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AN EXACT SOLUTION OF THE BOLTZMANN EQUATION FOR A BINARY MIXTURE

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ABSTRACT

The set of coupled Boltzmann equations for a binary mixture of "colored" Maxwell molecules in a steady shear flow state has been solved. Color diffusion is generated in the system by means of an external field. The velocity moments can be expressed in terms of the solution of a quartic equation. In particular, the color conductivity and the shear viscosity coefficients have been obtained as nonlinear functions of the shear rate and the field strength.

1. INTRODUCTION

One of the main objectives in kinetic theory is the search for exact solutions of the nonlinear Boltzmann equation. Those solutions are generally hard to find, especially due to the mathematical difficulties embodied in the Boltzmann collision term. The interest for exact solutions has been greatly stimulated by the discovery of an explicit solution for Maxwell molecules in a spatially homogeneous situation, the so-called BKW-mode.[1] In the case of inhomogeneous states, the most physically interesting solutions correspond to planar shear flow at uniform temperature and density (usually referred to as "uniform shear flow")[2] and steady heat flow at constant pressure.[3] Both solutions refer to Maxwell molecules and are constructed in terms of the velocity moments of the distribution function.

Recently,[4] the hierarchy of moments of the Boltzmann equation for a binary mixture of Maxwell molecules has been exactly solved in the homogeneous color conductivity problem. Particles of both species are distinguished by a "color charge", but otherwise they are mechanically equivalent. The solution corresponds to a nonequilibrium homogeneous stationary state driven by an external force which accelerates particles of different colors along opposite directions, keeping the temperature constant. To the best of our knowledge, the only previous solution of the Boltzmann equation for a multicomponent system was obtained by Ernst and Hendriks for a 2D homogeneous and isotropic system of so-called "very hard particles".[5]

In this paper, we extend the previous color problem to an inhomogeneous situation. More concretely, the system as a whole is under uniform shear flow, so that the mean velocity has a linear profile. In addition, as in the homogeneous color case, an external field induces mutual diffusion in the system. Thus, there are two independent nonequilibrium parameters: the shear rate and the field strength. As a consequence, this problem exhibits a strong coupling between mass and momentum transport. The main generalized transport coefficients (shear viscosity and color conductivity) depend on both nonequilibrium parameters and are the quantities we are going to focus on. It is worth noticing that the solution we report here reduces to the cases of pure shear flow[2] and pure color[4] in the respective limits.

This paper is organized as follows. For the sake of completeness, the homogeneous color conductivity state is briefly described in Sect. 2. Section 3 is concerned with color conductivity under uniform shear flow. Exact expressions for the color conductivity, the shear viscosity, and the viscometric functions are explicitly obtained. Some final remarks are included in Sect. 4.

2. HOMOGENEOUS COLOR CONDUCTIVITY STATE

Let us consider a binary mixture constituted of mechanically equivalent particles of "color" 1 and "color" 2. The system is driven

to a steady homogeneous nonequilibrium state by the action of a constant external force that accelerates particles of different colors in opposite directions. This force plays the role of a chemical potential gradient. Further, a drag force is included to keep the temperature constant. This state has been simulated by molecular dynamics in dense systems.[6]

In a dilute system, all the physical information is contained in the velocity distribution functions $f_r(\vec{v})$, r=1, 2. These functions obey a coupled set of two Boltzmann equations:

$$\frac{\partial}{\partial \vec{v}} \cdot \left(\frac{\vec{F}_1(\vec{v})}{m} f_1(\vec{v}) \right) = J[f_1,f_1] + J[f_1,f_2] = J[f_1,f] , \tag{1}$$

and a similar equation for f_2. Here, m is the mass of a particle, $f=f_1+f_2$ is the total distribution function, J is the Boltzmann collision operator, which in standard notation reads[7]

$$J[f_r,f_s] = \int d\vec{v}_1 \int d\Omega |\vec{v}-\vec{v}_1| \sigma(|\vec{v}-\vec{v}_1|,\theta)[f_r(\vec{v}')f_s(\vec{v}_1')-f_r(\vec{v})f_s(\vec{v}_1)] , \tag{2}$$

and $\vec{F}_r(\vec{v})$ is the external force producing color diffusion:

$$\vec{F}_r(\vec{v}) = -k_B T \vec{\varepsilon}_r - \alpha \vec{v} . \tag{3}$$

In Eq. (3), T is the temperature, $\vec{\varepsilon}_r$ is a constant vector and α is a thermostat parameter identical for all the particles.

The first moments of f_r are given by

$$n_r = \int d\vec{v}\, f_r(\vec{v}) , \tag{4}$$

$$\vec{J}_r = \int d\vec{v}\, \vec{v}\, f_r(\vec{v}) , \tag{5}$$

and

$$\underline{\underline{P}}_r = \int d\vec{v}\, m\, \vec{v}\,\vec{v}\, f_r(\vec{v}) , \tag{6}$$

where n_r is the number density, $\vec{J}_r$ is the particle flux, and $\underline{\underline{P}}_r$ is the pressure tensor. In general, the coupled set of two Boltzmann equations does not seem to be solvable. However, the corresponding moment equations can be solved in a recursive way if one restricts oneself to Maxwell molecules (particles interacting via a potential $\varphi(r)=\kappa r^{-4}$). In this case, the first moments of the collision term are given by

$$\int d\vec{v}\, J[f_r,f_s] = 0 , \tag{7}$$

$$\int d\vec{v}\,\vec{v}\, J[f_r,f_s] = -\lambda(n_s\vec{J}_r - n_r\vec{J}_s) , \tag{8}$$

$$\int d\vec{v}\, m\,\vec{v}\,\vec{v}\, J[f_r,f_s] = \lambda'[\,(n_s p_r + n_r p_s + \tfrac{2}{3}m\vec{J}_r\cdot\vec{J}_s)\underline{\underline{1}} - (n_{s=r}\underline{\underline{P}} + n_{r=s}\underline{\underline{P}})$$

$$+ m(\vec{J}_s\vec{J}_r + \vec{J}_r\vec{J}_s)\,] - \lambda(n_{s=r}\underline{\underline{P}} - n_{r=s}\underline{\underline{P}}) . \tag{9}$$

Here, $\lambda=1.19\pi(\kappa/m)^{1/2}$, $\lambda'=0.777\,\lambda$, and $p_r=\frac{1}{3}\,\mathrm{tr}\,\underline{\underline{P}}_r$ is the partial hydrostatic pressure.

The most relevant transport properties have been obtained in Ref. 4. Here, we only quote the results that will be referred to in the next Section, namely the particle fluxes and the pressure tensor of the whole system. The particle fluxes are given by

$$\vec{J}_r = -\frac{k_B T}{mn\lambda}\,\sigma^*(\varepsilon^*)\, n_r\vec{\varepsilon}_r , \tag{10}$$

where $n=n_1+n_2$ is the total number density,

$$\sigma^*(\varepsilon^*) = \varepsilon^{*-2}\,[(1+2\varepsilon^{*2})^{1/2}-1] \tag{11}$$

is a dimensionless color conductivity coefficient and

$$\vec{\varepsilon}^* = \left(\frac{2}{3}\frac{k_B T}{mn^2\lambda^2}\frac{n_1}{n_2}\right)^{1/2}\vec{\varepsilon}_1$$

$$= -\left(\frac{2}{3}\frac{k_B T}{mn^2\lambda^2}\frac{n_2}{n_1}\right)^{1/2}\vec{\varepsilon}_2 \tag{12}$$

is a dimensionless measure of the field strength. The dimensionless pressure tensor of the whole system, $\underline{\underline{P}}^*=\underline{\underline{P}}/p$, where $\underline{\underline{P}}=\underline{\underline{P}}_1+\underline{\underline{P}}_2$ and $p=\frac{1}{3}\,\mathrm{tr}\,\underline{\underline{P}}=nk_BT$, is diagonal: $\underline{\underline{P}}^*=P_\perp^*\,\underline{\underline{1}}+(P_\parallel^*-P_\perp^*)\,\hat{\varepsilon}\hat{\varepsilon}$, with $P_\parallel^*=3-2P_\perp^*$ and

$$P_\perp^* = [1 + \frac{1}{2}\frac{\lambda}{\lambda'}\,\varepsilon^{*2}\sigma^*(\varepsilon^*)]^{-1} . \tag{13}$$

Proceeding in a similar way, higher order moments can also be obtained. In particular, the energy flux of the whole system vanishes in the equimolar case and is of third order in ε^*[4]. In order to get insight into the qualitative features of the velocity distribution function, information theory has been used to construct an approximate distribution from the knowledge of the moments up to the pressure tensor. Such a distribution is exact up to second order in ε^*. Also, it reduces to the exact form in the limit $|\varepsilon^*|\to\infty$, which corresponds to a situation where all the particles of the same species move with the same velocity. Thus, one can expect the information theory distribution to give a fair picture of the actual distribution for moderate values of ε^*.

3. COLOR CONDUCTIVITY UNDER SHEAR FLOW

The situation we have described in the previous Section corresponds to a homogeneous state which becomes that of equilibrium when the external field is switched off. Here, our aim is to extend the color conductivity problem to an inhomogeneous situation. More

concretely, we assume that the whole system is in a steady shear flow state characterized by the following hydrodynamic fields

$$n = \text{const.} , \tag{14}$$

$$T = \text{const.} , \tag{15}$$

$$u_i = a_{ij} r_j , \quad a_{ij} = a\, \delta_{ix}\delta_{jy} . \tag{16}$$

In Eq. (16), a is the constant shear rate and $\vec{u}$ is the mean velocity defined by

$$n\,\vec{u} = \int d\vec{v}\, \vec{v}\, f . \tag{17}$$

Under these conditions, the system is arbitrarily far from equilibrium even if the color field vanishes. This particular situation (uniform shear flow) has been extensively studied theoretically,[2,8] as well as by computer simulations.[9] Cummings *et al.*[10] have recently performed a molecular dynamics simulation of the color conductivity state in presence of shear flow.

We start from the stationary inhomogeneous Boltzmann equation:

$$\vec{v}\cdot\nabla f_1(\vec{r},\vec{v}) + \frac{\partial}{\partial \vec{v}}\cdot\left(\frac{\vec{F}_1}{m} f_1(\vec{r},\vec{v})\right) = J[f_1,f] , \tag{18}$$

and similarly for f_2. It is convenient to introduce the peculiar velocity $\vec{V}\equiv\vec{v}-\vec{u}$. Henceforth, the particle fluxes and the pressure tensors are understood to be defined by Eqs. (5) and (6), respectively, with $\vec{v}$ replaced by $\vec{V}$. One of the main advantages of the uniform shear flow state is that the distribution functions become uniform in the Lagrangian reference frame: $f_r(\vec{r},\vec{v})\to f_r(\vec{V})$. In order to keep this property under the color external field, we define it by

changing $\vec{v}$ into $\vec{V}$ in Eq. (3). Thus, Eq. (18) reduces to

$$-\frac{\partial}{\partial V_i}\left(\frac{\alpha}{m} V_i + a_{ij} V_j + \frac{k_B T}{m}\varepsilon_{1,i}\right) f_1 = J[f_1,f] . \tag{19}$$

From this equation and its counterpart for f_2, one easily gets the equation for the total distribution f:

$$-\frac{\partial}{\partial V_i}\left[\left(\frac{\alpha}{m} V_i + a_{ij}V_j\right)f - \frac{k_B T}{m}\frac{n_1}{n_2}\varepsilon_{1,i}\left(f - \frac{n}{n_1} f_1\right)\right] = J[f,f] . \tag{20}$$

Upon writing Eq. (20), we have taken into account that $n_1\vec{\varepsilon}_1 + n_2\vec{\varepsilon}_2 = 0$, as a consequence of the conservation of total momentum. On the other hand, the parameter α must be determined self-consistently by requiring the conservation of total energy. In this sense, it must be pointed out that the nonlinear character of Eqs. (19) and (20) is not only due to the collision terms, but also to the presence of α. The parameters measuring the deviation from equilibrium are the shear rate a and the strength ε_1 of the external field. As a matter of fact, this problem reduces to the homogeneous color conductivity case when $a=0$ and to the pure shear flow when $\vec{\varepsilon}_1 = 0$.

The set of coupled equations (19) and (20) can be solved recursively by the moment method when one considers the particular interaction of Maxwell molecules. In this case, a moment of a given order of the collision term only involves moments of order less than or equal to the given one. Further, from now on we restrict ourselves to a color field orthogonal to the gradient direction, i.e. $\varepsilon_{1,y} = 0$. Consequently, $j_{1,y} = 0$.

Multiplying both sides of Eq. (19) by $\vec{V}$ and integrating, one gets

$$\frac{k_B T}{m} n_1\vec{\varepsilon}_1 + \frac{\alpha}{m}\vec{J}_1 = -\lambda\, n\, \vec{J}_1 , \tag{21}$$

where use has been made of Eq. (8) with $\vec{v}$ replaced by $\vec{V}$ in the left side. Similarly, from Eq. (20) one obtains

$$\frac{1}{2}\frac{p}{n_2}(\vec{\varepsilon}_1\vec{J}_1+\vec{J}_1\vec{\varepsilon}_1)+\frac{\alpha}{m}\underline{\underline{P}}+\frac{1}{2}[\underline{\underline{a}}.\underline{\underline{P}}+(\underline{\underline{a}}.\underline{\underline{P}})^{\dagger}]=-\lambda'n(\underline{\underline{P}}-p\underline{\underline{1}}) , \tag{22}$$

where the dagger denotes the transpose operation and Eq. (9) has been used. The solution of Eq. (21) is given by Eq. (10), where now

$$\sigma^*=\frac{1}{1+\gamma\alpha^*} , \tag{23}$$

with $\alpha^*\equiv\alpha/(mn\lambda')$ and $\gamma\equiv\lambda'/\lambda$. Inserting Eqs. (10) and (23) into Eq. (22), one gets

$$P^*_{ij}=\frac{1}{1+\alpha^*}\left[\delta_{ij}-\frac{1}{1+\alpha^*}(a^*_{ij}+a^*_{ji})+\frac{2}{(1+\alpha^*)^2}a^*_{ik}a^*_{jk}\right.$$

$$\left.+\frac{3}{2\gamma(1+\gamma\alpha^*)}\varepsilon^*_i\varepsilon^*_j\right] , \tag{24}$$

where $a^*_{ij}=a^*\delta_{ix}\delta_{jy}$, $a^*\equiv a/(2\lambda'n)$ being the reduced shear rate, and $\vec{\varepsilon}^*$ is defined in Eq. (12). In the shear flow problem, it is adequate to introduce the generalized shear viscosity (η^*) and viscometric functions (Ψ_1, Ψ_2). According to Eq. (24), they are given by

$$\eta^*\equiv-\frac{P^*_{xy}}{a^*}=\frac{1}{(1+\alpha^*)^2} , \tag{25}$$

$$\Psi_1\equiv\frac{P^*_{yy}-P^*_{xx}}{a^{*2}}=-\frac{2}{(1+\alpha^*)^3}-\frac{3}{2}\frac{1}{\gamma(1+\alpha^*)(1+\gamma\alpha^*)}\frac{\varepsilon^{*2}_x}{a^{*2}} , \tag{26}$$

$$\Psi_2\equiv\frac{P^*_{zz}-P^*_{yy}}{a^{*2}}=\frac{3}{2}\frac{1}{\gamma(1+\alpha^*)(1+\gamma\alpha^*)}\frac{\varepsilon^{*2}_z}{a^{*2}} . \tag{27}$$

It must be noticed that in Eqs. (23)-(27) we still have to determine α^* as a function of a^* and ε^*. In order to close the problem, we must consider the consistency condition $P^*_{xx}+P^*_{yy}+P^*_{zz}=3$.

This gives rise to the following quartic equation for α^*:[11]

$$\alpha^*(1+\alpha^*)^2(1+\gamma\alpha^*)=\frac{2}{3}a^{*2}(1+\gamma\alpha^*)+\frac{\varepsilon^{*2}}{2\gamma}(1+\alpha^*)^2 . \tag{28}$$

In the particular case of homogeneous color state ($a^*=0$), Eq. (28) factorizes into two quadratic equations, whose physically meaningful solution is

$$\alpha^*(a^*=0,\varepsilon^*)=\frac{1}{2\gamma}[(1+2\varepsilon^{*2})^{1/2}-1] . \tag{29}$$

When this equation is substituted into Eqs. (23) and (24), with $a^*=0$, we reobtain the results given in Sect. 2. Furthermore, Eq. (29) allows us to get the ε^*-dependence of the shear viscosity in the limit of vanishing shear rate. Since $\alpha^*\geq 0$, Eq. (25) shows that $\eta^*(a^*=0,\varepsilon^*)\leq\eta^*(a^*=0,\varepsilon^*=0)=1$.

On the other hand, in absence of color field ($\varepsilon^*=0$), Eq. (28) reduces to a cubic equation, whose real solution is

$$\alpha^*(a^*,\varepsilon^*=0)=\frac{4}{3}\sinh^2\left[\frac{1}{6}\cosh^{-1}(1+9a^{*2})\right] . \tag{30}$$

Substitution of this equation into Eqs. (24)-(27), with $\varepsilon^*=0$, leads to the well-known uniform shear flow results for Maxwell molecules.[2,12] In addition, the color conductivity coefficient in the limit of zero field strength can be obtained from Eq. (23). We see that $\sigma^*(a^*,\varepsilon^*=0)\leq\sigma^*(a^*=0,\varepsilon^*=0)=1$.

Let us consider now the opposite limits, namely (i) large shear rate, but finite color field, and (ii) large color field, but finite shear rate. Asymptotic analysis of Eq. (28) shows that

$$\alpha^*(a^*,\varepsilon^*)=\left(\frac{2}{3}\right)^{1/3}a^{*2/3}\left[1-\left(\frac{2}{3}\right)^{2/3}a^{*-2/3}+\frac{1}{9}\left(\frac{2}{3}\right)^{-2/3}\left(1+\frac{3}{2\gamma^2}\varepsilon^{*2}\right)a^{*-4/3}\right.$$

$$\left.+O(a^{*-6/3})\right] , \tag{31}$$

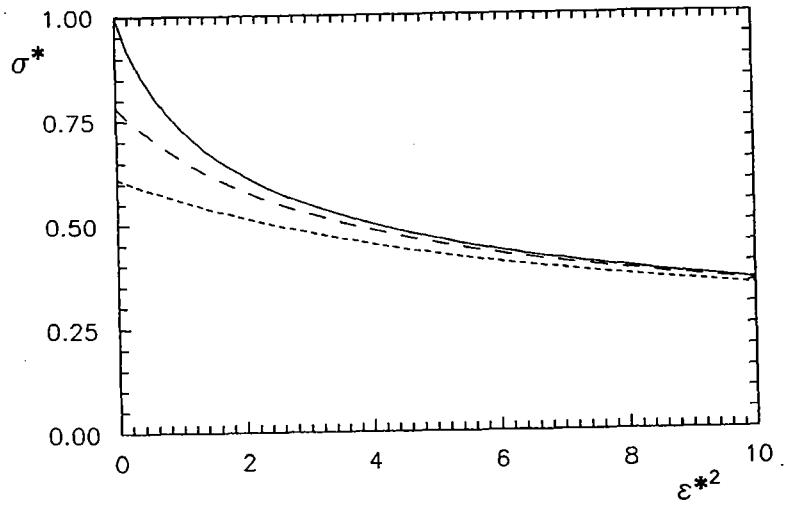

FIG. 1: Plot of the reduced color conductivity (σ^*) versus the square of the reduced field strength (ε^{*2}) for several values of the shear rate: $a^*=0$ (———), $a^*=1$ (– – –), $a^*=2$ (-----).

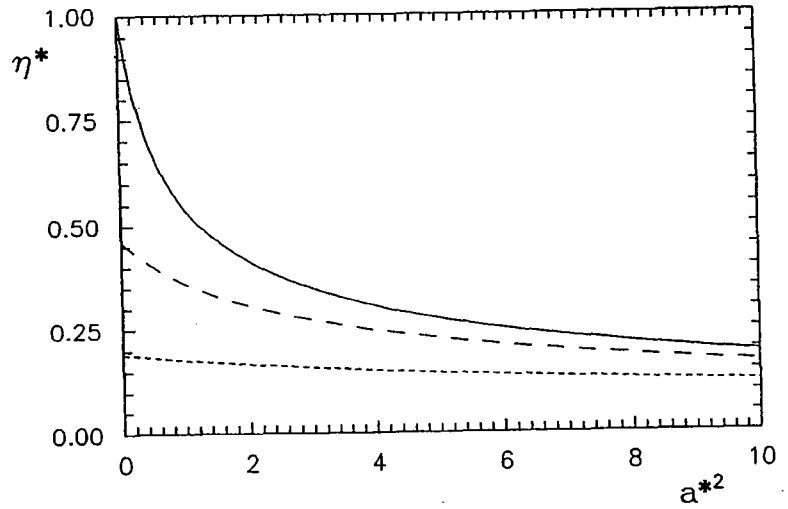

FIG. 2: Plot of the reduced shear viscosity (η^*) versus the square of the reduced shear rate (a^{*2}) for several values of the field strength: $\varepsilon^*=0$ (———), $\varepsilon^*=1$ (– – –), $\varepsilon^*=2$ (-----).

$$\alpha^*(a^*,\varepsilon^*) = \frac{\varepsilon^*}{\sqrt{2}\,\gamma}\left[1-\frac{1}{\sqrt{2}}\,\varepsilon^{*-1}+\frac{1}{4}\,\varepsilon^{*-2}+\frac{2\sqrt{2}}{3}\,\gamma^3 a^{*2}\varepsilon^{*-3} + O(\varepsilon^{*-4})\right]. \tag{32}$$

According to Eqs. (31) and (32), the behavior of α^* for large a^* is hardly sensitive to the value of ε^*, and vice versa.

In general, the solution of Eq. (28) is much more complicated to write explicitly and is given in the Appendix. Its insertion into Eqs. (23) and (25) gives the color conductivity and the shear viscosity, respectively. Figure 1 shows σ^* versus ε^{*2} for several values of a^*. At a given color field strength, we observe that the mass transport is inhibited as the shear rate increases. Nevertheless, this influence of the shear rate rapidly decays as ε^* increases. An analogous conclusion can be drawn from Fig. 2, where the shear viscosity is plotted versus a^{*2} for several values of ε^*. The presence of the color field hinders the momentum transport, this effect being more notorious in the region of small shear rates.

4. CONCLUDING REMARKS

In this paper, we have studied the coupling between mass and momentum transport in a binary mixture of mechanically identical Maxwell molecules described by the Boltzmann equation. Particles of each species are distinguished by a label or "color". The situation corresponds to a steady inhomogeneous state macroscopically characterized by a constant total density and pressure, a mean velocity along the x-direction with a constant gradient along the y-direction, and nonzero particle fluxes in the Lagrangian reference frame. Mutual diffusion is generated by a constant external force acting on particles of different colors in opposite directions. In addition, a nonconservative drag force is included to maintain the temperature constant. Therefore, the system is driven out of

equilibrium by the shearing as well as by the color field. This state includes the uniform shear flow[2] and the homogeneous color conductivity problem[4] as particular cases.

The hierarchy of moment equations can be solved in a recursive way. Here, we have been concerned with the particle fluxes and the total pressure tensor, although higher order moments can also be obtained. For the sake of simplicity, we have restricted ourselves to a color field orthogonal to the flow velocity gradient. Exact expressions for the color conductivity and shear viscosity coefficients have been obtained. They are nonlinear functions of both the shear rate and the field strength. The results show that both transport coefficients are smaller than the corresponding values given by the linear theory (Navier-Stokes regime). Competition between the shearing and the color field produces inhibition of mass and momentum transport. In other words, the shear flow gives rise to a decreasing of the color conductivity and the presence of the color field induces a decreasing of the shear viscosity.

It must be emphasized that our results hold for any molar fraction ratio. We expect to extend the analysis also to arbitrary mass ratio. On the other hand, it does not seem possible to explicitly get the distribution function from the Boltzmann equation. In this context, it would be interesting to study the problem by using kinetic models.[13]

APPENDIX

In this Appendix, we list the expressions leading to the physical root of Eq. (28). Following the standard method to solve a quartic equation,[14] we find

$$\alpha^* = \frac{1}{2}\left[(B_1^2-4B_0)^{1/2}-B_1\right], \tag{A1}$$

where

$$B_1 = \frac{2\gamma+1-(2\varepsilon^{*2}-4\gamma+1+4\gamma^2 w)^{1/2}}{2\gamma}, \tag{A2}$$

$$B_0 = \frac{3\gamma w-(24a^{*2}\gamma+18\varepsilon^{*2}+9\gamma^2 w^2)^{1/2}}{6\gamma}. \tag{A3}$$

In Eqs. (A2) and (A3), w is given by

$$w = -\frac{2}{3}D^{1/2}\cosh\left[\frac{1}{3}\cosh^{-1}\left(\frac{C}{D^{3/2}}\right)\right] - \frac{1}{3}\left(\frac{\varepsilon^{*2}}{2\gamma^2}-\frac{\gamma+2}{\gamma}\right) \tag{A4}$$

if $a^{*2}<[\gamma/2(3-2\gamma)][\varepsilon^{*2}/2\gamma^2+(1-\gamma)/\gamma]^2$, and by

$$w = -\frac{2}{3}|D|^{1/2}\sinh\left[\frac{1}{3}\sinh^{-1}\left(\frac{C}{|D|^{3/2}}\right)\right] - \frac{1}{3}\left(\frac{\varepsilon^{*2}}{2\gamma^2}-\frac{\gamma+2}{\gamma}\right) \tag{A5}$$

otherwise. In these equations,

$$C = \left(\frac{\varepsilon^{*2}}{2\gamma^2}+\frac{1-\gamma}{\gamma}\right)^3 - 3a^{*2}\left[2a^{*2}-\frac{\varepsilon^{*2}}{\gamma^3}\left(\frac{9}{2}-5\gamma\right)-\frac{1-\gamma}{\gamma^3}(2\gamma^2+3-3\gamma)\right], \tag{A6}$$

$$D = \left(\frac{\varepsilon^{*2}}{2\gamma^2}+\frac{1-\gamma}{\gamma}\right)^2 - 2\frac{3-2\gamma}{\gamma}a^{*2}. \tag{A7}$$

The solution (A1) has been chosen with the criterion that it reduces to Eqs. (29) and (30) in the appropriate limits.

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