Approach to a non-equilibrium steady state

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Abstract

We consider a non-interacting one-dimensional gas accelerated by a constant and uniform external field. The energy absorbed from the field is transferred via elastic collisions to a bath of scattering obstacles. At gas-obstacle encounters the particles of the gas acquire a fixed kinetic energy. The approach to the resulting stationary state is studied within the Boltzmann kinetic theory. It is shown that the long time behavior is governed by the hydrodynamic mode of diffusion superposed on a convective flow. The diffusion coefficient is analytically calculated for any value of the field showing a minimum at intermediate field intensities. It is checked that the properly generalized Green-Kubo formula applies in the non-equilibrium stationary state.

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1 Introduction

The problem of constructing adequate statistical ensembles for non-equilibrium stationary states (hereafter denoted by NESS) has a long history (see e.g. [1,2]). Related to it there are very interesting findings concerning the nature of fluctuations in the presence of spatial gradients inducing stationary flows [3]. The computation of exact expressions for the probability distribution of simple NESS allows to study different static properties as, for example, the

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long range density correlations [4]. The recent development of the theory of fluidized granular matter has also attracted a lot of attention to the structure of NESS (see for example [5,6,7]). Finally, there is at present an important research carried on in order to properly define the entropy production accompanying stationary dissipative currents (see e.g. [8]).

However, whereas the modes of approach of fluids to thermal equilibrium are well understood, there is still no satisfactory theory of the dynamics of reaching NESS. In both cases the final state is stationary, but in NESS, in contradistinction to equilibrium, there persist non-vanishing fluxes sustained by the coupling to environment.

The kinetic theory of fluids revealed the fundamental role of the separation between different time scales in the approach to equilibrium (see e.g. the presentation of Bogoliubov's ideas in [9]). In particular, in the evolution of the density of particles in the one-particle phase space all the degrees of freedom but those represented by the densities of globally conserved quantities relax at a short time scale producing a state close to local equilibrium. The subsequent slow evolution is essentially governed by changes of the hydrodynamic fields (an original construction of the hydrodynamic modes within the kinetic theory has been developed by P. Résibois [10]). One can wonder whether this kind of mechanism based on the time-scale separation still persists when the final state involves some dissipative stationary process related to the current flowing through the system. This is precisely the question we want to address in this paper.

Our object here is to exploit an analytically soluble one-dimensional model discussed in [11] in order to perform a detailed study of the evolution towards a NESS. Although the system is very simple indeed, we find that the possibility of a rigorous study of its dynamics is precious from the point of view of the search for the laws governing the approach to NESS. The coupling to the environment is represented in the model by the action of an external field. One of the original results of the paper is an explicit formula for the field dependent coefficient of diffusion governing the evolution of the only hydrodynamic mode in the approach to the stationary state.

In Sec. 2 we define the system and its dynamics. The following analysis of the approach to the stationary state is presented in Sec. 3. Finally, Sec. 4 contains the concluding comments.

2 One-dimensional system and its dynamics

We consider non-interacting point particles of mass m moving in one dimension with acceleration a under the influence of an external constant and uniform field. The particles are surrounded by a bath of point obstacles of mass mthat move with velocities $\pm U$, both directions being equally probable. At elastic collisions between the particles and the obstacles a simple interchange of velocities is taking place. The scattering obstacles are uniformly distributed with a number density n.

The statistical state of the particles is described by the probability density f(r, v, t) for finding a particle at time t at point r with velocity v. We assume that the evolution of the density f(r, v; t) is governed by the linear Boltzmann equation [11]

$$\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial r} + a\frac{\partial}{\partial v}\right)f(r, v, t) = n\int dc|v - c|\left[f(r, c, t)\phi(v) - f(r, v, t)\phi(c)\right],$$
(1)

putting

$$\phi(v) = \frac{1}{2} \left[\delta(v+U) + \delta(v-U) \right] \tag{2}$$

for the velocity distribution of the obstacles. When writing equation (1) it has been supposed that the particles always encountered obstacles with velocities distributed according to (2). The possibility of recollisions with obstacles perturbed by previous collisions with the particles is not taken into account by the Boltzmann collision term in (1).

In dimensionless variables w = v/U, x = nr, and $\tau = Unt$ equation (1) takes the form

$$\left(\frac{\partial}{\partial\tau} + w\frac{\partial}{\partial x} + \epsilon\frac{\partial}{\partial w} + \frac{1}{2}(|w+1| + |w-1|)\right)F(x,w,\tau) = \frac{1}{2}[\delta(w-1)\mu_{-}(x,\tau) + \delta(w+1)\mu_{+}(x,\tau)],$$
(3)

where $F(x, w, \tau) = f(x/n, Uw, \tau/nU)U/n$ is the dimensionless probability density, and

$$\mu_{\pm}(x,\tau) = \int dw |w \pm 1| F(x,w,\tau).$$
(4)

In equation (3) there appears the dimensionless intensity of the field $\epsilon = a/nU^2$.

Provided that appropriate boundary conditions are supplied at $\pm \infty$, equation (3) has a non-equilibrium stationary solution representing a homogeneous NESS whose velocity distribution $F_0(w; \epsilon)$, that can be chosen to be normalized as $\int dw F_0(w; \epsilon) = 1$, has been derived and analyzed in [11]. The NESS

is characterized by a constant current $V_{\text{NESS}}(\epsilon) = \int dw w F_0(w; \epsilon)$ that shows a linear response, $V_{\text{NESS}}(\epsilon) \sim \epsilon$, in the weak field limit $|\epsilon| \ll 1$ and a non-linear response, $V_{\text{NESS}}(\epsilon) \sim \text{sgn}(\epsilon) \sqrt{|\epsilon|}$, for strong fields $|\epsilon| \gg 1$.

Whereas the paper [11] focused on the properties of the stationary distribution, our aim here is to analyze the approach to the asymptotic homogeneous NESS starting from an arbitrary inhomogeneous initial condition. This requires solving the time-dependent Boltzmann equation. The way towards the construction of the solution has been already found in [11]. Using the Fourier-Laplace transformation

$$\tilde{F}(k,w,z) = \int_0^\infty d\tau \int dx e^{-z\tau - ikx} F(x,w,\tau)$$
(5)

one finds from (3) the integral equation

$$\tilde{F}(k,w,z) = \tilde{H}(k,w,z) + \frac{1}{2|\epsilon|} \exp\left[-\frac{\chi(w)}{\epsilon} - ik\frac{w^2 - 1}{2\epsilon}\right] \\ \times \left\{ \exp\left[\frac{1 - z(w-1)}{\epsilon}\right] \theta[\epsilon(w-1)]\tilde{\mu}_-(k,z) \\ + \exp\left[-\frac{1 + z(w+1)}{\epsilon}\right] \theta[\epsilon(w+1)]\tilde{\mu}_+(k,z) \right\},$$
(6)

where

$$\chi(w) = \left[(w+1)|w+1| + (w-1)|w-1| \right]/4, \tag{7}$$

that obey the relation $\chi(w) = -\chi(-w)$,

$$\tilde{\mu}_{\pm}(k,z) = \int dw |w \pm 1| \tilde{F}(k,w,z), \qquad (8)$$

and

$$\tilde{H}(k,w,z) = \int_0^\infty e^{-z\tau - ikx} H(x,w,\tau)$$
(9)

relates to the initial condition F(x, w, 0) through

$$H(x, w, t) = \exp[(\chi(w - \epsilon\tau) - \chi(w))/\epsilon]F(x - w\tau + \epsilon\tau^2/2, w - \epsilon\tau, 0)$$
(10)

Eq. (6) is implicit expressing $\tilde{F}(k, w, z)$ in terms of $\tilde{\mu}_{\pm}(k, z)$ that are linear functionals of $\tilde{F}(k, w, z)$. However, the solution can be made explicit in a straightforward way. Indeed, multiplying Eq. (6) by $|w \pm 1|$ and integrating with respect to w one obtains a closed system of linear equations for $\tilde{\mu}_{\pm}$ in the form

$$\mathbf{M}(k,z;\epsilon) \cdot \begin{bmatrix} \tilde{\mu}_{-}(k,z) \\ \tilde{\mu}_{+}(k,z) \end{bmatrix} = \begin{bmatrix} h_{-}(k,z) \\ h_{+}(k,z) \end{bmatrix}.$$
(11)

Here

$$h_{\pm}(k,z) = \int dw |w \pm 1| \tilde{H}(k,w,z)$$
 (12)

and $\mathbf{M}(k, z; \epsilon)$ is a two by two matrix analytic in z given by

$$\mathbf{M}(k, z; \epsilon) = \begin{pmatrix} M_{11}(k, z; \epsilon), \ M_{12}(k, z; \epsilon) \\ M_{21}(k, z; \epsilon), \ M_{22}(k, z; \epsilon) \end{pmatrix},$$
(13)

with

$$M_{11} = \frac{1}{2|\epsilon|} \int dw |w-1| \exp\left[-\frac{\chi(w)}{\epsilon} - ik\frac{w^2 - 1}{2\epsilon}\right] \exp\left[\frac{1 - z(w-1)}{\epsilon}\right] \theta[\epsilon(w-1)]$$

$$M_{12} = \frac{1}{2|\epsilon|} \int dw |w-1| \exp\left[-\frac{\chi(w)}{\epsilon} - ik\frac{w^2 - 1}{2\epsilon}\right] \exp\left[-\frac{1 + z(w+1)}{\epsilon}\right] \theta[\epsilon(w+1)]$$

$$M_{21} = \frac{1}{2|\epsilon|} \int dw |w+1| \exp\left[-\frac{\chi(w)}{\epsilon} - ik\frac{w^2 - 1}{2\epsilon}\right] \exp\left[\frac{1 - z(w-1)}{\epsilon}\right] \theta[\epsilon(w-1)]$$

$$M_{22} = \frac{1}{2|\epsilon|} \int dw |w+1| \exp\left[-\frac{\chi(w)}{\epsilon} - ik\frac{w^2 - 1}{2\epsilon}\right] \exp\left[-\frac{1 + z(w+1)}{\epsilon}\right] \theta[\epsilon(w+1)].$$

When $\epsilon > 0$, the matrix $\mathbf{M}(k, z; \epsilon)$ takes the form

$$\mathbf{M}(k,z;\epsilon) = \begin{pmatrix} 1 - (A-B)e^{(2z+1)/2\epsilon}, & C-D + (B-A)e^{-(2z+3)/2\epsilon} \\ -(A+B)e^{(2z+1)/2\epsilon}, & 1 - (A+B)e^{-(2z+3)/2\epsilon} - C - D \end{pmatrix},$$
(14)

where

$$A(k,z;\epsilon) = \frac{1}{2\epsilon} \int_{1}^{\infty} dw \, w \exp\left\{-\frac{1}{2\epsilon} \left[w^2(1+ik) + 2wz - ik\right]\right\} \tag{15}$$

$$B(k,z;\epsilon) = \frac{1}{2\epsilon} \int_{1}^{\infty} dw \exp\left\{-\frac{1}{2\epsilon} \left[w^2(1+ik) + 2wz - ik\right]\right\}$$
(16)

$$C(k,z;\epsilon) = \frac{1}{2\epsilon} \int_{-1}^{1} dw \, w \exp\left\{-\frac{1}{2\epsilon} \left[ikw^2 + 2(w+1)(z+1) - ik\right]\right\}$$
(17)

$$D(k,z;\epsilon) = \frac{1}{2\epsilon} \int_{-1}^{1} dw \exp\left\{-\frac{1}{2\epsilon} \left[ikw^2 + 2(w+1)(z+1) - ik\right]\right\}.$$
 (18)

The corresponding formulae for $\epsilon < 0$ follow from the important symmetry relations

$$M_{11}(k, z; \epsilon) = M_{22}(-k, z; -\epsilon)$$
(19)

$$M_{12}(k, z; \epsilon) = M_{21}(-k, z; -\epsilon).$$
(20)

3 Modes of Approach to the Non-Equilibrium Steady State

The linear equation (11) contains all information about the modes by which the system approaches the NESS. Whether these modes behave for long wavelengths as hydrodynamic modes is the question we want to study now. To this end we use the explicit solution of the Boltzmann equation. The structure of (6) and (11) implies that $\tilde{F}(k, w, z)$ is an analytic function in the complex plane except at points z where the inverse matrix \mathbf{M}^{-1} does not exist. Thus the zeros of the determinant $\text{Det}(\mathbf{M})$ define the singularities in the z-plane of the Fourier-Laplace transform $\tilde{F}(k, w, z)$. In particular, isolated zeros $z_i(k)$ corresponding to simple poles will produce after applying the inverse Laplace transformation an exponential time dependence of the form

$$\hat{F}(k, w, \tau) = \sum_{i} \alpha_i \, e^{z_i(k)\tau},\tag{21}$$

with coefficients α_i for each mode depending on the initial condition (\hat{F} denotes the spatial Fourier transform of F).

We performed a systematic numerical survey of the zeros of the determinant $\text{Det}(\mathbf{M})$ for different values of k and ϵ . It has been found that regardless of the value of ϵ there is a single isolated zero which behaves like $z_0 = -Dk^2 - ikV + O(k^3)$ for $k \ll 1$. All the other zeroes, both for finite k and in the limit $k \to 0$, have negative real parts and are located outside a band of a certain finite width around the imaginary axis. That is, these other zeros do not have an accumulation point with vanishing real part. Therefore, for long wavelengths, there is exactly one slow diffusive mode (coefficient D) combined with convective transport with velocity V. All the others are fast kinetic modes. The presence of an unique slow mode is related to the fact that the mass is the only conserved quantity. No zeroes with positive real part were found, reflecting the fact that the NESS is stable.

The slow mode can be obtained analytically by inserting the asymptotic formula $z = -D(\epsilon)k^2 - ikV(\epsilon)$ into the equation $Det(\mathbf{M}) = 0$ and then solving for D and V keeping only dominant terms in k. The relations (20) imply that the zeros of the determinant of the matrix $\mathbf{M}(k, z; \epsilon)$ coincide with the zeros of the determinant of the matrix $\mathbf{M}(-k, z; -\epsilon)$. It follows the symmetry relations

$$D(\epsilon) = D(-\epsilon) = \mathcal{D}(|\epsilon|), \qquad (22)$$

$$V(\epsilon) = -V(-\epsilon) = \operatorname{sgn}(\epsilon)\mathcal{V}(|\epsilon|).$$
(23)

One finds then a unique solution

$$\mathcal{V}(\epsilon) = \frac{\epsilon [1 + e^{-2/\epsilon}] + [\epsilon - 1 - (1 + \epsilon)e^{-2/\epsilon}]I(\epsilon)}{\epsilon [1 - e^{-2/\epsilon}] + [-\epsilon + 3 + (1 + \epsilon)e^{-2/\epsilon}]I(\epsilon)}$$
(24)

and

-

$$\mathcal{D}(\epsilon) = \left[e^{2/\epsilon} \Big(-2\epsilon^3 + \epsilon^4 + 2\epsilon^5 + 8\epsilon^2 I(\epsilon) + 2\epsilon^3 I(\epsilon) - 10\epsilon^4 I(\epsilon) - 8\epsilon^5 I(\epsilon) - 10\epsilon I(\epsilon)^2 - 11\epsilon^2 I(\epsilon)^2 - 2\epsilon^3 I(\epsilon)^2 + 7\epsilon^4 I(\epsilon)^2 + 6\epsilon^5 I(\epsilon)^2 + 4I(\epsilon)^3 + 8\epsilon I(\epsilon)^3 + 12\epsilon^2 I(\epsilon)^3 + 14\epsilon^3 I(\epsilon)^3 + 6\epsilon^4 I(\epsilon)^3 \Big) + e^{4/\epsilon} \Big(-4\epsilon^3 + 2\epsilon^4 - 4\epsilon^5 + 20\epsilon^2 I(\epsilon) - 8\epsilon^3 I(\epsilon) - 12\epsilon^4 I(\epsilon) + 16\epsilon^5 I(\epsilon) - 20\epsilon I(\epsilon)^2 - 2\epsilon^2 I(\epsilon)^2 + 20\epsilon^3 I(\epsilon)^2 + 22\epsilon^4 I(\epsilon)^2 - 12\epsilon^5 I(\epsilon)^2 + 4I(\epsilon)^3 + 16\epsilon^2 I(\epsilon)^3 + 8\epsilon^3 I(\epsilon)^3 - 12\epsilon^4 I(\epsilon)^3 \Big) + e^{6/\epsilon} \Big(-2\epsilon^3 - 3\epsilon^4 + 2\epsilon^5 + 12\epsilon^2 I(\epsilon) - 26\epsilon^3 I(\epsilon) + 22\epsilon^4 I(\epsilon) - 8\epsilon^5 I(\epsilon) - 10\epsilon I(\epsilon)^2 - 3\epsilon^2 I(\epsilon)^2 + 30\epsilon^3 I(\epsilon)^2 - 29\epsilon^4 I(\epsilon)^2 + 6\epsilon^5 I(\epsilon)^2 - 8\epsilon I(\epsilon)^3 + 20\epsilon^2 I(\epsilon)^3 - 22\epsilon^3 I(\epsilon)^3 + 6\epsilon^4 I(\epsilon)^3 \Big) \Big] / \Big[\epsilon \Big(\epsilon - I(\epsilon) - \epsilon I(\epsilon) + e^{2/\epsilon} (-\epsilon - 3I(\epsilon) + \epsilon I(\epsilon)) \Big)^3 \Big],$$

$$(25)$$

with

$$I(\epsilon) = e^{1/2|\epsilon|} \int_{1}^{\infty} dw \, e^{-w^{2}/2|\epsilon|}.$$
 (26)

The drift velocity $V(\epsilon)$ (24) coincides, as expected, with the stationary average velocity V_{NESS} found in [11]. In Fig. 1 we plotted its dependence on ϵ , showing the transition from a linear to a nonlinear response.

The explicit expression for the diffusion coefficient (25) is quite involved. A plot of it is presented in Fig. 1. It should be noticed that $D(\epsilon)$ has an interesting structure as a function of the intensity of the external field showing a minimum for $\epsilon \approx 1.60$. The asymptotic formulae for small and large intensities are

$$D(\epsilon) \approx \frac{1}{2} - \frac{15}{8} \epsilon^2$$
; $|\epsilon| \ll 1$, (27)

$$D(\epsilon) \approx \frac{4 - \pi}{\sqrt{2\pi^3}} \epsilon^{1/2} + \frac{9\pi - 20}{(2\pi)^{3/2}} \epsilon^{-1/2} \quad ; \quad \epsilon \gg 1.$$
 (28)

It should be remarked that in the limit of vanishing external field the value D(0) coincides with that following at equilibrium ($\epsilon = 0$) from the Green-Kubo formula. For large values of ϵ , the velocity of the obstacles becomes negligible compared to that acquired by accelerated motion and their action resembles that of stopping centers. Therefore by purely dimensional analysis one can predict the exponent 1/2 in the dependence of $D(\epsilon)$ in (28).

The appearance of a minimum in $D(\epsilon)$ shown in Fig. 1 is an interesting point which calls for interpretation. The minimum can be understood by analyzing the partial collision frequencies with obstacles moving with velocities +1 or



Fig. 1. Top: Average velocity $V_{\text{NESS}}(\epsilon)$ in the NESS as a function of the imposed acceleration ϵ . Bottom: Field dependent diffusion coefficient $D(\epsilon)$.

-1. In the NESS, these collision frequencies are given by

$$\mu_{0\pm}(\epsilon) = \int dw |w\pm 1| F_0(w;\epsilon), \qquad (29)$$

where the average is computed with the use of the NESS distribution $F_0(w;\epsilon)$ given in Eq.(40) of Ref. [11]. As shown in Fig. 2, the collision frequency μ_{0-} with obstacles moving to the right (in the direction of the accelerating field) has a minimum at $\epsilon = 1.37$. In order to understand this fact consider a particle that has just collided with an obstacle with velocity -1 getting instantaneously its velocity. If the field is weak, it will continue moving to the left encountering obstacles with velocity +1 and will be sent again towards those with velocity -1 the collision frequency μ_{0-} remaining high. Also if the field is large enough, the particle will turn rapidly to the right and gain a large velocity leading again to a large value of μ_{0-} . There are however intermediate values of acceleration where the particle remains a long time turning to the right under the action of the field before the next collision occurs without getting large velocities and thus reducing the collision rate. This fact explains the origin of the minimum in $\mu_{0-}(\epsilon)$. Finally, the presence of the minimum in μ_{0-} can be related to the observed minimum of $D(\epsilon)$ because the lowering of the collision rate for a range of values of ϵ produces an evolution that is closer to a deterministic one, and thus less diffusive.

Knowing the analytic solution of the initial value problem for the kinetic equation (3) we could also verify if the diffusion coefficient (25) follows from the Green-Kubo formula when the NESS distribution is used in the evaluation of



Fig. 2. Partial collision frequencies in the NESS, solid line μ_{0+} , dashed line μ_{0-} . the autocorrelation function. We thus considered the Green-Kubo expression

$$D_{\rm GK} = \lim_{z \to 0} \int_0^\infty d\tau e^{-z\tau} \langle (w - V)(\tau)(w - V)(0) \rangle_{\rm NESS}$$
(30)

$$= \lim_{z \to 0} \int_0^\infty d\tau e^{-z\tau} \int dw (w - V) F_{\rm GK}(w, \tau), \tag{31}$$

where $F_{\rm GK}(w,\tau)$ is the solution of the equation (3) with initial condition $F_{\rm GK}(w,0) = (w-V)F_0(w)$ and V is the NESS drift velocity. The computation process is as follows. Given the initial condition $F_{\rm GK}(w,0)$, the equation (11) is solved for $\tilde{\mu}_{\pm}$ (note that z must be nonzero because otherwise the inverse matrix $\mathbf{M}(k=0,z)^{-1}$ does not exist). Then, $\tilde{F}_{\rm GK}(w,z)$ is obtained and the coefficient $D_{\rm GK}$ can be found from the relation

$$D_{\rm GK} = \lim_{z \to 0} \int dw (w - V) \tilde{F}_{\rm GK}(w, z).$$
(32)

We performed the calculation obtaining a finite value which coincides with (25). We thus conclude that when the system is in the NESS, both in the linear and in the nonlinear response regimes, the diffusion coefficient is given by the Green-Kubo formula provided the NESS distribution is used in the averaging process and the fluctuations of the velocity around the non-zero mean value V_{NESS} are considered. This conclusion is also confirmed by an analogous result obtained for a simpler one-dimensional case where only nonlinear transport is present [12].

Finally, we have checked that beyond the linear response regime the system does not obey the fluctuation-dissipation theorem, relating the diffusion coefficient D and the mobility μ . The mobility is defined as $\mu = dV_{\text{NESS}}/d\epsilon$. Evaluating the non-equilibrium stationary temperature $T = \langle (w - V_{\text{NESS}})^2 \rangle$ using the stationary distribution F_0 , it is directly checked that $D(\epsilon) \neq T(\epsilon)\mu(\epsilon)$. The equality is only satisfied at the equilibrium case $\epsilon = 0$. A similar phenomenon has been predicted in granular gases [13].

4 Concluding comments

We have considered a one-dimensional system of particles absorbing energy from a constant and uniform external field, and dissipating it via collisions with a bath of scattering obstacles with a fixed velocity distribution (2). In this situation the appropriate linear Boltzmann equation (3) predicts the approach to a non-equilibrium steady state (NESS) characterized by a mass flux that can present both linear and nonlinear response depending on the strength of the field. It has been found that the evolution of arbitrary initial conditions toward the NESS involves short time scale kinetic modes producing the stationary velocity distribution followed by the slow long wavelength hydrodynamic diffusion superposed on a convective current flowing with the average velocity of the NESS.

Analytic calculations show an interesting structure in the dependence of the diffusion coefficient on the intensity of the external field, with a minimum at intermediate values of the field. The minimum is related to the presence of another minimum in the collision frequency between the particles and the obstacles, thus reducing the number of randomizing scattering processes. Furthermore, we have also shown that the value of the diffusion coefficient could be obtained from a Green-Kubo formula by considering the time displaced peculiar velocity correlation function (subtracting the average NESS velocity) averaged over the NESS distribution.

It thus appears that the modes of approach to the NESS when only the mass remains as a conserved quantity involve the corresponding single hydrodynamic mode which is the classical process of spatial diffusion. The diffusion coefficient does depend on the external field intensity and can be obtained at any value of the field from an appropriately generalized Green-Kubo formula. We conclude that the approach to NESS shows qualitative analogy to that of reaching equilibrium. Hopefully this conclusion remains valid for a large class of systems in which the stationary state results from the balance between the energy flow absorbed from an external field and collisional coupling to a kind of thermostat.

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