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Ordered motion of active colloids and effective temperature

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ABSTRACT

Using recent developments of non-equilibrium thermodynamics, we introduce an effective temperature for active colloidal systems, which is a product of two factors. The first one arises due to the motor activity and describes the randomized motion of the active particles, whereas the second one is a consequence of the ordered (collective) motion due to the alignment effects or initially ordered configuration. These factors depend on the corresponding characteristic velocities: the first one is expressed in terms of the propelled (swimming) velocity of an individual active particle, while the second one — in terms of the local drift velocity, which characterizes the collective motion of the active particles and plays a role analogous to that of an order parameter. The behavior of the active systems is governed by the interplay between these two factors, which leads to a hierarchy of anomalous diffusion regimes with different characteristic time scales and corresponding effective diffusion coefficients.

1. Introduction

The question of what precisely is a "local temperature", which has a well-established meaning only in global equilibrium, arises in any physical situation under far from equilibrium conditions, particularly, in granular matter, sheared fluids, amorphous semiconductors, glasses, shockwaves, biological and climate systems, turbulent fluids or chaotic systems or, in a spatially smaller scale, nuclear materials and nanoscale systems among others [1–18]. Different concepts of non-equilibrium temperature and entropy have been discussed in thermodynamic and microscopic approaches, including information theory, kinetic theory of gases, fluctuation–dissipation theorem (FDT) and computer simulations [1–18]. Several effective non-equilibrium temperatures may be defined, all of which reduce to a common value in equilibrium states, but which yield different results in non-equilibrium situations. For glassy systems, the definition of the equilibrium temperature has been extended to the non-equilibrium regime, showing up as an effective quantity in a modified version of the FDT [10]. Glasses are out-of-equilibrium systems in which thermal equilibrium is reached by work exchanged through thermal fluctuations and viscous dissipation exchange that happens at widely different timescales simultaneously.

Recently, active colloidal particles has emerged as a novel class of the active systems that is currently under intense scrutiny [19–28]. The active systems consume energy from environment or from internal fuel tanks and dissipate it by carrying out internal movements, which imply that their behavior is more ordered and thus intrinsically out of equilibrium. Realizations of active matter in biology are manifold and exist at different scales. Some of them are: active colloids, bacterial suspensions and cytoskeleton in living cells [19–28]. Understanding the generic properties of

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active systems and the collective motion of active colloidal suspensions poses fundamental and challenging questions of nonequilibrium thermodynamics and statistical physics. For the active colloidal systems, the definition of the effective (nonequilibrium) temperature has also come from the extensions of the FDT [19–28].

In this paper we use the definition of the effective temperature for the nonequilibrium systems taking into account the ordered motion of the energy carriers [6,7], which is briefly discussed in Section 2. In Section 3 we use this definition to describe the effective temperature of active system with allowance for the ordered effects and combine it with the effective temperature due to the FDT. Conclusion is made in Section 4. Appendix A briefly describes the effective diffusion coefficient of colloidal particles due to the system activity, which defines the FDT temperature. Appendix B demonstrates that the interplay between the Brownian diffusion of colloidal particles and the system activity leads to the minimum in the dependence of the effective diffusion coefficient on the particle size.

2. Effective temperature and entropy of passive systems with ordered motion

2.1. Effective temperature and entropy in systems with energy flux

Let us consider 1D system, which consists of two groups of energy carriers — one group moves on the left and another on the right [3,7,18]. This so-called two group (TG) approach yields the evolution equations for the temperature of the carriers as follows [7]

$$\frac{\partial T_1}{\partial t}+v\frac{\partial T_1}{\partial x}=\frac{T_2-T_1}{2\tau} \tag{1}$$

$$\frac{\partial T_2}{\partial t}-v\frac{\partial T_2}{\partial x}=\frac{T_1-T_2}{2\tau} \tag{2}$$

where $T_1(x,t)$ is the kinetic temperature of the heat carriers going to the right, $T_2(x,t)$ is the kinetic temperature of the heat carriers going to the left, v is the average velocity of heat carriers. Different formulations of the TG approach, similar to Eqs. (1)–(2), including Boltzmann transport equation with single relaxation time approximation, have been successfully used to study heat and mass transfer problems (see [2–7] and references therein). The corresponding average temperature T and heat flux q are given as

$$T=(T_1+T_2)/2 \tag{3}$$

$$q=vc_p(T_1-T_2)/2 \tag{4}$$

where c_p is heat capacity. After some algebra, Eqs. (1)–(4) give

$$\frac{\partial T}{\partial t}+\frac{\partial q}{\partial x}=0 \tag{5}$$

$$q+\tau\frac{\partial q}{\partial t}=-\tau v^2 c_p\frac{\partial T}{\partial x} \tag{6}$$

Eq. (5) represents the energy conservation law, whereas Eq. (6) is the modified Fourier law where $v^2\tau c_p=\lambda$ is thermal conductivity. Combining Eqs. (5) and (6), one obtains well-known hyperbolic heat conduction equation (HHCE) [1–7]

$$\frac{\partial T}{\partial t}+\tau\frac{\partial^2 T}{\partial t^2}=a\frac{\partial^2 T}{\partial x^2} \tag{7}$$

The temperatures of the heat carriers moving to the right, T_1, and moving to the left, T_2, can be represented as [7]

$$T_1=T+q/vc_p \tag{8}$$

$$T_2=T-q/vc_p \tag{9}$$

It should be stressed here that the temperatures T, T_1 and T_2 in Eqs. (1)–(9) characterize the corresponding local energy density, i.e. are so-called kinetic temperatures [7]. In particular, the kinetic temperature T, which space–time evolution is governed by the HHCE, Eq. (7), characterizes the local energy density of the nonequilibrium state — it is equal to the equilibrium temperature of the same system with the same internal energy in equilibrium. It implies that if a local volume element of the nonequilibrium system consisting of the two groups of the heat carriers with the temperatures T_1 and T_2 is suddenly isolated, i.e. bounded by adiabatic and rigid walls, and allowed to relax to equilibrium, after equilibration the equilibrium temperature of the local element will be $T_{eq}=(T_1+T_2)/2$. However, if the two groups of the heat carriers with T_1 and T_2 equilibrate reversibly, i.e. while producing work, their common equilibrium temperature θ will be [6,7]:

$$\theta=(T_1T_2)^{1/2} \tag{10}$$

Indeed, before equilibration the total equilibrium entropy of the two groups is equal to $S_{eq}=k_B\ln T_1+k_B\ln T_2=k_B\ln T_1T_2$, whereas after equilibration $\overline{S}_{eq}=2k_B\ln\theta$. The entropy change during the equilibration is

$$\Delta S=S_{neq}-S_{eq}=k_B\ln T_1T_2/\theta^2 \tag{11}$$

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