Effective temperature of active complex matter

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We use molecular dynamics simulations to study the dynamics of an ensemble of interacting self-propelled semi-flexible polymers in contact with a thermal bath. Our intention is to model complex systems of biological interest. We find that an effective temperature allows one to rationalize the out of equilibrium dynamics of the system. This parameter is measured in several independent ways – from fluctuation-dissipation relations and by using tracer particles – and they all yield equivalent results. The effective temperature takes a higher value than the temperature of the bath when the effect of the motors is not correlated with the structural rearrangements they induce. We show how to use this concept to interpret experimental results and suggest possible innovative research directions.

Introduction.- Active matter entities, be them particles, filaments or other, absorb energy from their environment or internal fuel tanks and use it to carry out motion. In this ubiquitous type of soft condensed matter, energy is partially transformed into mechanical work and partially dissipated in the form of heat. Units interact directly or through disturbances propagated in the medium. The effect of motors can be dictated by the state of the unit and/or its immediate neighborhood and it is not necessarily fixed by an external field. Active matter is thus kept in a non-equilibrium steady state and presents a number of interesting dynamical features, unusual mechanical properties, very large responses to small perturbations, and very large fluctuations. Realizations of active matter in biology are manifold and exist at different scales.

Surprisingly enough, studies of active matter have been mainly analytical so far, based on refined calculations using very stylized models [2–9], computer simulations of continuum models [10], and numerical studies of relatively simple lattice models [11,12]. Molecular dynamics simulations, that have proven to be so helpful to elucidate the behavior of complex passive systems, have not been much employed in this field yet.

Quite independently, passive systems with complex out of equilibrium dynamics have been the focus of much study. These are systems with competing interactions between their constituents and no external energy input that in some conditions (such as sufficiently low temperature or high density) cannot equilibrate with their environment. Glassy systems are the typical example. An important outcome of the theoretical modeling of these systems, later confirmed with numerical simulations, is the generation of an effective temperature, $T_{\text{eff}}$ [13]. $T_{\text{eff}}$ should be understood as a time-scales dependent parameter which takes a thermodynamic meaning in systems with slow dynamics only [13, 14]. Experimental measurements of $T_{\text{eff}}$ in different glassy systems [15, 20] have been performed.

In [21] we took a first step in the direction of analyzing $T_{\text{eff}}$ in active matter. We studied the dynamics of an ensemble of self-propelled particles, meant to be a reasonable model for real but simple active matter such as bacterial colonies, with molecular dynamics simulations. Here we get closer to more complex cases and we study a model of filamentous semi-flexible polymers [22]. We analyze its structure and dynamics and we study $T_{\text{eff}}$ by using a variety of independent measurements. In particular, we demonstrate that tracer particle techniques, that have already been exploited in the study of the mechanical properties of real biological systems [23, 24], can also be useful to obtain a direct characterization of the out-of-equilibrium state. Details of the calculations will be given in a forthcoming publication [25].

The model.- We consider the model for a passive semi-flexible linear polymers (filaments) of Ref. [26]. The optimal values of the parameters have been fixed by preliminary calculations [25, 26]. Polymers chains are coarse-grained and each segment is formed by identical beads, with mass $m$ and diameter $r_0$. Each bead is in contact with a thermal environment that is described by a random noise and a viscous drag. The dynamical evolution at a bath temperature $T$ is therefore controlled by a Langevin equation.

The deterministic mechanical conservative force among beads is given by intramolecular and intermolecular contributions. Connectivity of the chains is assured by harmonic springs acting between nearest-neighbor monomers. Chain rigidity is controlled by a purely repulsive interaction between next nearest-neighbor monomers. The actual choice of parameters allows one to control the flexibility of the chains, ranging from semi-rigid to completely flexible [26, 27].

Having in mind that no simple technique can take into

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account chemical activity in a molecular dynamics calculation, physical insight has been used to choose a reasonable model for motor action. Only a fixed fraction of polymers are provided with motors that have a gentle but still detectable effect on the behavior of the system. We localize the non-conservative motor activity on the monomer at the center of the polymer [27]. The motor effect is given by a time series of random isotropic kicks generated by a suitable stochastic process [21]. The action of the motors is independent of the structural rearrangements they induce (adamant [28] motors). The force of all motors, \( f^M \), is the same and a fraction of the mean conservative mechanical force acting on the equivalent passive system, \( \mathcal{F} \). We thus quantify the motor activity with the control parameter \( f = f^M / \mathcal{F} \). More details on the model are given in Refs. [21, 25].

We express all quantities in dimensionless reduced units [29] that we associate to reasonable values of the experimentally measured counterparts [30]. The typical unit of energy is \( 2k_BT \); typical lengths are measured in units of 0.4 nm implying forces of order 20 pN at ambient temperature, \( T = 300 \) K.

**Structure.** - We first investigate the structure of the semi-flexible active polymer melt by keeping all external macroscopic conditions fixed and varying the motor activity \( f \). The analysis of the static structure factors and pair distribution functions (not shown) is consistent with a picture in which the average nearest neighbor distance between beads pertaining to different polymers decreases upon increasing \( f \). Overall, the motors have the mixed effect of making the melt more compact and more disordered simultaneously. This picture is corroborated by the extremely complex probability distributions of the gyration radius, \( R_g \), which are highly non-Gaussian and very asymmetric (Fig. 1). Motor activity has the effect of pushing the filaments closer and these, at the same time, fold substantially. We interpret this behavior in terms of a competition between two effects: crowding, which is related to excluded volume effects and tends to slow down the dynamics, and folding of the chains, which dynamically lifts the topological constraints, therefore decreasing entanglement. These have important consequences on the long-time evolution of the system, as it is verified below.

**Dynamics.** - We next quantify the effect of motor activity on the long time dynamics. Figure 2 a) shows the self-intermediate scattering function, \( F_s(Q, t) \), at the wave-vector of the first maximum of the static structure factor (activities increase to the left). b) Diffusion coefficient, \( D \), and inverse structural (self-)relaxation time, \( \tau_s \), as a function of \( f \). Data are normalized to the value for the passive system and follow power laws (dashed lines), with the indicated exponents.

![Graph](image1.png)

**FIG. 1:** (Color online.) Probability distributions of the gyration radius, \( R_g \), at the investigated motor activities, \( f \). The structure is highly non trivial with an average value shifting towards lower values upon increasing \( f \). The passive case \( (f = 0) \) is also shown.

![Graph](image2.png)

**FIG. 2:** (Color online.) a) Time-dependence of the intermediate scattering function, \( F_s(Q, t) \), at the wave-vector of the first maximum of the static structure factor (activities increase to the left). b) Diffusion coefficient, \( D \), and inverse structural (self-)relaxation time, \( \tau_s \), as a function of \( f \). Data are normalized to the value for the passive system and follow power laws (dashed lines), with the indicated exponents.
Effective temperatures.- The analysis above proves that both structure and dynamics of an active system are influenced by motor activity in a very complex fashion. We ask now whether it is possible to embed all this complexity in a single parameter, also prone to be directly determined in experiments. The chosen quantity is the effective temperature \( T_{eff} \). One way of measuring the effective temperature in a non-equilibrium steady state consists in using the generalization of the fluctuation-dissipation theorem to out-of-equilibrium conditions \([13]\). The most visual way of analyzing the data is to construct a parametric relation between the integrated linear response, \( \chi(t) \), and the correlation \( C_{AB}(t) \) of a wisely chosen pair of observables, \( A \) and \( B \), and associating minus the inverse of its slope with a possibly time-dependent parameter \( T_{eff}(t) \) \([13, 34]\). Such measurements were performed in different out-of-equilibrium conditions \([35, 38]\) demonstrating that \( T_{eff}(t) \) is (asymptotically) piecewise constant taking, typically, two values: the one of the environmental bath at short times and an additional one characterizing the structural relaxation at long times, in cases with slow dynamics.

We performed these measurements for different values of the forcing \( f \) and the results are shown in Fig. 3. The needed observables are chosen such that the considered correlation functions are the \( F_s(Q,t) \) of Figure 2(a). Details can be found in Ref. \([35, 38]\). The curves clearly show two regimes. The first one, corresponding to high frequencies, represents the fast vibrations of the monomers, before any structural relaxation takes place. The second regime, at long times, describes the actual structural relaxation in the sample. In all cases, the parametric plot is rather well described by a straight line, implying that \( T_{eff} \) is a constant over this time-scale. These data are also shown in Fig. 4 with open (red) squares.

![FIG. 3: (Color online.) Fluctuation-Dissipation relations at the indicated values of \( f \). The red data on top (closed circles) are for the passive system and the dashed (red) line has slope \(-1/T\) confirming that FDT holds in this case. The solid lines are linear fits used to estimate the value of \( T_{eff} \).](image)

![FIG. 4: (Color online.) Summary of the entire set of data generated in this study. The power-law dependence of the effective temperature on motor activity, \( T_{eff}/T = 1 + \gamma f^2 \), is also shown (dashed line).](image)
To the Einstein relation, $T_{eff}$ should be the parameter linking the tracers’ mean-square displacement and their driven displacement under a weak external applied force, in the long time limit in which the dynamics is diffusive. Data for $T_{eff}$ obtained in this way are included in Fig. [I] as open (green) triangles.

Figure [II] collects all our results in the form $T_{eff}/T$ against $f$. We also include (diamonds) average values with error bars calculated from the entire set of data. The figure demonstrates that independent determinations of $T_{eff}$ yield consistent results and suggests that, in our system, there is a single frequency-independent $T_{eff}$ parameter, with a precise thermodynamic meaning. Data tend to $T_{eff} = T$ in the limit of vanishing activation, as they should, and the deviation from the environmental temperature monotonically increases with increasing forcing. Most importantly, data are represented by the empirical law $T_{eff}/T = 1 + \gamma f^2$, with $\gamma = 15.41$ (dashed line). Remarkably, this finding supports our conjecture that the parameter $f$ plays here a role analogous to the Peclet number for colloidal active particles considered in a few very recent experiments [31, 32].

In conclusion, we studied the out of equilibrium behavior of a system of active motorized filaments, a model for complex biological structures, using a genuine microscopic approach that is still quite innovative in the field. We described the influence of motor activity on both structure and dynamics, finding a rationale for very similar recent experimental observations. We confirmed the relevance of the effective temperature, a concept well established in statistical mechanics of glassy systems, for complex active matter. Most important, we demonstrated that this parameter, relatively simple to measure by micro rheology techniques, can be directly related to chemical activity, a process of extraordinary complexity. It would be interesting to explore the possibilities offered by the molecular dynamics approach used in this paper to clarify the extremely complex phenomenology of cell mechanical stability [33, 34]. In particular, one could try to give an answer to the question as to how mechanical properties (such as elastic moduli) change with motor activity and whether these changes can be rationalized in terms of an effective temperature.

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