Quantum drag forces on a sphere moving through a rarefied gas

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As an application of quantum fluid mechanics, we consider the drag force exerted on a sphere by an ultradilute gas. Quantum mechanical diffraction scattering theory enters in that regime wherein the mean free path of a molecule in the gas is large compared with the sphere radius. The drag force is computed in a model specified by the "sticking fraction" of events in which a gaseous molecule is adsorbed by the spherical surface. Classical inelastic scattering theory is shown to be inadequate for physically reasonable sticking fraction values. The quantum mechanical scattering drag force is exhibited theoretically and compared with experimental data.

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I. INTRODUCTION

Quantum fluid mechanical effects [1] are very often considered to be negligible. Except for some very special cases [2], such as the study of the superfluid phases of helium [3,4], quantum fluid mechanics is rarely considered. Here we wish to consider an important exception to this rule; i.e., the drag force exerted on a moving sphere by a highly rarified gas. We wish to consider the case in which the mean free path of a gas molecule is large, on the length scale of the sphere radius. For example, a very rarefied gas [5] exists above the upper atmosphere. Meteors or spaceships on first entering such an atmosphere [7,8] may approximate the situation to be studied in this work.

A rarified gas will exert a drag force on a moving sphere. If the mean free path of a molecule in the gas is small compared with the radius of the sphere, then the drag is due to the viscosity of the gas. If the gas is further diluted so that the mean free path of a molecule is much larger than the sphere radius, then the drag force in a kinetic theory picture depends on the notion of a sticking fraction f; i.e., the fraction $0<f<1$ of molecules incident on a surface that sticks and thermalizes to the temperature of the sphere before later evaporating. We shall later presume that those molecules which do not stick to the surface are specularly reflected. The central result of such a Knudsen model [6] is a relationship between the sticking fraction and the slip drag force on the sphere.

In past treatments of the scattering of molecules off the sphere, the classical scattering theory has been employed [9]. A central result of our work is that the classical scattering theory is inadequate and should be replaced by quantum scattering theory. The drag coefficient is proportional to the transport cross section for molecules to scatter off the sphere. Due to diffraction effects, the quantum mechanical cross section will differ appreciably from the classical cross section. The incoming molecules are sufficiently large and fast for their quantum wavelengths to be very small on the scale of the sphere radius. This is a necessary, but not sufficient condition for the classical limit to be obtained. The classical limit still fails to hold true due to diffractive shadow scattering which persists to even the smallest wavelengths. Diffraction effects increase the total cross section by roughly a factor of 2. The factor is exactly 2 for purely specular reflection. Millikan [10] made a series of experiments measuring the drag force on oil droplets by rarefied gases and found an effective transport cross section given by $\sigma_m \approx 1.37\pi a^2$, wherein a is the sphere radius. It is not very easy to understand why such an experimental cross section is larger than the standard classical geometric cross section πa^2. Unfortunately we do not know of any recent experiments, which attempt to measure the drag forces on spheres in a similar Knudsen regime [11,12]. We thereby use the reliable Millikan experimental results to compare with theory.

In Sec. II, we first review the classical kinetic theory of the drag coefficient on a sphere for the case of completely elastic classical specular reflection. Second, the completely absorptive limit is briefly discussed. In Sec. III we first review the kinetic theory of the drag coefficient on a sphere for the case of completely elastic *quantum* specular reflection. The quantum kinetic theory for the drag coefficient will be calculated. Second, the completely *quantum* absorptive limit is briefly discussed. In Sec. IV a general sticking fraction model will be discussed. The results obtained thereof will be compared to experiment. In the concluding Sec. V, the implication of these results for the picture of quantum turbulent backflow will be discussed. Quantum diffraction effects lead to a strong forward peak in the differential cross section. In quantum hydrodynamic terms, the forward scattering peak translates into a thin quantum trail of fluid which will flow behind a moving sphere. The trail is due to those particles which undergo specular reflection from the surface.

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II. CLASSICAL DRAG FORCE ON A SPHERE

Many of the kinetic models applied to drag forces in ultrararefied gases involve the notion of a sticking fraction f defined as follows: (i) $(1-f)$ is the probability that a molecule will elastically scatter off the surface in a specular fashion and (ii) f is the probability that a molecule will stick to the surface and thermalize to the substrate temperature before finally being evaporated back into the gas. Below, the drag force on a sphere of radius a will be reviewed using purely classical scattering theory and classical kinetic theory. Two opposite limits will be discussed; namely, (A) the purely elastic specular reflection limit, i.e., $f=0$ and (B) the purely inelastic absorption limit, i.e., $f=1$.

A. Classical elastic specular reflections

Consider a particle moving in the gas in the direction of a unit vector $\mathbf{u}$. If the particle hits the sphere and specularly scatters through an angle θ, then the component of the momentum transfer along the original direction is given by

$$\mathbf{u}\cdot(\mathbf{p}_i-\mathbf{p}_f)=|\mathbf{p}|(1-\cos\theta). \qquad (1)$$

If one now has n gas particles of mass m per unit volume with a distribution of momenta $\mathbf{p}=p\mathbf{u}$, then the momentum transfers give rise to a drag force

$$\mathbf{F}=\left\langle n\mathbf{p}\frac{p}{m}\int(1-\cos\theta)d\sigma\right\rangle_{\mathbf{p}}. \qquad (2)$$

In Eq. (2), $d\sigma$ is the differential cross section of scattering from the sphere into a solid angle $d\Omega$ about the angle θ. The brackets $\langle\cdots\rangle_{\mathbf{p}}$ denote averaging over all momenta $\mathbf{p}$ with a Maxwellian distribution corresponding to a mean gas “wind velocity” $\mathbf{v}$. The transport cross section is usually defined [13] as

$$\sigma_1=\int(1-\cos\theta)d\sigma, \qquad (3)$$

so that the drag force may be written as

$$\mathbf{F}=\left\langle n\mathbf{p}\frac{p}{m}\sigma_1\right\rangle_{\mathbf{p}}. \qquad (4)$$

For classical specular reflection from a spherical surface,

$$\left[\frac{d\sigma}{d\Omega}\right]_{specular}=\frac{a^2}{4}\quad(\text{classical hard sphere}), \qquad (5)$$

the transport cross section is the same as total cross section ([14]); i.e.,

$$\sigma_1=\sigma=\pi a^2\quad(\text{classical elastic hard sphere}). \qquad (6)$$

The drag force for the above cross sections is [15–20]

$$\mathbf{F}=\frac{\pi a^2 n}{m}\int p\mathbf{p}e^{-(\mathbf{p}-m\mathbf{v})^2/2mk_BT}\left[\frac{d^3\mathbf{p}}{(2\pi mk_BT)^{3/2}}\right],$$
$$F=\frac{1}{2}\rho\pi a^2C_Fv^2\quad(\rho=mn), \qquad (7)$$

where

$$C_F=\frac{e^{-s^2}}{\sqrt{\pi}s^3}(2s^2+1)+\frac{\text{erf}(s)}{2s^4}(4s^4+4s^2-1), \qquad (8)$$

$$s=v\sqrt{\frac{m}{2k_BT}}, \qquad (9)$$

and erf(s) is the error function [21]. When the velocity of the object is low, then the drag force obeys [22]

$$\lim_{v\to 0}\left[\frac{F}{v}\right]=\frac{4}{3}(\pi a^2)\rho\overline{c},\quad \text{where } \overline{c}=\sqrt{\frac{8k_BT}{\pi m}}. \qquad (10)$$

The mean speed of a gas particle is denoted by $\overline{c}$.

B. Classical purely inelastic absorption

By purely inelastic classical absorption, we mean that any incoming particle whose impact parameter is less than the sphere radius sticks to the spherical surface with probability 1; i.e., $f=1$. The particle may much later be re-emitted after thermal equilibrium with the sphere is established. This kind of evaporation implies the re-emission of gas particles with a Maxwellian distribution with zero mean velocity in the reference frame of the sphere. The spherical nature of the re-emission implies the equality of the transport cross section in Eq. (4) and the total cross section. Specifically,

$$\sigma_1(f=1)=\sigma_{in}=\pi a^2\quad(\text{classical}). \qquad (11)$$

It then follows that the drag force on a sphere due to purely classical elastic collisions coincides with the drag force due to purely classical inelastic collisions [22]. The drag force is again,

$$F=\frac{1}{2}\rho\pi a^2C_Fv^2, \qquad (12)$$

wherein C_F is defined in Eq. (8).

III. QUANTUM DRAG FORCE ON A SPHERE

The elastic amplitude for a gas molecule to scatter off a sphere may be expanded into partial waves as

$$f(\theta,p)=\left(\frac{\hbar}{2ip}\right)\sum_{l=0}^{\infty}(2l+1)[S_l(p)-1]P_l(\cos\theta). \qquad (13)$$

The total cross section can be decomposed into an elastic plus an inelastic part, as

$$\sigma_{tot}(p)=\sigma_{el}(p)+\sigma_{in}(p). \qquad (14)$$

The total cross section follows from the “optical theorem” as

$$\sigma_{tot}(p)=\left(\frac{4\pi\hbar}{p}\right)\text{Im}\,f(0,p)$$
$$\sigma_{tot}(p)=\left(\frac{2\pi\hbar^2}{p^2}\right)\sum_{l=0}^{\infty}(2l+1)[1-\text{Re}\,S_l(p)]. \qquad (15)$$

The elastic cross section is determined by

$$\frac{d\sigma_{el}}{d\Omega} = |f(\theta,p)|^2$$

$$\sigma_{el}(p) = \int |f(\theta,p)|^2 d\Omega = \left(\frac{\pi\hbar^2}{p^2}\right)\sum_{l=0}^{\infty}(2l+1)|1-S_l(p)|^2, \tag{16}$$

so that

$$\sigma_{in}(p) = \left(\frac{\pi\hbar^2}{p^2}\right)\sum_{l=0}^{\infty}(2l+1)[1-|S_l(p)|^2]. \tag{17}$$

Thus, the probability w_l^{el} of elastic scattering and the probability w_l^{in} of inelastic scattering in a given partial wave are determined, respectively, by

$$w_l^{el} = |S_l(p)|^2 \text{ and } w_l^{in} = 1 - |S_l(p)|^2. \tag{18}$$

A. Quantum pure elastic scattering

If the probability of elastic scattering in a partial wave is unity, then one may define phase shifts $\{\delta_l(p)\}$ via

$$w_l^{el} = 1 \text{ implies } S_l(p) = e^{2i\delta_l(p)}. \tag{19}$$

The elastic cross-section equation (16) yields the quantum result

$$\sigma(p) = \left(\frac{4\pi\hbar^2}{p^2}\right)\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l(p). \tag{20}$$

The quantum mechanical effect of the drag force is determined by the transport scattering cross section $\sigma_1(p)$. Equations (4), (16), and (19) imply [23]

$$\sigma_1(p) = \frac{(4\pi\hbar^2)}{p^2}\sum_{l=0}^{\infty} l\sin^2[\delta_{l-1}(p) - \delta_l(p)]. \tag{21}$$

The hard sphere phase shifts [24] are

$$\tan\delta_l(p) = \frac{j_l(pa/\hbar)}{n_l(pa/\hbar)}; \tag{22}$$

j_l and n_l are, respectively, the spherical Bessel and Neumann functions.

In the high-energy limit, $pa \gg \hbar$. First, the asymptotic form of the phase shift is given by

$$\delta_l(p) \to (-pa/\hbar) + (l\pi/2) \text{ as } p \to \infty. \tag{23}$$

Second, the partial wave summation cuts off at $\hbar l \approx pa$, where a is the radius of the sphere and p is the particle momentum. By inserting Eq. (23) into Eq. (21), one obtains

$$\lim_{p\to\infty}\sigma_1(p) = 2\pi a^2. \tag{24}$$

Comparing the classical specular reflection transport coefficient in Eq. (6) with the quantum specular reflection Eq. (24), one finds the drag force ratio

$$\frac{\sigma_1(\text{quantum specular})}{\sigma_1(\text{classical specular})} = 2, \qquad \frac{F(\text{quantum specular})}{F(\text{classical specular})} = 2. \tag{25}$$

The argument for the famous factor of 2 [25] between the quantum and classical cross sections is that there exists an interference of amplitudes between the scattered wave and the incoming wave. This interference creates a peak in the forward direction. This effect is closely analogous to Fresnel diffraction in optics, wherein the limit to geometric optics cannot really be achieved. Our point here is that the so-called classical limit $\hbar \to 0$ cannot really be achieved because of diffraction effects when the particle scatters off the sphere. From Eq. (4) one gets the final equation (25). The drag force on a sphere due to elastic scattering is twice as large as the classical value if quantum mechanical diffraction effects are taken into account.

B. Quantum pure absorptive scattering

Pure absorptive scattering takes place when the inelastic cross section is at a maximum. Equations (17) and (18) imply that pure absorptive scattering in the lth partial wave occurs [26] when $S_l=0$. If all the partial waves scatter in a purely absorptive manner, then $S_{(l<ka)} \approx 0$ and $S_{(l>ka)} \approx 1$. The total cross section becomes $\sigma_{tot} \approx 2\pi a^2$. The elastic cross section is thereby equal to the inelastic cross section; i.e.,

$$\sigma_{el} = \sigma_{in} = \pi a^2 \text{ and } \sigma_{tot} = 2\pi a^2. \tag{26}$$

As in the classical result, the inelastic cross section is equal to the inelastic transport cross section. The ratio between the force due to quantum scattering and classical scattering is

$$\frac{\sigma_1(\text{quantum absorptive})}{\sigma_1(\text{classical absorptive})} = 2, \qquad \frac{F(\text{quantum absorptive})}{F(\text{classical absorptive})} = 2. \tag{27}$$

The drag force due to quantum purely inelastic scattering is twice as large as the classical drag force.

IV. STICKING FRACTION MODEL

For purely elastic scattering, the S-matrix eigenvalues obey the unitary condition $|S_l|^2=1$. In terms of the Heitler K-matrix eigenvalues [27,28],

$$S_l = \left[\frac{1 - i\pi K_l}{1 + i\pi K_l}\right], \tag{28}$$

the unitary condition is enforced by requiring that K_l be real. In the most simple sticking fraction model, the inelastic processes are described with imaginary K-matrix eigenvalues,

$$\pi K_l = -i\eta_l, \quad \text{where } \eta_l \geq 0. \tag{29}$$

In the lth partial wave, a fraction w_l^{in} of incident particles "stick" to the sphere and a fraction w_l^{el} specularly reflect from the sphere. In detail, Eqs. (18), (28), and (29) imply

$$w_l^{el} = \frac{(1-\eta_l)^2}{(1+\eta_l)^2} \text{ (nonsticking)},$$
$$w_l^{in} = \frac{4\eta_l}{(1+\eta_l)^2} \text{ (sticking)}. \tag{30}$$

Finally, we presume a single value for the sticking fraction:

$$w_l^{in} \approx f \text{ if } \hbar l < pa,$$
$$w_l^{in} \approx 0 \text{ if } \hbar l > pa. \tag{31}$$

Equations (16)–(18) and (28)–(31) imply the central results of the simple sticking fraction model; i.e.,

$$\sigma^{el} = (\pi a^2)[1-\sqrt{1-f}]^2,$$
$$\sigma^{in} = (\pi a^2) f. \tag{32}$$

The physical significance of the central quantum scattering Eq. (32) is as follows. (i) The cross section for the incident particle to stick to the sphere is simply the classical cross section times sticking probability, i.e., $\sigma^{in}=(\pi a^2)f$, which would also be valid in a classical scattering context. (ii) The elastic cross section $\sigma^{el}=(\pi a^2)[1-\sqrt{1-f}]^2$ is in part due to diffractive scattering which is a purely quantum mechanical process having *no classical counterpart*. (iii) The total cross section in the sticking fraction model is

$$\sigma^{tot} = 2\pi a^2[1-\sqrt{1-f}] \text{ (quantum sticking)}. \tag{33}$$

On the other hand, for a classical sticking model, the total cross section is geometrical:

$$\sigma^{tot}_{classical} = \pi a^2 \text{ (classical sticking)}. \tag{34}$$

The physical kinetics of sticking and specular reflection are such that the mean momenta transferred to the sphere are equal for elastic and inelastic events. The friction drag coefficient is thereby

$$\lim_{v\to 0}\left[\frac{F}{v}\right] \equiv \Gamma = \left(\sqrt{\frac{128 k_B T}{9\pi m}}\right)\rho\sigma^{tot}. \tag{35}$$

The quantum expression for the drag coefficient in the sticking model is thereby

$$\Gamma = (2\pi a^2)\sqrt{\frac{128 k_B T}{9\pi m}}[1-\sqrt{1-f}]. \tag{36}$$

The sticking fraction for very dilute air molecules bouncing off an oil surface had been measured by two different methods. (i) In the rolling cylinder method [29], the drag force on one rotating cylinder due to the dilute gas between it and another nearby concentric stationary cylinder is employed to measure the sticking fraction f. (ii) In the falling drop method [30], the drag coefficient Γ on a falling spherical oil droplet is measured. Γ then determines the sticking fraction f. The droplet should have a small radius compared with the mean free path length of an atom in the gas. Agreement between these two methods is obtained if the fully quantum mechanical scattering theoretical equation (36) is used in the analysis of the data. The experimental results are shown in the table below:

Experimental method	Sticking fraction f
Rotating cylinder	0.893
Falling droplet	0.901

More recently, methods [31,32], similar to the rolling cylinder method have been developed. For the case of air on polished spheres [33], sticking fractions in the range

$$0.85 < f < 0.95 \tag{37}$$

were observed. The close agreement corresponds to a measured total cross section for a droplet in which the Knudsen number $\mathrm{Kn} \gg 1$. Recall the conventional definition [6] of this number,

$$\mathrm{Kn} = \frac{\Lambda}{a}, \tag{38}$$

where Λ is the mean free path of a molecule in the rarified gas. The experimental number deduced from Eq. (35) is

$$\sigma^{tot} \approx 1.37\pi a^2 \tag{39}$$

from which f may be deduced from Eq. (33). The experimental cross section σ^{tot} is larger than the classical total cross section $\sigma^{tot}_{classical}=\pi a^2$ due to quantum diffraction effects. The agreement between the experimental methods is not *entirely* satisfactory since only for one oil droplet is data available to us in which $\mathrm{Kn}\approx 10^2 \gg 1$. However, the data that do exist seem to demand quantum diffraction effects for the scattering of a molecule off the sphere. Further experiments would be of interest for probing the accuracy of these results.

V. CONCLUSION

The drag force on a sphere moving through a highly rarefied gas with large Knudsen number has been discussed. It was found that quantum mechanics substantially alters the drag force. Quantum mechanics enters into the computation via diffraction effects in the cross section for molecules scattering from the sphere. In the extreme case, it was found that if the molecules of the gas are completely elastic or completely inelastic, then the cross section is twice that found if only classical mechanics is taken into account. On the other hand, when there are both elastic and inelastic processes, then the total cross section may be only somewhat higher than the classical result. When collisions are mostly inelastic and absorptive, the cross sections are determined mainly by the sticking fraction f for the molecule to thermalize on the oil drop surface. Whereas classical elastic scattering is roughly isotropic, leaving an "empty shadow" behind the sphere, the elastic quantum cross section exhibits diffraction patterns strongly peaking in the forward direction of the gas flow. A quantum wake with a narrow stream of particles will thus appear behind the sphere.

By independent measurements of the sticking fraction and the drag force, quantum mechanical theory has been experimentally shown to be a more accurate description of the flow than the classical cross section. However, experimental data available to us in the $\mathrm{Kn} \gg 1$ regime are somewhat limited. Further experiments would be of great importance.

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