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Local *H*-Theorem for the Revised Enskog Equation

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A simple derivation of the local *H*-theorem for the revised Enskog equation is presented.

KEY WORDS: *H*-theorem; Enskog's equation.

1. INTRODUCTION

I consider here a fluid composed of identical hard spheres of diameter a. Within Enskog's kinetic theory the state of the fluid is described by the one-particle distribution $f_1(\mathbf{r}. \mathbf{v}; t)$, representing at time t the number density of particles at point $\mathbf{r}$ with velocity $\mathbf{v}$. In the course of time $f_1(\mathbf{r}, \mathbf{v}; t)$ changes due to free streaming and collisions. For hard spheres the duration of binary encounters is zero. When two particles of equal mass collide, their velocities $\mathbf{v}_1, \mathbf{v}_2$ take instantaneously postcollisional values

$$\mathbf{v}_1' = \mathbf{v}_1 - \hat{\boldsymbol{\varepsilon}}(\hat{\boldsymbol{\varepsilon}} \cdot \mathbf{v}_{12}), \qquad \mathbf{v}_2' = \mathbf{v}_2 + \hat{\boldsymbol{\varepsilon}}(\hat{\boldsymbol{\varepsilon}} \cdot \mathbf{v}_{12}) \tag{1.1}$$

where $\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2$, and $\hat{\boldsymbol{\varepsilon}}$ is a unit vector along the line passing through the centers of the spheres at the moment of impact. Correspondingly, the exact rate of change of the distribution $f_1(\mathbf{r}, \mathbf{v}; t)$ due to collisions is given by

$$\begin{aligned}\left(\frac{\partial f_1}{\partial t}\right)_{\text{coll}} (\mathbf{r}_1, \mathbf{v}_1; t) = \int d\mathbf{r}_2 \int d\mathbf{v}_2 \int d\hat{\boldsymbol{\varepsilon}}\, a^2(\hat{\boldsymbol{\varepsilon}} \cdot \mathbf{v}_{12})\, \vartheta(\hat{\boldsymbol{\varepsilon}} \cdot \mathbf{v}_{12})\\ \times [f_2(\mathbf{r}_1, \mathbf{v}_1', \mathbf{r}_2, \mathbf{v}_2'; t)\, \delta(\mathbf{r}_{12} - a\hat{\boldsymbol{\varepsilon}})\\ - f_2(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2; t)\, \delta(\mathbf{r}_{12} + a\hat{\boldsymbol{\varepsilon}})]\end{aligned} \tag{1.2}$$

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The step function ϑ and the distributions δ in Eq. (1.2) impose the conditions $\boldsymbol{\varepsilon}\cdot\mathbf{v}_{12}>0$ and $|\mathbf{r}_{12}|=|\mathbf{r}_1-\mathbf{r}_2|=a$, respectively, which must be satisfied at the moment of impact. The density of pairs of particles in collisional configurations is described by the two-particle distribution f_2 [Eq. (1.2) is the first of the infinite BBGKY hierarchy for hard spheres; see, e.g., Ref. 1].

The approximation leading to Enskog's theory consists in assuming that correlations between the particles entering into collision at time t coincide with those of an equilibrium inhomogeneous fluid whose density field equals

$$n(\mathbf{r},t)=\int d\mathbf{v}\, f_1(\mathbf{r},\mathbf{v};t) \tag{1.3}$$

Therefore, within Enskog's approach, one inserts into the exact formula (1.2) the approximation

$$\begin{aligned} f_2(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_2,\mathbf{v}_2;t)&\simeq f_2^{\mathrm{E}}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_2,\mathbf{v}_2;t)\\ &\equiv f_1(\mathbf{r}_1,\mathbf{v}_1;t)\, f_1(\mathbf{r}_2,\mathbf{v}_2;t)\, g_2(\mathbf{r}_1,\mathbf{r}_2\,|\,n(t)) \end{aligned} \tag{1.4}$$

Although no correlations between the velocities are retained, Eq. (1.4) takes correctly into account the mutual impenetrability of the spheres, and this in an inhomogeneous state corresponding to the momentary density field (1.3). The equilibrium pair distribution $g_2(\mathbf{r}_1,\mathbf{r}_2\,|\,n(t))$ is a functional of the density field.

Combining Eqs. (1.2) and (1.4), and taking into account the effect of free streaming, one obtains the revised Enskog equation$^{(2)}$

$$\begin{aligned} &\left(\frac{\partial}{\partial t}+\mathbf{v}_1\cdot\frac{\partial}{\partial \mathbf{r}_1}\right) f_1(\mathbf{r}_1,\mathbf{v}_1;t)\\ &\quad=\left(\frac{\partial f_1}{\partial t}\right)^{\mathrm{E}}_{\mathrm{coll}}(\mathbf{r}_1,\mathbf{v}_1;t)\\ &\quad=\int d\mathbf{r}_2\int d\mathbf{v}_2\int d\hat{\boldsymbol{\varepsilon}}\, a^2(\hat{\boldsymbol{\varepsilon}}\cdot\mathbf{v}_{12})\,\vartheta(\hat{\boldsymbol{\varepsilon}}\cdot\mathbf{v}_{12})\\ &\qquad\times[f_2^{\mathrm{E}}(\mathbf{r}_1,\mathbf{v}_1',\mathbf{r}_2,\mathbf{v}_2';t)\,\delta(\mathbf{r}_{12}-a\hat{\boldsymbol{\varepsilon}})\\ &\qquad-f_2^{\mathrm{E}}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_2,\mathbf{v}_2;t)\,\delta(\mathbf{r}_{12}+a\hat{\boldsymbol{\varepsilon}})] \end{aligned} \tag{1.5}$$

The term "revised" recalls the fact that in the original Enskog equation the function $g_2(\mathbf{r}_1,\mathbf{r}_2\,|\,n(t))$ was interpreted as corresponding to a homogeneous rather than inhomogeneous equilibrium state.$^{(3)}$

The global *H*-theorem for the kinetic equation (1.5) was proved (under periodic boundary conditions) by Résibois.[4] He found the appropriate generalization of the famous Boltzmann *H*-functional by using the relation

$$H(t) = -k_{\mathrm{B}}^{-1} S(t) \tag{1.6}$$

where k_{B} is Boltzmann's constant and $S(t)$ is the nonequilibrium entropy [a functional of $f_1(\mathbf{r}, \mathbf{v}; t)$], suitably defined to correspond to Enskog's approximate descrition of the fluid. $S(t)$ was shown to be an increasing function of time, yielding at equilibrium the exact entropy of the hard sphere fluid.

The aim of this paper is to provide a simple derivation of the local formulation of the *H*-theorem. The question is thus to define the nonequilibrium entropy density $s(\mathbf{r} \mid f_1(t))$ as a functional of the one-particle distribution $f_1(\mathbf{r}, \mathbf{v}; t)$ and show that it satisfies the local balance equation with a nonnegative source term, vanishing only at complete equilibrium. This has been already achieved by a rather complicated method involving formal series expansions,[5] a method inspired by Résibois' fundamental work.[4] No series expansions will be used here. The simplicity of the present derivation follows in fact from adopting the most natural definition of the nonequilibrium entropy density (Section 2), in full harmony with the physical content of the approximation that Enskog's theory represents.

2. ENTROPY DENSITY WITHIN ENSKOG'S THEORY

In view of the assumption (1.4) underlying Enskog's kinetic theory, I now define the entropy density (per particle) $s^{\mathrm{E}}(\mathbf{r} \mid f_1(t))$ by adopting simply the formula that applies to inhomogeneous equilibrium states (see the review article by Evans[6]). This most natural choice leads to the formula

$$s^{\mathrm{E}}(\mathbf{r} \mid f_1(t)) = s^{\mathrm{B}}(\mathbf{r} \mid f_1(t)) + s^{\mathrm{corr}}(\mathbf{r} \mid n(t)) \tag{2.1}$$

where the first term corresponds to Boltzmann's theory (ideal gas contribution)

$$\begin{aligned} & n(\mathbf{r}, t)\, s^{\mathrm{B}}(\mathbf{r} \mid f_1(t)) \\ & \quad = -k_{\mathrm{B}} \int d\mathbf{v}\, f_1(\mathbf{r}, \mathbf{v}; t)\{\ln[h^3 f_1(\mathbf{r}, \mathbf{v}; t)] - 1\} \end{aligned} \tag{2.2}$$

(h is Planck's constant), and the second term describes the effect of correlations

$$s^{\mathrm{corr}}(\mathbf{r} \mid n(t)) = k_{\mathrm{B}} \int_0^1 d\alpha\, c_1(\mathbf{r} \mid \alpha n(t)) \tag{2.3}$$

s^{corr} is expressed in Eq. (2.3) in terms of the equilibrium one-particle direct correlation function $c_1(\mathbf{r}\,|\,n(t))$, a functional of the density field $n(\mathbf{r}, t)$ related to the pair distribution $g_2(\mathbf{r}_1, \mathbf{r}_2\,|\,n(t))$ by the hard sphere equilibrium hierarchy equation

$$\frac{\partial}{\partial \mathbf{r}_1} c_1(\mathbf{r}_1\,|\,n(t)) = \int d\mathbf{r}_2 \int d\hat{\boldsymbol{\varepsilon}}\, a^2 \hat{\boldsymbol{\varepsilon}}\, \delta(\mathbf{r}_{12} - a\hat{\boldsymbol{\varepsilon}})\, n(\mathbf{r}_2, t)\, g_2(\mathbf{r}_1, \mathbf{r}_2\,|\,n(t)) \tag{2.4}$$

Formulas (2.3) and (2.4) are well known in the theory of inhomogeneous equilibrium fluids[6] [see also Eq. (25b) in Ref. 4]. The function c_1 appears as an effective chemical potential corresponding to the density field $n(\mathbf{r}, t)$.

3. LOCAL *H*-THEOREM

I proceed now to establish the local balance equation for the entropy density (2.1). Although the calculation involving the ideal gas contribution (2.2) has been already performed elsewhere,[3,4] I reproduce it briefly here for completeness.

The Enskog equation (1.5) implies the continuity equation

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{u} n) = 0 \tag{3.1}$$

where the mean velocity field $\mathbf{u}(\mathbf{r}, t)$ is defined by

$$n(\mathbf{r}, t)\, \mathbf{u}(\mathbf{r}, t) = \int d\mathbf{v}\, \mathbf{v} f_1(\mathbf{r}, \mathbf{v}, t) \tag{3.2}$$

Taking the time derivative of Eq. (2.2), one readily finds

$$\frac{\partial}{\partial t}(n s^{\mathrm{B}}) = \frac{\partial}{\partial \mathbf{r}_1} \cdot (-\mathbf{u} n s^{\mathrm{B}} - \mathbf{J}_s^{\mathrm{B}k}) - k_{\mathrm{B}} \int d\mathbf{v}_1 \left(\frac{\partial f_1}{\partial t}\right)^{\mathrm{E}}_{\text{coll}} \ln(h^3 f_1) \tag{3.3}$$

where $\mathbf{J}_s^{\mathrm{B}k}$ is the kinematic Boltzmann entropy current density,

$$J_s^{\mathrm{Bk}}(\mathbf{r}, t) = -k_{\mathrm{B}} \int d\mathbf{v}\, [\mathbf{v} - \mathbf{u}(\mathbf{r}, t)]\, f_1(\mathbf{r}, \mathbf{v}; t) \ln[h^3 f_1(\mathbf{r}, \mathbf{v}; t)] \tag{3.4}$$

Using Eq. (1.5) and the change of the integration variables $(\mathbf{v}_1, \mathbf{v}_2, \hat{\boldsymbol{\varepsilon}}) \to (\mathbf{v}_1', \mathbf{v}_2', -\hat{\boldsymbol{\varepsilon}})$, one can rewrite the last term in Eq. (3.3) in the form

$$k_{\mathrm{B}} \int d\mathbf{v}_2 \int d\mu\, \delta(\mathbf{r}_{12} + a\hat{\boldsymbol{\varepsilon}})\, f_2^{\mathrm{E}}(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2; t) \ln \frac{f_1(\mathbf{r}_1, \mathbf{v}_1; t)}{f_1(\mathbf{r}_1, \mathbf{v}_1'; t)} \tag{3.5}$$

where

$$d\mu = d\mathbf{v}_1\, d\mathbf{v}_2\, d\hat{\boldsymbol{\epsilon}}\, a^2(\hat{\boldsymbol{\epsilon}}\cdot\mathbf{v}_{12})\, \vartheta(\hat{\boldsymbol{\epsilon}}\cdot\mathbf{v}_{12}) \tag{3.6}$$

Now the crucial remark is that the antisymmetric part of the integrand in Eq. (3.5) with respect to the permutation of variables $\mathbf{r}_1$ and $\mathbf{r}_2$ contributes to the flow term due to the identity

$$\begin{aligned}&\int d\mathbf{r}_2\,[F(\mathbf{r}_1,\mathbf{r}_2)-F(\mathbf{r}_2,\mathbf{r}_1)]\\&\qquad = -\frac{\partial}{\partial\mathbf{r}_1}\cdot\left[\int_0^1 d\lambda \int d\mathbf{r}\,\mathbf{r}F(\mathbf{r}_1+(1-\lambda)\,\mathbf{r},\mathbf{r}_1-\lambda\mathbf{r})\right]\end{aligned} \tag{3.7}$$

The symmetric part will be interpreted as the source term. We thus rewrite Eq. (3.3) in the form

$$\frac{\partial}{\partial t}(ns^{\mathrm{B}})+\frac{\partial}{\partial\mathbf{r}}\cdot(\mathbf{u}ns^{\mathrm{B}}+\boldsymbol{J}_s^{\mathrm{Bk}}+\boldsymbol{J}_s^{\mathrm{Bp}})=\sigma_s^{\mathrm{B}} \tag{3.8}$$

where the "potential" part of the entropy current density is given by

$$\begin{aligned}\boldsymbol{J}_s^{\mathrm{Bp}}(\mathbf{r}_1,t)=\frac{k_{\mathrm{B}}}{2}\int_0^1 d\lambda \int d\mu\, a\hat{\boldsymbol{\epsilon}}\\ &\times f_2^{\mathrm{E}}(\mathbf{r}_1-\lambda a\hat{\boldsymbol{\epsilon}},\mathbf{v}_1,\mathbf{r}_1+(1-\lambda)\,a\hat{\boldsymbol{\epsilon}},\mathbf{v}_2;t)\\ &\times\ln\frac{f_1(\mathbf{r}_1-\lambda a\hat{\boldsymbol{\epsilon}},\mathbf{v}_1';t)}{f_1(\mathbf{r}_1-\lambda a\hat{\boldsymbol{\epsilon}},\mathbf{v}_1;t)}\end{aligned} \tag{3.9}$$

whereas the source term is given by

$$\begin{aligned}\sigma_s^{\mathrm{B}}(\mathbf{r}_1,t)=-\frac{k_{\mathrm{B}}}{2}\int d\mu\, f_2^{\mathrm{E}}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_1+a\hat{\boldsymbol{\epsilon}},\mathbf{v}_2;t)\\ &\times\ln\frac{f_1(\mathbf{r}_1,\mathbf{v}_1';t)\,f_1(\mathbf{r}_1+a\hat{\boldsymbol{\epsilon}},\mathbf{v}_2';t)}{f_1(\mathbf{r}_1,\mathbf{v}_1;t)\,f_1(\mathbf{r}_1+a\hat{\boldsymbol{\epsilon}},\mathbf{v}_2;t)}\end{aligned} \tag{3.10}$$

We now study the balance equation for the correlation part of the entropy density, defined by Eq. (2.3). Using the continuity equation (3.1) and the symmetry of the functional derivatives

$$\frac{\delta s^{\mathrm{corr}}(\mathbf{r}_1\,|\,n(t))}{\delta n(\mathbf{r}_2,t)}=\frac{\delta s^{\mathrm{corr}}(\mathbf{r}_2\,|\,n(t))}{\delta n(\mathbf{r}_1,t)} \tag{3.11}$$

one readily finds

$$\frac{\partial}{\partial t}(ns^{\mathrm{corr}})+\frac{\partial}{\partial \mathbf{r}_1}\cdot(\mathbf{u}ns^{\mathrm{corr}})=\int d\mathbf{r}_2\, n(\mathbf{r}_1,t)\,\mathbf{u}(\mathbf{r}_2,t) \times\frac{\delta}{\delta n(\mathbf{r}_1,t)}\left[n(\mathbf{r}_2,t)\frac{\partial}{\partial \mathbf{r}_2}s^{\mathrm{corr}}(\mathbf{r}_2\,|\,n(t))\right] \tag{3.12}$$

The gradient of s^{corr} can be evaluated with the help of Eqs. (2.3 and (2.4), yielding the formula

$$n(\mathbf{r}_2,t)\frac{\partial}{\partial \mathbf{r}_2}s^{\mathrm{corr}}(\mathbf{r}_2\,|\,n(t)) =k_{\mathrm{B}}\int d\mathbf{r}_3\int d\hat{\boldsymbol{\varepsilon}}\, a^2\hat{\boldsymbol{\varepsilon}}\,\delta(\mathbf{r}_{23}-a\hat{\boldsymbol{\varepsilon}})\,n(\mathbf{r}_2,t)\,n(\mathbf{r}_3,t) \times\int_0^1 d\alpha\,\alpha g_2(\mathbf{r}_2,\mathbf{r}_3\,|\,\alpha n(t)) \tag{3.13}$$

Substituting Eq. (3.13) into the right-hand side of Eq. (3.12), we find the sum of two terms. The first results from the action of the functional derivative on the product of densities $n(\mathbf{r}_2, r)\, n(\mathbf{r}_3, t)$. It reads

$$k_{\mathrm{B}}\int d\mathbf{r}_2\int d\hat{\boldsymbol{\varepsilon}}\, a^2\hat{\boldsymbol{\varepsilon}}[\mathbf{u}(\mathbf{r}_1,t)-\mathbf{u}(\mathbf{r}_2,t)]\,\delta(\mathbf{r}_{12}-a\hat{\boldsymbol{\varepsilon}})\,n(\mathbf{r}_1,t)\,n(\mathbf{r}_2,t) \times\int_0^1 d\alpha\,\alpha g_2(\mathbf{r}_1,\mathbf{r}_2\,|\,\alpha n(t)) \tag{3.14}$$

The second, in which the derivative acts on the distribution g_2 can be conveniently written as

$$\frac{k_{\mathrm{B}}}{2}\int d\mathbf{r}_2\int d\mathbf{r}_3\int d\hat{\boldsymbol{\varepsilon}}\, a^2\hat{\boldsymbol{\varepsilon}}\cdot[\mathbf{u}(\mathbf{r}_2,t)-\mathbf{u}(\mathbf{r}_3,t)]\,\delta(\mathbf{r}_{23}-a\hat{\boldsymbol{\varepsilon}}) \times n(\mathbf{r}_1,t)\,n(\mathbf{r}_2,t)\,n(\mathbf{r}_3,t)\int_0^1 d\alpha\,\alpha\frac{\delta g_2(\mathbf{r}_2,\mathbf{r}_3\,|\,\alpha n(t))}{\delta n(\mathbf{r}_1,t)} \tag{3.15}$$

Transforming then the term (3.14) with the help of the identity

$$\int_0^1 d\alpha\,\alpha g_2(\mathbf{r}_1,\mathbf{r}_2\,|\,\alpha n(t)) =\frac{1}{2}g_2(\mathbf{r}_1,\mathbf{r}_2\,|\,n(t)) -\frac{1}{2}\int d\mathbf{r}_3\, n(\mathbf{r}_3,t)\int_0^1 d\alpha\,\alpha\frac{\delta g_2(\mathbf{r}_1,\mathbf{r}_2\,|\,\alpha n(t))}{\delta n(\mathbf{r}_3,t)} \tag{3.16}$$

we can write the sum of (3.14) and (3.15) as

$$\begin{aligned}
&\frac{k_B}{2}\int d\mathbf{r}_2 \int d\hat{\boldsymbol{\varepsilon}}\, a^2\hat{\boldsymbol{\varepsilon}} \cdot [\mathbf{u}(\mathbf{r}_1, t) - \mathbf{u}(\mathbf{r}_2, t)] \\
&\quad \times \delta(\mathbf{r}_{12} - a\hat{\boldsymbol{\varepsilon}})\, n(\mathbf{r}_1, t)\, n(\mathbf{r}_2, t)\, g_2(\mathbf{r}_1, \mathbf{r}_2 \,|\, n(t)) \\
&\quad + \frac{k_B}{2}\int d\mathbf{r}_2 \int d\mathbf{r}_3 \int d\hat{\boldsymbol{\varepsilon}}\, a^2\hat{\boldsymbol{\varepsilon}} \cdot \{[\mathbf{u}(\mathbf{r}_2, t) - \mathbf{u}(\mathbf{r}_3, t)]\, \delta(\mathbf{r}_{23} - a\hat{\boldsymbol{\varepsilon}}) \\
&\quad - [\mathbf{u}(\mathbf{r}_1, t) - \mathbf{u}(\mathbf{r}_3, t)]\, \delta(\mathbf{r}_{13} - a\hat{\boldsymbol{\varepsilon}})\} \\
&\quad \times n(\mathbf{r}_1, t)\, n(\mathbf{r}_2, t)\, n(\mathbf{r}_3, t) \int_0^1 d\alpha\, \alpha \frac{\delta g_2(\mathbf{r}_2, \mathbf{r}_3 \,|\, \alpha n(t))}{\delta n(\mathbf{r}_1, t)} \qquad (3.17)
\end{aligned}$$

In the first term in Eq. (3.17) the integrand is symmetric with respect to variables $\mathbf{r}_1, \mathbf{r}_2$. We interpret it as a source term. With the notation (1.4) and (3.6) it takes the form

$$\begin{aligned}
\sigma_s^{\mathrm{corr}}(\mathbf{r}_1, t) = \frac{k_B}{2}\int d\mu\, [&f_2^{\mathrm{E}}(\mathbf{r}_1, \mathbf{v}_1', \mathbf{r}_1 + a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2'; t) \\
&- f_2^{\mathrm{E}}(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_1 + a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2; t)] \qquad (3.18)
\end{aligned}$$

In the second term in Eq. (3.17) the integrand is antisymmetric under the permutation $(\mathbf{r}_1, \mathbf{r}_2) \rightarrow (\mathbf{r}_2, \mathbf{r}_1)$. We can thus apply Eq. (3.7), finding the contribution to the entropy flow of the form

$$\begin{aligned}
&\mathbf{J}_s^{\mathrm{corr}}(\mathbf{r}_1, t) \\
&\quad = -\frac{k_B}{2}\int_0^1 d\lambda \int d\mathbf{r}\, \mathbf{r} \int d\mu\, \{f_1(\mathbf{r}_1 - \lambda\mathbf{r}, \mathbf{v}_1'; t)\, f_1(\mathbf{r}_1 - \lambda\mathbf{r} - a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2'; t) \\
&\quad\quad - f_1(\mathbf{r}_1 - \lambda\mathbf{r}, \mathbf{v}_1; t)\, f_1(\mathbf{r}_1 - \lambda\mathbf{r}_1 - a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2; t)\}\, n(\mathbf{r}_1 + (1-\lambda)\,\mathbf{r}, t) \\
&\quad\quad \times \frac{\delta}{\delta n(\mathbf{r}_1 + (1-\lambda)\,\mathbf{r}, t)} \int_0^1 d\alpha\, \alpha g_2(\mathbf{r}_1 - \lambda\mathbf{r}, \mathbf{r}_1 - \lambda\mathbf{r} - a\hat{\boldsymbol{\varepsilon}} \,|\, \alpha n(t)) \qquad (3.19)
\end{aligned}$$

where again the notation (3.6) has been used. In terms of quantities (3.18) and (3.19), Eq. (3.12) becomes

$$\frac{\partial}{\partial t}(ns^{\mathrm{corr}}) + \frac{\partial}{\partial \mathbf{r}_1} \cdot (\mathbf{u}ns^{\mathrm{corr}} + J_s^{\mathrm{corr}}) = \sigma_s^{\mathrm{corr}} \qquad (3.20)$$

Adding up Eq. (3.8) and (3.20), we arrive at the balance equation for the total entropy density (2.1):

$$\frac{\partial}{\partial t}(ns^{\mathrm{E}}) + \frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{u}ns^{\mathrm{E}} + \mathbf{J}_s^{\mathrm{E}}) = \sigma_s^{\mathrm{E}} \qquad (3.21)$$

The flow term is the sum of the convective current density $\mathbf{u}ns^{\mathrm{E}}$ and the three contributions given by Eqs. (3.4) and (3.19). We thus have

$$\begin{aligned}
\mathbf{J}_s^{\mathrm{E}}(\mathbf{r}_1, t) = & -k_{\mathrm{B}} \int d\mathbf{v}_1 [\mathbf{v}_1 - \mathbf{u}(\mathbf{r}_1, t)]\, f_1(\mathbf{r}_1, \mathbf{v}_1; t) \ln[h^3 f_1(\mathbf{r}_1, \mathbf{v}_1; t)] \\
& + \frac{k_{\mathrm{B}}}{2} \int_0^1 d\lambda \int d\mu \left\{ a\hat{\boldsymbol{\varepsilon}} f_2^{\mathrm{E}}(\mathbf{r}_1 - \lambda a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_1, \mathbf{r}_1 + (1-\lambda)\, a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2; t) \right. \\
& \times \ln \frac{f_1(\mathbf{r}_1 - \lambda a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_1'; t)}{f_1(\mathbf{r}_1 - \lambda a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_1; t)} \\
& - \int d\mathbf{r}\, \mathbf{r} [f_2^{\mathrm{E}}(\mathbf{r}_1 - \lambda \mathbf{r}, \mathbf{v}_1', \mathbf{r}_1 - \lambda \mathbf{r} - a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2'; t) \\
& - f_2^{\mathrm{E}}(\mathbf{r}_1 - \lambda \mathbf{r}, \mathbf{v}_1, \mathbf{r}_1 - \lambda \mathbf{r} - a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2; t)] \\
& \left. \times n(\mathbf{r}_1 + (1-\lambda)\, \mathbf{r}, t) \int_0^1 d\alpha\, \alpha \frac{\delta \ln g_2(\mathbf{r}_1 - \lambda \mathbf{r}, \mathbf{r}_1 - \lambda \mathbf{r} - a\boldsymbol{\varepsilon} \mid \alpha n(t))}{\delta n(\mathbf{r}_1 + (1-\lambda)\, \mathbf{r}, t)} \right\}
\end{aligned} \tag{3.22}$$

The source term σ_s^{E} is obtained by adding up the contributions (3.10) and (3.18). It is thus equal to

$$\begin{aligned}
\sigma_s^{\mathrm{E}}(\mathbf{r}_1, t) = & \frac{k_{\mathrm{B}}}{2} \int d\mu \left[f_2^{\mathrm{E}}(\mathbf{r}_1, \mathbf{v}_1', \mathbf{r}_1 + a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2'; t) \right. \\
& - f_2^{\mathrm{E}}(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_1 + a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2; t) \\
& \left. - f_2^{\mathrm{E}}(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_1 + a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2; t) \ln \frac{f_2^{\mathrm{E}}(\mathbf{r}_1, \mathbf{v}_1', \mathbf{r}_1 + a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2'; t)}{f_2^{\mathrm{E}}(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_1 + a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2; t)} \right]
\end{aligned} \tag{3.23}$$

As $x - y + y \ln(y/x) \geqslant 0$, for $x > 0$, $y > 0$, it follows from (3.23) that

$$\sigma_s^{\mathrm{E}}(\mathbf{r}, t) \geqslant 0 \tag{3.24}$$

The fundamental inequality (3.24) enables us indeed to consider the intuitive definition (2.1)–(2.3) as a proper generalization of the concept of the entropy density $s(\mathbf{r}, t)$ to nonequilibrium states whose evolution is described by the revised Enskog equation (1.5). With the entropy production nonnegative, Eq. (3.21) can be looked upon as a local formulation of the H-theorem for the kinetic equation (1.5). In fact, integrating the density $h(\mathbf{r}, t) = -k_{\mathrm{B}}^{-1} n(\mathbf{r}, t)\, s^{\mathrm{E}}(\mathbf{r}, t)$ over the volume of the fluid, one recovers the H-functional constructed by Résibois. The condition for H to reach a stationary value is equivalent to vanishing of the entropy source (3.23), i.e.,

$$f_1(\mathbf{r}_1, \mathbf{v}_1)\, f_1(\mathbf{r}_1 + a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2) \equiv f_1(\mathbf{r}_1, \mathbf{v}_1')\, f_1(\mathbf{r}_1 + a\hat{\boldsymbol{\varepsilon}}, \mathbf{v}_2') \tag{3.25}$$

The consequences of Eq. (3.25) [combined with the Enskog equation (1.5)] already have been discussed by Résibois (under periodic boundary conditions). Clearly, the equilibrium Maxwell distribution (with constant density) satisfies Eq. (3.25). Whether this is the only solution (for more general boundary conditions) remains to be clarified.

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