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Modified Sonine approximation for granular binary mixtures

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We evaluate in this work the hydrodynamic transport coefficients of a granular binary mixture in d dimensions. In order to eliminate the observed disagreement (for strong dissipation) between computer simulations and previously calculated theoretical transport coefficients for a monocomponent gas, we obtain explicit expressions of the seven Navier–Stokes transport coefficients by the use of a new Sonine approach in the Chapman–Enskog (CE) theory. This new approach consists of replacing, where appropriate in the CE procedure, the Maxwell–Boltzmann distribution weight function (used in the standard first Sonine approximation) by the homogeneous cooling state distribution for each species. The rationale for doing this lies in the well-known fact that the non-Maxwellian contributions to the distribution function of the granular mixture are more important in the range of strong dissipation we are interested in. The form of the transport coefficients is quite common in both standard and modified Sonine approximations, the distinction appearing in the explicit form of the different collision frequencies associated with the transport coefficients. Additionally, we numerically solve by the direct simulation Monte Carlo method the inelastic Boltzmann equation to get the diffusion and the shear viscosity coefficients for two and three dimensions. As in the case of a monocomponent gas, the modified Sonine approximation improves the estimates of the standard one, showing again the reliability of this method at strong values of dissipation.

1. Introduction

The success of the kinetic theory tools in describing granular gases has been widely recognized (Goldhirsch 2003; Brilliantov & Pöschel 2004). In particular, the Navier–Stokes (NS) constitutive equations for the stress tensor and the heat flux of a monocomponent gas have been derived (Brey *et al.* 1998; Sela & Goldhirsch 1998) by solving the inelastic Boltzmann equation by the Chapman–Enskog (CE) method to first order in the spatial gradients (Chapman & Cowling 1970). As in the elastic case, the NS transport coefficients are given in terms of the solutions of linear integral equations (Brey *et al.* 1998), which can be approximately solved to get the analytical dependence of these coefficients on dissipation. The standard method consists of

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approaching the solutions to these integral equations by the Maxwell–Boltzmann distribution f_M multiplied by the corresponding truncated Sonine polynomial expansion. For simplicity, usually only the lowest Sonine polynomial (first Sonine approximation) is retained. (We will refer henceforth to this procedure as the *standard* Sonine approximation.) In spite of this approximation, the results obtained from this approach (which formally apply for all values of the coefficient of restitution; see Brey *et al.* 1998) compare very well with Monte Carlo simulations (Brey, Ruiz-Montero & Cubero 1999; Brey *et al.* 2000; Garzó & Montanero 2002; Lutsko, Brey & Dufty 2002) for mild degrees of inelasticity; namely coefficients of restitution α that are larger than about 0.7. Specifically, while the self-diffusion and shear viscosity coefficients are well estimated by the first Sonine approximation (even for values of α smaller than 0.7), the transport coefficients associated with the heat flux present significant discrepancies with respect to computer simulations (Brey & Ruiz-Montero 2004; Brey *et al.* 2005*a*) for high dissipation ($\alpha \lesssim 0.7$). This fact has motivated the search for alternative methods which provide accurate estimates for the NS transport coefficients in the complete range of values of α. Thus, Noskowicz *et al.* (2007) used Borel resummation to obtain the distribution function of the homogeneous cooling state (HCS) and the NS transport coefficients. The method involves the solution of a system of algebraic equations that must be numerically solved. A different alternative consists of a slight modification of the Sonine polynomial approach, assuming that the isotropic part of the first-order distribution function is mainly governed by the HCS distribution $f^{(0)}$ rather than by the Maxwellian distribution f_M (Lutsko 2005) (and this is what we call *modified* Sonine approximation). Except for this, this modified Sonine approximation keeps the usual structure of the standard Sonine approximation. Comparison with computer simulations (Brey & Ruiz-Montero 2004; Brey *et al.* 2005*a*; Montanero, Santos & Garzó 2007) shows that this modified approximation significantly improves the accuracy of the NS transport coefficients of the single granular gas at strong dissipation (Garzó, Santos & Montanero 2007*c*), especially in the case of the heat flux transport coefficients. The improved agreement in the range of high inelasticities is of physical relevance, since it helps to put into proper context the discussion vividly maintained in the field (Goldhirsch 2003; Aranson & Tsimring 2006) about the existence (or not) of scale separation in granular gases. Moreover, interest in experimental works in the range of high inelasticities is growing (Clerc *et al.* 2008; Vega Reyes & Urbach 2008*a*). Thus, it is important from a fundamental point of view to understand the origin of the discrepancies between theory and simulation for $\alpha \lesssim 0.7$.

Motivated by the good agreement found between theory and simulation for a monocomponent granular gas, we extend in this work the modified Sonine approach to the case of a granular binary mixture. Early attempts to obtain the NS transport coefficients were carried out by the CE expansion around Maxwellians at the same temperature for each species (Jenkins & Mancini 1989; Zamankhan 1995; Arnarson & Willits 1998; Willits & Arnarson 1999; Serero *et al.* 2006). However, as confirmed by computer simulations (Barrat & Trizac 2002; Dahl *et al.* 2002; Montanero & Garzó 2002; Pagnani, Marconi & Puglisi 2002; Krouskop & Talbot 2003; Wang, Jin & Ma 2003; Brey, Ruiz-Montero & Moreno 2005*b*, 2006; Schröter *et al.* 2006) and experiments (Feitosa & Menon 2002; Wildman & Parker 2002), the equipartition assumption is not in general valid in granular mixtures, since it is only close to being fulfilled in the quasielastic limit. A kinetic theory for granular mixtures at low density which accounts for non-equipartition effects has been developed in the past few years by Garzó & Dufty (2002). As in the single-gas case, the above theory (Garzó & Dufty

2002) shows that the NS transport coefficients of the mixture are given in terms of the solutions of a set of linear integral equations, which are approximately solved (Garzó & Dufty 2002; Garzó, Montanero & Dufty 2006; Garzó & Montanero 2007) by the standard Sonine approximation. Furthermore, this theory has successfully predicted, as shown by computer simulations (Dahl *et al.* 2002; Montanero & Garzó 2002; Brey *et al.* 2005*b*; Schröter *et al.* 2006), a constant ratio between the granular temperatures of both species. Here, we revisit the theory of Garzó & Dufty (2002) and solve the corresponding linear integral equations defining the NS transport coefficients by taking the HCS distribution $f_i^{(0)} (i=1, 2)$ of each species as the weight function.

As expected, the problem for a binary mixture is much more involved than in the monocomponent case, since not only is the number of transport coefficients larger, but these coefficients are also functions of more parameters (masses, sizes, composition and three coefficients of restitution). In spite of these technical difficulties, explicit expressions for the seven relevant transport coefficients of the binary mixture (the mutual diffusion D, the pressure diffusion D_p, the thermal diffusion D', the shear viscosity η, the Dufour coefficient D'', the thermal conductivity λ and the pressure energy coefficient L) have been obtained in terms of the parameter space of the problem. The results show that the modified Sonine approximation at large inelasticities introduces significant, moderate and slight corrections to the transport coefficients associated with the heat flux (D'', λ, L), stress tensor (η) and mass flux (D, D_p, D'), respectively. In order to assess the degree of accuracy of the modified Sonine approximation, we have also performed Monte Carlo simulations for the mutual diffusion and the shear viscosity coefficients and used available simulation data for the heat flux coefficients in the monodisperse gas case (Brey & Ruiz-Montero 2004; Brey *et al.* 2005*a*). We show that, in the range of strong inelasticity, the modified Sonine approximation provides better agreement with simulations in all cases, this accuracy gain not being negligible for viscosity, thermal conductivity, pressure energy coefficient and Duffour coefficient. This clearly justifies the use of this new approximation in order to obtain accurate expressions for the NS transport coefficients of the mixture.

An important issue is the applicability of the NS equations for granular binary mixtures derived here. The expressions of the seven NS transport coefficients are not restricted to weak inelasticity and hold for arbitrary values of the degree of dissipation. In fact, our modified Sonine approximation turns to be more accurate than the previous one (Garzó & Dufty 2002) for very dissipative interactions. However, as already pointed out by Garzó *et al.* (2006), the NS hydrodynamic equations themselves may or may not be limited with respect to inelasticity, depending on the particular granular flows of real materials considered. It is important to recall that the CE method assumes that the relative changes of the hydrodynamic fields (partial densities, mean flow velocity and granular temperature) over distances of the order of the characteristic mean free path of the system are small. In the case of molecular or ordinary gas mixtures, the strength of the spatial gradients is controlled by external sources (the initial or boundary conditions, driving forces), and for a great variety of experimental conditions of practical interest the NS hydrodynamic equations describe adequately the hydrodynamics of the system. Unfortunately, the situation in the case of granular gases is more complex, since in most problems of practical interest (such as steady states) the boundary conditions cannot completely control by themselves the spatial gradients of the hydrodynamic fields. This is due to collisional cooling, which sets a minimum value for the relative size of the steady state gradients. An example of this situation corresponds to the well-known (steady) simple shear flow state (Goldhirsch 2003; Santos, Garzó & Dufty 2004). This type of flow can only occur when collisional cooling (which is fixed by the mechanical properties of the particles making up the fluid) is exactly balanced by viscous heating. Unfortunately, this occurs, except for the quasi-elastic limit, only for very extreme boundary conditions (high shear). The same applies for all steady states for a granular gas heated or sheared from the boundaries, although the behaviour of the gradients is qualitatively different for each type of flow (for a case by case study, please refer to the work by Vega Reyes & Urbach 2008*b*). Another example is the case of a granular gas bounded by two opposite walls at rest and at the same temperature. Recent comparisons (Hrenya, Galvin & Wildman 2008) between molecular dynamics simulations and kinetic theory provide evidence that higher order effects (i.e. beyond the NS description) can be measurable for moderate inelasticities.

In spite of the above cautions, the NS description is still accurate and appropriate for a wide class of flows. One of them corresponds to small spatial perturbations of the HCS for an isolated system (Brey *et al.* 1998; Garzó 2005). Both molecular dynamics and Monte Carlo simulations (Brey *et al.* 1999, 2000) have quantitatively confirmed the dependence of the NS transport coefficients on dissipation (even for strong values of the coefficient of restitution) and the applicability of the NS hydrodynamics with these transport coefficients to describe cluster formation. Another interesting example consists of the application of the NS hydrodynamics from kinetic theory to characterize the symmetry breaking as well as the density and temperature profiles in vertically vibrated gases (Brey *et al.* 2002). In the case of dense gases, there is evidence of the good agreement found between the NS coefficients derived from the Enskog kinetic theory (Garzó & Dufty 1999*a*) and computer simulations (Dahl *et al.* 2002; Lutsko *et al.* 2002; Lois, Lemaître & Carlson 2007). Similar comparisons between NS hydrodynamics and real experiments of supersonic flow past a wedge (Rericha *et al.* 2002) and nuclear magnetic resonance (NMR) experiments of a system of mustard seeds vibrated vertically (Yang *et al.* 2002; Huan *et al.* 2004) have shown both qualitative and quantitative agreement. Furthermore, the NS hydrodynamics accounts for a variety of properties of granular flows that are preserved beyond the NS order; for instance, the curvature of the temperature profile: the same types of steady profiles predicted by NS hydrodynamics have been observed in direct simulation Monte Carlo (DSMC) simulations beyond the NS domain as reported in a recent theoretical work, where new steady states (exclusive to granular gases) have been found (Vega Reyes & Urbach 2008*b*). Therefore, the NS equations with the transport coefficients derived here can still be considered useful for a wide class of rapid granular flows although more limited than for ordinary gases.

The plan of the paper is as follows: In § 2, the full transport coefficients of the mixture are given in terms of the solutions of a set of coupled linear integral equations previously derived by Garzó & Dufty (2002). These integral equations are approximately solved by the modified first Sonine approximation in § 3, where explicit forms for the transport coefficients are provided. Technical details of the calculations carried out here are given in two Appendices and the supplementary material available in the online version of the paper. Next, in § 4 the results obtained for these seven transport coefficients from the standard and modified Sonine approximations are compared for several cases. In addition, both theoretical approaches are also compared with available and new simulation data obtained from numerical solutions of the Boltzmann equation by using the DSMC method (Bird 1994) in the cases of the diffusion and shear viscosity coefficients, both for two- and three-dimensional systems. The paper ends with a discussion of the results in § 5.

2. Navier–Stokes (NS) transport coefficients for a granular binary mixture

We consider a binary mixture composed of smooth inelastic disks ($d=2$) or spheres ($d=3$) of masses m_1 and m_2 and diameters σ_1 and σ_2. The inelasticity of collisions among all pairs is characterized by three independent constant coefficients of restitution α_{11}, α_{22} and $\alpha_{12}=\alpha_{21}$, where $\alpha_{ij}\leqslant 1$ is the coefficient of restitution for collisions between particles of species i and j. In the low-density regime, the one-particle velocity distribution functions $f_i(\boldsymbol{r},\boldsymbol{v},t)$ obey the set of (inelastic) Boltzmann equations (Goldshtein & Shapiro 1995; Brey, Dufty & Santos 1997). When the hydrodynamic gradients present in the system are weak, the CE method (Chapman & Cowling 1970) conveniently adapted to dissipative dynamics provides a solution to the Boltzmann equation based on the expansion

$$f_i = f_i^{(0)} + f_i^{(1)} + \cdots, \tag{2.1}$$

where $f_i^{(0)}$ is the *local* version of the HCS (Garzó & Dufty 1999*b*). Although the exact form of the distribution $f_i^{(0)}$ is not known (even in the one-component case), an indirect information of the behaviour of $f_i^{(0)}$ is given by its velocity moments. In particular, the deviation of $f_i^{(0)}$ from its Maxwellian form can be characterized by the fourth cumulant

$$c_i = 2\left[\frac{m_i^2}{n_i T_i^2}\frac{1}{d(d+2)}\int \mathrm{d}\boldsymbol{v}\; V^4 f_i^{(0)} - 1\right], \tag{2.2}$$

where $\boldsymbol{V}=\boldsymbol{v}-\boldsymbol{U}$ is the peculiar velocity;

$$n_i = \int \mathrm{d}\boldsymbol{v}\; f_i^{(0)} \tag{2.3}$$

is the number density of species i; and

$$\boldsymbol{U} = \frac{1}{\rho}\sum_{i=1}^{2}\int \mathrm{d}\boldsymbol{v}\; m_i \mathbf{v}\; f_i^{(0)} \tag{2.4}$$

is the mean flow velocity and $\rho = m_1 n_1 + m_2 n_2$ is the total mass density.

The first-order distribution $f_i^{(1)}$ has the form (Garzó & Dufty 2002)

$$f_i^{(1)} = \mathscr{A}_i\cdot\nabla x_1 + \mathscr{B}_i\cdot\nabla p + \mathscr{C}_i\cdot\nabla T + \mathscr{D}_{i,k\ell}\nabla_k U_\ell\;, \tag{2.5}$$

where $x_i = n_i/n$ is the mole fraction of species i;

$$T = \frac{1}{dn}\sum_{i=1}^{2}\int \mathrm{d}\boldsymbol{v}\; m_i V^2\; f_i^{(0)} \tag{2.6}$$

is the temperature; and $p=nT$ is the pressure. Here, $n=\sum_i n_i$ is the total number density. The coefficients $\mathscr{A}_i$, $\mathscr{B}_i$, $\mathscr{C}_i$ and $\mathscr{D}_i$ are functions of the peculiar velocity $\boldsymbol{V}=\boldsymbol{v}-\boldsymbol{U}$ and the hydrodynamic fields.

The knowledge of the distributions $f_i^{(1)}$ allows us to determine the NS transport coefficients. The analysis to obtain them has been worked out by Garzó and co-workers (Garzó & Dufty 2002; Garzó *et al.* 2006; Garzó & Montanero 2007). For the sake of completeness, the final results will be displayed in this section. The mass flux $\boldsymbol{j}_1^{(1)}$, the pressure tensor $\boldsymbol{P}_{k\ell}^{(1)}$ and the heat flux $\boldsymbol{q}^{(1)}$ are given, respectively, by (Garzó & Dufty 2002):

$$\boldsymbol{j}_1^{(1)} = -\frac{m_1 m_2 n}{\rho}D\nabla x_1 - \frac{\rho}{p}D_p\nabla p - \frac{\rho}{T}D'\nabla T, \qquad \boldsymbol{j}_2^{(1)} = -\boldsymbol{j}_1^{(1)}, \tag{2.7}$$

$$\mathsf{P}_{k\ell}^{(1)} = p\delta_{k\ell} - \eta\left(\nabla_\ell U_k + \nabla_k U_\ell - \frac{2}{d}\delta_{k\ell}\nabla\cdot U\right), \tag{2.8}$$

$$\boldsymbol{q}^{(1)} = -T^2 D''\nabla x_1 - L\nabla p - \lambda\nabla T. \tag{2.9}$$

It must be noted that the contribution to first order in the gradients of the collisional cooling vanishes ($\zeta^{(1)}=0$) by symmetry, and there is no need to consider here this term (Brey *et al.* 1998). This is due to the fact that the cooling rate is a scalar, and so corrections to first order in gradients can arise only from the divergence of the velocity field. However, as (2.5) shows, there is no contribution to $f_i^{(1)}$ proportional to $\nabla\cdot\boldsymbol{U}$ and consequently, $\zeta^{(1)}=0$. This is special to the low-density Boltzmann equation, and such terms occur at higher densities (Garzó & Dufty 1999*a*; Garzó, Hrenya & Dufty 2007*b*).

The transport coefficients appearing in (2.7)–(2.9) are the diffusion coefficient D, the pressure diffusion coefficient D_p, the thermal diffusion coefficient D', the shear viscosity η, the Dufour coefficient D'', the pressure energy coefficient L and the thermal conductivity λ. These coefficients are defined as

$$D = -\frac{\rho}{dm_2 n}\int \mathrm{d}\boldsymbol{v}\, \boldsymbol{V}\cdot\boldsymbol{\mathscr{A}}_1, \tag{2.10}$$

$$D_p = -\frac{m_1 p}{d\rho}\int \mathrm{d}\boldsymbol{v}\, \boldsymbol{V}\cdot\boldsymbol{\mathscr{B}}_1, \tag{2.11}$$

$$D' = -\frac{m_1 T}{d\rho}\int \mathrm{d}\boldsymbol{v}\, \boldsymbol{V}\cdot\boldsymbol{\mathscr{C}}_1, \tag{2.12}$$

$$\eta = -\frac{1}{(d-1)(d+2)}\sum_{i=1}^{2} m_i \int \mathrm{d}\boldsymbol{v}\, \boldsymbol{V}\boldsymbol{V} : \mathscr{D}_i, \tag{2.13}$$

$$D'' = -\frac{1}{dT^2}\sum_{i=1}^{2}\frac{m_i}{2}\int \mathrm{d}\boldsymbol{v}\, V^2\boldsymbol{V}\cdot\boldsymbol{\mathscr{A}}_i, \tag{2.14}$$

$$L = -\frac{1}{d}\sum_{i=1}^{2}\frac{m_i}{2}\int \mathrm{d}\boldsymbol{v}\, V^2\boldsymbol{V}\cdot\boldsymbol{\mathscr{B}}_i, \tag{2.15}$$

$$\lambda = -\frac{1}{d}\sum_{i=1}^{2}\frac{m_i}{2}\int \mathrm{d}\boldsymbol{v}\, V^2\boldsymbol{V}\cdot\boldsymbol{\mathscr{C}}_i. \tag{2.16}$$

As in the case of elastic collisions (Chapman & Cowling 1970), the unknowns are the solutions of a set of coupled linear integral equations. Their explicit forms are given in the supplementary material of this paper and (46)–(49) of Garzó & Dufty (2002).

3. Modified first Sonine approximation

The results presented above are still exact. However, to get the explicit dependence of the NS transport coefficients on the parameters of the mixture (masses, sizes, composition, coefficients of restitution), one has to solve the integral equations obeying $\boldsymbol{\mathscr{A}}_i$, $\boldsymbol{\mathscr{B}}_i$, $\boldsymbol{\mathscr{C}}_i$ and $\mathscr{D}_i$ as well as know the explicit forms of $f_i^{(0)}$ and of the HCS cooling rate $\zeta^{(0)}$ (see Appendix A and the work by Garzó & Dufty 1999*b*, for more details). With respect to the distribution $f_i^{(0)}$, except in the high-velocity region, it is accurately estimated by (Garzó & Dufty 1999*b*; Montanero & Garzó 2002)

$$f_i^{(0)}(\boldsymbol{V}) = f_{i,M}(\boldsymbol{V}) \left[1 + \frac{c_i}{4} \left(\theta_i^2 V^{*4} - (d+2)\theta_i V^{*2} + \frac{d(d+2)}{4} \right) \right], \tag{3.1}$$

where c_i is defined by (2.2); $V^* = V/v_0$, $\theta_i = m_i \gamma_i^{-1} \sum_j m_j^{-1}$; and

$$v_0 = \sqrt{\frac{2T(m_1+m_2)}{m_1 m_2}} \tag{3.2}$$

is a thermal speed. Further, $\gamma_i = T_i/T$ is the temperature ratio, and $f_{i,M}$ is the Maxwellian distribution:

$$f_{i,M}(\boldsymbol{V}) = n_i \left(\frac{m_i}{2\pi T_i} \right)^{d/2} \exp\left(-\frac{m_i V^2}{2T_i} \right). \tag{3.3}$$

The partial temperatures T_i are defined as

$$T_i = \frac{1}{dn_i} \int \mathrm{d}\boldsymbol{v} m_i V^2 f_i^{(0)}. \tag{3.4}$$

The cumulant c_i measures the departure of $f_i^{(0)}$ from $f_{i,M}$. The temperature ratios γ_i along with the coefficients c_i and the cooling rate $\zeta^{(0)}$ have been determined for inelastic hard spheres ($d=3$) (Garzó & Dufty 1999*b*). These calculations have been extended in Appendix A to an arbitrary number of dimensions.

With respect to the functions $\{\mathscr{A}_i, \mathscr{B}_i, \mathscr{C}_i, \mathscr{D}_i\}$, as in the elastic case, the simplest approximation consists of expanding them in a series of Sonine polynomials and consider only the leading terms in this expansion. Usually, for simplicity, the polynomials are defined with respect to a Gaussian weight factor. This alternative has been previously used (Garzó & Dufty 2002; Garzó & Montanero 2007) to get explicit forms for the NS transport coefficients. The accuracy of these theoretical predictions (based on the standard first Sonine approximation) over a wide range of inelasticities has been confirmed by Monte Carlo simulations of the Boltzmann equation in the cases of the tracer diffusion coefficient (Garzó & Montanero 2004, 2007) and the shear viscosity coefficient (Montanero & Garzó 2003; Garzó & Montanero 2007). However, as mentioned in the § 1, recent comparisons with computer simulations for the transport coefficients associated with the heat flux for a monocomponent gas have shown significant discrepancies for strong inelasticities (Brey & Ruiz-Montero 2004; Brey *et al.* 2005*a*; Montanero *et al.* 2007). This fact has motivated the search for new approaches, such as a modified first Sonine approximation (Garzó *et al.* 2007*c*).

As pointed out by Garzó *et al.* (2007*c*), one of the possible sources of discrepancy between the standard first Sonine approximation and computer simulations for the heat flux transport coefficients could be the emergence of the existing non-Gaussian features of the zeroth-order distribution function $f_i^{(0)}$. Although the Maxwellian distribution $f_{i,M}$ is a good approximation of $f_i^{(0)}$ in the region of thermal velocities relevant to low-degree velocity moments (hydrodynamic quantities, mass flux), quantitative discrepancies between $f_{i,M}$ and $f_i^{(0)}$ are expected to be important when one evaluates higher degree velocity moments, such as the pressure tensor and the heat flux, specially for strong dissipation. However, the behaviour of the first-order distribution $f_i^{(1)}$ in the standard Sonine approximation (Garzó & Dufty 2002) is mainly governed by the Maxwellian distribution $f_{i,M}$ and not by the HCS distribution $f_i^{(0)}$. A possible way of mitigating the discrepancies between the standard first Sonine approximation and simulations would be to incorporate more terms in the Sonine polynomial expansion

(Garzó & Montanero 2004), but the technical difficulties in evaluating these new contributions for general binary mixtures lead to the discarding of this method. Here, we follow the same route as in our previous work (Garzó *et al.* 2007*c*) for monocomponent gases and take the distribution $f_i^{(0)}$ instead of the simple Maxwellian form $f_{i,M}$ as the convenient weight function. In this case, care must be taken in the structure of the velocity polynomials chosen to preserve the solubility conditions of the CE method (Chapman & Cowling 1970; Garzó & Santos 2003). These conditions are given by

$$\int \mathrm{d}\boldsymbol{v}\, f_i^{(1)}(\boldsymbol{v}) = 0, \tag{3.5}$$

$$\sum_{i=1}^{2} m_i \int \mathrm{d}\boldsymbol{v}\, \boldsymbol{v} f_i^{(1)}(\boldsymbol{v}) = 0, \tag{3.6}$$

$$\sum_{i=1}^{2} \frac{m_i}{2} \int \mathrm{d}\boldsymbol{v}\, V^2 f_i^{(1)}(\boldsymbol{v}) = 0. \tag{3.7}$$

While the conditions (3.5) and (3.6) yield the same velocity polynomials as in the standard method, in order to preserve the solubility condition (3.7) one has to replace the polynomial

$$\boldsymbol{S}_i(\boldsymbol{V}) = \left(\frac{1}{2}m_i V^2 - \frac{d+2}{2}T_i\right)\boldsymbol{V} \tag{3.8}$$

appearing in the standard Sonine polynomial expansion (Garzó & Dufty 2002) by the modified polynomial

$$\begin{aligned}\overline{\boldsymbol{S}}_i(\boldsymbol{V}) &= \left(\frac{1}{2}m_i V^2 - \frac{d+2}{2}\left(1+\frac{1}{2}c_i\right)T_i\right)\boldsymbol{V} \\ &= \boldsymbol{S}_i(\boldsymbol{V}) - \frac{d+2}{4}c_i T_i \boldsymbol{V}.\end{aligned} \tag{3.9}$$

As will be shown later, this replacement gives rise to new contributions to the transport coefficients associated with the heat flux.

The determination of the NS transport coefficients in the *modified* first Sonine approximation follows mathematical steps similar to the ones previously used in the *standard* first Sonine approximation. More specific technical details on these calculations are available as a supplement to the online version of this paper and on request from the authors. Here, we only display the final expressions for the NS transport coefficients in terms of the parameter space of the problem.

3.1. *Mass flux transport coefficients*

The mass flux contains three transport coefficients: D, D_p and D'. Dimensionless forms are defined by

$$D = \frac{\rho T}{m_1 m_2 \nu_0}D^*, \quad D_p = \frac{p}{\rho\nu_0}D_p^*, \quad D' = \frac{p}{\rho\nu_0}D'^*, \tag{3.10}$$

where $\nu_0 = n\sigma_{12}^{d-1}v_0$ is an effective collision frequency and $\sigma_{12} = (\sigma_1+\sigma_2)/2$. The explicit forms are then

$$D^* = \left(\nu_D - \frac{1}{2}\zeta^*\right)^{-1}\left[\left(\frac{\partial}{\partial x_1}x_1\gamma_1\right)_{p,T} + \left(\frac{\partial \zeta^*}{\partial x_1}\right)_{p,T}\left(1-\frac{\zeta^*}{2\nu_D}\right)D_p\right], \tag{3.11}$$

$$D_p^* = x_1 \left(\gamma_1 - \frac{\mu}{x_2 + \mu x_1} \right) \left(\nu_D - \frac{3}{2}\zeta^* + \frac{\zeta^{*2}}{2\nu_D} \right)^{-1}, \tag{3.12}$$

$$D'^* = -\frac{\zeta^*}{2\nu_D} D_p^*. \tag{3.13}$$

In these equations, $\zeta^* = \zeta^{(0)}/\nu_0$, $\mu = m_1/m_2$ is the mass ratio, and the expression of ν_D is given by (B 1). The definitions of collisional frequencies and the calculation of their integrals are given in the accompanying supplementary material.

3.2. *Shear viscosity coefficient*

The shear viscosity coefficient η is given by

$$\eta = \frac{p}{\nu_0} \left(x_1 T_1^2 \eta_1^* + x_2 T_2^2 \eta_2^* \right), \tag{3.14}$$

where the partial contributions η_i^* to the shear viscosity are

$$\eta_1^* = \frac{2\gamma_2(2\tau_{22} - \zeta^*) - 4\gamma_1\tau_{12}}{\gamma_1\gamma_2[\zeta^{*2} - 2\zeta^*(\tau_{11} + \tau_{22}) + 4(\tau_{11}\tau_{22} - \tau_{12}\tau_{21})]}, \tag{3.15a}$$

$$\eta_2^* = \frac{2\gamma_1(2\tau_{11} - \zeta^*) - 4\gamma_2\tau_{21}}{\gamma_1\gamma_2[\zeta^{*2} - 2\zeta^*(\tau_{11} + \tau_{22}) + 4(\tau_{11}\tau_{22} - \tau_{12}\tau_{21})]}, \tag{3.15b}$$

where the collision frequencies τ_{ij} are given by (B 3)–(B 6).

3.3. *Heat flux transport coefficients*

The transport coefficients D'', L and λ associated with the heat flux can be written as

$$D'' = -\frac{d+2}{2} \frac{n}{(m_1 + m_2)\nu_0} \left[\frac{x_1\gamma_1^3}{\mu_{12}} d_1^* + \frac{x_2\gamma_2^3}{\mu_{21}} d_2^* - \left(\frac{\gamma_1}{\mu_{12}} - \frac{\gamma_2}{\mu_{21}} \right) D^* \right], \tag{3.16}$$

$$L = -\frac{d+2}{2} \frac{T}{(m_1 + m_2)\nu_0} \left[\frac{x_1\gamma_1^3}{\mu_{12}} \ell_1^* + \frac{x_2\gamma_2^3}{\mu_{21}} \ell_2^* - \left(\frac{\gamma_1}{\mu_{12}} - \frac{\gamma_2}{\mu_{21}} \right) D_p^* \right], \tag{3.17}$$

$$\lambda = -\frac{d+2}{2} \frac{nT}{(m_1 + m_2)\nu_0} \left[\frac{x_1\gamma_1^3}{\mu_{12}} \lambda_1^* + \frac{x_2\gamma_2^3}{\mu_{21}} \lambda_2^* - \left(\frac{\gamma_1}{\mu_{12}} - \frac{\gamma_2}{\mu_{21}} \right) D'^* \right], \tag{3.18}$$

where $\mu_{ij} = m_i/(m_i + m_j)$ and the coefficients D^*, D_p^* and D'^* are given by (3.11)–(3.13), respectively. The expressions of the (dimensionless) coefficients d_i^*, ℓ_i^* and λ_i^* are

$$\begin{aligned} d_1^* = \frac{1}{\Lambda} \Bigg\{ & 2[2\nu_{12}Y_2 - Y_1(2\nu_{22} - 3\zeta^*)][\nu_{12}\nu_{21} - \nu_{11}\nu_{22} + 2(\nu_{11} + \nu_{22})\zeta^* - 4\zeta^{*2}] \\ & + 2\left(\frac{\partial \zeta^*}{\partial x_1} \right)_{p,T} (Y_3 + Y_5)\left[2\nu_{12}\nu_{21} + 2\nu_{22}^2 - \zeta^*(7\nu_{22} - 6\zeta^*)\right] \\ & - 2\nu_{12}\left(\frac{\partial \zeta^*}{\partial x_1} \right)_{p,T} (Y_4 + Y_6)(2\nu_{11} + 2\nu_{22} - 7\zeta^*) \Bigg\}, \end{aligned} \tag{3.19}$$

$$\ell_1^* = \frac{1}{\Lambda}\{-2Y_3[2(\nu_{12}\nu_{21}-\nu_{11}\nu_{22})\nu_{22}+\zeta^*(7\nu_{11}\nu_{22}-5\nu_{12}\nu_{21}+2\nu_{22}^2-6\nu_{11}\zeta^* - 7\nu_{22}\zeta^*+6\zeta^{*2})]+2Y_4\nu_{12}[2\nu_{12}\nu_{21}-2\nu_{11}\nu_{22}+2\zeta^*(\nu_{11}+\nu_{22})-\zeta^{*2}] + 2Y_5\zeta^*[2\nu_{12}\nu_{21}+\nu_{22}(2\nu_{22}-7\zeta^*)+6\zeta^{*2}]-2\nu_{12}\zeta^*Y_6[2(\nu_{11}+\nu_{22})-7\zeta^*]\}, \tag{3.20}$$

$$\lambda_1^* = \frac{1}{\Lambda}\{-Y_3\zeta^*[2\nu_{12}\nu_{21}+\nu_{22}(2\nu_{22}-7\zeta^*)+6\zeta^{*2}]+\nu_{12}\zeta^*Y_4[2(\nu_{11}+\nu_{22})-7\zeta^*] - Y_5[4\nu_{12}\nu_{21}(\nu_{22}-\zeta^*)+2\nu_{22}^2(5\zeta^*-2\nu_{11})+2\nu_{11}(7\nu_{22}\zeta^*-6\zeta^{*2})+5\zeta^{*2} \times(6\zeta^*-7\nu_{22})]+\nu_{12}Y_6[4\nu_{12}\nu_{21}+2\nu_{11}(5\zeta^*-2\nu_{22})+\zeta^*(10\nu_{22}-23\zeta^*)]\}. \tag{3.21}$$

Here, the various types of Y are defined by (B 7)–(B 12);

$$\Lambda = [4(\nu_{12}\nu_{21}-\nu_{11}\nu_{22})+6\zeta^*(\nu_{11}+\nu_{22})-9\zeta^{*2}] \times [\nu_{12}\nu_{21}-\nu_{11}\nu_{22}+2\zeta^*(\nu_{11}+\nu_{22})-4\zeta^{*2}]; \tag{3.22}$$

and the (reduced) collision frequencies ν_{ij} are given by (B 13) and (B 14). The corresponding expressions for d_2'', ℓ_2, λ_2, ν_{22} and ν_{21} can be deduced from (3.19)–(3.21) by interchanging $1 \leftrightarrow 2$. With these results, the coefficients D'', L and λ can be explicitly obtained from (3.16)–(3.18). In (3.19)–(3.21) it is understood that the coefficients D^*, D_p^* and D'^* are given by (3.11)–(3.13), respectively. Of course, our results show that D'' is antisymmetric with respect to the change $1 \leftrightarrow 2$, while L and λ are symmetric. Consequently, in the case of mechanically equivalent particles ($m_1 = m_2$, $\sigma_1 = \sigma_2$, $\alpha_{ij} = \alpha$), the coefficient $D'' = 0$.

The expressions for the NS transport coefficients derived here for a granular binary mixture reduce to those previously obtained (Garzó & Montanero 2007) when one takes Maxwellians distributions for the reference HCS $f_i^{(0)}$ ($c_1 = c_2 = 0$). In addition, for mechanically equivalent particles, the results obtained by Garzó *et al.* (2007*c*) for a single gas by using the modified Sonine method are also recovered. This confirms the self-consistency of the results reported in this paper.

4. Comparison with the standard first Sonine approximation and Monte Carlo simulations

The expressions for the transport coefficients derived in the previous section depend on many parameters: $\{x_1, m_1/m_2, \sigma_1/\sigma_2, \alpha_{11}, \alpha_{22}, \alpha_{12}\}$. Obviously, this complexity exists in the elastic limit as well, so that the primary new feature is the dependence of the transport coefficients on dissipation. Thus, to show more clearly the influence of inelasticity in collisions on transport, we normalize the transport coefficients with respect to their values in the elastic limit. Also, for simplicity, we take the simplest case of common coefficient of restitution ($\alpha_{11} = \alpha_{22} = \alpha_{12} \equiv \alpha$). This reduces the parameter space to four quantities: $\{x_1, m_1/m_2, \sigma_1/\sigma_2, \alpha\}$.

Let us start with the coefficients D, D_p and D' associated with the mass flux. In figure 1 the reduced coefficients $D(\alpha)/D(1)$, $D_p(\alpha)/D_p(1)$ and D'^*, defined by (3.13), are plotted as functions of the coefficient of restitution α for an equimolar mixture $x_1 = 1/2$ of hard spheres ($d = 3$) with the same size ratio $\omega \equiv \sigma_1/\sigma_2 = 1$ and three different values of the mass ratio $\mu \equiv m_1/m_2$. Here, $D(1)$ and $D_p(1)$ refer to the elastic values

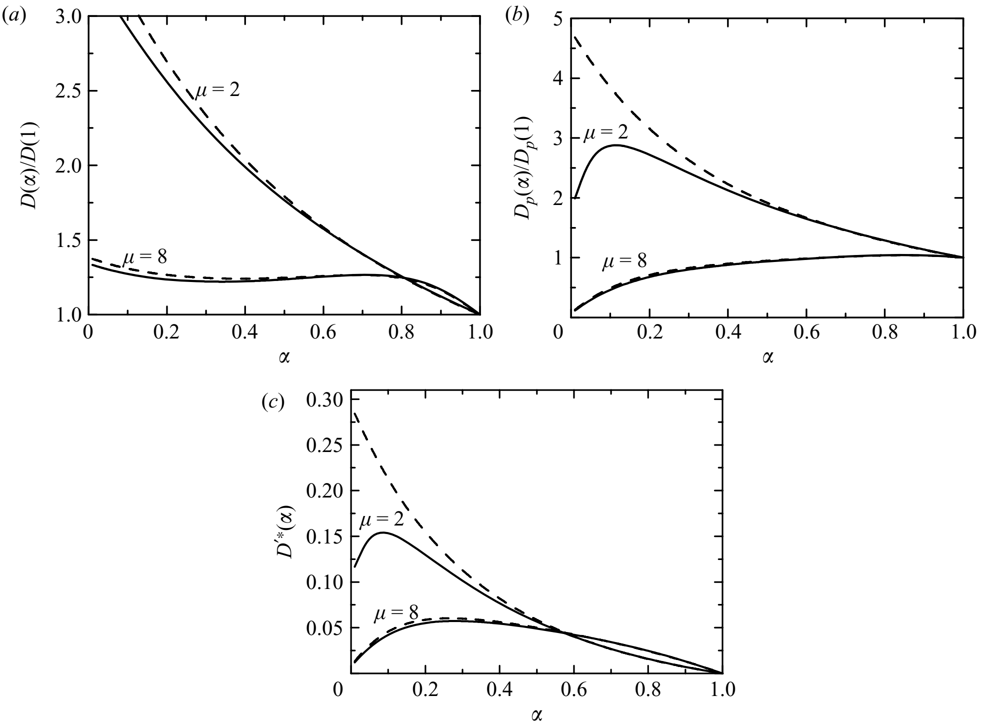

FIGURE 1. Plots of the reduced coefficients (*a*) $D(\alpha)/D(1)$, (*b*) $D_p(\alpha)/D_p(1)$ and (*c*) $D^{'*}(\alpha)$ as functions of the coefficient of restitution α for hard spheres with $x_1=1/2$, $\sigma_1=\sigma_2$ and two different values of the mass ratio $\mu=m_1/m_2$. The solid lines correspond to the results obtained from the modified first Sonine approximation, while the dashed lines refer to the results obtained from the standard first Sonine approximation.

of D and D_p, respectively. The coefficient $D^{'}$ has not been reduced with respect to its elastic value since $D'=0$ for $\alpha=1$. We observe that both Sonine approximations lead to identical results, except for extreme values of dissipation where both approaches present some discrepancies. This is especially important in the case $\mu=2$, where the disagreement is, for instance, about 15% and 32% for the coefficient D_p at $\alpha=0.1$ and 0.2, respectively. In order to test the accuracy of both Sonine approximations in the case of the diffusion coefficients, the dependence of the (reduced) diffusion coefficient $D(\alpha)/D(1)$ on α is plotted in figure 2 in the tracer limit ($x_1\to 0$) for two different cases when the tagged particle has the same mass density as the particles of the gas (i.e. $\mu=\omega^d$). The theoretical predictions of both Sonine approximations are compared with available (Garzó & Montanero 2004, 2007) and new Monte Carlo simulations (using the DSMC method; Bird 1994). Here, the tracer diffusion coefficient has been measured in computer simulations from the mean square displacement of a tagged particle in the HCS (Garzó & Montanero 2004). It is apparent that both Sonine approximations provide a good agreement with simulation data. However, the standard approximation slightly overestimates the diffusion coefficient at high inelasticity, this effect being corrected by the modified approximation.

The shear viscosity η is perhaps the most widely studied transport coefficient in granular fluids. Here, this coefficient has been measured in simulations by a new method proposed by the authors (Montanero, Santos & Garzó 2005). This method is based on the simple shear flow state modified by the introduction of (i) a deterministic

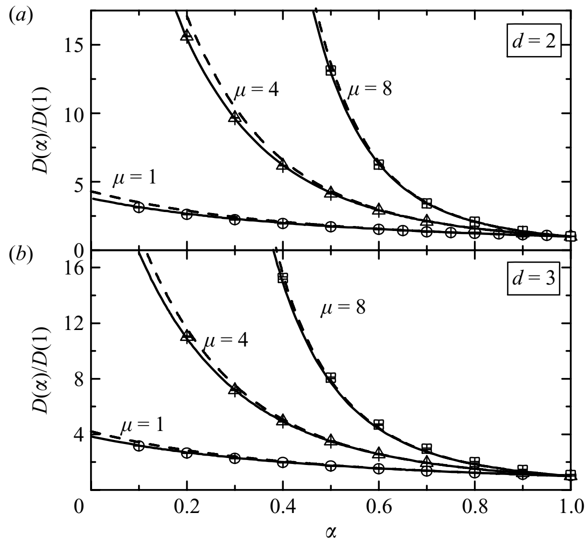

FIGURE 2. Plot of the reduced diffusion coefficient $D(\alpha)/D(1)$ as a function of the coefficient of restitution α for (a) hard disks and (b) hard spheres in the tracer limit ($x_1 \to 0$) when the tagged particle has the same mass density as the particles of the gas ($\mu = \omega^d$). Three different values of the mass ratio have been considered: $\mu = 1$, $\mu = 4$ and $\mu = 8$. The solid and dashed lines represent the modified and standard first Sonine approximations, respectively. The symbols are DSMC results obtained from the mean square displacement of the tagged particle. The DSMC results correspond to $\mu = 1$ (circles), $\mu = 4$ (triangles) and $\mu = 8$ (squares).

non-conservative force (Gaussian thermostat) that compensates for the collisional cooling and (ii) a stochastic process. While the Gaussian external force allows the granular mixture to reach a Newtonian regime in which the (true) NS shear viscosity can be identified, the stochastic process is introduced to reproduce the conditions appearing in the CE solution to NS order. More details on this procedure can be found in Montanero *et al.* (2005). The simulation data obtained from this method along with both Sonine approximations are presented in figure 3 for disks ($d = 2$) and spheres ($d = 3$). We have again considered mixtures constituted by particles of the same mass density. The simulation data corresponding to $d = 2$ for $\alpha \geqslant 0.5$ were reported by Garzó & Montanero (2007), while those corresponding to $d = 3$ and $d = 2$ for $\alpha \leqslant 0.5$ have been obtained in this work. As in the case of a single gas (Garzó *et al.* 2007c), we observe that up to $\alpha \simeq 0.6$ the simulation data agree quite well with both theories. On the other hand, for higher inelasticities and in the physical three-dimensional case, the standard first Sonine approximation overestimates the shear viscosity, while the modified first Sonine approximation compares well with computer simulations, even for low values of α. We also observe that the improvement of the modified Sonine method over the standard one is less clear for hard disks ($d = 2$), since the numerical data lie systematically between both theoretical approaches. However, even in this case the simulation results are closer to the modified ones than the standard ones. Therefore, according to the comparison carried out at the level of the coefficients D and η, we can conclude that while the standard Sonine approximation does quite good a job for not strong values of dissipation, it is fair to say that the modified Sonine approximation is still better (especially for hard spheres), since it agrees well with computer simulations in the full range of values of dissipation explored.

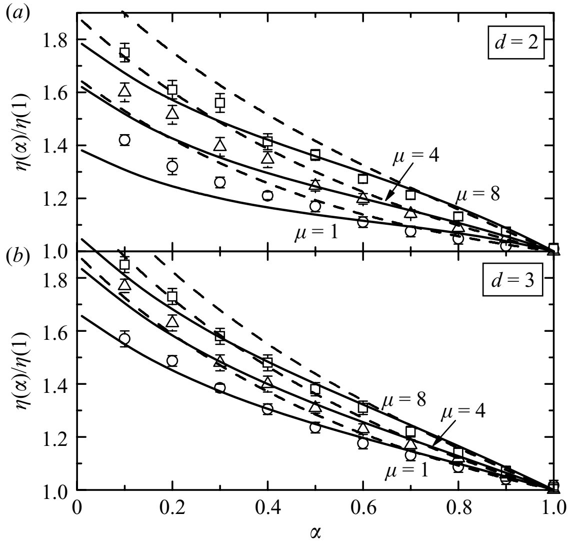

FIGURE 3. Plot of the reduced shear viscosity coefficient $\eta(\alpha)/\eta(1)$ as a function of the coefficient of restitution α for (*a*) hard disks and (*b*) hard spheres for an equimolar mixture ($x_1 = 1/2$) constituted by particles of the same mass density ($\mu = \omega^d$). Three different values of the mass ratio have been considered: $\mu = 1$, $\mu = 4$ and $\mu = 8$. The solid and dashed lines represent the modified and standard first Sonine approximations, respectively. The DSMC results correspond to $\mu = 1$ (circles), $\mu = 4$ (triangles) and $\mu = 8$ (squares).

Let us consider finally the heat flux. As mentioned in the § 1, recent studies for a monocomponent gas (Brey & Ruiz-Montero 2004; Brey *et al.* 2005*a*; Montanero *et al.* 2007) have shown that the standard first Sonine approximation dramatically overestimates the α dependence of the transport coefficients associated with the heat flux for high dissipation ($\alpha \lesssim 0.7$). This is the main reason why new alternative approximations (Noskowicz *et al.* 2007) have been proposed. However, in contrast to the single-gas case, the lack of available simulation data for granular mixtures for the coefficients D'', L and λ precludes a comparison between both Sonine approximations and computer simulations. Figures 4–6 show the α dependence of the reduced transport coefficients $\lambda(\alpha)/\lambda(1)$, $L(\alpha)n/\lambda(1)$ and $D''(\alpha)/D''(1)$, respectively, for $d = 3$, $x_1 = 1/2$, $\omega = 1$ and different values of the mass ratio. For comparison we show the theoretical results obtained by neglecting non-Gaussian corrections to the HCS distributions $f_i^{(0)}$ (i.e. the cumulants given in (2.2) are neglected: $c_i = 0$). Simulation results reported by Brey & Ruiz-Montero (2004) for a monocomponent granular gas are also included in the case $\mu = 1$, showing that the modified Sonine appoximation agrees with simulation data significantly better than the standard Sonine approximation, especially in the case of the pressure energy coefficient L. As expected, the standard and modified Sonine theories differ significantly for strong inelasticity, especially for mechanically *different* particles ($\mu \neq 1$). These discrepancies clearly justify the use of the modified Sonine approximation instead of the standard one to compute the dependence of the heat flux transport coefficients on dissipation. In addition, the standard approach leads to unphysical (negative) values for the thermal conductivity coefficient λ for low values of α, which is corrected by our modified Sonine approximation. This is of relevance, since it helps to clarify that the origin of unphysical values for the thermal conductivity at very high inelasticity

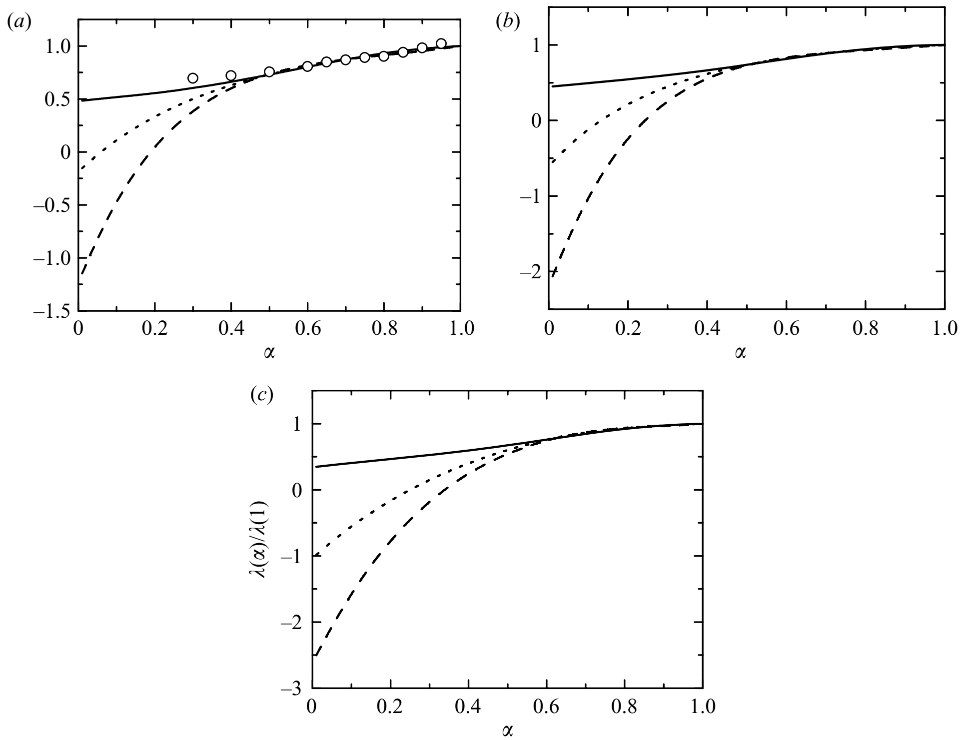

FIGURE 4. Plot of the reduced thermal conductivity coefficient $\lambda(\alpha)/\lambda(1)$ for hard spheres with $x_1 = 1/2$, $\sigma_1 = \sigma_2$ and three different values of the mass ratio μ: (*a*) $\mu = 1$, (*b*) $\mu = 2$ (*c*) and $\mu = 8$. The solid lines correspond to the results obtained from the modified first Sonine approximation; the dashed lines refer to the results obtained from the standard first Sonine approximation; and the dotted lines refer to the results derived by neglecting non-Gaussian corrections to the HCS distributions. The symbols in (*a*) are DSMC results obtained from the Green–Kubo relations for a monocomponent gas (Brey & Ruiz-Montero 2004).

is due to the mathematical accuracy of the Sonine approximation used and not a more fundamental reason; an inherent lack of scale separation, for instance. Note also that the simple theoretical results (Garzó & Montanero 2007) obtained by using Maxwellian forms for $f_i^{(0)}$ are even closer to the modified ones than those predicted by the standard approximation. The good agreement found in general between simulation (which yields the 'actual' values of the transport coefficients) and the modified Sonine approximation is the first evidence that the CE method may be safely extended down to very low values of the coefficient of normal restitution α.

5. Discussion

A modified Sonine approximation recently proposed (Garzó *et al.* 2007*c*) for monocomponent systems has been extended to granular mixtures in this paper. This theory has been mainly motivated by the disagreement found at high dissipation (Brey & Ruiz-Montero 2004; Brey *et al.* 2005*a*; Montanero *et al.* 2007) between the simulation data for the heat flux transport coefficients and the expressions derived from the standard first Sonine approximation for a single gas. As we have shown, important discrepancies between computer simulations and the standard Sonine approximation appear only in the region of strong inelasticity ($\alpha \lesssim 0.7$). Thus, it

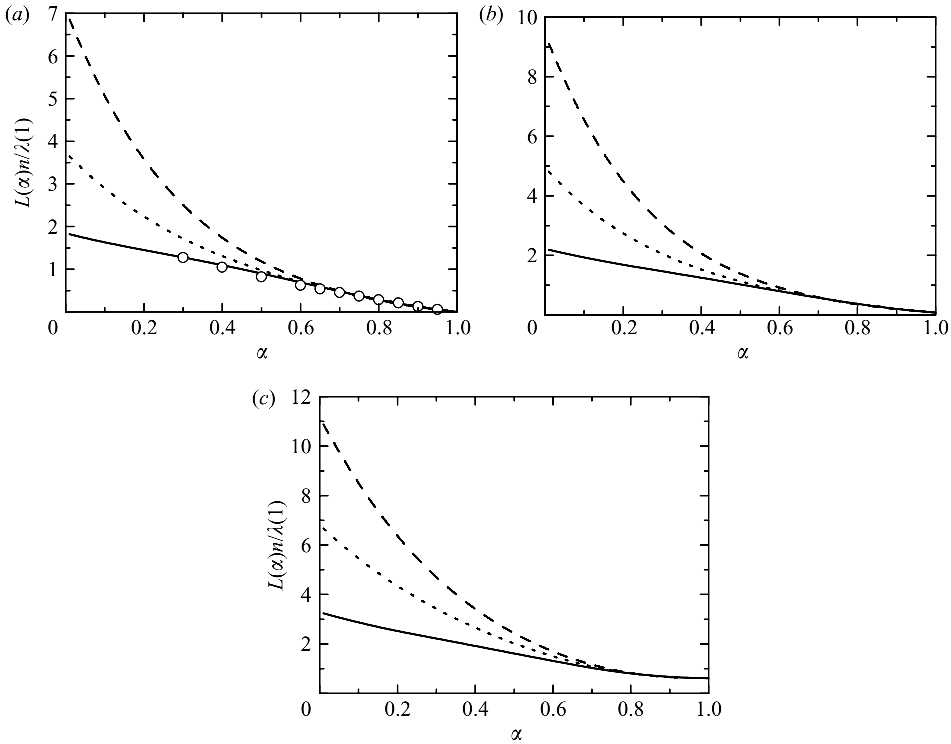

FIGURE 5. Plot of the reduced pressure energy coefficient $L(\alpha)n/\lambda(1)$ for hard spheres with $x_1 = 1/2$, $\sigma_1 = \sigma_2$ and three different values of the mass ratio μ: (*a*) $\mu = 1$, (*b*) $\mu = 2$ and (*c*) $\mu = 8$. The solid lines correspond to the results obtained from the modified first Sonine approximation; the dashed lines refer to the results obtained from the standard first Sonine approximation; and the dotted lines refer to the results derived by neglecting non-Gaussian corrections to the HCS distributions. The symbols in (*a*) are DSMC results obtained from the Green–Kubo relations for a monocomponent gas (Brey & Ruiz-Montero 2004).

could be argued that the search for new theoretical methods may admittedly be a more mathematical than physical endeavour. However, it is still physically relevant to propose methods (Garzó *et al.* 2007*c*; Noskowicz *et al.* 2007) that produce accurate results for the transport coefficients in the complete range of possible values of the coefficients of restitution. As in the case of a monocomponent gas (Garzó *et al.* 2007*c*), in the modified Sonine approximation the weight function for the unknowns $\mathscr{A}_i$, $\mathscr{B}_i$, $\mathscr{C}_i$ and $\mathscr{D}_i$ defining the first-order distribution $f_i^{(1)}$ is no longer the Maxwell–Boltzmann distribution $f_{i,M}$ but the HCS distribution $f_i^{(0)}$. Moreover, in order to preserve the solubility conditions (3.5)–(3.7), the polynomial $\boldsymbol{S}_i(\boldsymbol{V})$, defined by (3.8), appearing in the standard Sonine polynomial expansion must be replaced by the modified polynomial $\overline{\boldsymbol{S}}_i(\boldsymbol{V})$, defined by (3.9). The idea behind the modified method is that the deviation of $f_i^{(0)}$ from $f_{i,M}$ has an important influence on the NS distribution $f_i^{(1)}$. In this context, it is expected that the rate of convergence of the Sonine polynomial expansion is accelerated when $f_i^{(0)}$ rather than $f_{i,M}$ is used as weight function.

The extension of the modified Sonine approach to mixtures is not easy at all, since it involves the computation of new complex collision integrals. However, the structure of the NS transport coefficients is quite similar in the standard and

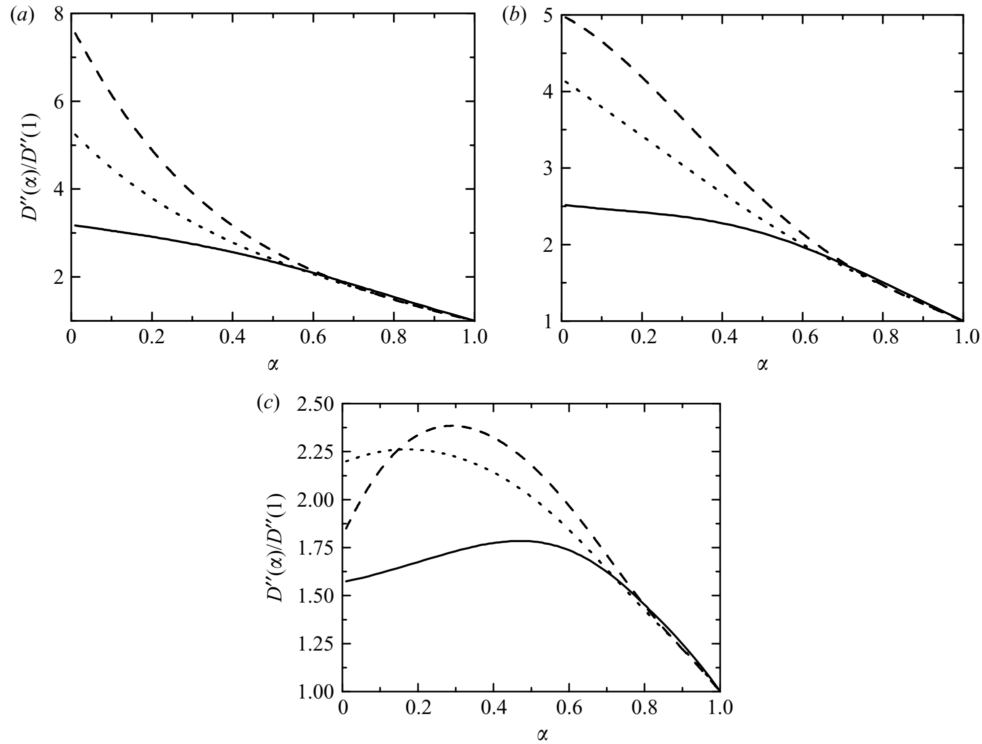

FIGURE 6. Plot of the reduced Duffour coefficient $D''(\alpha)/D(1)$ for hard spheres with $x_1 = 1/2$, $\sigma_1 = \sigma_2$ and three different values of the mass ratio μ: (*a*) $\mu = 2$, (*b*) $\mu = 4$ and (*c*) $\mu = 8$. The solid lines correspond to the results obtained from the modified first Sonine approximation; the dashed lines refer to the results obtained from the standard first Sonine approximation; and the dotted lines refer to the results derived by neglecting non-Gaussian corrections to the HCS distributions.

modified approximations (Garzó & Dufty 2002), since the distinction between both approximations occurs essentially in the α dependence of the characteristic collision frequencies of the transport coefficients ν_D, τ_{ij}, ω_{ij} and ν_{ij}. The forms of the NS coefficients are given by (3.10)–(3.13) for the mass flux transport coefficients D, D_p and D', (3.14)–(3.15*b*) for the shear viscosity η and (3.16)–(3.21) for the heat flux transport coefficients λ, L and D''. All the above expressions have the power to be explicit; that is they are explicitly given in terms of the parameters of the mixture. A *Mathematica* code providing the NS transport coefficients under arbitrary values of composition, masses, sizes and coefficients of restitution can be downloaded from http://www.unex.es/fisteor/vicente/granular_files.html/. The fact that our theory does not involve numerical solutions allows us to evaluate the transport coefficients within very short computing times. For instance, the code using our theoretical expressions for the NS transport coefficients takes just 5 seconds in a standard personal computer to produce a graph similar to those in figure 6 of the most complicated heat flux transport coefficients. Calculations were performed in a PC equipped with an $\times$ 86 64 bit Intel® processor and a RAM of 2 GB. These results contrast with the method devised by Noskowicz *et al.* (2007) for a monocomponent gas, where a system of algebraic equations must be numerically solved by employing the power of symbolic processors. This is perhaps another new added value of the method developed here for granular mixtures.

In order to check the accuracy of the modified Sonine approximation, computer simulations based on the DSMC method have been carried out in the cases of the tracer diffusion coefficient D and the shear viscosity coefficient η. Although some simulation data for these coefficients were previously reported by the authors (Garzó & Montanero 2004; Montanero *et al.* 2005), in this paper we extend those simulations to very low values of the coefficient of restitution (values of α typically larger than 0.1). This allows one to make a careful comparison between the modified and standard approximations with computer simulations. As expected, the discrepancies between simulation and the standard first Sonine estimates for D and η are partially corrected by the modified approximation, showing again the reliability of such approach for very strong values of dissipation. Unfortunately, the lack of available simulation data for the coefficients λ, L and D'' corresponding to the heat flux precludes a comparison between theory and simulation for these transport coefficients, except in the single-gas case (Brey & Ruiz-Montero 2004; Brey *et al.* 2005*a*) where figures 5 and 6 show the superiority of the modified Sonine approximation. We expect the present results for binary granular mixtures stimulate the performance of such simulations to assess the degree of accuracy of the modified Sonine method for the heat flux transport coefficients.

Hydrodynamic theories based on kinetic theory tools have not only been successful at predicting rapid granular flows (where the role of the interstitial fluid is assumed negligible) but have also been incorporated into models of high-velocity, gas–solid systems. These kinetic theory calculations are now standard features of commercial and research codes, such as Fluent® and MFIX (http://www.mfix.org/). These codes rely upon accurate expressions for the transport coefficients, and a first-order objective is to assure this accuracy from a careful treatment. As is shown in this paper, the price of this approach, in contrast to more phenomenological approaches, is an increasing complexity of the expressions for the transport coefficients as the system becomes more complex. In this context, we expect the theory reported here for granular binary mixtures to be quite useful for the above numerical codes.

The present results can also be applied to determine the dispersion relations for the hydrodynamic equations linearized about the HCS. Some previous results (Garzó *et al.* 2006) based on the standard Sonine method have shown that the resulting equations exhibit a long-wavelength instability for three of the modes. The objective now is to revisit the above problem by using the α dependence of the transport coefficients obtained in this paper. (If this should be done, then for consistency reasons, the linearized Burnett corrections to the cooling rate would need to be considered in the hydrodynamic equations, since $\nabla\cdot\boldsymbol{j}_1^{(1)}$, $\nabla_l\boldsymbol{P}_{kl}^{(1)}$ and $\nabla\cdot\boldsymbol{q}^{(1)}$ are of second order in the gradients, following the analysis by Brey *et al.* 1998.) Another possible open problem is to extend the present results (which are restricted to a low-density granular mixture) to finite densities in the framework of the Enskog kinetic theory. Given that the NS transport coefficients have recently been obtained from the Enskog equation (Garzó, Dufty & Hrenya 2007*a*; Garzó *et al.* 2007*b*) by the standard Sonine approximation, it would be interesting to compare again the above results with those derived from the modified first Sonine method. Finally, it would also be interesting to devise a method to measure by Monte Carlo simulations some of the NS transport coefficients of the heat flux in a granular binary mixture. This method could be based on the method proposed by Montanero *et al.* (2007) for a single gas, where the application of a homogeneous, anisotropic external force produces heat flux in the absence of gradients. We plan to carry out such extensions in the near future.

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Appendix A. Homogeneous cooling state (HCS)

In this appendix, the expressions of the cooling rate $\zeta^{(0)}$ and the fourth-degree cumulants c_i are given. These expressions were reported by Garzó & Dufty (1999*b*) for inelastic hard spheres ($d=3$). Here, we extend these expressions to an arbitrary number of dimensions d.

By using the leading Sonine approximation (3.1) for $f_1^{(0)}$ and neglecting nonlinear terms in c_1 and c_2, the (reduced) cooling rate $\zeta_1^* \equiv \zeta_1^{(0)}/\nu_0$ (where $\nu_0 = n\sigma_{12}^{d-1}v_0$) can be written as

$$\zeta_1^* = \zeta_{10} + \zeta_{11}c_1 + \zeta_{12}c_2, \tag{A 1}$$

where

$$\zeta_{10} = \frac{\sqrt{2}\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)}x_1\left(\frac{\sigma_1}{\sigma_{12}}\right)^{d-1}\theta_1^{-1/2}\left(1-\alpha_{11}^2\right) + \frac{4\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)}x_2\mu_{21} \times\left(\frac{1+\theta}{\theta}\right)^{1/2}(1+\alpha_{12})\theta_2^{-1/2}\left[1-\frac{1}{2}\mu_{21}(1+\alpha_{12})(1+\theta)\right], \tag{A 2}$$

$$\zeta_{11} = \frac{3\pi^{(d-1)/2}}{16\sqrt{2}d\Gamma\left(\frac{d}{2}\right)}x_1\left(\frac{\sigma_1}{\sigma_{12}}\right)^{d-1}\theta_1^{-1/2}\left(1-\alpha_{11}^2\right) + \frac{\pi^{(d-1)/2}}{8d\Gamma\left(\frac{d}{2}\right)}x_2\mu_{21} \times\frac{(1+\theta)^{-3/2}}{\theta^{1/2}}(1+\alpha_{12})\theta_2^{-1/2}\left[2(3+4\theta)-3\mu_{21}(1+\alpha_{12})(1+\theta)\right], \tag{A 3}$$

$$\zeta_{12} = -\frac{\pi^{(d-1)/2}}{8d\Gamma\left(\frac{d}{2}\right)}x_2\mu_{21}\left(\frac{1+\theta}{\theta}\right)^{-3/2}(1+\alpha_{12})\theta_2^{-1/2} \times\left[2+3\mu_{21}(1+\alpha_{12})(1+\theta)\right]. \tag{A 4}$$

In the above equations, $\mu_{ij}=m_i/(m_i+m_j)$, $\theta_1=1/(\mu_{21}\gamma_1)$, $\theta_2=1/(\mu_{12}\gamma_2)$, $\theta=\theta_1/\theta_2$ and $v_0=\sqrt{2T(m_1+m_2)/m_1m_2}$. The expression for ζ_2^* can be easily inferred from (A 2)–(A 4) by interchanging 1 and 2 and setting $\theta\to\theta^{-1}$.

The coefficients c_1 and c_2 are determined from the Boltzmann equations by multiplying them by V^4 and integrating over the velocity. After some algebra, when only linear terms in c_1 and c_2 are retained, the result is

$$c_1 = \frac{AG-ED}{BG-DF}, \quad c_2 = \frac{BE-AF}{BG-DF}, \tag{A 5}$$

where

$$A = -\frac{d(d+2)}{2\theta_1^2}\zeta_{10} - \Lambda_1, \quad E = -\frac{d(d+2)}{2\theta_2^2}\zeta_{20} - \Lambda_2, \tag{A 6}$$

$$D = \frac{d(d+2)}{2\theta_1^2}\zeta_{12} + \Lambda_{12}, \quad F = \frac{d(d+2)}{2\theta_2^2}\zeta_{21} + \Lambda_{21}, \tag{A 7}$$

$$B=\frac{d(d+2)}{2\theta_1^2}\left(\zeta_{11}+\frac{1}{2}\zeta_{10}\right)+\Lambda_{11},\quad G=\frac{d(d+2)}{2\theta_2^2}\left(\zeta_{22}+\frac{1}{2}\zeta_{20}\right)+\Lambda_{22}. \tag{A 8}$$

In the above equations, Λ_1, Λ_{11} and Λ_{12} are given by

$$\begin{aligned}\Lambda_1 =& -\frac{\pi^{(d-1)/2}}{\sqrt{2}\Gamma\left(\frac{d}{2}\right)}\theta_1^{-5/2}x_1\left(\frac{\sigma_1}{\sigma_{12}}\right)^{d-1}\frac{3+2d+2\alpha_{11}^2}{2}\left(1-\alpha_{11}^2\right)\\ &+\frac{\pi^{(d-1)/2}}{\Gamma\left(\frac{d}{2}\right)}\theta_1^{-5/2}x_2(1+\theta)^{-1/2}\mu_{21}(1+\alpha_{12})\\ &\times\left\{-2[d+3+(d+2)\theta]+\mu_{21}(1+\alpha_{12})(1+\theta)\left(11+d+\frac{d^2+5d+6}{d+3}\theta\right)\right.\\ &\left.-8\mu_{21}^2(1+\alpha_{12})^2(1+\theta)^2+2\mu_{21}^3(1+\alpha_{12})^3(1+\theta)^3\right\},\end{aligned} \tag{A 9}$$

$$\begin{aligned}\Lambda_{11} =& -\frac{\pi^{(d-1)/2}}{\sqrt{2}\Gamma\left(\frac{d}{2}\right)}\theta_1^{-5/2}x_1\left(\frac{\sigma_1}{\sigma_{12}}\right)^{d-1}\left[\frac{d-1}{2}(1+\alpha_{11})+\frac{3}{64}\left(10d+39+10\alpha_{11}^2\right)\right.\\ &\left.\times\left(1-\alpha_{11}^2\right)\right]+\frac{\pi^{(d-1)/2}}{16\Gamma\left(\frac{d}{2}\right)}\theta_1^{-5/2}x_2(1+\theta)^{-5/2}\mu_{21}(1+\alpha_{12})\\ &\times\{-2[45+15d+(114+39d)\theta+(88+32d)\theta^2+(16+8d)\theta^3]\\ &+3\,\mu_{21}(1+\alpha_{12})(1+\theta)[55+5d+9(10+d)\theta+4(8+d)\theta^2]\\ &-24\mu_{21}^2(1+\alpha_{12})^2(1+\theta)^2(5+4\theta)+30\mu_{21}^3(1+\alpha_{12})^3(1+\theta)^3\},\end{aligned} \tag{A 10}$$

$$\begin{aligned}\Lambda_{12} =& \frac{\pi^{(d-1)/2}}{16\Gamma\left(\frac{d}{2}\right)}\theta_1^{-5/2}x_2\theta^2(1+\theta)^{-5/2}\mu_{21}(1+\alpha_{12})\{2[d-1+(d+2)\theta]\\ &+3\mu_{21}(1+\alpha_{12})(1+\theta)[d-1+(d+2)\theta]-24\mu_{21}^2(1+\alpha_{12})^2(1+\theta)^2\\ &+30\mu_{21}^3(1+\alpha_{12})^3(1+\theta)^3\}.\end{aligned} \tag{A 11}$$

As before, the expressions for Λ_2, Λ_{22} and Λ_{21} are easily obtained from (A 9)–(A 11) by changing $1 \leftrightarrow 2$. In the case of a three-dimensional system ($d=3$), all the above expressions reduce to those previously obtained for hard spheres (Garzó & Dufty 1999*b*).

The dependence of the temperature ratio $\gamma=T_1/T_2$ on the parameters of the mixture is determined by requiring that the partial cooling rates $\zeta_i^{(0)}$ for the partial temperatures T_i be equal, i.e.

$$\zeta_1^{(0)}=\zeta_2^{(0)}=\zeta^{(0)}. \tag{A 12}$$

Once (A 12) is solved, the cumulants c_i are explicitly obtained by substituting γ into (A 5).

Appendix B. Expressions for the collision frequencies

The expressions of the different collision frequencies appearing in the NS transport coefficients are explicitly given in this appendix. For their definitions please refer to the supplementary material. The collision frequency ν_D associated with the mass flux is given by

$$\nu_D = \frac{2\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)}(1+\alpha_{12})\left(\frac{\theta_1+\theta_2}{\theta_1\theta_2}\right)^{1/2}\left\{x_2\mu_{21}\left[1+\frac{1}{16}\frac{\theta_2(3\theta_2+4\theta_1)c_1-\theta_1^2 c_2}{(\theta_1+\theta_2)^2}\right]\right.$$
$$\left.+\,x_1\mu_{12}\left[1+\frac{1}{16}\frac{\theta_1(3\theta_1+4\theta_2)c_2-\theta_2^2 c_1}{(\theta_1+\theta_2)^2}\right]\right\}. \quad \text{(B 1)}$$

It must be noted that the expression (B 1) for ν_D has been obtained by considering only linear terms in c_1 and c_2.

The expressions of the collision frequencies τ_{ij} corresponding to the shear viscosity are very long, and so, for the sake of clarity, we have presented them in terms of the operators Δ_i defined as

$$\Delta_i \equiv \theta_i^2\frac{\partial^2}{\partial\theta_i^2}+(d+2)\theta_i\frac{\partial}{\partial\theta_i}+\frac{d(d+2)}{4}. \quad \text{(B 2)}$$

Using (B 2), the collision frequencies τ_{11} and τ_{12} are given by

$$\tau_{11} = \frac{3\sqrt{2}\pi^{(d-1)/2}}{d(d+2)\Gamma\left(\frac{d}{2}\right)}x_1\left(\frac{\sigma_1}{\sigma_{12}}\right)^{d-1}(1+\alpha_{11})\theta_1^{-1/2}\left(1+\frac{2}{3}d-\alpha_{11}\right)\left(1+\frac{7}{32}c_1\right)$$
$$+\frac{2\pi^{(d-1)/2}}{d(d-1)(d+2)\Gamma\left(\frac{d}{2}\right)}x_2(1+\alpha_{12})\mu_{21}(\theta_1\theta_2)^{d/2}\theta_1^2$$
$$\times\left[1-\frac{c_1}{4}(2-\Delta_1)+\frac{c_2}{4}\Delta_2\right]I_\eta^{(11)}(\theta_1,\theta_2), \quad \text{(B 3)}$$

$$\tau_{12} = \frac{2\pi^{(d-1)/2}}{d(d-1)(d+2)\Gamma\left(\frac{d}{2}\right)}x_2(1+\alpha_{12})\frac{\mu_{21}^2}{\mu_{12}}(\theta_1\theta_2)^{d/2}\theta_1^2$$
$$\times\left[1-\frac{c_2}{4}(2-\Delta_2)+\frac{c_1}{4}\Delta_1\right]I_\eta^{(12)}(\theta_1,\theta_2), \quad \text{(B 4)}$$

where

$$I_\eta^{(11)}(\theta_1,\theta_2) = (\theta_1\theta_2)^{-\frac{d+1}{2}}\left\{2(d+3)(d-1)(\mu_{12}\theta_2-\mu_{21}\theta_1)\theta_1^{-2}(\theta_1+\theta_2)^{-1/2}\right.$$
$$+3(d-1)\mu_{21}\left(1+\frac{2d}{3}-\alpha_{12}\right)\theta_1^{-2}(\theta_1+\theta_2)^{1/2}$$
$$\left.+\,[2d(d+1)-4]\,\theta_1^{-1}(\theta_1+\theta_2)^{-1/2}\right\}, \quad \text{(B 5)}$$

$$I_\eta^{(12)}(\theta_1,\theta_2) = (\theta_1\theta_2)^{-\frac{d+1}{2}}\left\{2(d+3)(d-1)(\mu_{12}\theta_2-\mu_{21}\theta_1)\theta_2^{-2}(\theta_1+\theta_2)^{-1/2}\right.$$
$$+3(d-1)\mu_{21}\left(1+\frac{2d}{3}-\alpha_{12}\right)\theta_2^{-2}(\theta_1+\theta_2)^{1/2}$$
$$\left.-\,[2d(d+1)-4]\,\theta_2^{-1}(\theta_1+\theta_2)^{-1/2}\right\}. \quad \text{(B 6)}$$

The corresponding expressions for τ_{22} and τ_{21} can easily be inferred from (B 4)–(B 6).

Let us consider now the NS transport coefficients d_i^*, ℓ_i^* and λ_i^* of the heat flux. The quantities Y_i appearing in the expressions (3.19)–(3.20) for these coefficients are given by

$$Y_1 = \frac{D^*}{x_1\gamma_1^2}\left[\omega_{12} - \zeta^*\left(1+\frac{c_1}{2}\right)\right] - \frac{1}{\gamma_1^2}\left(\frac{\partial \gamma_1}{\partial x_1}\right)_{p,T}\left(1+\frac{c_1}{2}\right) - \frac{1}{2\gamma_1}\left(\frac{\partial c_1}{\partial x_1}\right)_{p,T}, \tag{B 7}$$

$$Y_2 = -\frac{D^*}{x_2\gamma_2^2}\left[\omega_{21} - \zeta^*\left(1+\frac{c_2}{2}\right)\right] - \frac{1}{\gamma_2^2}\left(\frac{\partial \gamma_2}{\partial x_1}\right)_{p,T}\left(1+\frac{c_2}{2}\right) - \frac{1}{2\gamma_2}\left(\frac{\partial c_2}{\partial x_1}\right)_{p,T}, \tag{B 8}$$

$$Y_3 = \frac{D_p^*}{x_1\gamma_1^2}\left[\omega_{12} - \zeta^*\left(1+\frac{c_1}{2}\right)\right] - \frac{m_1 n}{\rho}\frac{c_1}{2\gamma_1^2}, \tag{B 9}$$

$$Y_4 = -\frac{D_p^*}{x_2\gamma_2^2}\left[\omega_{21} - \zeta^*\left(1+\frac{c_2}{2}\right)\right] - \frac{m_2 n}{\rho}\frac{c_2}{2\gamma_2^2}, \tag{B 10}$$

$$Y_5 = \frac{D'^*}{x_1\gamma_1^2}\left[\omega_{12} - \zeta^*\left(1+\frac{c_1}{2}\right)\right] - \frac{1}{\gamma_1}\left(1+\frac{c_1}{2}\right), \tag{B 11}$$

$$Y_6 = -\frac{D'^*}{x_2\gamma_2^2}\left[\omega_{21} - \zeta^*\left(1+\frac{c_2}{2}\right)\right] - \frac{1}{\gamma_2}\left(1+\frac{c_2}{2}\right), \tag{B 12}$$

where

$$\begin{aligned}
\nu_{11} = {}& \frac{8\pi^{(d-1)/2}}{d(d+2)\Gamma\left(\frac{d}{2}\right)} x_1 \left(\frac{\sigma_1}{\sigma_{12}}\right)^{d-1}(1+\alpha_{11})(2\theta_1)^{-1/2}\left[\frac{d-1}{2} + \frac{3}{16}(d+8)\right. \\
& \left.\times(1-\alpha_{11}) + \frac{296+217d-3(160+11d)\alpha_{11}}{512}c_1\right] + \frac{\pi^{(d-1)/2}}{d(d+2)\Gamma\left(\frac{d}{2}\right)} \\
& \times x_2\mu_{21}(1+\alpha_{12})(\theta_1\theta_2)^{d/2}\theta_1^3\left\{\left[1-\frac{c_1}{4}(d+8-\Delta_1)+\frac{c_2}{4}\Delta_2\right]\right. \\
& \times(\theta_1\theta_2)^{-\frac{d+3}{2}}(\theta_1+\theta_2)^{-3/2}E - (d+2)\theta_1^{-1}\left[1-\frac{c_1}{4}(d+8-\Delta_1)+\frac{c_2}{4}\Delta_2\right] \\
& \left.\times\theta_1^{-\frac{d+5}{2}}\theta_2^{-\frac{d+1}{2}}(\theta_1+\theta_2)^{-1/2}[(d+2)\theta_1+(d+3)\theta_2]\right\} \\
& - \frac{\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)} x_2\mu_{21}(1+\alpha_{12})(\theta_1\theta_2)^{d/2}\theta_1^2\left\{\left[1-\frac{c_1}{4}(d+8-\Delta_1)+\frac{c_2}{4}\Delta_2\right]\right. \\
& \times(\theta_1\theta_2)^{-\frac{d+3}{2}}(\theta_1+\theta_2)^{-1/2}A - (d+2)\theta_1^{-1}\left[1-\frac{c_1}{4}(d+8-\Delta_1)+\frac{c_2}{4}\Delta_2\right] \\
& \left.\times\theta_1^{-\frac{d+3}{2}}\theta_2^{-\frac{d+1}{2}}(\theta_1+\theta_2)^{1/2}\right\} - \frac{c_1}{2}\frac{\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)}x_2\mu_{21}(1+\alpha_{12}) \\
& \times(\theta_1+\theta_2)^{-1/2}\theta_1^{1/2}\theta_2^{-3/2}\left[A-(d+2)\theta_2-(d+1)\theta_1^{-1}\theta_2^2\right],
\end{aligned} \tag{B 13}$$

$$\begin{aligned}
\nu_{12} = {}& -\frac{\pi^{(d-1)/2}}{d(d+2)\Gamma\left(\frac{d}{2}\right)} x_2\frac{\mu_{21}^2}{\mu_{12}}(1+\alpha_{12})(\theta_1\theta_2)^{d/2}\theta_1^3\left\{\left[1-\frac{c_2}{4}(d+8-\Delta_2)+\frac{c_1}{4}\Delta_1\right]\right. \\
& \times(\theta_1\theta_2)^{-\frac{d+3}{2}}(\theta_1+\theta_2)^{-3/2}F - (d+2)\theta_1^{-1}\left[1-\frac{c_2}{4}(d+8-\Delta_2)+\frac{c_1}{4}\Delta_1\right] \\
& \left.\times\theta_1^{-\frac{d+1}{2}}\theta_2^{-\frac{d+5}{2}}(\theta_1+\theta_2)^{-1/2}[(d+3)\theta_1+(d+2)\theta_2]\right\} \\
& - \frac{\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)} x_2\frac{\mu_{21}^2}{\mu_{12}}(1+\alpha_{12})\theta_1^{3+\frac{d}{2}}\theta_2^{\frac{d}{2}-1}\left\{\left[1-\frac{c_2}{4}(d+8-\Delta_2)+\frac{c_1}{4}\Delta_1\right]\right.
\end{aligned}$$

$$\times(\theta_1\theta_2)^{-\frac{d+3}{2}}(\theta_1+\theta_2)^{-1/2}B+(d+2)\theta_1^{-1}\left[1-\frac{c_2}{4}(d+8-\Delta_2)+\frac{c_1}{4}\Delta_1\right]$$
$$\times\theta_1^{-\frac{d+1}{2}}\theta_2^{-\frac{d+3}{2}}(\theta_1+\theta_2)^{1/2}\Big\}-\frac{\pi^{(d-1)/2}}{2d\Gamma\left(\frac{d}{2}\right)}x_2\frac{\mu_{21}^2}{\mu_{12}}(1+\alpha_{12})(\theta_1+\theta_2)^{-1/2}\theta_1^{3/2}\theta_2^{-5/2}$$
$$\times\ [c_2B+c_2(d+2)(\theta_1+\theta_2)-c_1\theta_2]\,, \tag{B 14}$$

$$\omega_{12}=\frac{\sqrt{2}\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)}x_1\left(\frac{\sigma_1}{\sigma_{12}}\right)^{d-1}\theta_1^{-1/2}(1+\alpha_{11})\left[1-\alpha_{11}+\frac{70+47d-3(34+5d)\alpha_{11}}{32(d+2)}c_1\right]$$
$$+\frac{2\pi^{(d-1)/2}}{d(d+2)\Gamma\left(\frac{d}{2}\right)}\mu_{21}(1+\alpha_{12})\theta_1^2(\theta_1\theta_2)^{d/2}\left[x_2\left(1+\frac{c_1}{4}\Delta_1+\frac{c_2}{4}\Delta_2\right)\right.$$
$$\times(\theta_1\theta_2)^{-\frac{d+3}{2}}(\theta_1+\theta_2)^{-1/2}A-x_1\frac{\mu_{12}}{\mu_{21}}\theta_2\theta_1^{-1}\left(1+\frac{c_1}{4}\Delta_1+\frac{c_2}{4}\Delta_2\right)(\theta_1\theta_2)^{-\frac{d+3}{2}}$$
$$\times(\theta_1+\theta_2)^{-1/2}B-(d+2)\theta_1^{-1}x_2\left(1+\frac{c_1}{4}\Delta_1+\frac{c_2}{4}\Delta_2\right)\theta_1^{-\frac{d+3}{2}}\theta_2^{-\frac{d+1}{2}}(\theta_1+\theta_2)^{1/2}$$
$$\left.-(d+2)x_1\frac{\mu_{12}}{\mu_{21}}\theta_2\theta_1^{-2}\left(1+\frac{c_1}{4}\Delta_1+\frac{c_2}{4}\Delta_2\right)\theta_1^{-\frac{d+1}{2}}\theta_2^{-\frac{d+3}{2}}(\theta_1+\theta_2)^{1/2}\right]$$
$$-c_1\frac{\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)}(1+\alpha_{12})\left(\frac{\theta_1+\theta_2}{\theta_1\theta_2}\right)^{1/2}(x_2\mu_{21}+x_1\mu_{12})\,. \tag{B 15}$$

In the above equations we have introduced the quantities

$$A(\theta_1,\theta_2)=(d+2)(2\beta_{12}+\theta_2)+\mu_{21}(\theta_1+\theta_2)\big\{(d+2)(1-\alpha_{12})$$
$$-[(11+d)\alpha_{12}-5d-7]\beta_{12}\theta_1^{-1}\big\}+3(d+3)\beta_{12}^2\theta_1^{-1}$$
$$+2\mu_{21}^2\left(2\alpha_{12}^2-\frac{d+3}{2}\alpha_{12}+d+1\right)\theta_1^{-1}(\theta_1+\theta_2)^2, \tag{B 16}$$

$$B(\theta_1,\theta_2)=(d+2)(2\beta_{12}-\theta_1)+\mu_{21}(\theta_1+\theta_2)\big\{(d+2)(1-\alpha_{12})$$
$$+[(11+d)\alpha_{12}-5d-7]\beta_{12}\theta_2^{-1}\big\}-3(d+3)\beta_{12}^2\theta_2^{-1}$$
$$-2\mu_{21}^2\left(2\alpha_{12}^2-\frac{d+3}{2}\alpha_{12}+d+1\right)\theta_2^{-1}(\theta_1+\theta_2)^2, \tag{B 17}$$

$$E(\theta_1,\theta_2)=2\mu_{21}^2\theta_1^{-2}(\theta_1+\theta_2)^2\left(2\alpha_{12}^2-\frac{d+3}{2}\alpha_{12}+d+1\right)[(d+2)\theta_1+(d+5)\theta_2]$$
$$-\mu_{21}(\theta_1+\theta_2)\big\{\beta_{12}\theta_1^{-2}[(d+2)\theta_1+(d+5)\theta_2][(11+d)\alpha_{12}-5d-7]$$
$$-\theta_2\theta_1^{-1}[20+d(15-7\alpha_{12})+d^2(1-\alpha_{12})-28\alpha_{12}]-(d+2)^2(1-\alpha_{12})\big\}$$
$$+3(d+3)\beta_{12}^2\theta_1^{-2}[(d+2)\theta_1+(d+5)\theta_2]$$
$$+2\beta_{12}\theta_1^{-1}[(d+2)^2\theta_1+(24+11d+d^2)\theta_2]$$
$$+(d+2)\theta_2\theta_1^{-1}[(d+8)\theta_1+(d+3)\theta_2], \tag{B 18}$$

$$F(\theta_1,\theta_2)=2\mu_{21}^2\theta_2^{-2}(\theta_1+\theta_2)^2\left(2\alpha_{12}^2-\frac{d+3}{2}\alpha_{12}+d+1\right)[(d+5)\theta_1+(d+2)\theta_2]$$
$$-\mu_{21}(\theta_1+\theta_2)\big\{\beta_{12}\theta_2^{-2}[(d+5)\theta_1+(d+2)\theta_2][(11+d)\alpha_{12}-5d-7]$$
$$+\theta_1\theta_2^{-1}[20+d(15-7\alpha_{12})+d^2(1-\alpha_{12})-28\alpha_{12}]+(d+2)^2(1-\alpha_{12})\big\}$$
$$+3(d+3)\beta_{12}^2\theta_2^{-2}[(d+3)\theta_1+(d+2)\theta_2]$$

$$-2\beta_{12}\theta_2^{-1}[(24+11d+d^2)\theta_1+(d+2)^2\theta_2]$$
$$+(d+2)\theta_1\theta_2^{-1}[(d+3)\theta_1+(d+8)\theta_2]. \quad \text{(B 19)}$$

Here, $\beta_{12}=\mu_{12}\theta_2-\mu_{21}\theta_1$. From (B 13) to (B 19), one easily gets the expressions for ω_{21}, ν_{22} and ν_{21} by interchanging $1 \leftrightarrow 2$.

Finally, note that the expressions (B 1), (B 3), (B 4), (B 13), (B 14) and (B 15) reduce to those previously obtained (Garzó & Montanero 2007) when one takes Maxwellians distributions for the reference HCS $f_i^{(0)}$, i.e. when $c_1=c_2=0$. Moreover, in the case of mechanically equivalent particles, the expressions of ν_D, τ_{ij} and ν_{ij} are consistent with those recently obtained for a monocomponent gas by using the modified Sonine approximation (Garzó *et al.* 2007*c*).

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