Color conductivity induced by a shear-rate dependent color field

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(Received 23 November 1992; accepted 4 January 1993)

Nonlinear mass and momentum transport in a binary mixture subject to steady uniform shear flow has been recently analyzed.[1] Diffusion is generated by the action of a constant external force (color field)[2] that accelerates particles of different "color" along opposite directions. The results were derived for a dilute gas in the context of the Boltzmann equation for Maxwell molecules by using the moment method. The relevant transport properties, namely the color conductivity tensor and the shear viscosity coefficient, were obtained. These transport coefficients turn out to be nonlinear functions of both the color field and the shear rate.

From a computer simulation point of view, the color field algorithm[2] seems to be an efficient alternative to molecular dynamics methods based on the Green-Kubo formula for measuring the self-diffusion coefficient. Thus, in absence of shear rate, the self-diffusion coefficient can be defined as the zero-field limit of the color conductivity coefficient. However, this agreement between both methods cannot be extended when the system as a whole is in a uniform shear flow state with arbitrary shear rate.[1,3] In order to avoid the above discrepancy, a modified external field was suggested in Ref. 1. With this choice, and by using the Boltzmann equation for a dilute gas of Maxwell molecules, it was proved that the color conductivity tensor coincides with the generalized self-diffusion tensor[4] in the limit of small color field.

The aim of this Note is to analyze the general coupling between color and momentum transport under uniform shear flow in presence of the modified color field. Since we are interested basically in the influence of this force on the particle fluxes, here we will focus on the derivation of the color conductivity tensor for finite shear rate and color field strength.

Let us consider a binary mixture of mechanically equivalent particles in steady uniform shear flow. Particles of color r ($r=1,2$) are accelerated by the action of the color field

$$\mathscr{F}_r=-k_BT\mathsf{P}^*\cdot\epsilon_r. \tag{1}$$

Henceforth, we will generally use the same notation as in Ref. 1. The field strengths ϵ_r play the role of chemical potential gradients. In Eq. (1), P^* is the reduced pressure tensor in the pure uniform shear flow. For Maxwell molecules, its non-zero components are[5] $P^*_{xx}=(1+3\beta)/(1+\beta)$, $P^*_{yy}=P^*_{zz}=1/(1+\beta)$, and $P^*_{xy}=P^*_{yx}=-a^*/(1+\beta)^2$. Here, $\beta=\frac{4}{3}\sinh^2[\frac{1}{6}\cosh^{-1}(1+9a^{*2})]$, a^* being the reduced shear rate. As said above, the color field $\mathscr{F}_r$ defined by Eq. (1) leads to equivalent results for the self-diffusion and the color conductivity tensors in the limit of vanishing color field. This is not true in the usual color field method,[1,2] where P^* is replaced by the unity tensor. For arbitrary values of the shear rate, Eq. (1) takes into account the anisotropy induced by the shear flow, since $\mathscr{F}_r$ and ϵ_r are no longer parallel.

Under the above conditions, the hierarchy of moments corresponding to the set of Boltzmann equations can be solved recursively in the particular case of Maxwell molecules. Further, it is straightforward to show that this set of Boltzmann equations can be obtained from the set given by Eqs. (2.19) and (2.20) of Ref. 1 by formally making the change $\epsilon_r\to\mathsf{P}^*\cdot\epsilon_r$. Therefore, the reduced conductivity tensor σ^*_{ij} can be written in the form

$$\sigma^*_{ij}=\frac{1}{1+\gamma\alpha^*}\left(\delta_{ik}-\frac{2\gamma}{1+\gamma\alpha^*}a^*\delta_{ix}\delta_{ky}\right)P^*_{kj}, \tag{2}$$

where $\gamma\simeq 0.777$. The parameter α^* is defined through the following implicit algebraic equation:

$$\begin{aligned}\alpha^*(1+\alpha^*)^2(1+\gamma\alpha^*)^2&=\frac{2}{3}a^{*2}(1+\gamma\alpha^*)^2+\frac{1}{2\gamma}(1+\alpha^*)^2(1+\gamma\alpha^*)\\&\times P^*_{kj}P^*_{kl}\epsilon^*_j\epsilon^*_l+\frac{1+\gamma(1+2\alpha^*)}{\gamma}\\&\times a^*[a^*\delta_{iy}\delta_{ky}-(1+\alpha^*)\delta_{ix}\delta_{ky}]P^*_{ij}P^*_{kl}\epsilon^*_j\epsilon^*_l,\end{aligned} \tag{3}$$

where ϵ^* is the reduced color field strength. In the limit of large shear rate, $\alpha^*\approx(\frac{2}{3})^{1/3}a^{*2/3}$. For large field strength, $\alpha^*\approx\gamma^{-1}(\frac{1}{2}P^*_{kj}P^*_{kl}\epsilon^*_j\epsilon^*_l)^{1/2}$. On the other hand, in linear order in ϵ^*, Eq. (3) implies that $\alpha^*=\beta$, and then Eq. (2) gives the shear-rate dependent self-diffusion tensor.[4]

The solution of Eq. (3) gives α^* for arbitrary a^* and ϵ^*. Here, in order to compare with the results of Ref. 1, we choose the case $\epsilon^*_x=\epsilon^*_z=0$. In Fig. 1 , we have plotted some of the components of σ^*_{ij} as functions of ϵ^{*2} for $a^*=1$. We observe that the diagonal components decrease as the color field increases. On the other hand, we have verified that, for a given value of the field strength, an increasing in the shear rate gives rise to an increasing of σ^*_{xx} and to a decreasing of σ^*_{yy} and the trace σ^*_{kk}. The influence of the shear rate on the off-diagonal component σ^*_{xy} is much less noticeable.

The behavior of σ^*_{ij} as a function of ϵ^{*2} is similar to that of the color conductivity tensor $\tilde{\sigma}^*_{ij}$ derived in Ref. 1 .

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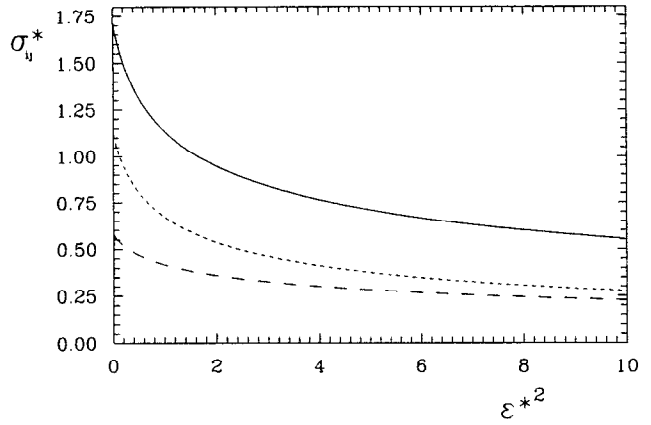

FIG. 1. Plot of some components of the reduced color conductivity tensor σ_{ij}^* versus the reduced field strength square ϵ^{*2} for $a^* = 1$: σ_{xx}^* (—); σ_{yy}^* (– – –); $-\sigma_{xy}^*$ (- - -).

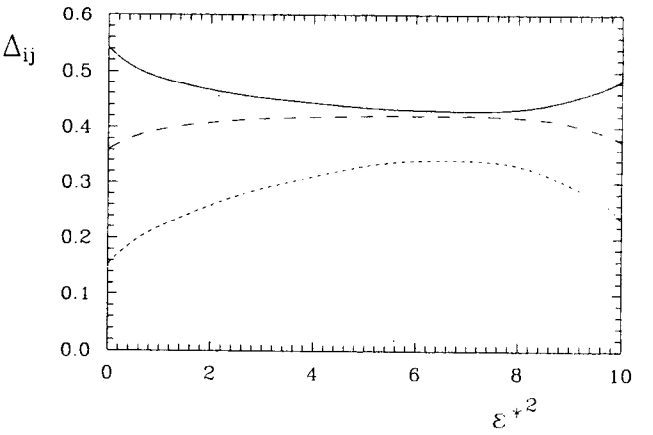

FIG. 2. Plot of some components of the tensor Δ_{ij} versus the reduced field strength square ϵ^{*2} for $a^* = 1$: $-\Delta_{xx}$ (—); Δ_{yy} (– – –); $-\Delta_{xy}$ (- - -).

Nevertheless, both tensors have different qualitative features. In particular, $\sigma_{xx}^* > \tilde{\sigma}_{xx}^* = \tilde{\sigma}_{yy}^* = \tilde{\sigma}_{zz}^* > \sigma_{yy}^* = \sigma_{zz}^*$ and $\sigma_{xy}^* < \tilde{\sigma}_{xy}^* < \sigma_{yx}^* < \tilde{\sigma}_{yx}^* = 0$. In order to perform a more detailed comparison between both quantities, we define the functions $\Delta_{ij} = (\tilde{\sigma}_{ij}^*/\sigma_{ij}^*) - 1$. Figure 2 shows $-\Delta_{xx}$, Δ_{yy}, and $-\Delta_{xy}$ as functions of ϵ^{*2} for $a^* = 1$. In the range of field strengths considered, the relative deviation Δ_{yy} is less sensitive to the value of ϵ^{*2} than Δ_{xx} and Δ_{xy}. In fact, in the limit of large ϵ^{*2}, one has $-\Delta_{xx} \approx 0.40$, $\Delta_{yy} \approx 0.24$, and $-\Delta_{xy} \approx 1$.

In summary, the adequate choice of a shear-rate dependent color field yields a color conductivity tensor that reduces in the zero-field limit to the generalized self-diffusion tensor. In addition, for nonzero shear rate and any value of the field strength, the discrepancy between the conductivity tensor obtained here and the one derived from the original choice of the color field is quite remarkable. Finally, although the exact results reported in this Note have been obtained from the Boltzmann equation for Maxwell molecules, we think that the color field algorithm based on the use of the force defined by Eq. (1) could lead to the self-diffusion tensor even in the regime of dense fluids. In this context, it would be very interesting to carry out computer simulations in order to check the above conjecture.

Partial support from the Dirección General de Investigación Científica y Técnica (Spain) through Grant No. PB91-0316 is gratefully acknowledged.

[1] V. Garzó and A. Santos, J. Chem. Phys. **97**, 2039 (1992). Notice a misprint in Eq. (3.2): the term $+\frac{2}{3}m\mathbf{j}_r\cdot\mathbf{j}_s$ should read $-\frac{2}{3}m\mathbf{j}_r\cdot\mathbf{j}_s$.

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