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Dynamical self-structure factor $S_s(q,\omega)$ for inverse-power-law interactions in the Rayleigh and Lorentz limits

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For purely repulsive $r^{-\nu}$ potentials the three-dimensional linear Boltzmann equation is solved for two limiting cases. In the Rayleigh limit ($m_A \rightarrow \infty$) the Boltzmann collision operator reduces to the Fokker-Planck differential operator, which is independent of the potential index ν. In the Lorentz limit ($m_A \rightarrow 0$) the eigenvalue problem of the Boltzmann collision operator is solved analytically yielding speed-dependent eigenvalues and the Legendre polynomials as eigenfunctions. For the particular case of a hard-sphere interaction potential ($\nu=\infty$) the Lorentz collision operator reduces to the well-known projection operator, which averages the distribution function over all directions in velocity space. Either of the above limits allows an analytical solution of the Boltzmann equation for the dynamical self-structure factor $S_s(q,\omega)$ in terms of a scalar continued fraction. Finally, for the particular case of a Maxwell interaction potential ($\nu=4$), the dependence of $S_s(q,\omega)$ on the mass ratio m_A/m_B is studied using our previous result of the infinite matrix-continued-fraction representation of $S_s(q,\omega)$. It turns out that for $m_A/m_B \rightarrow 0$ and $m_A/m_B \rightarrow \infty$ the matrix-continued-fraction representation of $S_s(q,\omega)$ converges to the same values as do the respective scalar-continued-fraction representations mentioned above. From a physical point of view two interesting results should be mentioned here: First, it turns out that in the Lorentz limit the dynamical self-structure factor does not approach the well-known Lorentz line shape in the hydrodynamic limit ($q \rightarrow 0$), which means that the two limiting processes, $m_A \rightarrow 0$ and $q \rightarrow 0$, must not be interchanged. Second, by scaling $S_s(q,\omega)$ to the customary dimensionless quantity $R(q,x)$, the dependence of $R(q,x)$ on both the potential index ν and the mass ratio $M := m_A/(m_A+m_B)$ is rather weak. This statement, however, is only true for mass ratios $M > 0.05$, whereas for very small mass ratios ($M < 0.05$) one observes for all potential indices a strong dependence of $R(q,x)$ on the mass ratio.

I. INTRODUCTION

In a previous paper[1] we have presented a new derivation of the dynamical self-structure factor $S_s(q,\omega)$. The starting point was the Boltzmann equation for a dilute gas mixture of particles interacting via a Maxwellian (r^{-4}) potential. It turned out that the dynamical self-structure factor can be represented by an infinite matrix continued fraction. The result is valid for the entire (q,ω) range and for arbitrary mass (m_A/m_B) and concentration (n_A/n_B) ratios. Although the numerical evaluation of the infinite matrix continued fraction does not cause any problem, we only studied the convergence of the truncated matrix continued fraction in the free-gas limit ($q \rightarrow \infty$) and compared it with the well-known Gaussian limit (see Table II of Ref. 1).

In this paper we pursue two objectives. First, we want to investigate the dependence of $S_s(q,\omega)$ on the potential index ν for purely repulsive $r^{-\nu}$ potentials. Second, for the special case of the Maxwell potential ($\nu=4$) we compare our previous matrix continued fraction (see Ref. 1) with a completely different representation, namely, a scalar-continued fraction, which—as will be outlined below—is obtained from the Boltzmann equation in the Lorentz limit ($n_A \rightarrow 0$, $m_A \rightarrow 0$) and the Rayleigh limit ($n_A \rightarrow 0$, $m_A \rightarrow \infty$), respectively.

For the case of a hard-sphere gas a Gross-Jackson[2] modeling procedure was used by Lindenfeld[3] in order to calculate the dependence of $S_s(q,\omega)$ on the mass ratio m_A/m_B. That paper also contains a careful analytical treatment of the Lorentz and the Rayleigh limit. However, the results are restricted to a hard-sphere interaction potential only. In particular, for the interesting case of the Lorentz gas[4] the Boltzmann collision operator is replaced by a projection operator, which averages the distribution function over all directions in velocity space, and the generalization of this Lorentz collision operator to other interaction potentials is not obvious.

This paper is organized as follows. In Sec. II we briefly summarize the definitions concerning the dynamical self-structure factor $S_s(q,\omega)$ in a suitable scaling of the variables. In Sec. III we derive the Rayleigh limit ($n_A \rightarrow 0$, $m_A \rightarrow \infty$) of the Boltzmann collision operator and present the dynamical self-structure factor in terms of an infinite scalar continued fraction. As expected, the Rayleigh collision operator is equivalent to the linear Fokker-Planck operator.[5,6] It should be stressed that for calculating $S_s(q,\omega)$ this second-order differential

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operator is the exact limit of the Boltzmann collision operator as the mass ratio of the tagged particle A and the bath particles B tends to infinity. At a first glance this seems surprising, since a systematic expansion of the linear Boltzmann equation in powers of the mass ratio[7–9] yields the Fokker-Planck equation, where the fluctuations (or equivalently, the second-order partial derivative with respect to the velocity) are controlled by the mass ratio. These fluctuations tend to zero as the mass of the tagged particle becomes larger, and an initially sharply peaked distribution function will remain unchanged over time. However, when calculating $S_s(q,\omega)$, an average over the equilibrium Maxwell-Boltzmann velocity distribution is performed, and the mass ratio which controls the fluctuations can be scaled out. As expected, the Rayleigh collision operator is independent of the potential index ν considered.

In Sec. IV we treat the Lorentz limit ($n_A \rightarrow 0$, $m_A \rightarrow 0$) for an arbitrary repulsive interaction potential. It turns out that the eigenfunctions of the Lorentz collision operator are given by the Legendre polynomials, and in general one obtains distinct eigenvalues ($\mu_l \neq \mu_{l'}$ for $l \neq l'$), except for the hard-sphere gas, where the Lorentz operator reduces to a projection operator, which averages the distribution function over all directions in velocity space. In the Lorentz limit the dynamical self-structure factor can be represented by a single integral over an infinite scalar continued fraction. This representation comprises the entire range of the potential index ν, which for the hard-sphere interaction reduces to an elementary function.[3,4]

Both the hydrodynamic limit ($q \rightarrow 0$) and the free-gas limit ($q \rightarrow \infty$) of the dynamical self-structure factor are discussed for the Rayleigh and the Lorentz gas. It should be stressed that the hydrodynamic limit of $S_s(q,\omega)$ for the Lorentz gas does not approach the usual Lorentz line shape, which means that the two limits, $m_A \rightarrow 0$ and $q \rightarrow 0$, must not be interchanged. For a hard-sphere Lorentz gas this was already pointed out by Lindenfeld.[3] Finally, the peak height and the full width at half maximum of $S_s(q,\omega)$ are presented for different values of the potential index ν (see Figs. 1 and 2).

In Sec. V we study the dependence of $S_s(q,\omega)$ on the mass ratio, confining ourselves to the Maxwell interaction potential. To this end we compare our previous results[1] for $S_s(q,\omega)$ in terms of an infinite matrix continued fraction with the ones obtained in this paper. We first study the mass dependence of $S_s(q,\omega)$ calculated via a truncated matrix continued fraction. It turns out that much of the mass dependence has been removed by scaling. In Fig. 3 the variation of the scaled peak height $R(q,0)$ as function of the mass ratio is plotted for different values of q. For a large range of mass ratios $[0.05 \leq M = m_A/(m_A+m_B) \leq 1]$ one gets a rather weak dependence on M, whereas for $M<0.05$ a steep increase of $R(q,0)$ to the Lorentz limit is observed. The same features are found in Fig. 4 for the full width at half maximum. Comparing our results (Maxwell potential, $\nu=4$) with those obtained by Lindenfeld (hard-sphere potential, $\nu=\infty$) one also finds that for $M>0.05$ the dependence of $R(q,x)$ on the potential index is rather weak, whereas, when approaching the Lorentz limit ($M \rightarrow 0$) the results differ considerably. In Figs. 5(a)–5(c) the dynamical self-structure factor $S_s(q,\omega)$ is plotted for the particular mass ratios $m_A/m_B = 0, 1, \infty$.

Finally, we study the accuracy of the truncated matrix continued fraction, comparing it with the scalar continued fractions derived in Secs. III and IV. To put it differently, we compare two completely different representations for the same physical quantity, namely, $S_s(q,\omega)$, and find an excellent numerical agreement for the entire (q,ω) range (see Tables I and II).

II. BOLTZMANN EQUATION FOR INVERSE-POWER-LAW INTERACTIONS

We consider a dilute binary gas mixture of particles with masses m_A and m_B and assume that the number density of the tagged particles A is low ($n_A \approx 0$) so that A-A collisions can be neglected. Our starting point is the Fourier transform of the linear Boltzmann equation for the tagged particle A

$$\frac{\partial}{\partial t}\tilde{h}(\mathbf{q},\mathbf{v},t) - i\mathbf{q}\cdot\mathbf{v}\tilde{h}(\mathbf{q},\mathbf{v},t) = \int [\omega_{AB}(\mathbf{v}'\rightarrow\mathbf{v})\tilde{h}(\mathbf{q},\mathbf{v}',t) - \omega_{AB}(\mathbf{v}\rightarrow\mathbf{v}')\tilde{h}(\mathbf{q},\mathbf{v},t)] \times d^3v' , \quad (2.1)$$

where $\omega_{AB}(\mathbf{v}\rightarrow\mathbf{v}')$ is the probability for an A particle to change its velocity from $\mathbf{v}$ to $\mathbf{v}'$ due to a collision with a B particle. This transition probability can be written in the following form:[10]

$$\int \omega_{AB}(\mathbf{v}\rightarrow\mathbf{v}')\varphi(\mathbf{v}')d^3v' = n_B \int \varphi(\mathbf{v}')f_B(v_1)\,|\mathbf{v}_1-\mathbf{v}|\,b\,db\,d\epsilon\,d^3v_1 , \quad (2.2)$$

where φ is an arbitrary function, b and ϵ denote the collision variables, $\mathbf{v}$ and $\mathbf{v}_1$ are the velocities of the colliding particles before the collision, and the primed quantities are the postcollision velocities. Furthermore, n_B is the number density of the bath particles B and

$$f_B(v) = (\sqrt{\pi}v_{T_B})^{-3}e^{-v^2/v_{T_B}^2} , \quad (2.3)$$

with $v_{T_B}^2 = 2kT/m_B$ the equilibrium Maxwell-Boltzmann velocity distribution. In the right-hand side of Eq. (2.2) one calculates the average of φ with the aid of Boltzmann's *Stosszahlansatz,* where $\mathbf{v}'$ has to be expressed in terms of $\mathbf{v}$, $\mathbf{v}_1$, b, and ϵ, while in the left-hand side $\mathbf{v}'$ is an integration variable. Since we are interested in the dynamical self-structure factor $S_s(q,\omega)$, we are looking for a solution of (2.1) subject to the initial condition,[11,12]

$$\tilde{h}(\mathbf{q},\mathbf{v},0) = f_A(v) = (\sqrt{\pi}v_{T_A})^{-3}\exp(-v^2/v_{T_A}^2) . \quad (2.4)$$

Then by definition, the dynamical self-structure factor is given by

$$S_s(q,\omega) = \frac{2}{\pi}\,\mathrm{Re}Q(q,i\omega) , \quad (2.5a)$$

where we have introduced the auxiliary function,

$$Q(q,s)=\int_0^\infty e^{-st}F_s(q,t)dt \tag{2.5b}$$

as the Laplace transform of the intermediate scattering function,

$$F_s(q,t)=\int \tilde{h}(\mathbf{q},\mathbf{v},t)d^3v \ . \tag{2.5c}$$

Next we want to rewrite the collision term in (2.1). To this end we define

$$\psi(\mathbf{q},\mathbf{v},t):=\tilde{h}(\mathbf{q},\mathbf{v},t)/f_A(v) \ , \tag{2.6}$$

(where $a:=b$ represents a defined by b) and making use of detailed balance, i.e.,

$$f_A(v_1)\omega_{AB}(\mathbf{v}_1\rightarrow\mathbf{v})=f_A(v)\omega_{AB}(\mathbf{v}-\mathbf{v}_1) \ , \tag{2.7}$$

we can write (2.1) as

$$\frac{\partial}{\partial t}\psi-i\mathbf{q}\cdot\mathbf{v}\psi=\int \omega_{AB}(\mathbf{v}\rightarrow\mathbf{v}')[\psi(\mathbf{q},\mathbf{v}',t)-\psi(\mathbf{q},\mathbf{v},t)]d^3v' \ , \tag{2.8a}$$

with the initial condition

$$\psi(\mathbf{q},\mathbf{v},0)=1 \ . \tag{2.8b}$$

The solution of Eq. (2.8) for a Maxwell interaction potential can be found in Ref. 1. Here we are interested in a solution for an arbitrarily repulsive interaction potential for the limiting cases of the Lorentz ($m_A\rightarrow 0$) and the Rayleigh gas ($m_A\rightarrow\infty$). To this end we introduce the dimensionless variables t^*, $\mathbf{q}^*$, and $\mathbf{v}^*$ by

$$t=\frac{2[D_{AB}]^{\mathrm{I}}}{v_{T_A}^2}t^* \ , \tag{2.9a}$$

$$\mathbf{q}=\frac{v_{T_A}}{2[D_{AB}]^{\mathrm{I}}}\mathbf{q}^* \ , \tag{2.9b}$$

$$\mathbf{v}=v_{T_A}\mathbf{v}^* \ , \tag{2.9c}$$

where $[D_{AB}]^{\mathrm{I}}$ is the first Chapman-Enskog approximation to the diffusion coefficient D_{AB} which is given by[8]

$$[D_{AB}]^{\mathrm{I}}=\frac{3v_{T_A}}{16\sqrt{\pi}\Gamma(3-2/\nu)A_1(\nu)n_B\sigma^2_{AB}}\times\left[\frac{kT}{\nu}\right]^{2/\nu}\left[\frac{m_A+m_B}{m_B}\right]^{1/2} . \tag{2.10}$$

For the coefficients $A_l(\nu)$ see Appendix. In the scaled variables Eqs. (2.5a)–(2.5c) take the following form:

$$\psi(\mathbf{q},\mathbf{v},t)=\psi^*(\mathbf{q}^*,\mathbf{v}^*,t^*) \ , \tag{2.11a}$$

$$F_s^*(q^*,t^*)=\pi^{-3/2}\int e^{-v^{*2}}\psi^*(\mathbf{q}^*,\mathbf{v}^*,t^*)d^3v^* \ , \tag{2.11b}$$

and

$$Q^*(q^*,s)=\int_0^\infty e^{-st^*}F_s^*(q^*,t^*)dt^* \ . \tag{2.11c}$$

The dynamical self-structure factor $S_s(q,\omega)$ is usually calculated in the following dimensionless form:[1,3]

$$R(q^*,x)=\frac{2}{\pi}q^*\mathrm{Re}Q^*(q^*,ixq^*) \ . \tag{2.11d}$$

For typographical convenience we drop the stars from the variables and functions for the remainder of this paper. In the scaled variables Eq. (2.8a) can be written as

$$\frac{\partial}{\partial t}\psi-i\mathbf{q}\cdot\mathbf{v}\psi=-K_{\alpha,\nu}\psi \ , \tag{2.12a}$$

where the action of the integral operator $K_{\alpha,\nu}$ on an arbitrary function φ is given by

$$K_{\alpha,\nu}\varphi(\mathbf{v}):=-\frac{3(1+\alpha)^{2/\nu+1/2}}{8\sqrt{\pi}\Gamma(3-2/\nu)A_1(\nu)}\times\frac{1}{(\alpha\pi)^{3/2}}\int e^{-v_1^2/\alpha}|\mathbf{v}_1-\mathbf{v}|^{\mu}\times[\varphi(\mathbf{v}')-\varphi(\mathbf{v})]z\,dz\,d\epsilon\,d^3v_1 \ . \tag{2.12b}$$

In Eq. (2.12b) we have introduced the reduced potential index μ

$$\mu:=1-\frac{4}{\nu} \ , \tag{2.13a}$$

and the mass ratio α

$$\alpha:=\frac{m_A}{m_B} \ . \tag{2.13b}$$

Furthermore, the postcollisional velocity is now given by

$$\mathbf{v}'=\frac{1}{1+\alpha}(\mathbf{g}-\mathbf{g}')+\mathbf{v} \ , \tag{2.14}$$

where $\mathbf{g}=\mathbf{v}_1-\mathbf{v}$ and $\mathbf{g}'=\mathbf{v}_1'-\mathbf{v}'$ denote the relative velocities of the colliding particles before and after the collision, respectively. The angle $\chi(z,\nu)$ between $\mathbf{g}$ and $\mathbf{g}'$,

$$\mathbf{g}\cdot\mathbf{g}'=g^2\cos\chi(z,\nu) \ , \tag{2.15}$$

is uniquely defined by the interaction law (see Appendix). In what follows we shall study the Rayleigh limit ($\alpha\rightarrow\infty$) and the Lorentz limit ($\alpha\rightarrow 0$) of the integral operator $K_{\alpha,\nu}$ defined by Eq. (2.12b).

III. THE RAYLEIGH LIMIT ($m_A\rightarrow\infty$)

In the Introduction we already anticipated that the Fokker-Planck differential operator as an approximation to the Boltzmann collision operator for large α is well established.[5,8] Regardless of the special structure of the collision kernel one can formally transform the Boltzmann equation to a differential equation of infinite order. In the terminology of master equations this is called the Kramers-Moyal expansion.[13] Taking into account only the first and second derivative one obtains the Fokker-Planck equation. However, the conditions allowing the passage from the Boltzmann equation to its approximate Fokker-Planck equation are not obvious, and some of the assumptions concerning the initial conditions were investigated by Ferrari.[6] Another way of deriving the Fokker-Planck equation from a master equation was given by van Kampen,[7] who expanded the distribution function around the solution of the macroscopic equation. In the linear noise approximation, one obtains a Fokker-Planck equation with time-dependent coefficients. In the limit of large mass ratios ($\alpha \to \infty$) the fluctuations tend to zero, and the Green's function of the Fokker-Planck equation is a δ function, shifted by the mean velocity. Under these circumstances one can say that the motion of the heavy particle is described by a macroscopic equation with a velocity-dependent friction coefficient.

In what follows we will sketch a derivation of the Fokker-Planck equation as the exact large-α limit of the Boltzmann equation for the particular initial condition (2.8b). The arguments above should demonstrate that such a derivation is not superfluous, since commonly the Fokker-Planck equation is an approximation to the Boltzmann equation only and is not obtained as the large-α limit.

Let us first perform the following variable transformation in (2.12b):

$$\mathbf{v}_1 = \sqrt{\alpha}\mathbf{u} + \mathbf{v} , \tag{3.1a}$$

which implies

$$\mathbf{v}' = \frac{\sqrt{\alpha}}{1+\alpha}(\mathbf{u}-\mathbf{u}') + \mathbf{v} , \tag{3.1b}$$

with

$$\mathbf{u}\cdot\mathbf{u}' = u^2 \cos\chi(z,\nu) . \tag{3.1c}$$

In these new variables the collision operator $K_{\alpha,\nu}$ reads

$$K_{\alpha,\nu}\varphi(\mathbf{v}) = -\frac{3(1+1/\alpha)^{2/\nu-1/2}}{8\sqrt{\pi}\Gamma(3-2/\nu)A_1(\nu)} \frac{1+\alpha}{\pi^{3/2}} \times \int |\mathbf{u}|^{\mu} e^{-[\mathbf{u}+(1/\sqrt{\alpha})\mathbf{v}]^2} \times \left[\varphi\left[\frac{\sqrt{\alpha}}{1+\alpha}(\mathbf{u}-\mathbf{u}')+\mathbf{v} \right] - \varphi(\mathbf{v}) \right] \times z\, dz\, d\epsilon\, d^3u , \tag{3.2}$$

where, in order to obtain the Rayleigh limit, we have to consider Eq. (3.2) for large α. Therefore we expand the difference in the square brackets into a Taylor series yielding

$$\frac{\sqrt{\alpha}}{1+\alpha}(\mathbf{u}-\mathbf{u}')\cdot\frac{\partial}{\partial\mathbf{v}}\varphi(\mathbf{v}) + \frac{1}{2}\frac{\alpha}{(1+\alpha)^2}(\mathbf{u}-\mathbf{u}')(\mathbf{u}-\mathbf{u}'):\frac{\partial}{\partial\mathbf{v}}\frac{\partial}{\partial\mathbf{v}}\varphi(\mathbf{v}) + O\left[\frac{1}{\alpha^{3/2}}\right] , \tag{3.3}$$

where the colon denotes the scalar product of two tensors. This shows immediately, that the higher than second derivatives vanish in the limit $\alpha \to \infty$. It remains to consider the above terms in connection with Eq. (3.2).

First we evaluate the integral

$$\mathbf{I}_1 := \lim_{\alpha\to\infty} \frac{\sqrt{\alpha}}{\pi^{3/2}} \int u^{\mu} e^{-[\mathbf{u}+(1/\sqrt{\alpha})\mathbf{v}]^2}(\mathbf{u}-\mathbf{u}')z\, dz\, d\epsilon\, d^3u . \tag{3.4}$$

In order to perform the integration over z and ϵ we introduce an orthogonal reference frame $\{\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3\}$ with $\mathbf{u}$ parallel to the $\mathbf{e}_3$ axis; we then have

$$\mathbf{u} = u\mathbf{e}_3 , \tag{3.5a}$$

$$\mathbf{u}' = u[\mathbf{e}_1 \sin\chi(z,\nu)\cos\epsilon + \mathbf{e}_2 \sin\chi(z,\nu)\sin\epsilon + \mathbf{e}_3\cos\chi(z,\nu)] , \tag{3.5b}$$

which yields

$$\int (\mathbf{u}-\mathbf{u}')z\, dz\, d\epsilon = 2\pi\mathbf{u}\int_0^\infty dz\, z[1-\cos\chi(z,\nu)] = 2\pi A_1(\nu)\mathbf{u} . \tag{3.6}$$

This leaves us with the three-dimensional integration over $\mathbf{u}$. Again using spherical coordinates with $\mathbf{v}$ in the $\mathbf{e}_3$ axis one obtains the following integral for $\mathbf{I}_1$:

$$\mathbf{I}_1 = 4\sqrt{\pi}A_1(\nu)\mathbf{e}_3 \lim_{\alpha\to\infty}\sqrt{\alpha}\int_0^\infty du\, u^{3+\mu}e^{-u^2-(1/\alpha)v^2} \times \int_{-1}^{1} d\xi\, \xi\, e^{-(2/\sqrt{\alpha})uv\xi} . \tag{3.7}$$

Carrying out the integration over ξ by expanding the exponential function in a power series in ξ and performing the limit $\alpha \to \infty$ yields

$$\mathbf{I}_1 = -\tfrac{16}{3}\sqrt{\pi}A_1(\nu)\mathbf{v}\int_0^\infty du\, u^{4+\mu}e^{-u^2} = -\tfrac{8}{3}\sqrt{\pi}\Gamma(3-2/\nu)A_1(\nu)\mathbf{v} . \tag{3.8}$$

Next, inserting the second term of (3.3) into (3.2), the limit $\alpha \to \infty$ can be readily performed, leaving us with the tensor integral

$$I_2 := \frac{1}{2\pi^{3/2}}\int u^{\mu}e^{-u^2}(\mathbf{u}-\mathbf{u}')(\mathbf{u}-\mathbf{u}')z\, dz\, d\epsilon\, d^3u . \tag{3.9}$$

Using (3.5a) and (3.5b) the integration over z and ϵ can be easily carried out, yielding

$$I_2 = \frac{1}{2\sqrt{\pi}}\int u^{\mu}e^{-u^2}[4A_1(\nu)\mathbf{u}\mathbf{u} + 3A_2(\nu)(\mathbf{u}\mathbf{u}-\tfrac{1}{3}Iu^2)]d^3u , \tag{3.10}$$

where $I = (\delta_{ij})$ denotes the unit tensor. While the integral over the symmetric traceless tensor $\mathbf{u}\mathbf{u}-\frac{1}{3}Iu^2$ vanishes, the first one yields

$$I_2 = \tfrac{4}{3}\sqrt{\pi}\Gamma(3-2/\nu)A_1(\nu)I . \tag{3.11}$$

Inserting (3.8) and (3.11) into (3.2) yields the Rayleigh limit of the Boltzmann collision operator

$$\lim_{\alpha\to\infty} K_{\alpha,\nu}\varphi = \mathbf{v}\cdot\frac{\partial}{\partial\mathbf{v}}\varphi - \frac{1}{2}\frac{\partial}{\partial\mathbf{v}}\cdot\frac{\partial}{\partial\mathbf{v}}\varphi , \tag{3.12a}$$

and in connection with Eq. (2.12a),

$$\frac{\partial}{\partial t}\psi - i\mathbf{q}\cdot\mathbf{v}\psi = -\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{v}}\psi + \frac{1}{2}\frac{\partial}{\partial}\cdot\frac{\partial}{\partial \mathbf{v}}\psi . \quad (3.12b)$$

This Fokker-Planck equation is independent of the interaction law and emerged as the exact large-α limit of the Boltzmann equation for the initial condition (2.8b). In order to solve Eq. (3.12b) subject to the initial condition $\psi(\mathbf{q},\mathbf{v},0)=1$ the *ansatz*

$$\psi(\mathbf{q},\mathbf{v},t) = \varphi(q,t)\psi_1(\mathbf{q},\mathbf{v},t) \quad (3.13)$$

turns out to be useful, where ψ_1 denotes the solution of (3.12b) when dropping the second derivative. After some straightforward manipulations one obtains[14]

$$\psi(\mathbf{q},\mathbf{v},t) = \exp[i\mathbf{q}\cdot\mathbf{v}(1-e^{-t}) - \tfrac{1}{2}q^2(t+2e^{-t}-\tfrac{1}{2}e^{-2t}-\tfrac{3}{2})] . \quad (3.14)$$

The average of ψ over the Maxwell-Boltzmann equilibrium distribution function is readily performed, yielding for $Q(q,s)$ [see (2.11c)]

$$Q(q,s) = \int_0^\infty e^{-st}e^{-(1/2)q^2(t-1+e^{-t})}dt . \quad (3.15)$$

This integral can be expressed in terms of a confluent hypergeometric function ${}_1F_1(a,c;z)$. Substituting $e^{-t} = \tau$ yields an integral which is proportional to the incomplete Γ function, which in turn can be expressed as a confluent hypergeometric function.[15] The final result is

$$Q(q,s) = \frac{1}{s+\frac{1}{2}q^2}\,{}_1F_1(1,1+s+\tfrac{1}{2}q^2;\tfrac{1}{2}q^2) . \quad (3.16)$$

For computing $S_s(q,\omega)$ via (2.5a) for the entire (q,ω) range, the representation of $Q(q,s)$ in terms of a continued fraction is more advantageous. To this end we consider the integrals

$$\varphi_n(z,s) := \int_0^\infty e^{-st}(1-e^{-t})^n e^{-z(t-1+e^{-t})}dt . \quad (3.17)$$

Integration by parts yields

$$s\varphi_0 = 1 - z\varphi_1 , \quad (3.18a)$$

$$(s+n)\varphi_n = n\varphi_{n-1} - z\varphi_{n+1}, \quad n \ge 1 . \quad (3.18b)$$

From (3.18b) we get the following one-step recursion relation for $c_n := \varphi_n/\varphi_{n-1}$:

$$c_n = \frac{n}{s+n+zc_{n+1}}, \quad n \ge 1 \quad (3.19)$$

and from (3.18a) we find

$$\varphi_0 = \frac{1}{s+zc_1} , \quad (3.20)$$

which yields the following continued fraction for $Q(q,s) = \varphi_0(q^2/2,s)$:

$$Q(q,s) = \cfrac{1}{s+\cfrac{\alpha_1 q^2}{s+1+\cfrac{\alpha_2 q^2}{s+2+\cdots}}}, \quad \alpha_k = \frac{k}{2} . \quad (3.21)$$

Although there exists a continued fraction representation for $1/{}_1F_1(1,c;z)$ (see, e.g., Ref. 16), we failed in deriving the simple continued fraction (3.21) from that more involved expression.

Finally let us study the free-gas limit $(q\to\infty)$ and the hydrodynamic limit $(q\to 0)$ of Eq. (3.21). For large q Eq. (3.21) simplifies to

$$\lim_{q\to\infty} qQ(q,qs) = \frac{1}{s}\cfrac{1}{1+\cfrac{\gamma_1}{1+\cfrac{\gamma_2}{1+\cdots}}}, \quad \gamma_k = \frac{k}{2s^2} . \quad (3.22)$$

This continued fraction can be expressed in terms of elementary functions[16] yielding

$$\lim_{q\to\infty} qQ(q,qs) = \sqrt{\pi}e^{s^2}\left[1-\frac{2}{\sqrt{\pi}}\mathrm{erf}(s)\right] . \quad (3.23)$$

Now, putting $s = ix$ we obtain with the aid of Eq. (2.11d)

$$\lim_{q\to\infty} R(q,x) = \frac{2}{\sqrt{\pi}}e^{-x^2} , \quad (3.24)$$

which is the well-known free-gas limit of the dynamical self-structure factor $S_s(q,\omega)$, expressed in terms of $R(q,x)$.

In the hydrodynamic limit $(q\to 0)$ Eq. (3.21) reduces to

$$Q(q,s) = \frac{1}{s+q^2/2} , \quad (3.25a)$$

which implies for $R(q,x)$

$$R(q,x) = \frac{2}{\pi}\frac{q/2}{x^2+(q/2)^2} . \quad (3.25b)$$

It should be noted that in Eq. (3.25b) the variable q is scaled to the first Chapman-Enskog approximation of the diffusion coefficient $[D_{AB}]^{\mathrm{I}}$ according to Eq. (2.9b). When deriving the hydrodynamic limit of $R(q,x)$ from the diffusion equation[3] one arrives at the same expression as given by (3.25b), the only difference being that the variable q is replaced by $\bar{q} = f_D(\alpha)q$. The function $f_D(\alpha)$ is defined as the ratio of the exact diffusion coefficient to its first Chapman-Enskog approximation and varies also with the potential index ν. For a Maxwell interaction potential one has $f_D(\alpha)=1$, since the first Chapman-Enskog approximation agrees with the exact diffusion coefficient. In the case of a hard-sphere interaction an approximation formula to $f_D(\alpha)$, reflecting the weak dependence on α $[1 \le f_D(\alpha) \le 32/9\pi$ for $\infty \ge \alpha \ge 0]$ can be found in Ref. 17, and numerical values for some mass ratios can be found in Table I of Ref. 3. In order to avoid confusion we will refer to Eq. (3.25b) as the hydrodynamic limit of $R(q,x)$.

IV. THE LORENTZ LIMIT $(m_A \to 0)$

We have seen in Sec. III that in the limit of large mass ratios the Boltzmann collision operator reduces to a second-order differential operator, which is equivalent to the Fokker-Planck operator. For the Lorentz limit, however, the reduction of the Boltzmann collision operator to a differential operator has only been shown for isotropic energy relaxation of a hard-sphere gas.[18] However, when studying the Lorentz limit of $S_s(q,\omega)$ one has to deal with an anisotropic relaxation process, since the action of the collision operator $K_{\alpha,\nu}$ [see (2.12b)] on an arbitrary function φ, which depends on q, v, and the angle between $\mathbf{q}$ and $\mathbf{v}$, has to be considered. In this section we will study the properties of the collision operator $K_{\alpha,\nu}$ in the Lorentz limit ($\alpha\to 0$), yielding for the particular case of the hard-sphere gas ($\nu=\infty$) the well-known projection operator, which averages a function over all directions in velocity space.[4] Furthermore, an explicit expression for $S_s(q,\omega)$ in terms of an integral over an infinite scalar continued fraction, valid for all ν, is presented.

In order to get the limit $\alpha\to 0$ of the Boltzmann collision operator $K_{\alpha,\nu}$, we make the following variable transformation:

$$\mathbf{v}_1=\mathbf{u}+\mathbf{v}\ , \tag{4.1a}$$

which implies for $\mathbf{v}'$

$$\mathbf{v}'=\frac{1}{1+\alpha}(\mathbf{u}-\mathbf{u}')+\mathbf{v}\ , \tag{4.1b}$$

where $\mathbf{u}$ and $\mathbf{u}'$ are related by (3.1c). Observing that the exponential function in (2.12b) approaches a δ function as $\alpha\to 0$, this limit can be performed easily, yielding

$$\lim_{\alpha\to 0}K_{\alpha,\nu}\varphi(\mathbf{v})=:L_\nu\varphi(\mathbf{v})=-\frac{3}{8\sqrt{\pi}\Gamma(3-2/\nu)A_1(\nu)}\int |\mathbf{u}|^{\mu}\delta(\mathbf{u}+\mathbf{v})[\varphi(\mathbf{u}-\mathbf{u}'+\mathbf{v})-\varphi(\mathbf{v})]z\,dz\,d\epsilon\,d^3u\ , \tag{4.2}$$

where we have introduced the Lorentz operator L_ν. For evaluating the integral in (4.2) it is advantageous to use spherical coordinates with $\mathbf{v}$ parallel to the $\mathbf{e}_3$ axis of the reference frame

$$\mathbf{v}=v\mathbf{e}_3\ , \tag{4.3a}$$

$$\mathbf{u}=u\,(\mathbf{e}_1\sin\theta\cos\varphi+\mathbf{e}_2\sin\theta\sin\varphi+\mathbf{e}_3\cos\theta)\ , \tag{4.3b}$$

$$\mathbf{u}'=u\,(\mathbf{e}_1\sin\theta'\cos\varphi'+\mathbf{e}_2\sin\theta'\sin\varphi'+\mathbf{e}_3\cos\theta')\ . \tag{4.3c}$$

Note that θ' and φ' are related by [see Eq. (3.1c)]

$$\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos(\varphi-\varphi')=\cos\chi(z,\nu)\ . \tag{4.4}$$

Evaluating the δ function in Eq. (4.2) means that $\mathbf{u}=-\mathbf{v}$, which in turn implies that $u=v$ and $\theta=\pi$ [see (4.3a) and (4.3b)]. Then, using (4.4), one obtains $\theta'=\chi(z,\nu)\pm\pi$ and, without loss of generality, $\varphi'=\epsilon$. Inserting these values for θ and φ and θ' and φ', respectively, into Eq. (4.3) yields

$$\bar{\mathbf{v}}:=\mathbf{u}-\mathbf{u}'+\mathbf{v}=v[\mathbf{e}_1\sin\chi(z,\nu)\cos\epsilon+\mathbf{e}_2\sin\chi(z,\nu)\sin\epsilon+\mathbf{e}_3\cos\chi(z,\nu)] \tag{4.5a}$$

and

$$\mathbf{v}=v\mathbf{e}_3\ . \tag{4.5b}$$

With the aid of (4.5a) and (4.5b) the Lorentz operator L_ν can be written as

$$L_\nu\varphi(\mathbf{v})=-\frac{3}{8\sqrt{\pi}\Gamma(3-2/\nu)A_1(\nu)}v^{\mu}\times\int[\varphi(\bar{\mathbf{v}})-\varphi(\mathbf{v})]z\,dz\,d\epsilon\ . \tag{4.6}$$

It should be noted, that according to (4.5a) and (4.5b) one has $|\bar{\mathbf{v}}|=|\mathbf{v}|$ and therefore the Lorentz operator L_ν leaves the speed unaltered. That is to say, for an arbitrary function, which depends on $|\mathbf{v}|$ only, one has

$$L_\nu\varphi(|\mathbf{v}|)=0\ . \tag{4.7}$$

Next we use the fact that according to (2.12a) and due to the special initial condition (2.8b), the function $\psi(\mathbf{q},\mathbf{v},t)$ depends on $q=|\mathbf{q}|$, $v=|\mathbf{v}|$, and $\cos\eta=\mathbf{q}\cdot\mathbf{v}/qv$ only. Therefore we expand ψ into Legendre polynomials

$$\psi(\mathbf{q},\mathbf{v},t)=\sum_{l=0}^{\infty}\psi_l(q,v,t)P_l(\cos\eta)\ . \tag{4.8}$$

We study the action of L_ν on the Legendre polynomial $P_l(\cos\eta)$. To this end it suffices to consider the following operator:

$$QP_l(\cos\eta):=\int[P_l(\cos\bar{\eta})-P_l(\cos\eta)]z\,dz\,d\epsilon\ , \tag{4.9a}$$

with

$$\cos\bar{\eta}:=\frac{\mathbf{q}\cdot\bar{\mathbf{v}}}{q\bar{v}}\ . \tag{4.9b}$$

Next we expand $P_l(\cos\bar{\eta})$ into spherical harmonics

$$P_l(\cos\bar{\eta})=\frac{4\pi}{2l+1}\sum_{m=-l}^{l}Y_{l,m}(\eta,\varphi)Y^*_{l,m}(\chi(z,\nu),\epsilon)\ , \tag{4.10}$$

where we have used the fact that according to (4.5b) $\mathbf{v}$ lies in the $\mathbf{e}_3$ axis and therefore the angle between $\mathbf{q}$ and the $\mathbf{e}_3$ axis is θ and the angle between $\bar{\mathbf{v}}$ and the $\mathbf{e}_3$ axis is $\chi(z,\nu)$. Integrating (4.10) over ϵ and taking into account

$$\int_0^{2\pi}Y_{l,m}(\chi,\epsilon)d\epsilon=2\pi Y_{l,0}(\chi,\epsilon)\delta_{m,0}\ , \tag{4.11a}$$

with

$$Y_{l,0}(\chi,\epsilon)=\left[\frac{2l+1}{4\pi}\right]^{1/2}P_l(\cos\chi)\ , \tag{4.11b}$$

one obtains instead of (4.9a)

$$QP_l(\cos\eta)=-2\pi P_l(\cos\eta)\int_0^{\infty}dz\,z[1-P_l(\cos\chi(z,\nu))]\ . \tag{4.12}$$

Inserting (4.12) into (4.6) we see that the Legendre polynomials are eigenfunctions of the Lorentz collision operator

$$L_\nu P_l(\cos\eta)=v^{1-4/\nu}B_l(\nu)P_l(\cos\eta)\ , \tag{4.13a}$$

with, in general velocity-dependent, eigenvalues $v^{1-4/\nu}B_l(\nu)$. The coefficients

$$B_l(\nu)=\frac{3\sqrt{\pi}}{4\Gamma(3-2/\nu)A_1(\nu)}\int_0^\infty dz\, z[1-P_l(\cos\chi(z,\nu))] \tag{4.13b}$$

are tabulated in the Appendix up to $l=30$ for some values of ν; it should be noted that $B_0(\nu)=0$ for all ν.

For the particular case of a hard-sphere interaction one has $B_l(\infty)=3\sqrt{\pi}/8$ for $l\geq 1$, and L_∞ reduces to a projection operator

$$L_\infty\varphi(\mathbf{v})=\tfrac{3}{8}\sqrt{\pi}\,|\,\mathbf{v}\,|\,(1-P)\varphi(\mathbf{v})\ , \tag{4.14a}$$

with

$$P\varphi(\mathbf{v})=\frac{1}{4\pi}\int d\Omega\,\varphi(\mathbf{v})\ . \tag{4.14b}$$

Next, we make use of (4.13a) and calculate the dynamical self-structure factor $S_s(q,\omega)$ in the Lorentz limit $\alpha\to 0$. To this end we take the Laplace transform of Eq. (2.12a) yielding

$$s\hat{\psi}-1-i\mathbf{q}\cdot\mathbf{v}\hat{\psi}=-L_\nu\hat{\psi}\ . \tag{4.15}$$

Since the action of the operator L_ν is known explicitly (see above), we expand $\hat{\psi}$ into Legendre polynomials $P_l(\xi)$ with $\xi=\mathbf{q}\cdot\mathbf{v}/qv$

$$\hat{\psi}(\mathbf{q},\mathbf{v},s)=\sum_{l=0}^{\infty}\hat{\psi}_l(q,v,s)P_l(\xi)\ . \tag{4.16}$$

Making use of the well-known relation for the Legendre polynomials[15]

$$(2l+1)\xi P_l(\xi)=(l+1)P_{l+1}(\xi)+lP_{l-1}(\xi)\ , \tag{4.17}$$

we finally get the following recursion relation for the expansion coefficients $\hat{\psi}_l$:

$$s\hat{\psi}_0-iqv\tfrac{1}{3}\hat{\psi}_1=1\ , \tag{4.18a}$$

$$[s+v^\mu B_l(\nu)]\hat{\psi}_l-iqv\left[\frac{l}{2l-1}\hat{\psi}_{l-1}+\frac{l+1}{2l+3}\hat{\psi}_{l+1}\right]=0,\quad l\geq 1 \tag{4.18b}$$

where we used again the abbreviation $\mu=1-4/\nu$. When calculating $Q(q,s)$ via (4.16) and (2.11) one observes that only the term with $l=0$ contributes in the Legendre expansion of $\hat{\psi}$, yielding

$$Q(q,s)=\frac{4}{\sqrt{\pi}}\int_0^\infty e^{-v^2}v^2\hat{\psi}_0(q,v,s)dv\ . \tag{4.19}$$

In order to extract $\hat{\psi}_0$ from (4.18) we use the same method as applied in Sec. III for deriving Eq. (3.21). In doing so we arrive at the following representation of $\hat{\psi}_0$ in terms of an infinite scalar continued fraction:

$$\hat{\psi}_0(q,v,s)=\cfrac{1}{s+\cfrac{\beta_1(qv)^2}{s+v^\mu B_1(\nu)+\cfrac{\beta_2(qv)^2}{s+v^\mu B_2(\nu)+\cdots}}}\ , \tag{4.20a}$$

where

$$\beta_k=\frac{k^2}{(2k-1)(2k+1)}\ . \tag{4.20b}$$

The above representation of $\hat{\psi}_0$ and $Q(q,s)$, respectively, is valid for all purely repulsive interaction potentials $r^{-\nu}$. In the case of a hard-sphere interaction, however, a further simplification of (4.20a) is possible, since $B_l(\infty)$ are independent of l. Recalling the representation of the arc-tangent in terms of a continued fraction[16]

$$\arctan(z)=\cfrac{z}{1+\cfrac{\beta_1 z^2}{1+\cfrac{\beta_2 z^2}{1+\cdots}}}\ , \tag{4.21}$$

one finds for $Q(q,s)$

$$Q(q,s)=\frac{4}{\sqrt{\pi}}\int_0^\infty e^{-v^2}v\frac{\arctan\left[\dfrac{qv}{s+3\sqrt{\pi}v/8}\right]}{q-\frac{3}{8}\sqrt{\pi}\arctan\left[\dfrac{qv}{s+3\sqrt{\pi}v/8}\right]}dv\ . \tag{4.22}$$

The above expression for the hard-sphere interaction serves as a check for our general expressions (4.19), (4.20a), and (4.20b), since it can be derived in a different way,[3] making directly use of the projection operator property of L_∞.

Finally, we want to study both the hydrodynamic limit ($q\to 0$) and the free-gas limit ($q\to\infty$) of $R(q,x)$. In the free-gas limit we have to calculate $\hat{\psi}_0$ for large q. Using (4.20a) and (4.21) one readily finds

$$\lim_{q\to\infty}q\hat{\psi}_0(q,v,qs)=\frac{1}{v}\arctan\frac{v}{s}\ , \tag{4.23}$$

which implies for $Q(q,s)$ [see (4.19)]

$$\lim_{q\to\infty}qQ(q,qs)=\frac{4}{\sqrt{\pi}}\int_0^\infty e^{-v^2}v\arctan\frac{v}{s}dv=\sqrt{\pi}e^{s^2}\left[1-\frac{2}{\sqrt{\pi}}\text{erf}(s)\right]\ . \tag{4.24}$$

Putting $s=ix$ in (4.24) and taking the real part, one obtains

$$\lim_{q\to\infty} R(q,x)=\frac{2}{\sqrt{\pi}}e^{-x^2}, \tag{4.25}$$

which is the free-gas limit of $R(q,x)$ for a Lorentz gas. As expected, it coincides with the free-gas limit of the Rayleigh as [see (3.24)].

When calculating the hydrodynamic limit of $R(q,x)$, however, it will turn out that, first, it does not coincide with the hydrodynamic limit derived from the diffusion equation [see (3.25b)] and, second, it depends on the potential index ν. It is convenient to study the deviation of $R(q,x)$ (for small q) from the hydrodynamic limit (3.25b) with the aid of two quantities: the peak height $R(q,0)$ and the full width at half maximum (FWHM) $2\omega_{1/2}$. For sufficiently small q the continued fraction representation (4.20a) of $\hat{\psi}_0$ can be truncated after the first term, yielding for the peak height,

$$R(q,0)\approx\frac{4}{\pi q}c_\nu,\quad q\to 0, \tag{4.26a}$$

and for the FWHM,

$$2\omega_{1/2}\approx q d_\nu,\quad q\to 0, \tag{4.26b}$$

where

$$c_\nu=\frac{9\nu^2}{8(\nu-1)(\nu-2)} \tag{4.26c}$$

and d_ν denotes the deviation from the hydrodynamic limit (3.25b). It should be mentioned that the maximum deviation occurs for the Maxwell potential ($c_4=3$, $d_4=0.1396\ldots$), whereas for the hard-sphere potential the deviation from the hydrodynamic limit is rather small ($c_\infty=\frac{9}{8}$, $d_\infty=0.7835\ldots$).

In Fig. 1 we have plotted the peak height $R(q,0)$ for some values of ν, using Eqs. (4.19) and (4.20). In addition, we display the peak height of the Rayleigh gas which is independent of the potential index ν [see Eq. (3.21)]. Comparing the two extreme mass ratios, namely, the Lorentz gas ($\alpha\to 0$) and the Rayleigh gas ($\alpha\to\infty$), one observes an increasing difference in the peak height with decreasing potential index. For the same values of ν we have compared in Fig. 2 the FWHM for the Lorentz gas with that of the Rayleigh gas. Again, an increasing difference for $\omega_{1/2}$ is observed for a decreasing potential index. Comparing the Lorentz limit ($\alpha\to 0$) and the Rayleigh limit ($\alpha\to\infty$) we can also see that the mass dependence of $R(q,x)$ for a hard-sphere gas is rather weak, since the maximum height $R(q,0)$ and the half width $\omega_{1/2}$ differ only by about 10% for $\alpha\to 0$ and $\alpha\to\infty$, respectively. This has been already pointed out by Lindenfeld.[3] For a Maxwell interaction potential, however, this statement is not true, and in Sec. V we will study the mass dependence of $R(q,x)$, using its infinite matrix-continued-fraction representation.[1]

V. $S_s(q,\omega)$ FOR THE MAXWELL POTENTIAL

In this section we limit ourselves to a detailed study of $S_s(q,\omega)$ for the Maxwell interaction potential ($\nu=4$).

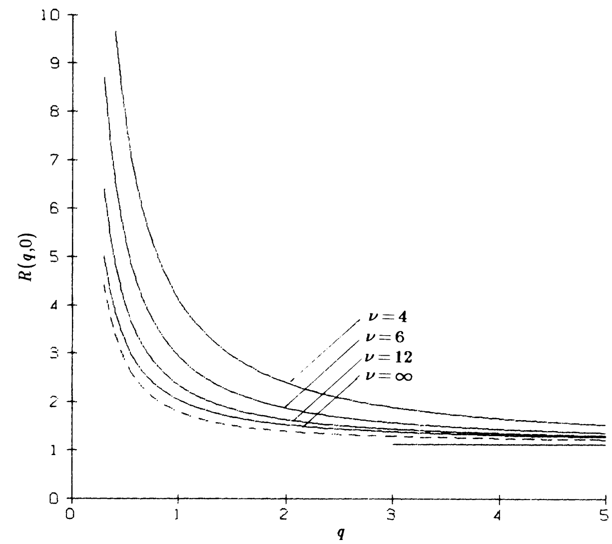

FIG. 1. Peak height $R(q,0)$ in the Lorentz limit ($\alpha\to 0$) for different values of the potential matrix ν ($\nu=4,6,12,\infty$). The dashed line shows the peak height of the Rayleigh gas ($\alpha\to\infty$), which is independent of the potential index. The straight line indicates the free-gas limit [$\lim_{q\to\infty}R(q,0)=2/\sqrt{\pi}$].

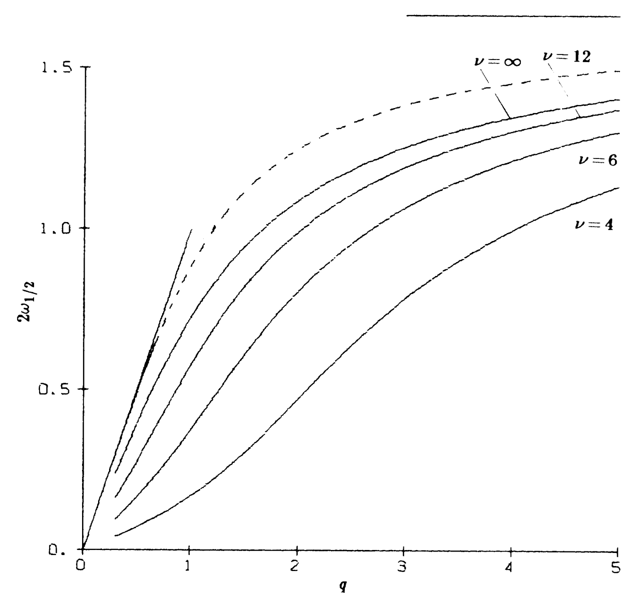

FIG. 2. Full width at half maximum (FWHM) $2\omega_{1/2}$ in the Lorentz limit ($\alpha\to 0$) for different values of the potential index ν ($\nu=4,6,12,\infty$). The dashed line shows the FWHM of the Rayleigh gas ($\alpha\to\infty$), which is independent of the potential index. The line $2\omega_{1/2}=q$ indicates the hydrodynamic limit, and the constant line $2\omega_{1/2}=2\sqrt{\ln 2}$ shows the free-gas limit.

The starting point for our considerations is the matrix-continued-fraction representation of $S_s(q,\omega)$, the derivation of which can be found in Ref. 1. In what follows we pursue two objectives. First, we want to study the mass dependence of $S_s(q,\omega)$ for a Maxwell gas comparing it with the rather weak mass dependence of the hard-sphere gas.[3] Second, for the Lorentz and the Rayleigh gas, we shall compare two completely different representations for $S_s(q,\omega)$, namely the matrix-continued-fraction representation, which is valid for the entire α range (including $\alpha=0$ and $\alpha=\infty$), and the two expressions already derived in Secs. III and IV [see Eqs. (3.21) and (4.19)]. Let us briefly recall the main results of Ref. 1. We have shown that the dynamical self-structure factor $R(q,x)$, which is related to $Q(q,s)$ via (2.11b), can be expressed in terms of the following infinite matrix continued fraction [we drop the asterisk appearing in Eq. (4.3b) of Ref. 1]:

$$Q(q,s)=\frac{1}{s}\mathbf{e}_1^T A_0 \mathbf{e}_1 , \tag{5.1}$$

where the matrix A_0 is defined by the recursion relation

$$A_l=(1+q^2N_l A_{l+1}M_l)^{-1}, \quad l=0,1,2,\ldots \tag{5.2}$$

and $\mathbf{e}_1^T=(1,0,0,\ldots)$ denotes the transpose of the unit vector. The infinite matrices N_l and M_l, respectively, are given by

$$N_l=\frac{2(l+1)^2}{(2l+1)(2l+3)}\begin{bmatrix} \beta_{0,l} & 0 & 0 & \cdots \\ -\alpha_{1,l} & \beta_{1,l} & 0 & \cdots \\ 0 & -2\alpha_{2,l} & \beta_{2,l} & \cdots \\ 0 & 0 & -3\alpha_{3,l} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \tag{5.3a}$$

and

$$M_l=\frac{1}{2}\begin{bmatrix} \alpha_{0,l+1} & -\alpha_{0,l+1} & 0 & 0 & \cdots \\ 0 & \alpha_{1,l+1} & -\alpha_{1,l+1} & 0 & \cdots \\ 0 & 0 & \alpha_{2,l+1} & -\alpha_{2,l+1} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}, \tag{5.3b}$$

with

$$\alpha_{k,l}=\frac{1}{s+\mu_{k,l}} \tag{5.4a}$$

and

$$\beta_{k,l}=\frac{k+l+\frac{3}{2}}{s+\mu_{k,l}} . \tag{5.4b}$$

An explicit expression for the eigenvalues $\mu_{k,l}$ can be found in the Appendix. Note that in order to get the infinite matrix A_0 explicitly, one has to "solve" Eq. (5.2) successively, yielding just an infinite matrix-continued fraction. According to Eq. (5.1), $Q(q,s)$ is then determined by the first element of A_0. Let us first consider the Lorentz and the Rayleigh limit of $Q(q,s)$. In the Appendix it is shown that for the Lorentz gas the eigenvalues $\mu_{k,l}$ become independent of the index k (which implies an extra conservation law)

$$\lim_{\alpha\to 0}\mu_{k,l}=B_l(4) , \tag{5.5a}$$

and for the Rayleigh limit one gets

$$\lim_{\alpha\to\infty}\mu_{k,l}=2k+l . \tag{5.5b}$$

For these values of $\mu_{k,l}$ we have computed $Q(q,s)$ via the matrix-continued fraction (5.2). In Table I(a) one finds the values for $R(q,x)$ for the Lorentz gas ($\alpha=0$). Throughout the computations we truncated the infinite

TABLE I. The Lorentz limit ($\alpha\to 0$) of the dynamical self-structure factor $R(q,x)$ for $\nu=4$ (Maxwell gas) and different values of $q=1/y$ and x (a) computed via the matrix continued fraction (5.1), (b) computed via the integral (4.19). Note that the same values for $y=1/q$ were selected in Figs. 3 and 4.

			x		
$y=1/q$	0.0	0.5	1.0	1.5	2.0
			(a)		
0.5	2.2301	0.7647	0.2903	0.0928	0.0275
1.0	3.7493	0.6347	0.2170	0.0765	0.0282
1.5	5.3808	0.5328	0.1699	0.0642	0.0268
2.0	7.0527	0.4553	0.1380	0.0546	0.0247
3.0	10.4432	0.3483	0.0988	0.0412	0.0204
4.0	13.8588	0.2797	0.0763	0.0326	0.0169
			(b)		
0.5	2.4037	0.7631	0.2902	0.0928	0.0275
1.0	4.1164	0.6347	0.2170	0.0765	0.0282
1.5	5.9378	0.5329	0.1699	0.0642	0.0268
2.0	7.7989	0.4553	0.1380	0.0546	0.0247
3.0	11.5671	0.3483	0.0988	0.0412	0.0204
4.0	15.3603	0.2797	0.0763	0.0326	0.0169

TABLE II. The Rayleigh limit ($\alpha \to \infty$) of the dynamical self-structure factor $R(q,x)$ for different values of $q=1/y$ and x computed via the matrix continued fraction (5.1). The respective computation via the scalar continued fraction (3.21) yields identical results. Note that the same values for $y=1/q$ were selected in Figs. 3 and 4.

			x		
$y=1/q$	0.0	0.5	1.0	1.5	2.0
0.5	1.3971	0.8808	0.2976	0.0830	0.0243
1.0	1.7961	0.7796	0.2176	0.0688	0.0253
1.5	2.2944	0.6497	0.1694	0.0592	0.0245
2.0	2.8468	0.5402	0.1375	0.0514	0.0231
3.0	4.0263	0.3924	0.0986	0.0398	0.0196
4.0	5.2497	0.3042	0.0762	0.0319	0.0165

matrix-continued fraction after at most ten terms and the size of the matrices N_l and M_l was always less than 10×10 except for the peak values $R(q,0)$, where the convergence is rather poor. In the first column of Table I(a) ($x=0$) we used 80×80 matrices and it tuned out that the results are not yet converged. In Table I(b) we have also evaluated the scalar continued fraction of Sec. IV [see Eq. (4.19)] and found a very good agreement with the corresponding matrix continued fraction [see Table I(a)], except for $x=0$. It should be mentioned that the values of Table I(b) are numerically converged and can therefore be used as a check for the convergence of the matrix continued fraction [Table I(a)]. In Table II the dynamical self-structure factor $R(q,x)$ for the Rayleigh gas is shown, again calculated via the matrix continued fraction (5.2). We also compared these values with a numerical evaluation of the scalar continued fraction (3.12), and found an agreement up to the last digit displayed. This excellent agreement between the two independent calculations for the Lorentz and the Rayleigh gas, respectively, proves—in a numerical sense—the convergence of our infinite matrix continued fraction.

In Fig. 3 the dependence of the peak height $R(q,0)$ on the mass ratio $M:=\alpha/(\alpha+1)$ is shown for different values of q. In order to evaluate the matrix continued fraction (5.2) for different values of M the dependence of the eigenvalues $\mu_{k,l}$ on the mass ratio has to be considered. Since the computation of the $\mu_{k,l}$'s via their definition [Eq. (A10a) in the Appendix] is too time consuming, we used the relation (A13), where the eigenvalues for different mass ratios are expressed as linear combinations of the $A_l(4)$. The coefficients $A_l(4)$ do not depend on the mass ratio and are tabulated in Table III up to $l=30$. It can be seen from Fig. 3 that the peak height is a monotonous function of M and does not show a minimum as observed for the hard-sphere gas.[3] We want to stress that in contrast to the calculations by Lindenfeld,[3] we did not encounter any convergence problems for small α with the exception $\alpha=0$. The limiting values for $\alpha=0$ were computed via the scalar continued fraction (4.19). Comparing the Maxwell and the hard-sphere gas quantitatively one observes that for $M>0.05$ the peak values do not differ by more than 10%, whereas for the Lorentz limit ($M\to 0$) the peak values differ considerably depending on $y=1/q$ (e.g., for $y=4$ the peak height of the Maxwell gas is approximately three times the peak height of the hard-sphere gas[3]).

In Fig. 4 we have plotted the full width at half maximum versus M for different values of q. It can be seen, that for $M>0.05$ the dependence of the FWHM on the mass ratio is rather weak, whereas for $M<0.05$ a rather steep descent to the Lorentz limit is observed. The rather weak dependence of the FWHM on the mass ratio for $M>0.05$ was also observed for the hard-sphere potential.[3]

In Figs. 5(a)–5(c) the dynamical self-structure factor $R(q,x)$ is displayed for three extreme mass ratios. In particular, in Fig. 5(a) we have plotted $R(q,x)$ in the Lorentz limit ($\alpha=0$) using Eq. (4.19). In Fig. 5(b) the matrix continued fraction (5.1) has been used to evaluate $R(q,x)$ for equal masses ($\alpha=1$). In Fig. 5(c) we computed $R(q,x)$ in the Rayleigh limit ($\alpha=\infty$) with the aid of the scalar continued fraction (3.21). It can be seen from Figs. 5(b) and 5(c) that for $q\approx 0.5$ the Lorentz line shape

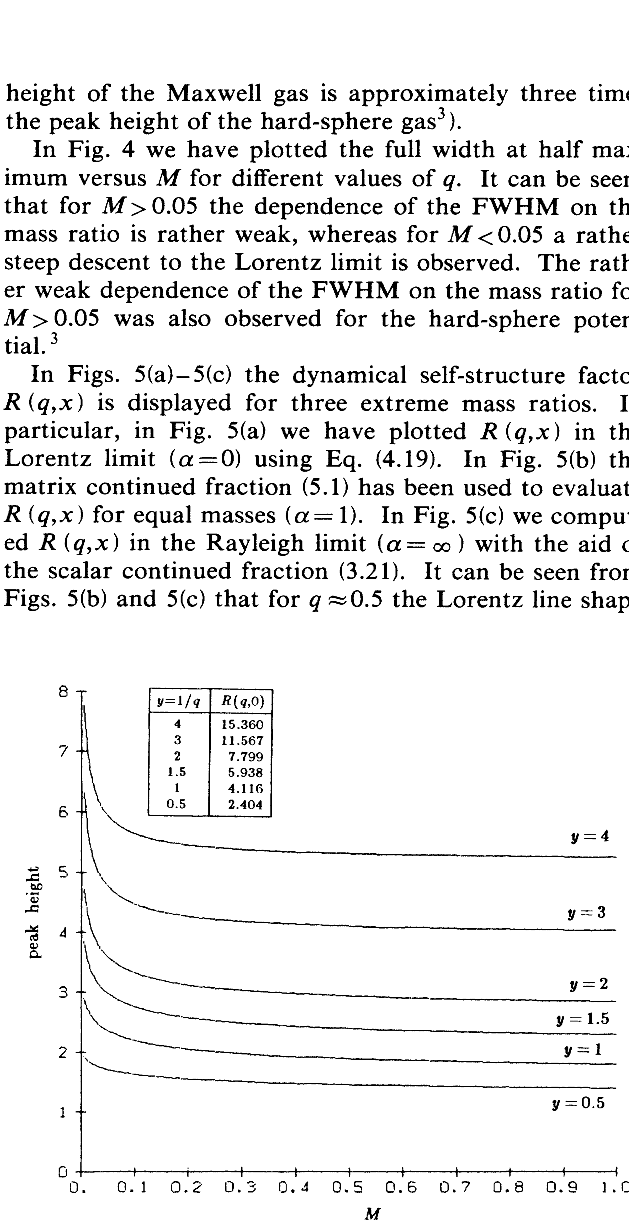

FIG. 3. Dependence of the peak height $R(q,0)$ on the mass ratio $M=m_A/(m_A+m_B)$ for different values of $y=1/q$. The limiting values for the Lorentz gas ($M=0$) are given in the table indicating the steep increase of $R(q,0)$ for $M\to 0$.

TABLE III. The coefficients $A_l(4)$ and $B_l(\nu)$ ($\nu=4,6,12$) as defined in Eq. (A17) for $l=1,\ldots,30$.

l	$A_l(4)$	$B_l(\nu)$ $\nu=4$	$\nu=6$	$\nu=12$
1	0.298 36	1.	0.884	0.771
2	0.308 44	1.551	1.227	0.932
3	0.413 80	1.967	1.458	1.028
4	0.422 21	2.314	1.637	1.097
5	0.487 91	2.618	1.785	1.150
6	0.495 27	2.890	1.913	1.194
7	0.543 61	3.139	2.026	1.232
8	0.550 21	3.371	2.128	1.264
9	0.588 72	3.587	2.221	1.293
10	0.594 76	3.791	2.307	1.320
11	0.626 93	3.985	2.387	1.344
12	0.632 51	4.170	2.462	1.366
13	0.660 22	4.348	2.533	1.386
14	0.665 43	4.518	2.600	1.405
15	0.689 84	4.682	2.664	1.423
16	0.694 74	4.840	2.725	1.440
17	0.716 58	4.994	2.784	1.455
18	0.721 22	5.143	2.840	1.470
19	0.741 02	5.288	2.893	1.485
20	0.745 43	5.429	2.945	1.498
21	0.763 57	5.566	2.996	1.511
22	0.767 77	5.700	3.044	1.524
23	0.784 52	5.831	3.091	1.536
24	0.788 54	5.959	3.137	1.548
25	0.804 11	6.085	3.181	1.559
26	0.807 98	6.207	3.225	1.570
27	0.822 53	6.328	3.267	1.580
28	0.826 26	6.446	3.308	1.590
29	0.839 94	6.562	3.348	1.600
30	0.843 53	6.676	3.387	1.609

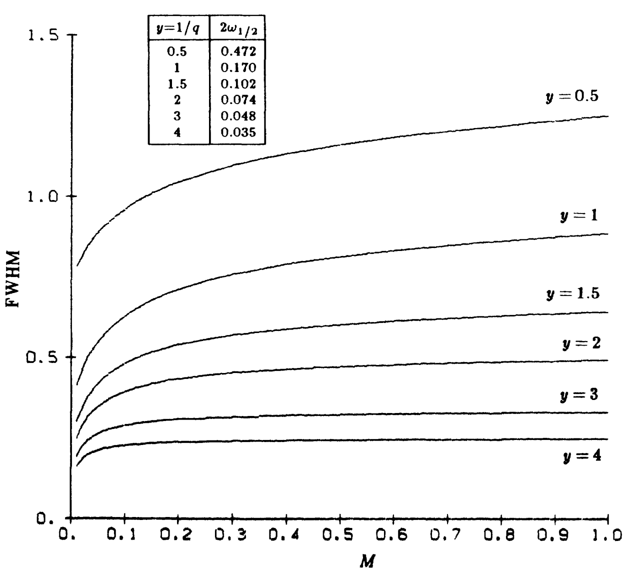

FIG. 4. Dependence of the full width at half maximum $2\omega_{1/2}$ on the mass ratio $M=m_A/(m_A+m_B)$ for different values of $y=1/q$. The limiting values for the Lorentz gas ($M=0$) are given in the table indicating the steep decrease of the FWHM for $M\to 0$.

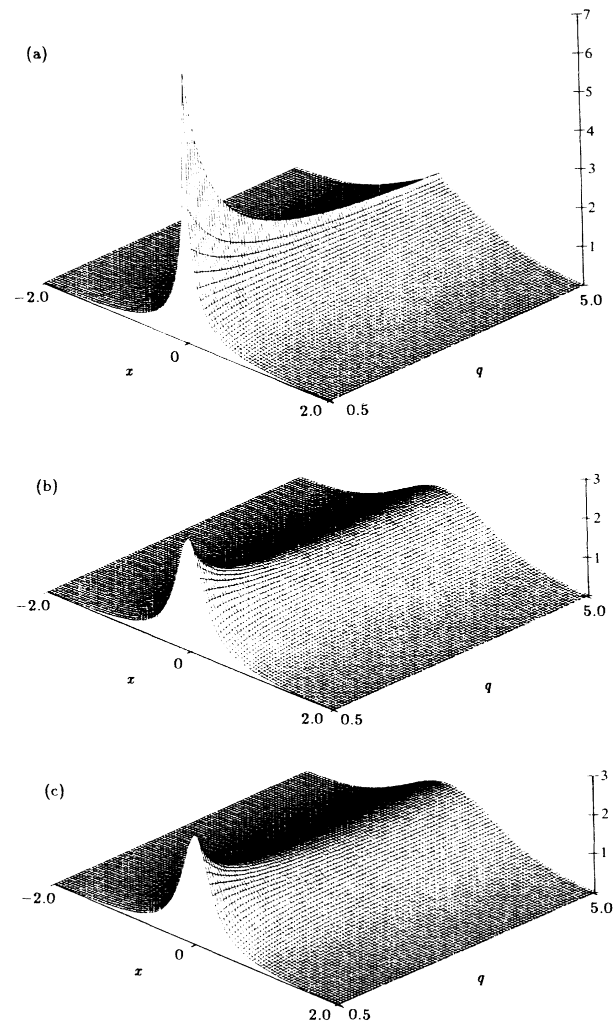

FIG. 5. The dynamical self-structure factor $R(q,x)$ of the Maxwell gas ($\nu=4$) for $0.5\le q\le 5.0$ and $-2.0\le x\le 2.0$. (a) Lorentz gas ($\alpha=0$) computed via the integral (4.19), (b) equal masses ($\alpha=1$) computed via the matrix continued fraction (5.1), (c) Rayleigh gas ($\alpha=\infty$) computed via the scalar continued fraction (3.21). Note that the Rayleigh limit is independent of the potential index ν.

(3.25b) of the hydrodynamic limit and for $q\approx 5$ the Gaussian distribution of the free-gas limit are almost reached. In contrast, Fig. 5(a) shows the exceptional behavior of $R(q,x)$ for the Lorentz gas already discussed in Sec. IV.

Finally, we want to comment upon the hydrodynamic limit ($q\to 0$) and the free-gas limit ($q\to\infty$) of our matrix-continued-fraction representation of $R(q,x)$. In our previous paper[1] it was shown that for large q the matrix continued fraction (5.1) yields the correct free-gas limit. Furthermore, for small q it was shown that the matrix continued fraction approaches the Lorentz line shape of the hydrodynamic limit. This statement, however, seems to be in contradiction to our results of Sec. IV, where we have proven that the Lorentz limit ($\alpha\to 0$)

of $R(q,x)$ differs considerably from the hydrodynamic limit derived from the diffusion equation [see (4.26a) and (4.26b)]. This discrepancy can be resolved easily, when looking at the assumptions made in Ref. 1 for deriving the hydrodynamic limit from the matrix continued fraction. There we assumed [see Eq. (4.20) of Ref. 1] that $\mu_{k,l}>0$ for $(k,l)\neq(0,0)$ and only $\mu_{0,0}=0$. In the Lorentz limit ($\alpha\to 0$), however, one has $\mu_{k,0}=0$ for all k [see Eq. (5.5a)], and therefore the assumptions made in Ref. 1 are violated. In other words, the memory matrix $D^*_{\rm hyd}$ [see Eq. (4.21) of Ref. 1], which has only two nonzero elements for $\alpha\neq 0$, has to be replaced by a regular infinite band matrix, if the limit $\alpha\to 0$ is performed first. This means that the limits $\alpha\to 0$ and $q\to 0$ must not be interchanged.

VI. CONCLUSION

In this paper we pursued two objectives. First, we studied the dynamical self-structure factor $S_s(q,\omega)$—expressed in terms of $R(q,x)$—for different values of the potential index ν, restricting ourselves to the Lorentz limit ($\alpha\to 0$) and the Rayleigh limit ($\alpha\to\infty$). Second, for the Maxwell potential ($\nu=4$) we investigated the mass dependence of $R(q,x)$, using the previously derived matrix-continued-fraction representation of the dynamical self-structure factor. Furthermore, both in the Lorentz limit and the Rayleigh limit we compared the matrix continued fraction with the respective scalar-continued-fraction representation derived in Secs. III and IV, and found an excellent numerical agreement confirming once more the convergence of the infinite matrix-continued-fraction representation of $S_s(q,\omega)$.

With the exception of very small mass ratios we can summarize that both the mass dependence and the dependence of $R(q,x)$ on the potential index ν ($4\leq\nu\leq\infty$) are rather weak. For the Maxwell potential ($\nu=4$) the mass dependence of the peak height $R(q,0)$ and the full width-at-half maximum $2\omega_{1/2}$ is almost independent of the mass ratio [for $M=m_A/(m_A+m_B)>0.05$]. This weak dependence was also found by Lindenfeld,[3] who investigated the mass dependence of $S_s(q,\omega)$ for a hard-sphere gas ($\nu=\infty$). Comparing $R(q,x)$ for the two extreme potential indices, namely $\nu=\infty$ (hard-sphere gas) and $\nu=4$ (Maxwell gas) one finds for the FWHM both a qualitative and quantitative agreement for $M>0.05$, whereas for the peak height $R(q,0)$ a quantitative agreement, but a different qualitative behavior (see the occurrence of a minimum in Fig. 7 of Ref. 3) for $0<M<1$ and small values of q is observed.

Therefore, when calculating the dynamical self-structure factor for purely repulsive interaction potentials ($4\leq\nu\leq\infty$) and not too small mass ratios ($M>0.05$), the Boltzmann collision operator can be replaced by the Fokker-Planck collision operator to obtain acceptable results (see also Ref. 19).

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APPENDIX

In this appendix we show how the eigenvalues of the Boltzmann collision operator for a mixture of Maxwellian particles can be calculated from a recursion relation involving only polynomials in the mass ratio and the numbers $A_l(4)$. For completeness we also briefly repeat some well-established formulas concerning the evaluation of the collision integrals.

For inverse-power-law interactions, i.e., for potentials of the form

$$V(r)=\left[\frac{\sigma_{AB}}{r}\right]^{\nu}, \tag{A1}$$

where σ_{AB} is the force constant for an A-B interaction, the deflection angle χ between the precollisional and postcollisional velocity is given by[10]

$$\chi=\pi-2\int_{r_0}^{\infty}\left[1-\frac{b^2}{r^2}-\frac{2}{m_{AB}g^2}\left[\frac{\sigma_{AB}}{r}\right]^{\nu}\right]^{-1/2}\frac{b}{r^2}dr\ , \tag{A2}$$

where $1/m_{AB}=1/m_A+1/m_B$ is the reduced mass, g is the relative speed, b the impact parameter, and r_0 is the only positive root of the expression in the square brackets. Introducing new variables

$$y=\frac{b}{r},\quad z=\frac{b}{\sigma_{AB}}\left[\frac{m_{AB}g^2}{2\nu}\right]^{1/\nu}, \tag{A3}$$

the deflection angle can be written as

$$\chi=\pi-2\int_0^{y_0}\left[1-y^2-\frac{1}{\nu}\left[\frac{y}{z}\right]^{\nu}\right]^{-1/2}dy\ , \tag{A4}$$

with $y_0=b/r_0$, and $\chi=\chi(z,\nu)$ does not depend on the mass ratio. The expression $gbdb$, which enters the Boltzmann collision operator, is now given by

$$gbdb=\sigma_{AB}^2\left[\frac{2\nu}{m_{AB}}\right]^{2/\nu}g^{1-4/\nu}z\,dz\ , \tag{A5}$$

indicating the simplification obtained for Maxwellian particles ($\nu=4$). For hard spheres ($\nu\to\infty$) we have instead of (A4) and (A5)

$$\tfrac{1}{4}\sin\chi d\chi=\frac{1}{\sigma_{AB}^2}bdb=z\,dz\ . \tag{A6}$$

In studies of the Boltzmann equation for inverse-power-law interactions the following quantities are frequently encountered:

$$A_l(\nu):=\int_0^\infty dz\, z[1-\cos^l\chi(z,\nu)] \ . \tag{A7}$$

To get an estimate of the convergence of these integrals we consider the asymptotic behavior of $\chi(z,\nu)$ for $z\rightarrow\infty$; one gets[20]

$$\chi(z,\nu)=\sqrt{\pi}\frac{\Gamma\left[\frac{\nu+1}{2}\right]}{\nu\Gamma\left[\frac{\nu}{2}\right]}\frac{1}{z^\nu}+O\left[\frac{1}{z^{2\nu}}\right], \quad z\rightarrow\infty \tag{A8}$$

which allows the following representation of $A_l(\nu)$:

$$A_l(\nu)=\int_0^B dz\, z[1-\cos^l\chi(z,\nu)] +\frac{l}{2}\pi\left[\frac{\Gamma[(\nu+1)/2]}{\nu\Gamma(\nu/2)}\right]^2\frac{1}{(2\nu-2)B^{2\nu-2}} +O\left[\frac{1}{B^{3\nu-2}}\right], \quad B\rightarrow\infty \tag{A9}$$

showing that the $A_l(\nu)$ exists for $\nu>1$. Numerical values for A_1 to A_{30} for the Maxwell interaction potential ($\nu=4$) are tabulated in Table III.

Next we want to show that the eigenvalues of the collision operator for a binary mixture of Maxwellian particles, which are given by[21] ($\alpha=m_A/m_B$)

$$\mu_{r,l}=2\pi n_B\sigma_{AB}^2\sqrt{8/m_{AB}}\int_0^\infty dz\, z\left[1-\frac{1}{(1+\alpha)^{2r+l}}(1+2\alpha\cos\chi+\alpha^2)^{r+l/2}P_l(\xi)\right], \quad r,l=0,1,2,\ldots \tag{A10a}$$

with

$$\xi=(\alpha+\cos\chi)(1+2\alpha\cos\chi+\alpha^2)^{-1/2} \ , \tag{A10b}$$

can be written in the form

$$(1+\alpha)^{-2r-l}\sum_{k=1}^{r+l}b_{r,l}^{(k)}A_k(4) \ ,$$

where the $A_k(4)$ are the numbers given in Eq. (A7) and the coefficients $b_{r,l}^{(k)}$ are polynomials in α. To prove this, it suffices to show that

$$(1+2\alpha\cos\chi+\alpha^2)^{r+l/2}\times P_l[(\alpha+\cos\chi)(1+2\alpha\cos\chi+\alpha^2)^{-1/2}] =\sum_{k=0}^{r+l}b_{r,l}^{(k)}\cos^k\chi \tag{A11}$$

because for $\chi=0$ we get from (A11)

$$\sum_{k=0}^{r+l}b_{r,l}^{(k)}=(1+\alpha)^{2r+l} \ , \tag{A12}$$

which allows for $\mu_{r,l}$ the representation

$$\mu_{r,l}=2\pi n_B\sigma_{AB}^2\sqrt{8/m_{AB}}\frac{1}{(1+\alpha)^{2r+l}}\sum_{k=1}^{r+l}b_{r,l}^{(k)}A_k(4) \ . \tag{A13}$$

To prove (A11) we start with $l=0$. Binomial expansion leads to

$$b_{r,0}^{(k)}=\begin{bmatrix} r \\ k\end{bmatrix}(2\alpha)^k(1+\alpha^2)^{r-k}, \quad k=0,\ldots,r \ . \tag{A14}$$

For $l\geq1$ we make use of the recursion relation for the Legendre polynomials and get after some straightforward manipulations

$$b_{r,l}^{(k)}=\frac{2l-1}{l}[\alpha b_{r,l-1}^{(k)}+b_{r,l-1}^{(k-1)}] -\frac{l-1}{l}[(1+\alpha^2)b_{r,l-2}^{(k)}+2\alpha b_{r,l-2}^{(k-1)}] \ , \quad k=0,\ldots,r+l \tag{A15}$$

where it is understood that

$$b_{r,l}^{(k)}=0 \quad \text{for } k<0 \text{ or } k>r+l \ . \tag{A16}$$

Equation (A15) allows the successive calculation of the eigenvalues $\mu_{r,l}$ and also proves—together with (A14)—the representation (A13). From the explicit form of the Legendre polynomials it is also possible to derive an explicit expression for the coefficients $b_{r,l}^{(k)}$. However, since this rather involved explicit form is of little use for practical computations, it is not presented here.

Of interest in this paper are also the following coefficients (see Sec. IV):

$$B_l(\nu)=\frac{3\sqrt{\pi}}{4\Gamma(3-2/\nu)A_1(\nu)}\int_0^\infty dz\, z[1-P_l(\cos\chi(z,\nu))] \ , \tag{A17}$$

which can, of course, be expressed in terms of the $A_l(\nu)$. For hard-spheres the integral in (A17) can be transformed with the aid of (A6), yielding

$$B_l(\infty)=\tfrac{3}{8}\sqrt{\pi}=0.664\,67\ldots \ , \tag{A18}$$

which are independent of the index l. For other interaction laws the $B_l(\nu)$ have to be computed numerically and in Table III we present B_1 to B_{30} for $\nu=4,6,12$.

Finally, for Maxwellian particles ($\nu=4$), we want to relate the coefficients $B_l(\nu)$ to the limiting values of the eigenvalues of the collision operator. To be consistent we scale the eigenvalues to the first nonzero eigenvalue $v_{T_A}^2/2[D_{AB}]^{\text{I}}=\mu_{0,1}$ [compare Eq. (2.9a)]. The scaled eigenvalues $\mu_{r,l}^*:=\mu_{r,l}/\mu_{0,1}$ are then given by (see above)

$$\mu^*_{r,l}=\frac{1+\alpha}{A_1(4)}\int_0^\infty dz\, z\left[1-\frac{1}{(1+\alpha)^{2r+l}}\times(1+2\alpha\cos\chi+\alpha^2)^{r+l/2}\times P_l(\xi)\right], \tag{A19}$$

with ξ given by Eq. (A10b).

In the Lorentz limit one immediately obtains

$$\lim_{\alpha\to 0}\mu^*_{r,l}=B_l(4)\ . \tag{A20}$$

In the Rayleigh limit ($\alpha\to\infty$), one has to use de l'Hospital's rule and gets, after some calculations,

$$\lim_{\alpha\to\infty}\mu^*_{r,l}=2r+l\ . \tag{A21}$$

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