Diffusion of an intruder in a molecular/granular gas as a random walk

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It is well known that by using elementary random walk (RW) arguments it is possible to obtain a rough estimate of the mean square displacement (MSD) of a molecule moving in a gas of elastic hard spheres. However, this result is not very good: the difference between the diffusion coefficient thus obtained, $D=\lambda v/3$, and the diffusion coefficient obtained from the standard kinetic theory (e.g. Chapman-Enskog expression in the so-called first Sonine approximation) or simulation results is remarkable, exceeding 40%. (Here λ is the mean free path of the molecule and v is its mean speed.) The origin of this large discrepancy lies in the fact that the above simple random walk calculation neglects the correlation between the directions of the particle velocities before and after each binary collision. In fact, it is known that if this sort of correlation were rigorously taken into account, the results derived from the RW theory would be consistent with those obtained by solving the Boltzmann equation with the Chapman-Enskog method.

Here we estimate the MSD of an intruder (or walker) immersed in an ordinary gas using a RW (or free path) method that considers the correlations between the directions of the molecules before and after each collision. In the case of an elastic intruder moving in an ordinary gas of elastic hard spheres, our method gives results for the self-diffusion coefficient that differ by less than 4% from those obtained by the Sonine approximation of order 9. When the intruder and particles of the gas are mechanically different, we find that the RW results for the corresponding diffusion coefficient do not differ by more than 15%, and this happens only in the extreme case when the mass of intruder is much larger than that of the particles of the gas. Our procedure can also be generalized to the case of a grain moving in a gas of elastic hard spheres (i.e., when grain-gas particle collisions are inelastic and characterized by a constant coefficient of restitution). In this case, the difference between the RW results and those derived in the second Sonine approximation is typically a few percent units. Finally, it is also possible to extend the method to the case of an intruder (grain) moving in a freely cooling granular gas (modelled as a gas of smooth inelastic hard spheres). In this situation, we analyze how the inelasticity of collisions modifies the MSD of the intruder. The results are generally very good (in some cases even excellent) when compared with simulation results and with the first and second Sonine approximations.