

A Note on the Nonequilibrium Stationary State in Continuous-Activity Thermostatted Models

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Abstract: The present paper addresses uniqueness of the nonequilibrium stationary state of a continuous-activity thermostatted kinetic theory framework. Specifically, a sufficient condition for the existence and uniqueness of the nonequilibrium stationary state is established. The sufficient condition defines a relation between the interaction rate and the magnitude of the external force. The proof of the main result is obtained by employing fixed-point arguments.

Keywords: Complexity, Nonlinearity, Thermostat, Integro-differential Equation, Kinetic Theory

1 Introduction

Mathematical structures [1–5], computational tools [6–10] and simulators [11, 12] have been the main interest of the scholars in the last and the present century. The main aim is the possibility to understand and predict the evolution of a phenomenon related to a complex system [13]. In particular, a mathematical structure, based on differential and/or algebraic equations, has been of great interest for the researchers due to the possibility to make efficient probabilistic forecasts towards a complex phenomenon. However, also the mathematical structures can show limitations related to the difficulty to gain the mathematical proof of the results, especially the comparison between the real data. The latter subject has been the target of the development of computational methods, which show how the interplay between different scholars is at the base of achievement.

Recently, the thermostatted kinetic theory has been proposed and employed for modeling large particle systems characterized by particles which can perform inner and outer interactions according to an internal and external strategy (active particles), see [14]. The systems under consideration, which usually share the same characteristics of a complex system, are divided into

different subsystems composed of particles which manifest the same strategy (functional subsystems). The function expressed by an active particle is modeled by introducing a scalar variable (called activity) which has a discrete or a continuous structure. Accordingly, a continuous [15] or a discrete [16] thermostatted kinetic theory structure, which is based on the definition of interaction rates and transition probability functions, is derived.

The system is also assumed to be subject to an external force at the macroscopic scale which moves the system out-of-equilibrium and a mathematical thermostat (a dissipative term) [17–19] is coupled to the framework to ensure reaching a nonequilibrium stationary state.

This paper addresses the continuous-activity thermostatted kinetic theory framework under the assumption of constant interaction rates and a constant magnitude external force. The mathematical analysis has already addressed the well-posedness of the related initial boundary value problem, the existence of the nonequilibrium stationary state and the convergence of the transient state to the nonequilibrium stationary state (the interested reader is referred to the recent papers [20, 21]). Uniqueness of the nonequilibrium stationary state is the main interest of the present paper. Specifically, a

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sufficient condition for the uniqueness of the nonequilibrium stationary state is proposed. The sufficient condition is based on the relation between the interaction rate and the magnitude of the external force. The proof of the main result is obtained by employing fixed-point arguments.

The present paper is organized, as follows: Section 2 handles the presentation of the stationary thermostatted framework and the statement of the main theorem. Section 3 is devoted to the mathematical proof of the main result. Conclusion is presented in Section 4.

2 The stationary thermostatted framework

A function $f : D_u \rightarrow \mathbb{R}^+$, where $D_u \subseteq \mathbb{R}$, is a nonequilibrium stationary state of the continuous-activity thermostatted kinetic theory framework if it is solution of the following nonlinear integro-differential equation with quadratic nonlinearity:

$$\begin{aligned} \partial_u \left(\left(1 - u \int_{D_u} f(u) du \right) f(u) \right) &= \\ &= \frac{\eta}{F} \left(\int_{D_u \times D_u} \mathcal{A}(u_*, u^*, u) f(u_*) f(u^*) du_* du^* \right. \\ &\left. - f(u) \int_{D_u} f(u^*) du^* \right), \end{aligned} \quad (1)$$

where $\eta, F > 0$ and $\mathcal{A} : D_u \times D_u \times D_u \rightarrow \mathbb{R}^+$.

The existence of a nonequilibrium stationary state $f \in C\left(\mathbb{R} \setminus \left\{ \frac{1}{\mathbb{E}_1^+} \right\}\right)$, where $\mathbb{E}_1^+ := \frac{-\eta + \sqrt{\eta^2 + 4F^2}}{2F}$, has been proved in [20] under the following assumptions:

A1 $D_u = \mathbb{R}$;

A2 $\|\mathcal{A}(\cdot, \cdot, u)\|_{L^1(D_u)} = 1$;

A3 $\int_{D_u} u^2 \mathcal{A}(u_*, u^*, u) du = u_*^2$, for all $u_*, u^* \in D_u$;

A4 $\int_{D_u} u \mathcal{A}(u_*, u^*, u) du = 0$, for all $u_*, u^* \in D_u$;

A5 $\|f(u)\|_{L^1(D_u)} = 1$;

A6 $\|u^2 f(u)\|_{L^1(D_u)} du = 1$.

Remark. The integro-differential equation (1) is the nonequilibrium stationary problem of the following continuous-activity thermostatted kinetic theory framework:

$$\begin{aligned} \partial_t f(t, u) + F \partial_u \left(\left(1 - u \int_{D_u} u f(t, u) du \right) f(t, u) \right) &= \\ &= J[f, f](t, u), \end{aligned} \quad (2)$$

where

$$\begin{aligned} J[f, f] &:= \int_{D_u \times D_u} \eta \mathcal{A}(u_*, u^*, u) f(t, u_*) f(t, u^*) du_* du^* \\ &\quad - f(t, u) \int_{D_u} \eta f(t, u^*) du^* \end{aligned}$$

denotes the operator which models the net-flux of active particles with state u , η is the interaction rate, F the external force field and \mathcal{A} the transition probability function.

A sufficient condition for the uniqueness of the nonequilibrium stationary state of the integro-differential equation (1) is established in the next theorem.

Theorem 1. Assume that A1-A6 hold true. If

$$\frac{\eta}{F} < \frac{1}{\sqrt{12}} \quad (3)$$

then there exists, for almost every $u \in \mathbb{R}$, a unique nonequilibrium stationary state f of the integro-differential equation (1).

3 Proof of Theorem 1

The equation (1) can be rewritten, as follows:

$$\begin{aligned} \eta \int_{D_u \times D_u} \mathcal{A}(u_*, u^*, u) f(u_*) f(u^*) du_* du^* - \eta f(u) &= \\ &= F \partial_u \left((1 - u \mathbb{E}_1^+) f(u) \right) \\ &= F \partial_u f(u) - F \mathbb{E}_1^+ f(u) - F u \mathbb{E}_1^+ \partial_u f(u). \end{aligned} \quad (4)$$

Let D_u be a compact subset of \mathbb{R} . Without loss of generality, we can assume that $f(u) = 0$ for $u \in \partial D_u$. If \bar{D}_u is a compact subset which contains D_u , we can consider the function $\bar{f} : \bar{D}_u \rightarrow \mathbb{R}^+$ defined, as follows:

$$\bar{f}(u) = \begin{cases} f & u \in D_u \\ 0 & u \in \bar{D}_u \setminus D_u. \end{cases}$$

Let $f_1, f_2 \in C\left(\mathbb{R} \setminus \left\{ \frac{1}{\mathbb{E}_1^+} \right\}\right)$ be two nonequilibrium stationary states of the equation (1). Rewriting the equation (4) for f_1 and f_2 , one has:

$$\begin{aligned} (F \mathbb{E}_1^+ - \eta) f_1(u) &= (1 - u \mathbb{E}_1^+) F \partial_u f_1(u) \\ &\quad - \eta \int_{D_u \times D_u} \mathcal{A}(u_*, u^*, u) f_1(u_*) f_1(u^*) du_* du^*, \end{aligned} \quad (5)$$

and

$$(F \mathbb{E}_1^+ - \eta) f_2(u) = (1 - u \mathbb{E}_1^+) F \partial_u f_2(u) - \eta \int_{D_u \times D_u} \mathcal{A}(u_*, u^*, u) f_2(u_*) f_2(u^*) du_* du^* \tag{6}$$

Subtracting equations (5) and (6), one has:

$$(F \mathbb{E}_1^+ - \eta) (f_1(u) - f_2(u)) = F (1 - u \mathbb{E}_1^+) \partial_u (f_1(u) - f_2(u)) - \eta \int_{D_u \times D_u} \mathcal{A}(u_*, u^*, u) f_1(u_*) f_1(u^*) du_* du^* + \eta \int_{D_u \times D_u} \mathcal{A}(u_*, u^*, u) f_2(u_*) f_2(u^*) du_* du^* \tag{7}$$

From equation (7), it follows:

$$|F \mathbb{E}_1^+ - \eta| |f_1(u) - f_2(u)| \leq F |(1 - u \mathbb{E}_1^+) \partial_u (f_1(u) - f_2(u))| + \eta \int_{D_u \times D_u} |f_1(u_*) f_1(u^*) - f_2(u_*) f_2(u^*)| du_* du^* \tag{8}$$

Integrating inequality (8) with respect to $u \in D_u$, one has:

$$|F \mathbb{E}_1^+ - \eta| \|f_1(u) - f_2(u)\|_{L^1(D_u)} \leq F \int_{D_u} |(1 - u \mathbb{E}_1^+) \partial_u (f_1(u) - f_2(u))| du + \eta \int_{D_u^3} |f_1(u_*) f_1(u^*) - f_2(u_*) f_2(u^*)| du du_* du^* \tag{9}$$

For the first term of the right hand side of the inequality (9), one has:

$$\int_{D_u} |(1 - u \mathbb{E}_1^+) \partial_u (f_1(u) - f_2(u))| du \leq \int_{D_u} |\partial_u (f_1(u) - f_2(u))| du + \mathbb{E}_1^+ \int_{D_u} |u \partial_u (f_1(u) - f_2(u))| du \tag{10}$$

The first term of the right hand side of inequality (10) equals to 0 because $f = 0$ on the boundary ∂D_u and the assumption **A5**. Moreover, the second term of the right hand side of inequality (10) equals zero because:

$$\int_{D_u} |u \partial_u (f_1(u) - f_2(u))| du \leq c \int_{D_u} |\partial_u (f_1(u) - f_2(u))| du = 0, \tag{11}$$

where c is the diameter of the compact subset D_u .

By using the equation (11), the first term of the right hand side of the inequality (9) rewrites:

$$\int_{D_u} |(1 - \mathbb{E}_1^+) \partial_u (f_1(u) - f_2(u))| du = 0. \tag{12}$$

Observe that:

$$|f_1(u_*) f_1(u^*) - f_2(u_*) f_2(u^*)| = |f_1(u_*) f_1(u^*) - f_1(u_*) f_2(u^*) + f_1(u_*) f_2(u^*) - f_2(u_*) f_2(u^*)| \leq |f_1(u_*)| |f_1(u^*) - f_2(u^*)| + |f_2(u^*)| |f_1(u_*) - f_2(u_*)|. \tag{13}$$

By (13), the second term of the right hand side of inequality (9) rewrites:

$$\int_{D_u} \int_{D_u \times D_u} |f_1(u_*) f_1(u^*) - f_2(u_*) f_2(u^*)| du \leq \int_{D_u} (u_*, u^*, u) \int_{D_u \times D_u} |f_1(u_*)| |f_1(u^*) - f_2(u^*)| du + \int_{D_u} (u_*, u^*, u) \int_{D_u \times D_u} |f_2(u^*)| |f_1(u_*) - f_2(u_*)| du \leq 2 \|f_1(u) - f_2(u)\|_{L^1(D_u)}. \tag{14}$$

Using equation (12) and inequality (14), inequality (9) writes:

$$|F \mathbb{E}_1^+ - \eta| \|f_1(u) - f_2(u)\|_{L^1(D_u)} \leq 2 \eta \|f_1(u) - f_2(u)\|_{L^1(D_u)}. \tag{15}$$

By straightforward calculations inequality (15) rewrites:

$$(|F \mathbb{E}_1^+ - \eta| - 2 \eta) \|f_1(u) - f_2(u)\|_{L^1(D_u)} \leq 0. \tag{16}$$

Since $\mathbb{E}_1^+ = \frac{-\eta + \sqrt{\eta^2 + 4F^2}}{2F}$, one has:

$$F \mathbb{E}_1^+ = \frac{-\eta + \sqrt{\eta^2 + 4F^2}}{2} \tag{17}$$

$$F \mathbb{E}_1^+ - \eta = \frac{-3\eta + \sqrt{\eta^2 + 4F^2}}{2}. \tag{18}$$

By equations (17) and (18), the first factor of the left hand side of inequality (16) rewrites:

$$(|F \mathbb{E}_1^+ - \eta| - 2 \eta) = \left(\frac{|-3\eta + \sqrt{\eta^2 + 4F^2}| - 4\eta}{2} \right), \tag{19}$$

which is a positive constant because of inequality (3). The right hand side of equation (19) rewrites, as follows:

$$(|F\mathbb{E}_1^+ - \eta| - 2\eta) = \frac{\eta}{2} \left[-3 + \sqrt{1 + 4\frac{F^2}{\eta^2}} - 4 \right],$$

and:

$$(|F\mathbb{E}_1^+ - \eta| - 2\eta) > 0 \Leftrightarrow \quad (20)$$

$$\Leftrightarrow \begin{cases} -3 + \sqrt{1 + 4\frac{F^2}{\eta^2}} > 0 \\ -3 + \sqrt{1 + 4\frac{F^2}{\eta^2}} - 4 > 0 \end{cases} \quad (21)$$

$$\cup \begin{cases} -3 + \sqrt{1 + 4\frac{F^2}{\eta^2}} < 0 \\ 3 - \sqrt{1 + 4\frac{F^2}{\eta^2}} - 4 > 0 \end{cases}$$

$$\Leftrightarrow \begin{cases} \frac{\eta}{F} < \frac{1}{\sqrt{2}} \\ \sqrt{1 + 4\frac{F^2}{\eta^2}} > 7 \end{cases} \cup \begin{cases} \frac{\eta}{F} > \frac{1}{\sqrt{2}} \\ -\sqrt{1 + 4\frac{F^2}{\eta^2}} - 1 > 0 \end{cases}$$

$$\Leftrightarrow \begin{cases} \frac{\eta}{F} < \frac{1}{\sqrt{2}} \\ \frac{\eta^2}{F^2} < \frac{1}{12} \end{cases} \Leftrightarrow \frac{\eta}{F} < \frac{1}{\sqrt{12}}.$$

Accordingly,

$$\|f_1(u) - f_2(u)\|_{L^1(D_u)} = 0,$$

which means $f_1(u) = f_2(u)$ for a.e. $u \in D_u$. Thus, uniqueness of the nonequilibrium stationary state is proved for a compact domain D_u .

Let $D_u = \mathbb{R}$ and $k \in \mathbb{N}$. Using the first step of the proof, there exists a unique nonequilibrium stationary state $f(u) \in L^1([-k, k])$ of the problem (1), i.e. if $f_1(u), f_2(u) \in L^1([-k, k])$ are two nonequilibrium stationary states, then

$$\|f_1(u) - f_2(u)\|_{L^1([-k, k])} = 0. \quad (22)$$

Then, by using the continuity of the norm:

$$\|f_1(u) - f_2(u)\|_{L^1([-k, k])} \xrightarrow{k \rightarrow \infty} 0.$$

Thus, the proof is gained.

Remark. As shown in the proof of Theorem 1, uniqueness of the nonequilibrium stationary state f is also ensured if D_u is a compact subset of \mathbb{R} .

4 Conclusion

The objective of the present paper has been another important step in the formal validation of the thermostatted kinetic theory proposed in [14]. Existence and uniqueness of the solution have been already proved in [14] and the dependence on the initial data has been proved in [22]. However, the important step obtained in this paper has been the possibility to ensure the existence and uniqueness of the nonequilibrium stationary state. The main result has been obtained by assuming that the interaction rate and the magnitude of the external force are constants. This assumption can be relaxed and it appears possible to ensure the uniqueness of the nonequilibrium stationary state by constructing a suitable upper bound for the interaction rate function and the external force field.

To the authors' knowledge, this is the first paper that investigates the conditions of uniqueness for the nonequilibrium stationary state within the thermostatted kinetic theory framework.

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Conflict of Interest.

The authors declare that there is no conflict of interest regarding the publication of this article

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