Torque on a Small Particle in a Nonhomogeneous Monatomic Gas

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Z. Naturforsch. **36a**, 559–567 (1981); received December 27, 1980

The torque a particle experiences in a monatomic gas in non-equilibrium is calculated with the method Waldmann originally used to compute the force. For a particle which is much smaller than the mean free path in the gas this method involves the following two essential steps:

i) with the help of a boundary condition the torque is expressed by the velocity distribution function of the gas atoms approaching the particle;

ii) this undisturbed distribution function is approximated by a moments-expansion, restricted here to thirteen moments.

In the resulting expression for the torque the pressure tensor and the local vorticity in the gas occur. The geometrical factors are given for particles shaped as spheroids, cylinders and spherocylinders.

Forces on particles suspended in a nonhomogeneous gas are of wide interest, in particular for the physics of aerosols, and have fascinated scientists from Tyndall's time [1] up to now [2]. Over a period of twenty years the theoretical and experimental aspects of this topic again and again played a role in Waldmann's work. The general method for calculating the forces on particles much smaller than the mean free path in the gas had been developed in 1959 [3]. Its basic ideas can be summarized as follows. By the use of a boundary condition the velocity distribution function of gas atoms leaving the particle is expressed by the distribution f_{inc} of atoms approaching it. Consequently, the force per unit area of the particle is determined by f_{inc} only. Since the particle is small, its presence does not essentially influence f_{inc}. For the undisturbed distribution function an expansion is inserted, and the force is obtained as a sum over several terms each of which is a product of a gas-moment times a geometrical shape factor of the particle. In particular, results are stated [3] for a sphere in monatomic gases, viz. in a streaming and heat conducting pure gas and in a diffusing binary mixture. Epstein's expression [4] for the friction force was confirmed, and instead of Einstein's approximate formula [5] the exact result for the thermal force was obtained. Experimental data on thermophoresis by Schmidt [6] and on diffusiophoresis by Schmitt and Waldmann [7] established the range of applicability of the theoretical work [8], [9]. More recent thermophoresis measurements by Davis and Adair [10] clearly revealed the practical importance of the "Waldmann limit".

Waldmann's work has been extended to polyatomic gases containing small spheroidal particles [11]. This concept has also been used to calculate the thermomagnetic force [12], [13], [14], i.e. the influence of a magnetic field on the force experienced by a particle in a heat conducting polyatomic gas. Experiments by Davis [15] confirmed the theoretically predicted connection between the thermomagnetic force and the Senftleben-Beenakker effect of thermal conductivity [16].

For particles which are much larger than the mean free path in the gas the hydrodynamic results apply; the expressions for the friction force on an ellipsoid [17], [18] can easily be extended to thermophoresis (see e.g. [11]), thus generalizing Epstein's formula for the thermal force on a sphere [19].

The rather complex situation in the transition regime between hydrodynamics and the "Waldmann limit" attracted Waldmann's attention in the last decade. As it turned out, the consequent use of generalized hydrodynamics and thermodynamically consistent boundary conditions [20] led to a satisfactory description of friction force and thermal force data over a wide pressure range [21], [22].

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In this paper, Waldmann's method [3] is applied to the calculation of the torque on a small particle immersed in a monatomic gas. The boundary condition for the distribution function is taken in a form containing two accommodation coefficients [23]. For the distribution function f_{inc} a "thirteen moments" expansion is used as an approximate solution of the linearized Boltzmann equation [24], i.e. the state of the gas is described by the local density, temperature, flow velocity, heat flux and symmetric traceless pressure tensor. The resulting torque consists of two contributions: the first one is proportional to the pressure tensor in the gas and leads to an orientation of the particle in a shear flow; the second one is determined by the local vorticity $\boldsymbol{\omega}$ in the gas and causes the particle to rotate with the fluid. With $\boldsymbol{\omega} = -\boldsymbol{\Omega}$ the second term essentially reduces to the expression obtained by Halbritter [25] for the torque on a spheroid rotating with angular velocity $\boldsymbol{\Omega}$. The geometrical shape factors given in both cases for spheroids, cylinders and spherocylinders are of the order a^3, respectively a^4 where a is a typical length of the particle.

In the Appendix, the hydrodynamic formulae for the torque on spheroids as calculated by Gans [26] are listed for convenience.

1. Basic Relations

A monatomic gas exerts the force

$$\mathrm{d}\boldsymbol{K} = \left[\int P_+(c)\, m\, c\, \boldsymbol{c} f\, \mathrm{d}^3c + \int P_+(-c)\, m\, c\, \boldsymbol{c} f\, \mathrm{d}^3c\right] \mathrm{d}\sigma \tag{1.1}$$

and the torque

$$\mathrm{d}\boldsymbol{M} = \boldsymbol{x} \times \mathrm{d}\boldsymbol{K} \tag{1.2}$$

on the surface element $\mathrm{d}\sigma$ of a particle at rest. The distribution function $f(t, \boldsymbol{x}, \boldsymbol{c})$ of the gas atoms of mass m depends on time t, space coordinate $\boldsymbol{x}$ and velocity $\boldsymbol{c}$. With the help of the Heaviside function

$$P_+(c) = \begin{cases} 1 & \text{for } c > 0 \\ 0 & \text{for } c < 0 \end{cases}$$

the force in (1.1) has been split up into the contributions from the atoms approaching the surface, i.e. with positive normal velocity

$$c = \boldsymbol{c} \cdot \boldsymbol{n}, \quad \boldsymbol{n}\text{: outer unit normal of the gas,}$$

and from those leaving the surface (i.e. $c < 0$). Utilizing a boundary condition, the distribution of outgoing atoms, $P_+(-c)\, f$, is expressed by the distribution of incoming atoms, $P_+(c)\, f$. In a simple model with two accommodation coefficients [23] this relation at the particle's surface σ has the following form ($\boldsymbol{x} \in \sigma$):

$$P_+(-c) f(t, \boldsymbol{x}, \boldsymbol{c}) = P_+(-c) \cdot [\alpha f_p(\boldsymbol{c}) + \beta(1-\alpha) f(t, \boldsymbol{x}, -\boldsymbol{c}) + (1-\beta)(1-\alpha) f(t, \boldsymbol{x}, \boldsymbol{c} - 2c\boldsymbol{n})]. \tag{1.3}$$

The coefficient α characterizes the fraction of gas atoms leaving the surface with the local Maxwellian

$$f_p(\boldsymbol{c}) = n_p \left(\frac{m}{2\pi k T_p}\right)^{3/2} \exp\left(-\frac{m\, \boldsymbol{c} \cdot \boldsymbol{c}}{2 k T_p}\right) \tag{1.4}$$

corresponding to the temperatur T_p of the particle (k is Boltzmann's constant); the "density" n_p is determined by the incoming flux according to

$$n_p = \left(\frac{2\pi m}{k T_p}\right)^{1/2} \int P_+(c')\, c' f(t, \boldsymbol{x}, \boldsymbol{c}')\, \mathrm{d}^3c'. \tag{1.5}$$

Whereas α ($0 \leqq \alpha \leqq 1$) is the probability of thermalization of atoms by the surface, $\beta(1-\alpha)$ and $(1-\beta)(1-\alpha)$ are the probabilities of backward and of specular reflection, respectively. The coefficient of backward reflection β ($0 \leqq \beta \leqq 1$) and the accommodation coefficient α for functions which are even in the tangential velocity

$$\boldsymbol{c}^{\tan} = \boldsymbol{c} - c\,\boldsymbol{n}$$

determine the accommodation coefficient α_{odd} for functions odd in $\boldsymbol{c}^{\tan}$ [23]:

$$\alpha_{\text{odd}} = 2 - \alpha - 2(1-\alpha)\beta. \tag{1.6}$$

Usually one puts $\beta = 0$, so that

$$\alpha_{\text{odd}} = 2 - \alpha$$

applies; notice $\alpha_{\text{odd}} = \alpha$ for $\beta = 1$.

After insertion of $P_+(-c)\, f$ from Eq. (1.3) into Eq. (1.1), the integration variables are changed, namely $\boldsymbol{c} \to -\boldsymbol{c}$ in the first two terms of Eq. (1.3) and $c \to -c$ in the third term. Then all integrals in $\mathrm{d}\boldsymbol{K}$ extend over the positive velocity half space $c > 0$. Next, the term proportional to αf_p is worked out in detail, using the relation

$$\int P_+(c)\, m\, c\, \boldsymbol{c} \exp\left(-\frac{m\, \boldsymbol{c} \cdot \boldsymbol{c}}{2 k T_p}\right) \mathrm{d}^3c = \tfrac{1}{2} k T_p \left(\frac{2\pi k T_p}{m}\right)^{3/2} \boldsymbol{n}$$

and replacing n_p by the integral from Equation (1.5).

In the resulting expression for the force,

$$\mathrm{d}\boldsymbol{K} = \Bigg[\alpha\left(\frac{\pi k T_p}{2m}\right)^{1/2} \int P_+(c)\, m c f \,\mathrm{d}^3 c\, \boldsymbol{n} + (2-\alpha)\int P_+(c)\, m c \boldsymbol{c} f \,\mathrm{d}^3 c\, \boldsymbol{n} + (2-\alpha_{\text{odd}})\int P_+(c)\, m c\, \boldsymbol{c}^{\tan} f \,\mathrm{d}^3 c\Bigg]\mathrm{d}\sigma, \quad (1.7)$$

only $P_+(c)f$ occurs, the distribution of gas atoms approaching the particle.

Since the particle is much smaller than the mean free path in the gas, its influence on the incoming distribution $f_{\text{inc}} = P_+(c)f$ will be negligible. Hence, in f_{inc} we will replace f by the distribution of a monatomic gas containing no particle at all. In particular, the undisturbed distribution is written as

$$f_{\text{inc}} = P_+(c)f = P_+(c) f_0 (1+\Phi), \quad (1.8)$$

and for the "small" deviation Φ from the equilibrium Maxwellian (density n_0, temperature T_0)

$$f_0 = n_0 \left(\frac{m}{2\pi k T_0}\right)^{3/2} \exp\left(-\frac{m\,\boldsymbol{c}\cdot\boldsymbol{c}}{2kT_0}\right)$$

an approximate solution of the linearized Boltzmann equation is used [24]

$$\Phi = \frac{n-n_0}{n_0} + (W^2 - \tfrac{3}{2})\frac{T-T_0}{T_0} + \frac{\sqrt{2}}{c_0}\boldsymbol{W}\cdot\boldsymbol{v} + \frac{2}{5}\frac{\sqrt{2}}{p_0 c_0}(W^2-\tfrac{5}{2})\boldsymbol{W}\cdot\boldsymbol{q} + \frac{1}{p_0}\overline{\boldsymbol{W}\boldsymbol{W}}:\overline{\mathsf{p}}, \quad (1.9)$$

which contains the thirteen moments (which are functions of $t, \boldsymbol{x}$) density n, temperature T, flow velocity $\boldsymbol{v}$, heat flux $\boldsymbol{q}$ and symmetric traceless pressure tensor $\overline{\mathsf{p}}$. The dimensionless velocity

$$\boldsymbol{W} = \frac{1}{\sqrt{2}\,c_0}\boldsymbol{c}, \quad c_0 = (kT_0/m)^{1/2}$$

and the equilibrium gas pressure

$$p_0 = n_0 k T_0$$

have been introduced.

Now, the expansion (1.8), (1.9) of f_{inc} is inserted into Eq. (1.7), and the integration over the velocity half space $c > 0$ is performed. After consequent linearization with respect to small deviations from equilibrium, the following expression for the force is obtained

$$\mathrm{d}\boldsymbol{K} = \{\boldsymbol{n}[X^{(0)} + \boldsymbol{n}\cdot\boldsymbol{X}^{(0)} + \boldsymbol{n}\boldsymbol{n}:\mathsf{X}^{(0)}] + \boldsymbol{X}^{(1)} + \boldsymbol{n}\cdot\mathsf{X}^{(1)}\}\,\mathrm{d}\sigma, \quad (1.10)$$

where the quantities $X^{(r)}_{\mu_1\ldots\mu_l}$ are combinations of moments:

$$X^{(0)} = p + \frac{\alpha}{4}\frac{p_0}{T_0}(T_p - T), \quad (1.11)$$

$$\boldsymbol{X}^{(0)} = (1 - \alpha + \tfrac{1}{2}\alpha_{\text{odd}})\frac{1}{\pi}\frac{p_0}{\hat{c}_0}\cdot\left(\boldsymbol{v} + \frac{1}{5}\frac{1}{p_0}\boldsymbol{q}\right) + \frac{\alpha}{4}\frac{p_0}{\hat{c}_0}\boldsymbol{v}, \quad (1.12)$$

$$\boldsymbol{X}^{(1)} = (1 - \tfrac{1}{2}\alpha_{\text{odd}})\frac{1}{\pi}\frac{p_0}{\hat{c}_0}\left(\boldsymbol{v} + \frac{1}{5}\frac{1}{p_0}\boldsymbol{q}\right), \quad (1.13)$$

$$\mathsf{X}^{(0)} = \left(\frac{1}{2}\alpha_{\text{odd}} - \frac{\alpha}{4}\right)\overline{\mathsf{p}}, \quad (1.14)$$

$$\mathsf{X}^{(1)} = (1 - \tfrac{1}{2}\alpha_{\text{odd}})\overline{\mathsf{p}}; \quad (1.15)$$

$\hat{c}_0$ is an abbreviation for

$$\hat{c}_0 = c_0/\sqrt{2\pi}.$$

In order to get the force and the torque, Eqs. (1.10) and (1.2) have to be integrated over the surface σ. At σ, the "moments" $X^{(r)}_{\mu_1\ldots\mu_l}$ will vary only very little since the particle is small. Hence it certainly is sufficient to use a first order Taylor series expansion

$$X^{(r)}_{\mu_1\ldots\mu_l}(\boldsymbol{x}) \approx X^{(r)}_{\mu_1\ldots\mu_l}(0) + x_\nu(\partial/\partial x_\nu X^{(r)}_{\mu_1\ldots\mu_l})(0) \equiv Y^{(r)}_{\mu_1\ldots\mu_l} + x_\nu Z^{(r)}_{\nu,\mu_1\ldots\mu_l} \quad (1.16)$$

with the origine $\boldsymbol{x} = 0$ chosen to coincide with the center of mass of the particle. Accordingly, the force $\boldsymbol{K}$ and torque $\boldsymbol{M}$,

$$\boldsymbol{K} = \boldsymbol{K}^{(0)} + \boldsymbol{K}^{(1)}, \quad \boldsymbol{M} = \boldsymbol{M}^{(0)} + \boldsymbol{M}^{(1)}, \quad (1.17)$$

consist of two contributions $\boldsymbol{K}^{(0)}$, $\boldsymbol{M}^{(0)}$ and $\boldsymbol{K}^{(1)}$, $\boldsymbol{M}^{(1)}$ which are derived from $Y^{(r)}_{\mu_1\ldots\mu_l}$ and $Z^{(r)}_{\nu,\mu_1\ldots\mu_l}$, respectively. Integration over σ now only involves products of $\boldsymbol{n}$ and $\boldsymbol{x}$ leading to geometrical shape factors.

2. The Force

The force $\boldsymbol{K}^{(0)}$ is obtained from Eq. (1.10) by using the first term in the expansion (1.16), i.e. in replacing $X^{(r)}_{\mu_1\ldots\mu_l}(\boldsymbol{x})$ by the constant $X^{(r)}_{\mu_1\ldots\mu_l}(0) = Y^{(r)}_{\mu_1\ldots\mu_l}$. Since the relation

$$\int n_\mu \,\mathrm{d}\sigma = 0$$

applies for any closed surface σ, the first and the last term in Eq. (1.10) give no contribution to $\boldsymbol{K}^{(0)}$:

$$K_\mu^{(0)} = Y_\nu^{(0)} \int n_\nu n_\mu \, d\sigma + Y_{\nu\lambda}^{(0)} \int n_\nu n_\lambda n_\mu \, d\sigma + Y_\mu^{(1)} F_1 ;$$

here F_1 denotes the surface of the particle

$$F_1 = \int d\sigma . \tag{2.1}$$

Now we assume that the particle has a symmetry axis $\boldsymbol{s}$, then all integrals containing an odd number of n_ν vanish, e.g.

$$\int n_\nu n_\lambda n_\mu \, d\sigma = 0 ,$$

and all integrals over an even number of n_ν can be expressed by an even number of s_ν, e.g.

$$\int n_\mu n_\nu \, d\sigma = F_1 \tfrac{1}{2} (\delta_{\mu\nu} - s_\mu s_\nu) + F_2 \tfrac{3}{2} \overline{s_\mu s_\nu} ,$$

with F_1 from Eq. (2.1) and F_2 given by

$$F_2 = \int (\boldsymbol{n} \cdot \boldsymbol{s})^2 \, d\sigma . \tag{2.2}$$

Hence, for a symmetric body the force $\boldsymbol{K}^{(0)}$ is determined by the two vectors $\boldsymbol{Y}^{(0)}$ and $\boldsymbol{Y}^{(1)}$

$$\boldsymbol{K}^{(0)} = \boldsymbol{s}\boldsymbol{s} \cdot [F_2 \boldsymbol{Y}^{(0)} + F_1 \boldsymbol{Y}^{(1)}] + (\boldsymbol{\delta} - \boldsymbol{s}\boldsymbol{s}) \cdot [\tfrac{1}{2}(F_1 - F_2) \boldsymbol{Y}^{(0)} + F_1 \boldsymbol{Y}^{(1)}] ,$$

and with Eqs. (1.12), (1.13) its components $\boldsymbol{K}_\parallel^{(0)}$, $\boldsymbol{K}_\perp^{(0)}$ parallel and perpendicular to the figure axis $\boldsymbol{s}$ are obtained in the following form (the moments have to be taken at $\boldsymbol{x} = 0$):

$$\boldsymbol{K}_\parallel^{(0)} = \frac{1}{\pi} \frac{p_0}{\hat{c}_0} \boldsymbol{s}\boldsymbol{s} \cdot \left\{ \left(\boldsymbol{v} + \frac{1}{5} \frac{1}{p_0} \boldsymbol{q} \right) \cdot [F_2 (1 - \alpha + \tfrac{1}{2} \alpha_{\text{odd}}) + F_1 (1 - \tfrac{1}{2} \alpha_{\text{odd}})] + \boldsymbol{v} F_2 \alpha \frac{\pi}{4} \right\} , \tag{2.3}$$

$$\boldsymbol{K}_\perp^{(0)} = \frac{1}{\pi} \frac{p_0}{\hat{c}_0} (\boldsymbol{\delta} - \boldsymbol{s}\boldsymbol{s}) \cdot \left\{ \left(\boldsymbol{v} + \frac{1}{5} \frac{1}{p_0} \boldsymbol{q} \right) [\tfrac{1}{2} (F_1 - F_2)(1 - \alpha + \tfrac{1}{2} \alpha_{\text{odd}}) + F_1 (1 - \tfrac{1}{2} \alpha_{\text{odd}})] + \boldsymbol{v} \tfrac{1}{2} (F_1 - F_2) \alpha \frac{\pi}{4} \right\} . \tag{2.4}$$

With $\alpha_{\text{odd}} = 2 - \alpha$, Eqs. (2.3), (2.4) reduce to the expressions stated in [11]. Results for $F = F_1$ and $N = \frac{1}{2}(F_1 - F_2)/F_1$ are given in [11] for prolate and oblate spheroids; for a *cylinder* of radius a and length h one has

$$F_1 = 2\pi a (a + h) , \quad F_2 = 2\pi a^2 ,$$

and for a *spherocylinder* consisting of a cylinder (radius a, length h) with spherical caps

$$F_1 = 2\pi a (2a + h) , \quad F_2 = (4\pi/3) a^2 .$$

For a *sphere* of radius a

$$F_2 = \tfrac{1}{3} F_1 = (4\pi/3) a^2$$

applies, and the force

$$\boldsymbol{K}^{(0)} = \frac{8}{3} a^2 \frac{p_0}{\hat{c}_0} \left[(1 + \beta(1 - \alpha)) \cdot \left(\boldsymbol{v} + \frac{1}{5} \frac{1}{p_0} \boldsymbol{q} \right) + \frac{\pi}{8} \alpha \boldsymbol{v} \right] \tag{2.5}$$

differs from Waldmann's result [3] only if the coefficient of back reflection β is different from zero.

The force $\boldsymbol{K}^{(1)}$ is calculated from Eq. (1.10) by using the second term in the expansion (1.16). First, the relation ($-\boldsymbol{n}$ is the outer unit normal of the body)

$$\int x_\nu (-n_\lambda) \, d\sigma = V_1 \delta_{\nu\lambda} ,$$
$$V_1 = \int \tfrac{1}{3} \boldsymbol{x} \cdot (-\boldsymbol{n}) \, d\sigma = \int_\tau d\tau \tag{2.6}$$

is noted which is valid for any closed surface σ of a particle with volume V_1. For a body with symmetry axis $\boldsymbol{s}$, the integrals

$$\int n_\mu n_\nu x_\lambda \, d\sigma = 0 , \quad \int x_\nu \, d\sigma = 0 \tag{2.7}$$

vanish, hence the force is given by

$$K_\mu^{(1)} = - V_1 (Z_\mu^{(0)} + Z_{\nu,\nu\mu}^{(1)}) + \int n_\mu x_\nu \overline{n_\lambda n_\varkappa} \, d\sigma \, Z_{\nu,\lambda\varkappa}^{(0)} .$$

According to Eqs. (1.11), (1.14) and (1.15), $\boldsymbol{K}^{(1)}$ is determined by gradients of temperature, pressure and symmetric traceless pressure tensor. Compared to terms in $\boldsymbol{K}^{(0)}$, the contributions to $\boldsymbol{K}^{(1)}$ are smaller by a factor of $a/l \ll 1$ where a is a characteristic dimension of the particle and l is the mean free path in the gas. Therefore, the force $\boldsymbol{K}^{(1)}$ will not be discussed further.

3. The Contribution $\boldsymbol{M}^{(0)}$ to the Torque

According to Eq. (1.17), the torque $\boldsymbol{M}$ consists of two contributions,

$$\boldsymbol{M} = \boldsymbol{M}^{(0)} + \boldsymbol{M}^{(1)} .$$

The first contribution $\boldsymbol{M}^{(0)}$ is obtained from Eqs. (1.2) and (1.10) with the first term

$$Y_{\mu_1 \ldots \mu_l}^{(r)} = X_{\mu_1 \ldots \mu_l}^{(r)}(0)$$

in the Taylor series expansion (1.16). Due to the relation (2.6), the first and the last term in Eq. (1.10) do not contribute to $\boldsymbol{M}^{(0)}$ and we are left with

$$M^{(0)}_\mu = \int \varepsilon_{\mu\nu\lambda} \{x_\nu n_\lambda n_\varkappa Y^{(0)}_\varkappa + x_\nu n_\lambda n_\varkappa n_\tau Y^{(0)}_{\varkappa\tau} + x_\nu Y^{(1)}_\lambda\} \, \mathrm{d}\sigma .$$

In particular, for a body with symmetry axis $\boldsymbol{s}$ the first and the third integral vanish (see Eq. (2.7)), and the second integral can be written as

$$-\int (\boldsymbol{x} \times \boldsymbol{n})_\mu n_\varkappa n_\tau \, \mathrm{d}\sigma = \tfrac{1}{2} V_0 (\varepsilon_{\mu\lambda\tau} s_\varkappa + \varepsilon_{\mu\lambda\varkappa} s_\tau) s_\lambda$$

with

$$V_0 = V_1 - V_2 . \tag{3.1}$$

Here V_1 is the volume of the particle given already in Eq. (2.6), and V_2 is calculated from

$$V_2 = \int (-\boldsymbol{n}) \cdot \boldsymbol{x} (\boldsymbol{n} \cdot \boldsymbol{s})^2 \, \mathrm{d}\sigma . \tag{3.2}$$

Then, the torque

$$\boldsymbol{M}^{(0)} = - V_0 \boldsymbol{s} \times (\mathsf{Y}^{(0)} \cdot \boldsymbol{s})$$

with Eqs. (1.16), (1.14) is determined by the symmetric traceless part $\overline{\mathsf{p}}$ of the pressure tensor p:

$$\boldsymbol{M}^{(0)} = -\left(\frac{1}{2} \alpha_{\text{odd}} - \frac{\alpha}{4}\right) V_0 \boldsymbol{s} \times (\overline{\mathsf{p}} \cdot \boldsymbol{s}) . \tag{3.3}$$

Obviously, $\overline{\mathsf{p}}$ can also be replaced by $\mathsf{p} = p \boldsymbol{\delta} + \overline{\mathsf{p}}$. The torque $\boldsymbol{M}^{(0)}$ is perpendicular to the figure axis $\boldsymbol{s}$ of the particle and to the "local force per unit area" $\mathsf{p} \cdot \boldsymbol{s}$ in the gas. In a steady state, the thirteen moments ansatz [20]

$$\overline{\mathsf{p}} = -2\eta \left(\overline{\boldsymbol{\nabla} \boldsymbol{v}} + \frac{2}{5} \frac{1}{p_0} \overline{\boldsymbol{\nabla} \boldsymbol{q}}\right) \tag{3.4}$$

with

$$\boldsymbol{q} = -\lambda \left(\boldsymbol{\nabla} T - \frac{2}{5} \frac{T_0}{p_0} \boldsymbol{\nabla} p\right) \tag{3.5}$$

may be used in Equation (3.3). Consequently, the torque $\boldsymbol{M}^{(0)}$ contains a first order derivative of flow velocity, and second order derivatives of temperature and of pressure, all taken at $\boldsymbol{x} = 0$. Furthermore, $\boldsymbol{M}^{(0)}$ is proportional to the transport constants η (shear viscosity) and λ (thermal conductivity).

In a steady state particles subject to stresses will preferentially be oriented such that the torque $\boldsymbol{M}^{(0)}$ vanishes. In particular, in a plane Couette flow with

$$\overline{\mathsf{p}} = -2\eta \left(\frac{\mathrm{d} v_x}{\mathrm{d} z}\right) \overline{\boldsymbol{e}_x \boldsymbol{e}_z} ,$$

the axis of the particle has to be oriented under 45^0 with respect to the unit vectors $\boldsymbol{e}_x$ and $\boldsymbol{e}_z$,

$$\boldsymbol{s} = \pm \frac{1}{\sqrt{2}} (\boldsymbol{e}_x \pm \boldsymbol{e}_z) ,$$

or it has to be perpendicular to both

$$\boldsymbol{s} = \pm \boldsymbol{e}_x \times \boldsymbol{e}_z ,$$

in order to have $\boldsymbol{M}^{(0)} = \boldsymbol{0}$.

For a *sphere* and for a *cylinder*, due to

$$V_1 = V_2 , \quad V_0 = 0 , \tag{3.6}$$

the torque vanishes from geometrical reasons

$$\boldsymbol{M}^{(0)} = \boldsymbol{0} .$$

If the particle is shaped as a *spherocylinder* (radius a, length h), the torque is nonzero since

$$V_0 = \tfrac{1}{2} \pi a^2 h \tag{3.7}$$

applies.

Spheroids with semi-axes $a_\parallel$ and $a_\perp$ parallel and perpendicular to $\boldsymbol{s}$, respectively, have the volume

$$V_1 = \frac{4\pi}{3} a_\parallel a_\perp^2 ;$$

the quantity V_2 has to be calculated separately for prolate and for oblate spheroids. A *prolate spheroid* ($a_\parallel \geqq a_\perp$) with nonsphericity

$$\varepsilon = [1 - (a_\perp / a_\parallel)^2]^{1/2}$$

has the shape factor

$$V_0 = \frac{4\pi}{3} a_\parallel^3 (1 - \varepsilon^2) \cdot \left\{1 - \frac{3(1-\varepsilon^2)}{\varepsilon^2} \left[\frac{1}{2\varepsilon} \ln \frac{1+\varepsilon}{1-\varepsilon} - 1\right]\right\} , \tag{3.8}$$

which vanishes with $\varepsilon \to 0$:

$$V_0 \approx (8\pi/15) a_\parallel^3 \varepsilon^2 = (8\pi/15) a_\parallel (a_\parallel^2 - a_\perp^2) .$$

For a rod, $\varepsilon \to 1$, V_0 also goes to zero, viz.

$$V_0 \approx V_1 \approx (4\pi/3) a_\parallel^3 (1 - \varepsilon^2) .$$

The maximum value (for fixed $a_\parallel$)

$$V_{0\text{m}} = (4\pi/3) a_\parallel^3 * 0.134479$$

of V_0 is obtained for

$$\varepsilon_\text{m} = 0.7695 .$$

On the other hand, an *oblate spheroid* ($a_\perp \geqq a_\parallel$) with nonsphericity

$$\varepsilon = [1 - (a_\parallel / a_\perp)^2]^{1/2}$$

has the shape factor

$$V_0 = \frac{4\pi}{3} a_\perp{}^3 \sqrt{1-\varepsilon^2} \cdot \left\{1 - \frac{3}{\varepsilon^2}\left[1 - \frac{\sqrt{1-\varepsilon^2}}{\varepsilon} \arcsin\varepsilon\right]\right\}, \tag{3.9}$$

which vanishes with $\varepsilon \to 0$:

$$V_0 \approx -(8\pi/15)\, a_\perp{}^3 \varepsilon^2 = -(8\pi/15)\, a_\perp (a_\perp{}^2 - a_\parallel{}^2).$$

Also for a disc, $\varepsilon \to 1$, V_0 goes to zero

$$V_0 \approx -V = -(4\pi/3)\, a_\perp{}^3 \sqrt{1-\varepsilon^2}.$$

For

$$\varepsilon_{\mathrm{m}} = 0.9222$$

V_0 reaches its minimum value (for fixed $a_\perp$)

$$V_{0\mathrm{m}} = -(4\pi/3)\, a_\perp{}^3 * 0.306013.$$

4. The Contribution $\boldsymbol{M}^{(1)}$ to the Torque

The second contribution $\boldsymbol{M}^{(1)}$ to the torque $\boldsymbol{M}$ is calculated from Eqs. (1.2) and (1.10) by using the second term

$$x_\nu Z^{(r)}_{\nu,\mu_1\ldots\mu_l} = x_\nu \left(\frac{\partial}{\partial x_\nu} X^{(r)}_{\mu_1\ldots\mu_l}\right)(0)$$

in the expansion (1.16):

$$M^{(1)}_\mu = \int \varepsilon_{\mu\nu\lambda} x_\nu x_\varkappa \{n_\lambda [Z^{(0)}_\varkappa + Z^{(0)}_{\varkappa,\tau} n_\tau + Z^{(0)}_{\varkappa,\tau\varrho} n_\tau n_\varrho] + Z^{(1)}_{\varkappa,\lambda} + Z^{(1)}_{\varkappa,\lambda\tau} n_\tau\}\, \mathrm{d}\sigma.$$

For a particle with symmetry axis $\boldsymbol{s}$, three terms vanish due to

$$\int x_\nu x_\varkappa n_\lambda \,\mathrm{d}\sigma = 0, \quad \int x_\nu x_\varkappa n_\lambda n_\tau n_\varrho \,\mathrm{d}\sigma = 0,$$

and two terms remain,

$$M^{(1)}_\mu = \int [(\boldsymbol{x}\times\boldsymbol{n})_\mu x_\varkappa n_\lambda Z^{(0)}_{\varkappa,\lambda} + \varepsilon_{\mu\nu\lambda} x_\nu x_\varkappa Z^{(1)}_{\varkappa,\lambda}]\, \mathrm{d}\sigma.$$

Now, the second rank tensor $Z^{(r)}_{\varkappa,\lambda}$ is split up into its irreducible components, the isotropic, symmetric traceless and the antisymmetric parts:

$$Z^{(r)}_{\varkappa,\lambda} = (\partial/\partial x_\varkappa) X^{(r)}_\lambda = \tfrac{1}{3}\delta_{\varkappa\lambda} \boldsymbol{\nabla}\cdot\boldsymbol{X}^{(r)} + \overline{\boldsymbol{\nabla} X^{(r)}_{\varkappa\lambda}} + \tfrac{1}{2}\varepsilon_{\varkappa\lambda\tau} (\operatorname{rot}\boldsymbol{X}^{(r)})_\tau.$$

Because of the relations

$$\int \boldsymbol{x}\times\boldsymbol{n}\, \boldsymbol{x}\cdot\boldsymbol{n}\,\mathrm{d}\sigma = 0, \quad \boldsymbol{x}\times\boldsymbol{x} = \boldsymbol{0},$$

the isotropic terms (which are proportional to $\delta_{\varkappa\lambda}$) do not contribute to $\boldsymbol{M}^{(1)}$. According to Eqs. (1.12), (1.13) the symmetric traceless components $\overline{\boldsymbol{\nabla}\boldsymbol{X}^{(r)}}$ contain $\overline{\boldsymbol{\nabla}\boldsymbol{v}}$ and $\overline{\boldsymbol{\nabla}\boldsymbol{q}}$, hence, the ensuing contributions to $\boldsymbol{M}^{(1)}$ are of the same type as those occurring in $\boldsymbol{M}^{(0)}$ (via Eqs. (3.3), (3.4)), but are smaller in magnitude by a factor of $a/l \ll 1$. Consequently they are dropped in the following. We are only interested in contributions to $\boldsymbol{M}^{(1)}$ which are different from the terms in $\boldsymbol{M}^{(0)}$, i.e. in the rot $\boldsymbol{X}^{(r)}$ components of the antisymmetric part of $Z^{(r)}_{\varkappa,\lambda}$:

$$M^{(1)}_\mu = \tfrac{1}{2}\int [(\boldsymbol{x}\times\boldsymbol{n})_\mu (\boldsymbol{x}\times\boldsymbol{n})_\nu (\operatorname{rot}\boldsymbol{X}^{(0)})_\nu + (\delta_{\mu\nu}\boldsymbol{x}\cdot\boldsymbol{x} - x_\mu x_\nu)(\operatorname{rot}\boldsymbol{X}^{(1)})_\nu]\,\mathrm{d}\sigma + \cdots.$$

The surface integrals

$$\int x_\mu x_\nu \,\mathrm{d}\sigma = G_1 \tfrac{1}{2}(\delta_{\mu\nu} - s_\mu s_\nu) + G_2 \tfrac{3}{2}\overline{s_\mu s_\nu},$$

$$\int (\boldsymbol{x}\times\boldsymbol{n})_\mu (\boldsymbol{x}\times\boldsymbol{n})_\nu \,\mathrm{d}\sigma = H_1 \tfrac{1}{2}(\delta_{\mu\nu} - s_\mu s_\nu) + H_2 \tfrac{3}{2}\overline{s_\mu s_\nu}$$

are characterized by four geometrical factors:

$$G_1 = \int \boldsymbol{x}\cdot\boldsymbol{x}\,\mathrm{d}\sigma, \tag{4.1}$$

$$G_2 = \int (\boldsymbol{x}\cdot\boldsymbol{s})^2 \,\mathrm{d}\sigma, \tag{4.2}$$

$$H_1 = \int (\boldsymbol{x}\times\boldsymbol{n})\cdot(\boldsymbol{x}\times\boldsymbol{n})\,\mathrm{d}\sigma, \tag{4.3}$$

$$H_2 = \int [(\boldsymbol{x}\times\boldsymbol{n})\cdot\boldsymbol{s}]^2 \,\mathrm{d}\sigma. \tag{4.4}$$

In particular, for spheroids, cylinders and spherocylinders the relation

$$(\boldsymbol{x}\times\boldsymbol{n})\cdot\boldsymbol{s} = 0$$

leads to

$$H_2 = 0. \tag{4.5}$$

According to Eqs. (1.12) and (1.13), rot $\boldsymbol{X}^{(r)}$ is a linear combination of rot $\boldsymbol{v}$ and rot $\boldsymbol{q}$; if we use the ansatz (3.5), the heat flux is irrotational, rot $\boldsymbol{q} = \boldsymbol{0}$. Then, the particle experiences a torque

$$\boldsymbol{M}^{(1)} = w_\parallel \boldsymbol{s}\boldsymbol{s}\cdot\boldsymbol{\omega} + w_\perp (\boldsymbol{\delta} - \boldsymbol{s}\boldsymbol{s})\cdot\boldsymbol{\omega} \tag{4.6}$$

due to the local vorticity (taken at $\boldsymbol{x} = 0$)

$$\boldsymbol{\omega} = \tfrac{1}{2}\operatorname{rot}\boldsymbol{v} \tag{4.7}$$

of the gas:

$$w_\parallel = \frac{p_0}{\pi \hat{c}_0}[(G_1 - G_2)(1 - \tfrac{1}{2}\alpha_{\mathrm{odd}}) + H_2(1 - \alpha + \alpha(\pi/4) + \tfrac{1}{2}\alpha_{\mathrm{odd}})], \tag{4.8}$$

$$w_\perp = \frac{p_0}{\pi \hat{c}_0}[\tfrac{1}{2}(G_1 + G_2)(1 - \tfrac{1}{2}\alpha_{\mathrm{odd}}) + \tfrac{1}{2}(H_1 - H_2)(1 - \alpha + \alpha(\pi/4) + \tfrac{1}{2}\alpha_{\mathrm{odd}})]. \tag{4.9}$$

This torque is independent of the transport coefficients η and λ; it causes the particle to rotate locally with the angular velocity $\boldsymbol{\Omega}=\boldsymbol{\omega}$, where the corresponding "rotational relaxation times" $\tau_\parallel, \tau_\perp$ are determined by the coefficients $w_\parallel, w_\perp$ and by the moments of inertia $\Theta_\parallel, \Theta_\perp$:

$$\tau_\parallel = \frac{\Theta_\parallel}{w_\parallel}, \quad \tau_\perp = \frac{\Theta_\perp}{w_\perp}.$$

In a plane Couette flow with

$$\boldsymbol{v} = v_x(z)\, \boldsymbol{e}_x,$$

the local vorticity in the gas is parallel to the y-direction:

$$\boldsymbol{\omega} = \frac{1}{2}\frac{\mathrm{d}v_x}{\mathrm{d}z}\, \boldsymbol{e}_z \times \boldsymbol{e}_x.$$

Consequently, under the combined action of $\boldsymbol{M}^{(0)}$ and $\boldsymbol{M}^{(1)}$ the particle preferentially will rotate with $\boldsymbol{\omega}$ around its axis $\boldsymbol{s}$ which will be aligned parallel to $\boldsymbol{\omega}$.

With $\alpha_{\text{odd}}=2-\alpha$, $H_2=0$ and $\boldsymbol{\omega}=-\boldsymbol{\Omega}$ the torque $\boldsymbol{M}^{(1)}$ from Eqs. (4.6)—(4.9) is identical to the expression derived in a quite different way [25] for spheroids rotating with angular velocity $\boldsymbol{\Omega}$. The form factors for *prolate spheroids* are given by the following formulae:

$$G_1 = \pi a_\parallel^4 \sqrt{1-\varepsilon^2}\left[(\tfrac{3}{2}-\varepsilon^2)\sqrt{1-\varepsilon^2} + (5-4\varepsilon^2)\frac{1}{2\varepsilon}\arcsin\varepsilon\right], \tag{4.10}$$

$$G_2 = \pi a_\parallel^4 \sqrt{1-\varepsilon^2}\,\frac{1}{\varepsilon^2}\left[(\varepsilon^2-\tfrac{1}{2})\sqrt{1-\varepsilon^2} + \frac{1}{2\varepsilon}\arcsin\varepsilon\right], \tag{4.11}$$

$$H_1 = \pi a_\parallel^4 \sqrt{1-\varepsilon^2}\left[(\tfrac{3}{2}-\varepsilon^2)\sqrt{1-\varepsilon^2} + (4\varepsilon^2-3)\frac{1}{2\varepsilon}\arcsin\varepsilon\right]. \tag{4.12}$$

In the limit of a rod, $\varepsilon \to 1$ i.e. $a_\perp/a_\parallel \to 0$, one has

$$G_1 = G_2 = H_1 = \frac{\pi^2}{4} a_\parallel^3 a_\perp \to 0, \tag{4.13}$$

i.e. the torque has no component parallel to the axis $\boldsymbol{s}$,

$$w_\parallel = 0, \quad w_\perp = \frac{\pi}{4}\frac{p_0}{\hat{c}_0} a_\parallel^3 a_\perp \left(\frac{3}{2} - \frac{1}{4}\alpha_{\text{odd}} - \frac{\alpha}{2} + \alpha\frac{\pi}{8}\right),$$

as one would expect.

For *oblate spheroids* the geometrical shape factors are

$$G_1 = \pi a_\perp^4 \left[\tfrac{3}{2} - \tfrac{1}{2}\varepsilon^2 + (1-\varepsilon^2)(\tfrac{5}{2}-\tfrac{1}{2}\varepsilon^2)\frac{1}{2\varepsilon}\ln\frac{1+\varepsilon}{1-\varepsilon}\right], \tag{4.14}$$

$$G_2 = \pi a_\perp^4 \frac{1-\varepsilon^2}{2\varepsilon^2}\left[1+\varepsilon^2 - (1-\varepsilon^2)^2\frac{1}{2\varepsilon}\ln\frac{1+\varepsilon}{1-\varepsilon}\right], \tag{4.15}$$

$$H_1 = \pi a_\perp^4 \left[\tfrac{3}{2} - \tfrac{1}{2}\varepsilon^2 - (1-\varepsilon^2)(\tfrac{3}{2}+\tfrac{1}{2}\varepsilon^2)\frac{1}{2\varepsilon}\ln\frac{1+\varepsilon}{1-\varepsilon}\right]. \tag{4.16}$$

In particular, for a disc, $\varepsilon \to 1$ i.e. $a_\parallel/a_\perp \to 0$, one gets

$$G_1 = H_1 = \pi a_\perp^4, \quad G_2 = 0, \tag{4.17}$$

and the components of the torque have the simple form

$$w_\parallel = \frac{p_0}{\hat{c}_0} a_\perp^4 (1 - \tfrac{1}{2}\alpha_{\text{odd}}),$$

$$w_\perp = \frac{p_0}{\hat{c}_0} a_\perp^4 \left(1 - \frac{1}{2}\alpha + \alpha\frac{\pi}{8}\right).$$

Due to the inequality [23]

$$\alpha \leqq \alpha_{\text{odd}} \leqq 2-\alpha \quad \text{or} \quad \tfrac{1}{2}\alpha \leqq 1 - \tfrac{1}{2}\alpha_{\text{odd}} \leqq 1 - \tfrac{1}{2}\alpha$$

the components $w_\parallel$ and $w_\perp$ are different for $\alpha > 0$; only in the unrealistic case of complete backreflection, $\alpha_{\text{odd}}=\alpha=0$ (i.e. $\beta=1$, see Eqs. (1.3), (1.6)), the torque $\boldsymbol{M}^{(1)}$ is "isotropic", viz.

$$\boldsymbol{M}^{(1)} = \frac{p_0}{\hat{c}_0} a_\perp^4 \boldsymbol{\omega}.$$

It should be noted, that in the hydrodynamic limit the torque on a rotating disc is isotropic [26], see Appendix.

In the limit $\varepsilon = 0$ i.e. $a_\parallel = a_\perp = a$, Eqs. (4.10) — (4.12) and (4.14)—(4.16) yield the result for a sphere of radius a:

$$H_1 = 0, \quad G_2 = \tfrac{1}{3} G_1 = (4\pi/3)\, a^4, \qquad (4.18)$$

hence the torque is simply given by

$$\boldsymbol{M}^{(1)} = \frac{p_0}{\hat{c}_0} \frac{8}{3} a^4 (1 - \tfrac{1}{2}\alpha_{\text{odd}})\, \boldsymbol{\omega}.$$

Finally, the form factors are listed for a *cylinder* of radius a and height h,

$$G_1 = \pi a [a^3 + 2a^2 h + \tfrac{1}{2} a h^2 + \tfrac{1}{6} h^3], \qquad (4.19)$$

$$G_2 = \tfrac{1}{2} \pi a h^2 [a + \tfrac{1}{3} h], \qquad (4.20)$$

$$H_1 = \pi a [a^3 + \tfrac{1}{6} h^3], \qquad (4.21)$$

and for a *spherocylinder* (cylinder of radius a, height h with two spherical caps),

$$G_1 = 4\pi a [a^3 + \tfrac{1}{2} a^2 h + \tfrac{1}{4} a h^2 + \tfrac{1}{24} h^3], \qquad (4.22)$$

$$G_2 = 4\pi a [\tfrac{1}{3} a^3 + \tfrac{1}{2} a^2 h + \tfrac{1}{4} a h^2 + \tfrac{1}{24} h^3], \qquad (4.23)$$

$$H_1 = \pi a (h^2/6) [h + 4a]. \qquad (4.24)$$

Now, let us look at the torque on a particle of size a as a function of gas pressure p_0 or mean free path $l = \eta c_0 / p_0$. In the hydrodynamic regime (see Appendix) the torque

$$\boldsymbol{M}^{\text{h}} \propto \eta a^3 \operatorname{rot} \boldsymbol{v}, \quad l \ll a,$$

is independent of pressure (rot $\boldsymbol{v}$ has to be taken at infinity). If the mean free path is increased, the torque decreases to

$$\boldsymbol{M}^{(1)} \propto \frac{p_0}{c_0} a^4 \operatorname{rot} \boldsymbol{v} = \eta a^3 \operatorname{rot} \boldsymbol{v}\, a/l, \quad l \gg a,$$

which is by a factor of $a/l \ll 1$ smaller than at high pressure. At "low pressure" there is also a torque which is determined by the shear stresses $\eta\, \overline{\nabla \boldsymbol{v}}$,

$$\boldsymbol{M}^{(0)} \propto \eta a^3 \overline{\nabla \boldsymbol{v}}, \quad l \gg a,$$

and which is independent of p_0. This is due to the fact that the distribution function for a dilute gas has been used in calculating $\boldsymbol{M}^{(0)}$. With the distribution function of a rarefied gas also $\boldsymbol{M}^{(0)}$ will get proportional to the pressure.

Appendix

The Torque in the Hydrodynamic Limit

For convenience the formulae calculated by Gans [26] for the torque on a spheroidal particle much larger than the mean free path in the fluid are given below. The solution of the linearized hydrodynamic equations for a fluid with vorticity

$$\boldsymbol{\omega} = \tfrac{1}{2} \operatorname{rot} \boldsymbol{v}$$

far away from the particle (which is at rest) leads to the expression

$$\boldsymbol{M}^{\text{h}} = w_\parallel{}^{\text{h}}\, \boldsymbol{s}\boldsymbol{s} \cdot \boldsymbol{\omega} + w_\perp{}^{\text{h}} (\boldsymbol{\delta} - \boldsymbol{s}\boldsymbol{s}) \cdot \boldsymbol{\omega}$$

for the torque. In the case of a *prolate spheroid* the "resistivity coefficients" parallel and perpendicular to the figure axis $\boldsymbol{s}$ are given by

$$w_\parallel{}^{\text{h}} = \frac{16}{3} \pi \eta a_\parallel{}^3 \varepsilon^2 (1 - \varepsilon^2) \cdot \left[1 - \frac{1-\varepsilon^2}{2\varepsilon} \ln \frac{1+\varepsilon}{1-\varepsilon} \right]^{-1},$$

$$w_\perp{}^{\text{h}} = \frac{16}{3} \pi \eta a_\parallel{}^3 \varepsilon^2 (2 - \varepsilon^2) \cdot \left[\frac{1+\varepsilon^2}{2\varepsilon} \ln \frac{1+\varepsilon}{1-\varepsilon} - 1 \right]^{-1}.$$

In particular, for a rod ($\varepsilon \to 1$, $a_\perp / a_\parallel \to 0$) only the component $w_\perp{}^{\text{h}}$ is important

$$w_\parallel{}^{\text{h}} \approx \frac{16}{3} \pi \eta a_\parallel a_\perp{}^2 \to 0,$$

$$w_\perp{}^{\text{h}} \approx \frac{8}{3} \pi \eta a_\parallel{}^3 \left[\ln 2 - \frac{1}{2} + \ln \frac{a_\parallel}{a_\perp} \right]^{-1}.$$

For an *oblate spheroid* the following result is obtained:

$$w_\parallel{}^{\text{h}} = \frac{16}{3} \pi \eta a_\perp{}^3 \varepsilon^2 \left[\frac{1}{\varepsilon} \arcsin \varepsilon - \sqrt{1-\varepsilon^2} \right]^{-1},$$

$$w_\perp{}^{\text{h}} = \frac{16}{3} \pi \eta a_\perp{}^3 \varepsilon^2 (2 - \varepsilon^2) \cdot \left[\sqrt{1-\varepsilon^2} + \frac{2\varepsilon^2 - 1}{\varepsilon} \arcsin \varepsilon \right]^{-1}.$$

In the limit $\varepsilon \to 1$, $a_\parallel / a_\perp \to 0$ of a disc both shape factors are equal,

$$w_\parallel{}^{\text{h}} = w_\perp{}^{\text{h}} = \tfrac{32}{3} \eta a_\perp{}^3.$$

With $\varepsilon = 0$, $a_{\parallel} = a_{\perp} = a$ the wellknown expression [17], [18]

$$w_{\parallel}{}^{\mathrm{h}} = w_{\perp}{}^{\mathrm{h}} = 8\,\pi\,\eta\,a^3$$

for a sphere is obtained.

Acknowledgement

We thank Prof. S. Hess for stimulating discussions.

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