Comment on "Microscopic kinetic theory of the mean collision force of a particle moving in rarefied gases"

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In a recent paper [T. Wei *et al.*, Phys. Rev. E **106**, 034101 (2022)] a derivation of the resistance force acting on a small classical particle moving through a rarefied gas has been presented. Unfortunately, the obtained expression is inaccurate. The purpose of this Comment is to provide the accurate expression and to discuss several related aspects.

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In a recent paper [1] an expression for the resistance force acting on a small classical test particle moving through a rarefied gas has been reported. The authors focused on the regime where the particle size is much smaller than the mean free path; that is, the Knudesen number is large (free molecular regime). This is where Stokes' law is not applicable. They used an elastic hard-sphere collision model and assumed that the background gas is in equilibrium and characterized by the Maxwellian velocity distribution. Under these assumptions they derived a general expression for the collision (resistance) force and analyzed two limiting cases: low speed (test particle drift velocity is much lower than the thermal velocity of background gas atoms) and high speed (test particle drift velocity is much higher than the thermal velocity of background gas atoms). The force derived in Ref. [1] is proportional to the reduced mass, which is generally not correct. In the following, the correct expression is first derived, the origin of the inaccuracy is identified, and a few related remarks are made.

Let us consider a test particle of mass m_1 moving through a gas of field atoms having mass m_2, number density n_2, and an isotropic Maxwellian distribution of velocities. The key ingredient in evaluating the properties of collision processes is the distribution function over relative velocities [2]. The kinetic energy of any two particles in the laboratory reference frame is the sum of the energy of their relative motion, $\mu v^2/2$, and the energy of the center of mass $(m_1+m_2)V^2/2$. Here $\mathbf{v}=\mathbf{v}_1-\mathbf{v}_2$ is the relative velocity, $\mathbf{V}=(m_1\mathbf{v_1}+m_2\mathbf{v_2})/(m_1+m_2)$ is the velocity of the center of mass, and $\mu=m_1m_2/(m_1+m_2)$ is the reduced mass. If a test particle is in thermal equilibrium with the gas (sometimes this is not the case, like, for instance, in nonequilibrium plasmas, where different species can have different temperatures) the distribution of the relative velocities can be derived as [3]

$$\begin{aligned}\frac{dN(v)}{N} &= \iint_{|\mathbf{v}_1-\mathbf{v}_2|=\text{const}} f_1(\mathbf{v}_1)d\mathbf{v}_1 f_2(\mathbf{v}_2)d\mathbf{v}_2 \\ &= \int_{|\mathbf{v}|=\text{const}} \left(\frac{\mu}{2\pi T}\right)^{3/2} e^{-\mu v^2/2T} d\mathbf{v} \int \left(\frac{m_1+m_2}{2\pi T}\right)^{3/2} \\ &\quad \times e^{-(m_1+m_2)V^2/2T} d\mathbf{V} \\ &= 4\pi\left(\frac{\mu}{2\pi T}\right)^{3/2} e^{-\mu v^2/2T} v^2 dv = 4\pi v^2 f_M(v)dv, \quad (1)\end{aligned}$$

where T is the temperature (energy units are used so that $k_BT \to T$), $d\mathbf{v}=4\pi v^2 dv$, $d\mathbf{V}=4\pi V^2 dV$, and $d\mathbf{v}_1 d\mathbf{v}_2 = d\mathbf{v}\,d\mathbf{V}$. The distribution of relative velocities is therefore just the Maxwellian distribution taken with the reduced mass instead of the bare mass of field atoms. When a test particle is heavy so that $m_1 \gg m_2$, its thermal motion can be neglected and the use of the bare mass m_2 in the relative velocity distribution would be appropriate. The same follows from Eq. (1), because $\mu \simeq m_2$ in this limit. For comparable masses $m_1 \simeq m_2$, the use of the reduced mass is essential.

Assuming that the test particle is drifting with the velocity $\mathbf{v}_1$, it is convenient to work in the reference frame moving with the test particle. Relative velocity distribution function of field atoms becomes a shifted Maxwellian distribution [4,5]

$$f_M(\mathbf{v}+\mathbf{v}_1) = \left(\frac{\mu}{2\pi T}\right)^{3/2} \exp\left[-\frac{\mu(\mathbf{v}+\mathbf{v}_1)^2}{2T}\right]. \quad (2)$$

It is further convenient to introduce a characteristic thermal velocity $v_T=\sqrt{T/\mu}$. An expression for the resistance force in the free-molecular regime for simple scatering trajectories can be written as [4]

$$\mathbf{F}_r = \mu n_2 \int \mathbf{v} v f_M(\mathbf{v}+\mathbf{v}_1)\sigma(v)d^3v, \quad (3)$$

where $\sigma(v)$ is the velocity-dependent momentum transfer cross section. Equation (3) is rather general and can be applied to systems with quite disparate interactions. The properties of interaction govern the functional form of $\sigma(v)$. A first calculation of this kind was apparently performed by Langevin, who focused on the "low speed" regime $v_1 \ll v_T$ and considered special cases of Maxwell molecules with $\sigma(v) \propto 1/v$ and elastic scattering of rigid spheres with $\sigma(v)=\text{const}$ [6]. Examples related to plasma-related systems such as dusty or complex plasma can be found in Refs. [7–9]. A useful summary of momentum transfer rate coefficients for collisions between various species (including charged and uncharged particles) can be found in Ref. [10].

For the elastic hard-sphere collision model, the momentum transfer cross section σ is simply determined by the geometrical cross section, $\sigma=\pi d^2=\pi(r_1+r_2)^2$, where r_1 and r_2 are the radii of the test sphere and background gas spheres (atoms), respectively. The integral (3) can be

relatively straightforwardly evaluated, leading to

$$F_r = -\mu n_2 \sigma v_T^2 \left(\frac{v_\mathrm{T}}{v_1}\right)^2 \left\{ \sqrt{\frac{2}{\pi}} \frac{v_1}{v_\mathrm{T}} \left(1 + \frac{v_1^2}{v_\mathrm{T}^2}\right) e^{-v_1^2/2v_\mathrm{T}^2} + \left(\frac{v_1^4}{v_\mathrm{T}^4} + 2\frac{v_1^2}{v_\mathrm{T}^2} - 1\right) \mathrm{erf}\left(\frac{v_1}{\sqrt{2} v_\mathrm{T}}\right) \right\}. \quad (4)$$

The minus sign implies that the resistance force is acting against the direction of motion of the test particle.

The expression of this kind was derived by Baines *et al.* in relation to the behavior of dust grains in interstellar gas [see Eq. (4.5) from Ref. [11]]. The only difference is that the case when the mass of the sphere is large in comparison with the mass of the gas atoms (and hence $\mu = m_2$) was considered there. Equation (4) is similar to the key result of Eq. (21) from Ref. [1], but with an important difference. The background gas thermal velocity $\sqrt{T/m_2}$ appears in Ref. [1] in place of the relative thermal velocity $v_\mathrm{T} = \sqrt{T/\mu}$. The reason behind this difference is that in Ref. [1] the averaging is performed over the velocity distribution function of the background gas and not over the distribution of relative velocities. As already pointed out, when a heavy particle moves through a gas of lighter particles (like, e.g., in Ref. [11]), this point is not important since $\mu \simeq m_2$. For comparable masses, Eq. (21) from Ref. [1] is inaccurate.

For a low relative speed $v_1 \ll v_\mathrm{T}$ we obtain in the first approximation

$$F_r \simeq -\frac{8\sqrt{2}}{3\sqrt{\pi}} \mu n_2 \sigma v_\mathrm{T} v_1 = -\frac{8\sqrt{2}}{3\sqrt{\pi}} n_2 \sigma \sqrt{\mu T} v_1. \quad (5)$$

This result coincides with that derived by Langevin [6], but not with that from Ref. [1]. The force is proportional to $\mu^{1/2}$ rather than μ. This has important direct consequences. Equation (5) defines the mobility, b, of a test particle from $\mathbf{F} = b\mathbf{v}$, where $\mathbf{F}$ is the external force and $\mathbf{v}$ is the equilibrium velocity [4]. The mobility is related to the diffusion coefficient via the Einstein relation $D = T/b$. In the special case when $m_1 = m_2 = m$ (and thus $\mu = m/2$), we obtain the classical expression for the self-diffusion coefficient of a rarefied gas of hard spheres of diameter d and density n [4,6]:

$$D = \frac{3}{8nd^2} \sqrt{\frac{T}{\pi m}}. \quad (6)$$

This corroborates the presented derivation.

In the opposite limit of high relative speed, $v_1 \gg v_\mathrm{T}$, we get in the first approximation

$$F_r \simeq -\mu n_2 \sigma v_1^2. \quad (7)$$

In this regime the force is proportional to the reduced mass. This agrees with the first-order terms from Ref. [1], because thermal motion can be ignored compared to the drift in the first approximation. Higher terms are, however, incorrect.

The interest in the resistance force experienced by a sphere (spherical droplet) moving through a gas was particularly triggered by experiments of Millikan and coworkers, who used the oil-drop method for measuring the elementary electric charge [12] and coefficients of slip in gases [13]. Among the outstanding observations he made was the fact that the nature of droplet surface and the exact properties of gas-surface interactions exert a very important influence upon the resistance force. The assumption of specular reflection is generally inappropriate. An excellent theoretical account of this problem was provided by Epstein [14]. For a sphere that is much larger and heavier than atomic scales, but is much smaller than the atomic mean free path, he derived the expression, which reads (using the present notation)

$$F_r = -\delta \frac{8\sqrt{2\pi}}{3} n_2 a^2 \sqrt{m_2 T} v_1, \quad (8)$$

where a is the radius of the sphere (and $\sigma = \pi a^2$ is the momentum transfer cross section for specular reflection). This is identical to Eq. (5), except the numerical factor δ, which depends on the details of how atoms interact with the sphere surface (the high-speed regime was not considered at this time as irrelevant for the regime of Millikan experiments). Epstein considered various scenarios for atom-sphere interactions and obtained $\delta = 1$ for specular reflection (interestingly, $\delta = 1$ also for atom sticking and remaining on the sphere surface); $\delta = \frac{13}{9} \simeq 1.444$ for diffuse reflection with conservation of velocity; $\delta = 1 + \frac{9\pi}{64} \simeq 1.442$ for a sphere that is a perfect thermal nonconductor; and $\delta = 1 + \frac{\pi}{8} \simeq 1.393$ for a sphere that is a perfect thermal conductor. This can be compared with the experimental value $\delta \simeq 1.368$ found by Millikan.

The force of resistance acting on a particle moving through a rarefied gas is also very important in the field of complex (dusty) plasma [15–19]. This is the main mechanism responsible for friction when a particle is moving through a stationary low-ionized plasma. This force is often called the neutral drag force, but it is also not uncommon to use the term "Epstein drag," recognizing Epstein's pioneering contribution. As a main mechanism of dissipation, neutral drag severely affects particle transport and dynamics, as well as dominates damping of waves. Equation (8) has been verified experimentally. For melamine-formaldehyde micron-size microspheres in an argon gas the coefficient δ has been measured as $\delta \simeq 1.26 \pm 0.13$ using the single-particle laser acceleration method, and $\delta = 1.44 \pm 0.19$ using the vertical resonance method [20].

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