consider the self-diffusion process of a hard sphere fluid confined by two parallel plates separated by a distance on the order of the particle diameter is studied. The starting point is a closed kinetic equation for the distribution function that takes into account the effects of the confinement and that is valid in the low-density limit. From it, the Boltzmann-Lorentz equation that describes the dynamics of some tagged particles when the whole system is in equilibrium is derived. An equation that describes the diffusion in the directions parallel to the walls is deduced by applying the Zwanzig-Mori projection technique to the Boltzmann-Lorentz equation, obtaining an explicit expression for the self-diffusion coefficient that depends on the height of the system. A very good agreement between its theoretical prediction and Molecular Dynamics simulation results is obtained for the whole range of heights [4].

References:

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