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On the Initial-Boundary-Value Problem and Moments Evolution in a Thermostatted Framework with Nonhomogeneous Boundary Conditions

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Abstract: This paper is devoted to the construction of a generalized termostat term for a kinetic theory framework of the thermostatted theory for active particles. Specifically the novelty of this paper with respect the pertinent literature is the relaxation of the homogeneous boundary conditions assumption. The existence and uniqueness of the related initial-boundary-value problem is presented and the time evolution of the low-order moments is investigated. The new framework constitutes a background paradigm for the derivation of specific models for complex living systems.

Keywords: Kinetic theory, Thermostas, Nonlinearity, Macroscopic equations, Complex systems

1 Introduction

The analysis and numerical simulation of the solution of an initial-boundary-value problem for nonlinear evolution equations is an important research field in engineering and fluid dynamics, see the review paper [1]. In particular many attention has been payed to the Korteweg-de Vries equation [2], the Schrodinger equations [3], the Navier-Stokes-Fourier system [4] and the Boltzmann equation [5]. Differently from the pure initial-value problems, in the analysis of initial-boundary-value problems homogeneous or nonhomogeneous boundary conditions can be defined and the regularity demanded of the boundary data can strongly affect the existence and uniqueness of the solution [6,7].

This paper aims at deriving a new mathematical framework of the thermostatted kinetic theory for activity particles [8]. Differently from the previous thermostatted frameworks proposed in the pertinent literature, see among others [9,10,11,12], in this paper the homogeneous boundary conditions assumption is relaxed. In particular the selected primitive framework of the thermostatted kinetic theory consists in a nonlinear integro-partial differential equation fulfilled by the distribution function that describes the time evolution of the system. The microscopic state of the particles, called active particles, is composed by a continuous scalar variable (activity) and the mutual binary interactions are modeled by introducing the following operators:
- the conservative operator, which models the transition of the state of the active particle;
- the nonconservative operator, which represents the proliferation or destruction of active particles and thus modifying the number of active particles involved in the evolution of the system;
- the thermostat operator, which is derived by imposing the conservation of the activity energy by following the methods of non equilibrium statistical mechanics, see the papers [13,14] and the references cited therein.

The introduction of the thermostat term strongly influences the time evolution of the moments of the distribution function. It is worth stressing that the activity variable can be also defined for attaining discrete values (discrete thermostatted framework); however this is not

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within the scope of the present paper. The new thermostatted framework is mathematically analyzed and specifically the existence and uniqueness of solution of the initial-boundary-value problem is investigated and the result is gained by employing the same steps of the proof in [8]. Moreover the evolution equations of the density and the linear-momentum of the system are derived (low-order moments). In particular the evolution equations are nonlinear ordinary differential equations with quadratic nonlinearity. As the evolution equations show, the functions at the boundary strongly affect the time evolution of the low-order moments and then their definition assumes an important role. To the best of our knowledge, this is the first time that these investigations are performed in the context of the thermostatted kinetic theory for active particles.

The present paper is organized into four more sections which follow this introduction. Specifically:
- Section 2 deals with the presentation of the underlying framework and the main assumptions. The new mathematical framework contains conservative and conservative interactions and the new thermostat term is established.
- Section 3 is devoted to the mathematical analysis and specifically to the existence and uniqueness of the solution of the related initial-boundary-value problem.
- Section 4 is concerned with the derivation of the evolution equations for the low-order moments (density and linear-momentum).
- Section 5 summarizes the paper and presents the future research directions and applications.

2 The thermostatted kinetic theory framework in nonhomogeneous boundary conditions

This section is devoted to the derivation of a new mathematical framework of the thermostatted kinetic theory. Specifically the homogeneous boundary conditions assumption is relaxed and consequently the thermostat term is modified.
According to the general kinetic theory for active particles, the whole system is modeled by introducing a distribution function $f = f(t,u)$ where $t \in [0,+\infty[$ denotes the time variable and $u \in D_u = [a,b]$, a, $b \in \mathbb{R}$, denotes the activity variable. The particles of the system, called active particles, are able to interact each others with a constant interaction rate η and are able to proliferate with a constant proliferation/destruction rate μ. The probability that an active particle u_* acquires the state u after an interaction with the active particle u_* is modeled by introducing the function $\mathscr{A}(u,u_*,u^*)$ which is assumed to satisfy the following assumptions:

$\mathbf{A_1}$: $\int_{D_u} \mathscr{A}(u,u_*,u^*)\,du = 1$, for all u_*, $u^* \in D_u$;

$\mathbf{A_2}$: $\int_{D_u} u\,\mathscr{A}(u,u_*,u^*)\,du = 0$, for all u_*, $u^* \in D_u$;

$\mathbf{A_3}$: $\int_{D_u} u^2\,\mathscr{A}(u,u_*,u^*)\,du = u_*^2$, for all u_*, $u^* \in D_u$.

Moreover the system is assumed to be subjected to a constant external force F.
Assume that $f_a(t), f_b(t) : [0,+\infty[\to \mathbb{R}^+$ are suitable functions. Let $(t,u) \in [0,+\infty[\times[a,b]$, the underlying thermostatted framework of the kinetic theory for active particles reads:

$$\begin{cases} \partial_t f + \partial_u((F - \alpha_F[f]\,u)f) = \eta J[f] + \eta\mu P[f], \\ f(t,a) = f_a(t), \quad t \in [0,+\infty[, \\ f(t,b) = f_b(t), \quad t \in [0,+\infty[, \end{cases} \tag{1}$$

where

$$\begin{aligned} J[f](t,u) &= G[f](t,u] - L[f](t,u) \\ &= \int_{D_u\times D_u} \mathscr{A}(u,u_*,u^*)\,f(t,u_*)f(t,u^*)\,du_*\,du^* \\ &\quad - f(t,u)\int_{D_u} f(t,u^*)\,du^*, \end{aligned} \tag{2}$$

and

$$P[f](t,u) = f(t,u)\int_{D_u} f(t,u^*)\,du^*.$$

The operators $J[f]$ and $P[f]$ model the conservative and conservative interactions, respectively.
The density $\mathbb{E}_0[f]$ and the linear-momentum $\mathbb{E}_1[f]$ of the system are defined as follows:

$$\mathbb{E}_0[f](t) = \int_{D_u} f(t,u)\,du, \quad \mathbb{E}_1[f](t) = \int_{D_u} uf(t,u)\,du.$$

The thermostat operator $\alpha_F[f]$ of the (1) is derived by imposing the conservation of the activity-energy defined as follows:

$$\mathbb{E}_2[f](t) = \int_{D_u} u^2 f(t,u)\,du,$$

and in particular it is assumed that $\mathbb{E}_2[f](t) = 1$, $\forall t > 0$.
Bearing all above in mind, one has:

$$\frac{d}{dt}(\mathbb{E}_2[f](t)) = 0, \qquad \forall t > 0.$$

Multiplying the both sides of the equation $(1)_1$ by u^2 and by integrating with respect to the variable $u \in D_u = [a,b]$, one has:

$$\begin{aligned} &\partial_t \int_a^b u^2 f(t,u)\,du + \int_a^b u^2\partial_u((F - \alpha_F[f]\,u)f(t,u))\,du \\ &= \eta\int_a^b u^2 J[f](t,u)\,du + \eta\mu\int_a^b u^2 P[f](t,u)\,du. \end{aligned} \tag{3}$$

Since $\mathbb{E}_2[f](t)$ is assumed to be constant during the evolution, the (3) rewrites:

$$\begin{aligned}&\int_a^b u^2\partial_u\left((F-\alpha_F[f]\,u)f(t,u)\right)du\\&=\eta\int_a^b u^2 J[f](t,u)\,du+\eta\mu\int_a^b u^2 P[f](t,u)\,du.\end{aligned}\tag{4}$$

By integrating by parts the left hand side of the equation (4), one has:

$$\begin{aligned}&\int_a^b u^2\partial_u\left((F-\alpha_F[f]\,u)f(t,u)\right)du\\&=u^2\left[(F-\alpha_F[f]\,u)\right]f(t,u)\big]_a^b\\&-\int_a^b 2u\left[(F-\alpha_F[f]\,u)\,f(t,u)\right]du\\&=b^2\left[(F-\alpha_F[f]\,b)\,f_b(t)\right]-a^2\left[(F-\alpha_F[f]\,a)\,f_a(t)\right]\\&-\int_a^b 2u\left[(F-\alpha_F[f]\,u)\,f(t,u)\right]du.\end{aligned}\tag{5}$$

Let

$$\begin{aligned}\Theta[f](t):=\;&b^2\left[(F-\alpha_F[f]\,b)\,f_b(t)\right]\\&-a^2\left[(F-\alpha_F[f]\,a)\,f_a(t)\right]\\&=\alpha_F[f](a^3f_a(t)-b^3f_b(t))\\&-F(a^2f_a(t)-b^2f_b(t)).\end{aligned}\tag{6}$$

The right hand side of the equation (5) rewrites:

$$\begin{aligned}&\Theta[f](t)-2\int_a^b u\left[(F-\alpha_F[f]\,u)\,f(t,u)\right]du\\&=\Theta[f](t)-2\left[F\int_a^b u\,f\,du-\alpha_F[f]\int_a^b u^2\,f\,du\right]\\&=\Theta[f](t)-2\left[F\mathbb{E}_1[f](t)-\alpha_F[f]\mathbb{E}_2[f](t)\right]\\&=\Theta[f](t)-2F\mathbb{E}_1[f](t)+2\,\alpha_F[f].\end{aligned}\tag{7}$$

The right hand side of the equation (4) rewrites:

$$\begin{aligned}&\eta\int_a^b u^2 J[f](t,u)\,du+\eta\mu\int_a^b u^2 P[f](t,u)\,du\\&=\eta\int_a^b\int_a^b\int_a^b u^2\mathscr{A}\,f(t,u_*)f(t,u^*)\,du_*\,du^*\,du\\&-\eta\int_a^b u^2 f(t,u)\left(\int_a^b f(t,u^*)\,du^*\right)du\\&+\eta\mu\int_a^b u^2 f(t,u)\left(\int_a^b f(t,u^*)\,du^*\right)du\\&=\eta\,\mathbb{E}_0[f](t)\mathbb{E}_2[f](t)-\eta\,\mathbb{E}_0[f](t)\mathbb{E}_2[f](t)\\&+\eta\mu\,\mathbb{E}_0[f](t)\mathbb{E}_2[f](t)\\&=\eta\mu\,\mathbb{E}_0[f](t)\mathbb{E}_2[f](t).\end{aligned}\tag{8}$$

Since $\mathbb{E}_2[f](t)=1$ and by using the (7) and the (8), the (5) writes:

$$\begin{aligned}&\alpha_F[f](a^3f_a(t)-b^3f_b(t))-F(a^2f_a(t)-b^2f_b(t))\\&-2F\mathbb{E}_1[f](t)+2\,\alpha_F[f]=\eta\mu\,\mathbb{E}_0[f](t).\end{aligned}\tag{9}$$

Let $\beta(t)=a^3f_a(t)-b^3f_b(t)$ and $\gamma(t)=F(a^2f_a(t)-b^2f_b(t))$. The thermostat term α_F thus reads:

$$\alpha_F[f,f_a,f_b,P](t)=\frac{\eta\mu\mathbb{E}_0[f](t)+2F\mathbb{E}_1[f](t)-\gamma(t)}{2+\beta(t)}.\tag{10}$$

Bearing all above in mind, the *thermostatted kinetic theory framework* with *nonhomogeneous boundary conditions* reads:

$$\begin{cases}\partial_t f+\partial_u\left(F\left(1-\dfrac{2u}{2+\beta(t)}\displaystyle\int_a^b uf(t,u)\,du\right)f(t,u)\right)+\\\partial_u\left(\dfrac{u}{2+\beta(t)}\left(\gamma(t)-\eta\mu\displaystyle\int_a^b f(t,u)\,du\right)f(t,u)\right)\\=\eta J[f](t,u)+\eta\mu P[f](t,u),\quad (t,u)\in[0,+\infty[\times[a,b],\\\\f(t,a)=f_a(t),\quad t\in[0,+\infty[,\\\\f(t,b)=f_b(t),\quad t\in[0,+\infty[.\end{cases}\tag{11}$$

The new thermostatted framework (11) allows the modeling of complex systems where nonconservative interactions occur (biological systems) and a specific model is derived when the interaction rate η and the proliferation/destruction rate μ are selected. In particular the function $\mathscr{A}$ and the boundary conditions need to be defined.

The thermostat operator $T_F=T_F[f,f_a,f_b,P](t,u)$ writes:

$$\begin{aligned}T_F=&\partial_u\left(F\left(1-\frac{2u}{2+\beta(t)}\int_a^b uf(t,u)\,du\right)f(t,u)\right)+\\&\partial_u\left(\frac{u}{2+\beta(t)}\left(\gamma(t)-\eta\mu\int_a^b f(t,u)\,du\right)f(t,u)\right)\end{aligned}\tag{12}$$

*Remark.*If the boundary conditions are homogeneous, namely $f_a(t)=f_b(t)=0$, then $\alpha(t)=\beta(t)=0$, for all $t\in[0,+\infty[$, and the thermostat term $\alpha_F[f,f_a,f_b,P]$ equals the thermostat of the paper [15]:

$$\alpha_F[f,f_a,f_b,P](t)=\alpha_F[f,P](t).$$

Moreover if the system is not subjected to nonconservative interactions namely $\mu=0$, then the thermostat term $\alpha_F[f,f_a,f_b,P]$ equals the thermostat of the paper [8]:

$$\alpha_F[f,f_a,f_b,P](t)=\alpha_F[f](t).$$

2.1 The initial-boundary-value problem

This section deals with a preliminary mathematical analysis of the new thermostatted framework (11) and specifically with the existence and uniqueness of solution of the related initial-boundary-value problem.
Assume that $f_a(t) : [0,+\infty[\to \mathbb{R}^+$ and $f_b(t) : [0,+\infty[\to \mathbb{R}^+$ are suitable functions, and $f^0(u) : [a,b] \to \mathbb{R}^+$, $f^0(u) \in L^1([a,b])$. The initial-boundary-value problem related to the mathematical framework (11) reads:

$$\begin{cases} \partial_t f(t,u) + T_F[f,f_a,f_b,P](t,u) \\ = \eta J[f](t,u) + \eta\mu P[f](t,u), & (t,u) \in [0,+\infty[\times[a,b], \\ f(t,a) = f_a(t), & t \in [0,+\infty[, \\ f(t,b) = f_b(t), & t \in [0,+\infty[, \\ f(0,u) = f^0(u) & u \in [a,b]. \end{cases} \tag{13}$$

Since

$$\begin{aligned} &\eta J[f](t,u) + \eta\mu P[f](t,u) \\ &= \eta G[f](t,u) - \eta L[f](t,u) + \eta\mu P[f](t,u) \\ &= \eta G[f](t,u) - \eta\mathbb{E}_0[f](t) f(t,u) + \eta\mu\mathbb{E}_0[f](t) f(t,u) \\ &= \eta G[f](t,u) - \eta(1-\mu)\mathbb{E}_0[f](t,u) f(t,u), \end{aligned} \tag{14}$$

the equation $(11)_1$ rewrites:

$$\begin{aligned} &\partial_t f(t,u) + \partial_u\left((F - \alpha_F[f,f_a,f_b,P](t)\,u) f(t,u)\right) \\ &+ \left[\eta(1-\mu)\mathbb{E}_0[f](t) - \alpha_F[f,f_a,f_b,P](t)\right] f(t,u) \\ &= \eta G[f](t,u). \end{aligned} \tag{15}$$

The (15) is a first-order semilinear equation. In order to solve it, the following characteristics are considered:

$$U(t,u) = \varphi_t(u) = u e^{-\lambda(t)} + F e^{-\lambda(t)} \int_0^t e^{\lambda(s)}\, ds,$$

where

$$\lambda(t) = \int_0^t \alpha_F[f,f_a,f_b,P](s)\, ds.$$

Since

$$\begin{aligned} \frac{\partial U}{\partial t} &= \left[-\dot\lambda(t) e^{-\lambda(t)} u + F e^{-\lambda(t)}(-\dot\lambda(t)) + F\right] \\ &= \left[F - \dot\lambda(t)\left(u e^{-\lambda(t)} + F e^{-\lambda(t)} \int_0^t e^{\lambda(s)}\, ds\right)\right] \\ &= \left[F - \alpha_F[f,f_a,f_b,F](t)\, U\right], \end{aligned} \tag{16}$$

the equation (15) writes:

$$\begin{aligned} &\frac{d}{dt} f_U(t,u) + \\ &\left[\eta(1-\eta)\mathbb{E}_0[f](t) - \alpha_F[f,f_a,f_b,P](t)\right] f_U(t,u) \\ &= \eta G_U[f](t,u), \end{aligned} \tag{17}$$

where

$$f_U(t,u) = f(t,U(t,u)).$$

Let now

$$\begin{aligned} \Lambda(t) &= \int_0^t \left(\eta(1-\mu)\mathbb{E}_0[f](s) - \alpha_F[f,f_a,f_b,P](s)\right) ds \\ &= \eta(1-\mu)\int_0^t \mathbb{E}_0[f](s)\, ds - \lambda(t). \end{aligned} \tag{18}$$

Then the (17) rewrites in integral form as follows:

$$f_U(t,u) = e^{-\Lambda(t)} f_U^0(u) + \eta e^{-\Lambda(t)} \int_0^t e^{\Lambda(t)} G_U[f](\tau,u)\, d\tau, \tag{19}$$

where $f_U^0(u) = f^0(U(t,u))$. Then the equation (19) rewrites in terms of f as follows:

$$f(t,u) = \Phi_{f^0}[f](t,u), \tag{20}$$

where

$$\begin{aligned} &\Phi_{f^0}[f](t,u) = e^{-\Lambda(t)} f_U^0(\varphi_t^{-1}) \\ &+ \eta e^{-\Lambda(t)} \int_0^t e^{\Lambda(t)} G[f](\tau, \varphi_\tau \circ \varphi_t^{-1}(u))\, d\tau. \end{aligned} \tag{21}$$

The proof can be obtained by following the same steps of [8].

3 The low-order moments evolution

This section is devoted to the derivation of the time evolution of the low-order moments, and specifically the density and the linear-momentum:

$$\rho(t) := \mathbb{E}_0[f](t), \quad m(t) := \mathbb{E}_1[f](t).$$

Let $\varphi(u)$ be a *test function*. Multiply both sides of the $(11)_1$ by $\varphi(u)$ and by integrating with respect to the variable $u \in [a,b]$, we have:

$$\begin{aligned}
&\partial_t \int_a^b \varphi(u) f(t,u)\,du \\
&+\int_a^b \varphi(u)\,\partial_u\left((F-u\alpha_F[f,f_a,f_b,P](t))\,f(t,u)\right)du \\
&=\eta\int_a^b\int_a^b\int_a^b \varphi(u)\mathscr{A}f(t,u_*)f(t,u^*)\,du_*\,du^*\,du \\
&-\eta\int_a^b \varphi(u)f(t,u)\left(\int_a^b f(t,u^*)\,du^*\right)du \\
&+\eta\mu\int_a^b \varphi(u)f(t,u)\left(\int_a^b f(t,u^*)\,du^*\right)du \\
&=\eta\int_a^b\int_a^b\int_a^b \varphi(u)\mathscr{A}f(t,u_*)f(t,u^*)\,du_*\,du^*\,du \\
&-\rho\left(\int_a^b \varphi(u)f(t,u)\,du-\eta\mu\int_a^b \varphi(u)f(t,u)\,du\right). \qquad (22)
\end{aligned}$$

• Let now $\varphi(u)=1$. Then by straightforward calculations the (22) writes:

$$\begin{aligned}
&\dot\rho(t)+\int_a^b \partial_u\left((F-u\alpha_F[f,f_a,f_b,P](t))\,f(t,u)\right)du \\
&=\eta\int_a^b\int_a^b\int_a^b \mathscr{A}(u,u_*,u^*)\,f(t,u_*)f(t,u^*)\,du_*\,du^*\,du \\
&-\eta\rho(t)\int_a^b f(t,u)\,du+\eta\mu\rho(t)\int_a^b f(t,u)\,du. \qquad (23)
\end{aligned}$$

The second term on the left hand side of the (23) writes:

$$\begin{aligned}
&\int_a^b \partial_u\left((F-u\alpha_F[f,f_a,f_b,P](t))\,f(t,u)\right)du= \\
&=\left(F-b\left[\frac{\eta\mu\mathbb{E}_0[f](t)+2F\mathbb{E}_1[f](t)-\gamma(t)}{2+\beta(t)}\right]\right)f_b(t) \\
&-\left(F-a\left[\frac{\eta\mu\mathbb{E}_0[f](t)+2F\mathbb{E}_1[f](t)-\gamma(t)}{2+\beta(t)}\right]\right)f_a(t) \\
&=F\left[f_b(t)-f_a(t)\right] \\
&-\left(\frac{\eta\mu\mathbb{E}_0[f](t)+2F\mathbb{E}_1[f](t)-\gamma(t)}{2+\beta(t)}\right)\left[b\,f_b(t)-a\,f_a(t)\right]. \qquad (24)
\end{aligned}$$

The right hand side of the (23) writes:

$$\begin{aligned}
&\eta\int_a^b\int_a^b\int_a^b \mathscr{A}(u,u_*,u^*)\,f(t,u_*)f(t,u^*)\,du_*\,du^*\,du \\
&-\eta\int_a^b f(t,u^*)\int_a^b f(t,u)\,du^*\,du \\
&+\eta\mu\int_a^b\int_a^b f(t,u^*)f(t,u)\,du^*\,du \\
&=\eta\mu\,\rho^2(t). \qquad (25)
\end{aligned}$$

By using the (24) and (25), the *evolution equation of the density* (23) reads:

$$\begin{aligned}
\dot\rho(t)&=\eta\mu\,\rho^2(t)+\left(\frac{\eta\mu\left[b\,f_b(t)-a\,f_a(t)\right]}{2+\beta(t)}\right)\rho(t) \\
&+\left(\frac{2F\left[b\,f_b(t)-a\,f_a(t)\right]}{2+\beta(t)}\right)m(t)+L[f_a,f_b](t), \qquad (26)
\end{aligned}$$

where

$$\begin{aligned}
L[f_a,f_b](t):=&-\left(\frac{\gamma(t)}{2+\beta(t)}\right)\left[b\,f_b(t)-a\,f_a(t)\right] \\
&-F\left[f_b(t)-f_a(t)\right]. \qquad (27)
\end{aligned}$$

• Let now $\varphi(u)=u$, the (22) writes:

$$\begin{aligned}
&\partial_t \int_a^b u\,f(t,u)\,du \\
&+\int_a^b u\,\partial_u\left((F-u\alpha_F[f,f_a,f_b,P](t))\,f(t,u)\right)du \\
&=\eta\int_a^b\int_a^b\int_a^b u\mathscr{A}f(t,u_*)f(t,u^*)\,du_*\,du^*\,du \\
&-\eta\int_a^b u\,f(t,u)\left(\int_{D_u} f(t,u^*)\,du^*\right)du \\
&+\eta\mu\int_a^b u\,f(t,u)\left(\int_{D_u} f(t,u^*)\,du^*\right)du \\
&=\eta\int_a^b\int_a^b\int_a^b u\mathscr{A}f(t,u_*)f(t,u^*)\,du_*\,du^*\,du \\
&-\eta\left(\int_a^b f(t,u^*)\,du^*\right)\left(\int_a^b uf(t,u)\,du\right) \\
&+\eta\mu\left(\int_a^b f(t,u^*)\,du^*\right)\left(\int_a^b uf(t,u)\,du\right) \\
&=-\eta\rho(t)m(t)+\eta\mu\rho(t)m(t). \qquad (28)
\end{aligned}$$

By integrating by parts, the second term of the left hand side of the (28) writes:

$$\begin{aligned}
&\int_a^b u\,\partial_u\left((F-u\alpha_F[f,f_a,f_b,P](t))\,f(t,u)\right)du= \\
&=b\left(F-b\alpha_F[f,f_a,f_b,P](t)\right)f_b(t) \\
&-a\left(F-a\alpha_F[f,f_a,f_b,P](t)\right)f_a(t) \\
&-\int_a^b\left(F-\alpha_F[f,f_a,f_b,P](t)\,u\right)f(t,u)\,du \\
&=b\left(F-b\left(\frac{\eta\mu\mathbb{E}_0[f](t)+2F\mathbb{E}_1[f](t)-\gamma(t)}{2+\beta(t)}\right)\right)f_b(t) \\
&-a\left(F-a\left(\frac{\eta\mu\mathbb{E}_0[f](t)+2F\mathbb{E}_1[f](t)-\gamma(t)}{2+\beta(t)}\right)\right)f_a(t) \\
&-F\rho(t)+\left(\frac{\eta\mu\mathbb{E}_0[f](t)+2F\mathbb{E}_1[f](t)-\gamma(t)}{2+\beta(t)}\right)m(t). \qquad (29)
\end{aligned}$$

Let

$$\begin{aligned}
S[f_a,f_b](t):=&-b\left(F+b\left(\frac{\gamma(t)}{2+\beta(t)}\right)\right)f_b(t) \\
&+a\left(F+a\left(\frac{\gamma(t)}{2+\beta(t)}\right)\right)f_a(t), \qquad (30)
\end{aligned}$$

then the (28) writes:

$$\begin{aligned}\dot{m}(t) = F\rho(t) - \left(\frac{\eta\mu\rho(t)+2Fm(t)-\gamma(t)}{2+\beta(t)}\right)m(t)\\ +b^2\left(\frac{\eta\mu\rho(t)+2Fm(t)}{2+\beta(t)}\right)f_b(t)\\ -a^2\left(\frac{\eta\mu\rho(t)+2Fm(t)}{2+\beta(t)}\right)f_a(t)\\ -\eta\rho(t)m(t)+\eta\mu\rho(t)m(t)+S[f_a,f_b](t). \qquad (31)\end{aligned}$$

Bearing the (26) and (31) in mind, the density ρ and the linear-momentum m are solutions of the following system of nonlinear ordinary differential equations with quadratic nonlinearity:

$$\begin{cases}\dot{\rho}(t) = \eta\mu\,\rho^2(t) + \left(\frac{\eta\mu\,[b\,f_b(t)-a\,f_a(t)]}{2+\beta(t)}\right)\rho(t)\\ +\left(\frac{2F\,[b\,f_b(t)-a\,f_a(t)]}{2+\beta(t)}\right)m(t)+L[f_a,f_b](t),\\ \\ \dot{m}(t) = F\rho(t) - \left(\frac{\eta\mu\rho(t)+2Fm(t)-\gamma(t)}{2+\beta(t)}\right)m(t)\\ +b^2\left(\frac{\eta\mu\rho(t)+2Fm(t)}{2+\beta(t)}\right)f_b(t)\\ -a^2\left(\frac{\eta\mu\rho(t)+2Fm(t)}{2+\beta(t)}\right)f_a(t)-\eta\rho(t)m(t)\\ +\eta\mu\rho(t)m(t)+S[f_a,f_b](t).\end{cases} \qquad (32)$$

The system (32) needs to be coupled to the initial conditions $\rho(0)$ and $m(0)$, which are set when a specific model is derived.

It is worth stressing that the equations of the system (32) are nonlinear ordinary differential equations with quadratic nonlinearities and depend on the boundary functions.

4 Critical analysis and research perspectives

The derivation of a new mathematical structure of the thermostatted kinetic theory for active particles has been the main goal of the present paper. Specifically the homogeneous boundary conditions assumption has been relaxed and a new thermostat operator has been gained (see (10)). The paper has been also focused on a preliminary analysis of the related initial-boundary-value problem (11) and the time evolution of the low-order moments has been also established, see (32).

It is worth pointing out that the interaction rates η and μ, and the external force F have been assumed constants in the whole paper. The latter assumption has allowed the direct derivation of the evolution equations for the density and the linear-momentum. However the structure of the evolution equations still remains complicated even under the constant interaction rates assumption and their analysis requires a further investigation. Moreover the activity domain has been assumed bounded.

The initial-boundary-value problem (11) has been analyzed by assuming that the boundary and the initial functions are suitable functions; however the regularity properties of these functions have not been investigated in the present paper and it is an important research perspective.

The framework proposed in this paper can be also generalized to complex systems composed by many functional subsystems. Specifically the whole system is divided into n subsystems each of them composed by active particles expressing the same strategy modeled by the activity variable u. Accordingly a nonlinear integro-differential equation is defined for each functional subsystem f_i, for $i \in \{1,2,\ldots,n\}$, and the framework consists of a system of n coupled thermostatted kinetic equations. The derivation of the thermostat term should be straightforward; however the mathematical analysis needs to be adapted. In particular in this context the role of mutation can be introduced by considering the following operator [16]:

$$M_i[\mathbf{f}](t,u) = \sum_{h=1}^{n}\sum_{k=1}^{n}\eta\,\varphi^i_{hk}\,f_h(t,u_*)\,f_k(t,u_*)du_*du^*,$$

where $\mathbf{f} = (f_1, f_2, \ldots, f_n)$ and $\varphi^i_{hk} = \varphi^i_{hk}(u,u_*,u^*)$ denotes the net mutative rate into the ith functional subsystem, due to interactions that occur with rate η between the particle u_* of the hth functional subsystem and the particle u^* of the kth functional subsystem.

Bearing all above in mind, the thermostat operator (10) can be further developed by including the role of nonconservative interactions (proliferation/destruction events and mutations).

From the theoretical viewpoint, the mathematical framework $(11)_1$ could be futher mathematically analyzed for investigating the regularity properties of the solution and the suitable space functions. In particular the continuous dependence on the initial data needs to be investigated [17,18,19]. Moreover, as already mentioned, the whole analysis of the present paper could be generalized to the nonconstant interaction rates case and for a nonconstant external force.

An important issue to be taken into account is the introduction of external agents at the microscopic scale; a microscopic agent can be modeled by introducing a known distribution function (outer functional subsystem), see [20], which interacts with the (inner) functional subsystems.

The framework proposed in this paper refers to homogeneous complex systems where the dynamics of the space and velocity variables is neglected. The introduction of the space and velocity variables is an important research direction [21] and in particular the derivation of the macroscopic equations for the low-order moments can be performed by employing asymptotic

methods [22,23,24]. The asymptotic methods have at their basis the scaling of the time and space variables and the resulting macroscopic equations are of parabolic or hyperbolic type.

A future research direction is the introduction of fractional-order derivatives and time delays [25]. The latter issues have gained much attention recently, see, among others, the books [26,27].

From the application point of view, the mathematical framework derived in this paper can be proposed for the modeling of complex living systems composed by a large number of active particles. In particular the modeling refers to the complex phenomena occuring in biological systems [28,29,30,31].

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Conflict of Interest The authors declare that they have no conflict of interest.

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