Comments on nonlinear viscosity and Grad's moment method

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It is shown that the steady unidirectional flow with vanishing heat flux considered by B. C. Eu [Phys. Rev. E **65**, 031202 (2002)], and earlier by Uribe and García-Colín [Phys. Rev. E **60**, 4052 (1999)], is inconsistent with the exact conservation laws of mass, momentum, and energy. The inconsistency does not lie in the assumed symmetry properties of the flow but in the stationarity assumption. The unsteady problem is considered and its solution from the Boltzmann equation for Maxwell molecules is given.

In a recent paper [1], Eu analyzed a *steady* unidirectional flow at uniform temperature and derived the equations for the stress tensor elements from the Boltzmann equation by means of Grad's moment method. These are essentially the same state and the same method as those considered by Uribe and García-Colín [2], except that the transversal velocity gradients were assumed to vanish in Ref. [2], while they are included in the analysis of Ref. [1]. The major aim of this Comment is to show that the steady unidirectional flow at uniform temperature of Refs. [1,2] is inconsistent with the exact macroscopic conservation equations.

For a dilute monatomic gas, the macroscopic balance equations expressing the conservation of mass, momentum, and energy are [3,4]

$$D_t n + n \boldsymbol{\nabla} \cdot \mathbf{u} = 0, \tag{1}$$

$$D_t \mathbf{u} + \frac{1}{mn} \boldsymbol{\nabla} \cdot \mathsf{P} = \mathbf{0}, \tag{2}$$

$$D_t T + \frac{2}{3nk_B} (\boldsymbol{\nabla} \cdot \mathbf{q} + \mathsf{P}:\boldsymbol{\nabla}\mathbf{u}) = 0, \tag{3}$$

where $D_t \equiv \partial_t + \mathbf{u} \cdot \boldsymbol{\nabla}$ is the material time derivative, n is the local number density, $\mathbf{u}$ is the local flow velocity, T is the local temperature, m is the mass of a particle, k_B is the Boltzmann constant, $\mathbf{q}$ is the heat flux vector, and P is the pressure (or stress) tensor. The flow considered in Refs. [1,2] is characterized by the following properties (not necessarily independent): (a) it is a unidirectional flow, i.e., $\mathbf{u}(\mathbf{r}) = u_x(\mathbf{r})\hat{\mathbf{x}}$, where $\hat{\mathbf{x}}$ is the unit vector along the flow direction; (b) the temperature is uniform, $\boldsymbol{\nabla} T = \mathbf{0}$; (c) the heat flux vanishes, $\mathbf{q} = \mathbf{0}$; (d) the pressure tensor is uniform; and (e) the state is stationary, i.e., $\partial_t \rightarrow 0$. Let me consider first the geometrical properties (a)–(d) separately from the stationarity assumption (e). Application of assumptions (a)–(d) on the exact balance equations (1)–(3) yields

$$\partial_t n + \frac{\partial}{\partial x}(nu_x) = 0, \tag{4}$$

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$$\partial_t u_x + u_x \frac{\partial}{\partial x} u_x = 0, \tag{5}$$

$$\frac{3nk_B}{2} \partial_t T + P_{xx} \frac{\partial u_x}{\partial x} + P_{xy} \frac{\partial u_x}{\partial y} + P_{xz} \frac{\partial u_x}{\partial z} = 0. \tag{6}$$

Are Eqs. (4)–(6) consistent with a steady state? Equation (5) shows that the flow velocity is stationary if and only if the flow is incompressible, i.e., if $\partial u_x/\partial x = 0$. In that particular case, Eq. (4) is consistent with a stationary density if and only if the density is uniform as well. But, even if $\partial u_x/\partial x = 0$ and $n = $ const, energy balance equation (6) implies that the temperature cannot be stationary but monotonically increases with time due to viscous heating effects (note that $P_{xy}\partial u_x/\partial y < 0$ and $P_{xz}\partial u_x/\partial z < 0$ because of physical reasons). Therefore, the steady state assumption (e) is incompatible with assumptions (a)–(d), except in the trivial case $\boldsymbol{\nabla} u_x = \mathbf{0}$, i.e., at equilibrium. The *unsteady* Boltzmann equation for the incompressible unidirectional flow with $\partial u_x/\partial x = \partial u_x/\partial z = 0$, $\partial u_x/\partial y = $ const, usually referred to as uniform shear flow or homoenergetic simple shear flow, has been solved *exactly* for arbitrary shear rates in the case of Maxwell molecules [5–7]. An analogous solution has been obtained in the case of the BGK model kinetic equation for more general interactions [8–10].

In the case of a compressible flow in the absence of transversal gradients, i.e. $\boldsymbol{\nabla} u_x \| \hat{\mathbf{x}}$, Eq. (5) shows that the flow velocity is necessarily unsteady. According to continuity equation (4), it is still mathematically possible that $\partial_t n = 0$ if the product nu_x is uniform, i.e. $n(x)u_x(x,t) = K(t)$. Insertion of this condition into Eq. (5) yields $K^{-2}\dot{K}(t) = n^{-2}n'(x) = -A^{-1}$, where the dot denotes a time derivative, the prime denotes a spatial derivative, and A is a constant. The solution to these equations is simply $n(x) = A/(x-x_0)$, $u_x(x,t) = a(x-x_0)/(1+at)$, where x_0 and a are constants. This mathematical solution is unphysical unless the problem is restricted to the half domain $x > x_0$ ($x < x_0$) if $A > 0$ ($A < 0$). But even in that case the existence of a nonuniform density is in conflict with the uniformity assumptions (b) and (d) because in a dilute gas $n = p/k_B T$, where $p = \frac{1}{3}\mathrm{tr}\,\mathsf{P}$ is the hydrostatic pressure. In summary, assumptions (a)–(d) do not contradict the conservation laws (1)–(3) in the compressible flow with $\partial u_x/\partial x \neq 0$ if and only if the three hydrody-

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namic quantities (density, flow velocity, and temperature) are unsteady, so assumption (e) is again incompatible with (a)–(d).

Strictly speaking, assumptions (b) and (d), i.e., uniform temperature and pressure tensor, were not explicitly stated in Ref. [2]. Actually, assumption (b) is implicit in (c); otherwise, one would have a thermal gradient that does not produce any heat flux, what is at odds with the second principle of thermodynamics. As for assumption (d), it was replaced in Ref. [2] by a weaker one: (d′) the *irreversible* part of the pressure tensor is uniform, namely, $\partial(P_{xx}-p)/\partial x=0$. From a physical point of view it seems difficult to concile a uniform normal stress difference $P_{xx}-p$ with a nonuniform hydrostatic pressure p. In any case, let me drop conditions (b) and (d) for the moment and prove that conditions (a), (c), (d′), and (e) are also inconsistent with the conservation laws, except at equilibrium. Application of (a), (c), and (e) on Eqs. (1)–(3) gives

$$\frac{\partial}{\partial x}(nu_x)=0, \tag{7}$$

$$mnu_x\frac{\partial}{\partial x}u_x+\frac{\partial}{\partial x}P_{xx}=0, \tag{8}$$

$$\frac{3}{2}nk_Bu_x\frac{\partial}{\partial x}T+P_{xx}\frac{\partial}{\partial x}u_x=0, \tag{9}$$

where, as in Ref. [2], the case $\boldsymbol{\nabla}u_x\|\hat{\mathbf{x}}$ has been considered. Equations (7)–(9) can be easily integrated to get

$$nu_x=n_0u_0=\text{const}, \tag{10}$$

$$P_{xx}+mnu_x^2=P_0+mn_0u_0^2=\text{const}, \tag{11}$$

$$\left(\frac{3}{2}p+P_{xx}+\frac{m}{2}nu_x^2\right)u_x=\left(\frac{3}{2}p_0+P_0+\frac{m}{2}n_0u_0^2\right)u_0$$

$$=\text{const}, \tag{12}$$

where the subscript 0 denotes quantities evaluated at some reference point $x=x_0$. So far, assumption (d′) has not been used. This condition implies that $P_{yy}-p=P_0-p_0=\text{const}$, so that, according to Eq. (11),

$$p+mnu_x^2=p_0+mn_0u_0^2=\text{const}. \tag{13}$$

Insertion of Eqs. (11) and (13) into Eq. (12) yields

$$\left[\frac{3}{2}p_0+P_0+mn_0u_0\left(\frac{1}{2}u_0-2u_x\right)\right](u_x-u_0)=0. \tag{14}$$

Both solutions of this quadratic equation are constants (but the physical one is $u_x=u_0$). This closes the proof that assumptions (a), (c), (d′), and (e) are not consistent with the conservation equations except in the trivial case $u_x=\text{const}$.

On the other hand, there is nothing wrong with assumptions (a)–(d) in the unsteady case. What is then the right form of n and u_x if $\boldsymbol{\nabla}u_x\|\hat{\mathbf{x}}$? Since assumptions (b) and (d)

imply that n is uniform, Eq. (4) states that $-\partial u_x/\partial x=n^{-1}\dot{n}=-K(t)$, so $u_x(x,t)=K(t)(x-x_0)$. Substitution into Eq. (5) gives $K^{-2}\dot{K}=-1$, so we finally have $n(t)=n_0/(1+at)$, $u_x(x,t)=a(x-x_0)/(1+at)$. This simple flow is known as homoenergetic extension [6,11]. Again, the *unsteady* Boltzmann equation can be solved *exactly* for arbitrary values of the constant control parameter a in the case of Maxwell molecules [6,11,12], as well as with Grad's method [13] and in the case of the BGK model kinetic equation [12] for more general interactions. A situation where a transversal velocity gradient $\partial u_y/\partial x$ coexists with a longitudinal one $\partial u_x/\partial x$ has been studied by Galkin [11].

It is illustrative to recall the application of Grad's method to the *unsteady* unidirectional flow at uniform temperature with no transversal gradients [13]. We have seen above that conservation of mass and momentum imply that $n(t)=n_0/(1+at)$ and $\gamma_x(t)\equiv\partial u_x(x,t)/\partial x=an(t)/n_0$. Positive values of the longitudinal deformation rate γ_x represent some sort of "explosion" (or expansion) flow, while negative values represent an "implosion" (or condensation) flow [2]. The energy balance equation (3) becomes

$$\partial_t p+\left(p+\frac{2}{3}P_{xx}\right)\gamma_x=0. \tag{15}$$

In Grad's method, this equation is coupled to the (approximate) evolution equation for the stress element P_{xx} [13]:

$$\partial_t(P_{xx}-p)+\left(P_{xx}-p+\frac{4}{3}P_{xx}\right)\gamma_x=-\mu(P_{xx}-p), \tag{16}$$

where nonlinear terms have been neglected on the right-hand side and $\mu=p/\eta_{\text{NS}}$ is an effective collision frequency, η_{NS} being the Navier-Stokes shear viscosity. Equation (16) is equivalent to Eq. (21) of Ref. [2], except that the time derivative is absent in the latter. Without the time derivative operator, however, Eq. (16) cannot be made consistent with Eq. (15). After a transient regime, the system reaches a generalized hydrodynamic regime with $P_{ij}(t)=p(t)P_{ij}^*(\gamma_x^*(t))$, where $\gamma_x^*(t)\equiv\gamma_x(t)/\mu(t)$ is the *reduced* longitudinal deformation rate. In general, from Eqs. (15) and (16) one gets a nonlinear first-order ordinary differential equation for $P_{xx}^*(\gamma_x^*)$ [12,13]. In the special case of Maxwell molecules (i.e., $\mu\propto n$), γ_x^* (but not γ_x) is independent of time so one gets from Eqs. (15) and (16) an algebraic quadratic equation whose physical solution is $P_{xx}^*=3-2P_{yy}^*$, where

$$P_{yy}^*(\gamma_x^*)=\frac{3}{8\gamma_x^*}\left(\sqrt{1+\frac{4}{3}\gamma_x^*+4\gamma_x^{*2}}-1+2\gamma_x^*\right). \tag{17}$$

It turns out that this result for Maxwell molecules goes beyond the scope of Grad's method, since it can be exactly derived from the Boltzmann equation [6,11,12].

To the best of my knowledge, Grad's method has not been applied yet to the unsteady unidirectional flow at uniform

temperature with transversal gradients. For this flow, an analysis of Eqs. (4) and (5) shows that, in addition to $n(t) = n_0/(1+at)$ and $\gamma_x \equiv \partial u_x/\partial x = an(t)/n_0$, one generally has shear rates $\gamma_{yx} \equiv \partial u_x/\partial y = a_2 n(t)/n_0$ and $\gamma_{zx} \equiv \partial u_x/\partial z = a_3 n(t)/n_0$, where a, a_2, and a_3 are independent constants. Standard application of Grad's method yields the following evolution equation for the elements of the stress tensor:

$$\partial_t P_{ij} + P_{ij}\frac{\partial u_x}{\partial x} + \sum_{k=1}^{3}(P_{ik}\delta_{jx}+P_{jk}\delta_{ix})\frac{\partial u_x}{\partial x_k}$$

$$= -\mu(P_{ij}-p\,\delta_{ij}). \tag{18}$$

Taking the trace in this equation one recovers the energy conservation equation (6). It is worth noting that Eq. (18) can again be obtained exactly from the Boltzmann equation in the case of Maxwell molecules. For this interaction potential, the reduced rates $\gamma_x^* \equiv \gamma_x/\mu$, $\gamma_{yx}^* \equiv \gamma_{yx}/\mu$, and $\gamma_{zx}^* \equiv \gamma_{zx}/\mu$ are constants and Eq. (18) yields a coupled set of algebraic equations for $P_{ij}^* \equiv P_{ij}/p$. Without loss of generality [14] we can choose $\gamma_{zx}^* = \gamma_{yx}^*$, so that $P_{yy}^* = P_{zz}^*$ and $P_{xy}^* = P_{xz}^*$. In that case, Eq. (18) yields

$$\gamma_x^* = \frac{3P_{yy}^*(1-P_{yy}^*)-4P_{xy}^{*\,2}}{2P_{yy}^*[2P_{xy}^{*\,2}-P_{yy}^*(3-2P_{yy}^*)]}, \tag{19}$$

$$\gamma_{yx}^* = \frac{P_{xy}^*(3-P_{yy}^*)}{2P_{yy}^*[2P_{xy}^{*\,2}-P_{yy}^*(3-2P_{yy}^*)]}. \tag{20}$$

These two equations include as particular cases the homoenergetic extension flow ($\gamma_{yx}^* = 0$), in which case Eq. (17) is recovered, as well as the uniform shear flow ($\gamma_x^* = 0$), where $P_{xy}^{*\,2} = \frac{3}{4}P_{yy}^*(1-P_{yy}^*)$ and P_{yy}^* is the solution of the cubic equation $4\gamma_{yx}^{*\,2}P_{yy}^{*\,3} = 3(1-P_{yy}^*)$.

The inconsistency of assumption (e) on the stationarity of the flow geometrically characterized by (a)–(d) [or (a), (c), and (d′)] manifests itself in the results obtained in Refs. [1] and [2] for the stress tensor elements from Grad's method. Assuming cylindrical symmetry ($P_{xy} = P_{xz}$, $P_{yy} = P_{zz}$), Eu gets the following expression for the normal pressure element P_{yy} (neglecting nonlinear terms in the collisional integrals) [1]:

$$P_{yy}^* = 3\frac{(1+2\gamma_x^*)(1+3\gamma_x^*)}{(1+2\gamma_x^*)(3+7\gamma_x^*)+4\gamma_{yx}^{*\,2}}. \tag{21}$$

According to Eq. (21), P_{yy} becomes *negative* at least in the interval $-\frac{3}{7} < \gamma_x^* < -\frac{1}{3}$, regardless of the value of γ_{yx}^*. This is unphysical because the diagonal elements of the pressure tensor are positive definite quantities. Setting $\gamma_{yx}^* = 0$, Eq. (21) reduces to the result derived by Uribe and García-Colín in the linear approximation [2]. When the nonlinear terms are included, they get [2]

$$P_{yy}^* = 8 + \frac{49}{3}\gamma_x^* - 7\sqrt{1+\frac{94}{21}\gamma_x^* + \frac{49}{9}\gamma_x^{*\,2}}. \tag{22}$$
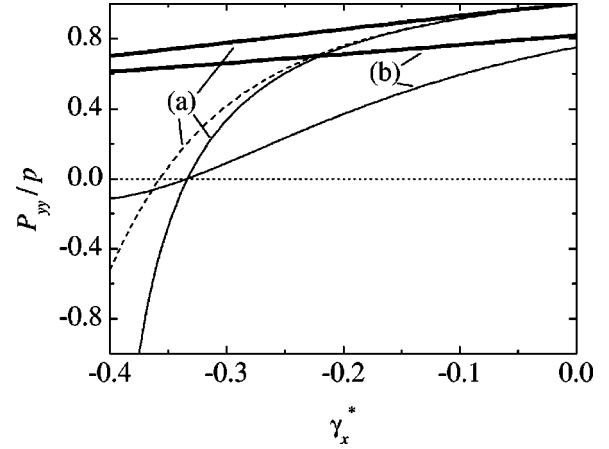

FIG. 1. Plot of the normal pressure element P_{yy} relative to the hydrostatic pressure p, as derived in Refs. [1,2], versus the longitudinal deformation rate in the range $-0.4 \leq \gamma_x^* \leq 0$ for (a) zero shear rate ($\gamma_{yx}^* = 0$) and (b) $\gamma_{yx}^* = \frac{1}{2}$. The thin solid lines correspond to the linear approximation, Eq. (21), while the dashed line in case (a) corresponds to the nonlinear approximation, Eq. (22). The thick solid lines represent the exact results for Maxwell molecules.

According to this expression, $P_{yy} < 0$ if $\gamma_x^* < -\frac{5}{14}$. The prediction of negative values of P_{yy} can be observed in Fig. 1, which shows the ratio P_{yy}/p given by Eqs. (21) and (22) in the range $-0.4 \leq \gamma_x^* \leq 0$ for vanishing shear rate ($\gamma_{yx}^* = 0$) and for $\gamma_{yx}^* = \frac{1}{2}$. Comparison with the exact results (17) for $\gamma_{yx}^* = 0$ and Eqs. (19) and (20) for $\gamma_{yx}^* \neq 0$ in the case of Maxwell molecules shows that predictions (21) and (22) are only valid in the Navier-Stokes domain of small gradients, where $P_{yy}/p \approx 1 + \frac{2}{3}\gamma_x^*$. It is worth noting that the application to the unidirectional flow of a rheological theory by Eu [15] also yields unphysical negative values for the diagonal elements of the pressure tensor [16].

In Ref. [1], Eu claims that Grad's moment method is not thermodynamically consistent [17]. Actually, Grad's method is not but an approximate scheme for (partially) solving the hierarchy of moment equations stemming from the Boltzmann equation. The point I want to emphasize is that the physical inconsistency of the equations for the stress tensor elements derived in Refs. [1,2] does not lie in the use of Grad's method (even if nonlinear terms are neglected), but in the wrong ansatz about the stationarity of the flow. In fact, as said before, the application of Grad's method to the unidirectional flow at uniform temperature for Maxwell molecules gives the same evolution equations for the stress elements as the Boltzmann equation. Therefore, at least in this instance, Grad's method is free from any thermodynamic inconsistency.

It might be argued that assumptions (a)–(e) [or (a), (c), (d′), and (e)] are used in Refs. [1,2] only as a tool to derive *rheological* constitutive equations relating the irreversible part of the stress tensor to the velocity gradients in a *nonlinear* way by means of Grad's method. Such constitutive equations could then be applied to the conservation equations (1)–(3) regardless of whether the flow is steady or not, whether the pressure is uniform or not, etc. However, it is doubtful that a constitutive equation derived from assump-

tions incompatible with the conservation laws can be acceptable beyond the Navier-Stokes regime, as Fig. 1 illustrates.

Before closing this paper, let me comment on a couple of remarks made in Ref. [1] which are not directly related to the discussion made so far. First, Eu states that "the shear viscosity is impossible to define" in the absence of transversal velocity gradients and, consequently, "it is impossible to measure a shear viscosity without shearing the fluid." This is misleading. To clarify this point, take the Navier-Stokes constitutive equations, namely [4],

$$P_{ij} = p\,\delta_{ij} - \eta_{\mathrm{NS}}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\boldsymbol{\nabla}\cdot\mathbf{u}\,\delta_{ij}\right). \quad (23)$$

In the special case of a unidirectional flow $\mathbf{u} = u_x\hat{\mathbf{x}}$, Eq. (23) yields

$$P_{xy} = -\eta_{\mathrm{NS}}\frac{\partial u_x}{\partial y}, \quad \frac{1}{2}(P_{xx} - P_{yy}) = -\eta_{\mathrm{NS}}\frac{\partial u_x}{\partial x}. \quad (24)$$

Thus, to Navier-Stokes order, the response of the shear stress P_{xy} to a shear rate $\partial u_x/\partial y$ is the same as the response of the normal stress difference $(P_{xx} - P_{yy})/2$ to a longitudinal deformation rate $\partial u_x/\partial x$. As a consequence, the Navier-Stokes shear viscosity can be measured from the normal stress difference, even in the absence of shearing ($\partial u_x/\partial y = 0$).

The second point refers to Eu's claim [1] that the velocity distribution function $f(\mathbf{r},\mathbf{v};t)$ obeying the Boltzmann equation must *always* depend on the three spatial coordinates despite the fact that the hydrodynamic variables may depend on one space coordinate only, e.g., $n(x,t)$, $\mathbf{u}(x,t)$, $T(x,t)$. In support of this claim, Eu recalls that "even if the fluid particle moves one dimensionally in its hydrodynamic configuration space, it does not mean that the molecules making up the fluid particle and contained in the elementary volume of the hydrodynamic configuration space $[\cdots]$ should be mov-

ing one dimensionally." While the quoted sentence is entirely correct, Eu's conclusion, namely, that one cannot have $f(\mathbf{r},\mathbf{v},t) = f(x,\mathbf{v},t)$, does not apply to the Boltzmann velocity distribution function $f(\mathbf{r},\mathbf{v},t)$ but to the *microscopic* one-body distribution function defined by

$$F(\mathbf{r},\mathbf{v},t) = \sum_{i=1}^{N}\delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{v} - \mathbf{v}_i(t)), \quad (25)$$

where $\{\mathbf{r}_i(t), i = 1,\ldots,N\}$ and $\{\mathbf{v}_i(t), i = 1,\ldots,N\}$ are the sets of positions and velocities of the particles of the system at time t. Actually, the velocity distribution function $f(\mathbf{r},\mathbf{v},t)$ is the *average* of $F(\mathbf{r},\mathbf{v},t)$,

$$f(\mathbf{r},\mathbf{v},t) = \langle F(\mathbf{r},\mathbf{v},t)\rangle = \int d\Gamma\, F(\mathbf{r},\mathbf{v},t)\rho(\Gamma), \quad (26)$$

where $\rho(\Gamma)$ is the probability density or ensemble for the initial state and the integration is carried out over all the points Γ of the phase space. While in a given microscopic realization of the system $F(\mathbf{r},\mathbf{v},t)$ is a highly nonuniform function, its statistical average $f(\mathbf{r},\mathbf{v},t)$ has a much smoother spatial dependence. In particular, it can depend on one coordinate only or it can even be uniform (e.g., at equilibrium). Of course, the fact that the hydrodynamic fields have a one-dimensional spatial dependence does not necessarily mean that the same holds to f, but there is nothing wrong if one restricts oneself to solutions to the Boltzmann equation with the same symmetry properties as the hydrodynamic fields. In fact, the so-called normal solutions are those that depend on space and time through a *functional* dependence on the hydrodynamic fields [4].

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[14] Note that if we perform a rotation on the y-z plane and define the new axes $y' = (\gamma_{yx}y + \gamma_{zx}z)/\sqrt{\gamma_{yx}^2 + \gamma_{zx}^2}$, $z' = (\gamma_{zx}y - \gamma_{yx}z)/\sqrt{\gamma_{yx}^2 + \gamma_{zx}^2}$, then we have the "canonical" form $\partial u_x/\partial y' = \sqrt{\gamma_{yx}^2 + \gamma_{zx}^2}$, $\partial u_x/\partial z' = 0$. Thus the true physical independent parameters are the longitudinal deformation rate γ_x and the shear rate $\sqrt{\gamma_{yx}^2 + \gamma_{zx}^2}$.

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[17] For a criticism of this statement, see Ref. [16].