

Effective temperature in non-equilibrium systems

Active Matter sub-group
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Why this doc exists: I'm trying to explain the non-equilibrium "freezing" and subsequent crystallization I see in my 2D active polygon systems (to borrow language from the literature [1,2]). This is by no means meant to be a complete overview, but I hope that writing down what I have found out so far and continuing to update it will be helpful for others looking to go down this literature rabbit hole.

1 First things first: what is temperature?

We traditionally approach the definition of temperature in equilibrium systems two ways: through either (1) a kinetic or (2) an entropic lens.

(1) For simple species that we can assume to have elastic collisions, we can think about temperature as a measure of the kinetic energy in the system. As we'll recall from freshman chemistry,

$$T_{\text{kinetic}} = \frac{2}{3k_B} \langle E_{\text{kinetic}} \rangle \quad (1)$$

For simply systems, this works well. However, many of the systems we deal with are more complicated; their internal energy cannot be primarily approximated by kinetic energy due to internal degrees of freedom (e.g. molecular rotation, vibration) or collective modes of a material.

(Note: (1) with some adjustments might actually be a reasonable approximation for temperature in point-disk systems, but I haven't seen an approach using a modified version of this in the literature.)

(2) More generally, then we can think of temperature as a measure of the tendency for of an object to spontaneously give up energy to its surroundings. Just to refresh all of

our memories, we define temperature in classical statistical mechanics in the following way:

$$T = \left(\frac{\partial U}{\partial S} \right)_{N,V} = \left(\frac{\partial H}{\partial S} \right)_{N,P} \quad (2)$$

Where U is the internal energy, H is the Helmholtz free energy, and S is the entropy.

In active systems, the typical approaches to find an effective temperature leverage definition (2) of temperature. I particularly like the intuition used in Ref. [3], which frames T_{eff} as the additional agitation caused by the nonconservative forces in active systems [3].

2 Why are we interested in defining an effective temperature in active systems?

The temperature of the bath the particles are in (plain old $k_B T$ in our systems) drives the magnitude of the thermal fluctuations.

However, active systems are characterized by having a driving force that drives motion and, generally, is \gg than the force of the thermal fluctuations. An effective temperature would allow us to compare the non-equilibrium behavior of the system to the equilibrium thermal fluctuations.

Of interest to our systems, having a defined framework for accounting for the role of various perturbations (...such as shape) in the non-equilibrium behavior of a system would then allow us to quantify the impact of these perturbations/influences.

(Whether temperature is the best method of approaching the issue of the role of shape remains to be seen, and is why this document exists.)

3 Summary of different approaches to calculating effective temperature in active systems

Some of the difficulty in calculating an effective temperature comes from the well-documented complications in calculating the thermodynamic properties in active systems [4–8]. Preisler sums this up well:

“... even basic thermodynamic properties such as non-equilibrium equivalents of temperature and pressure depend sensitively on the precise definitions at hand, e.g., the mechanical pressure (force per unit area exerted on a wall), thermodynamic pressure (derivative of the free energy with respect to volume),

or hydrodynamic pressure (trace of the bulk stress tensor) do not necessarily correspond to each other in out-of-equilibrium systems, the same is true for various definitions of temperature, e.g. using diffusion, fluctuation-dissipation theorem, and others... there is no consensus on how to define the pressure and temperature in active matter and there is yet no clear statistical mechanics framework for active systems.” [9]

With that kind of lead-in, Preisler and Dijkstra then go on to attempt to establish a statistical framework, as does the recent paper on the arxiv by Hancock and Baskaran [10] (in full disclosure, I haven’t read this one yet– ask Chengyu for details). They both seem to use a similar approach of attempting to fit an active matter system to a Boltzmann, and Priesler uses an effective temperature to achieve this.

As people who have been studying this much longer than I have are still disagreeing on the “best method” of defining temperature, I’m not going to attempt to do so. However, below are the key few papers for different methods I’ve seen used.

Approach	References
Diffusion	[11]
Fluctuation-Dissipation Theorem	[12–14]
Tracer particles	[13]
Tracer particles + active stress	[15]
Configurational entropy	[9]
Fitting activity/comparing to [a] Boltzmann distribution at T_{eff}	[9, 16, 17]
Comparison with glass transition	[18]

A few quick notes on what each approach is.

Diffusion

- I’m including this in the interest of attempted completeness; apparently Michael Cates makes a diffusion-driven argument for a T_{eff} in his review on whether biology needs statistical mechanics. I did not notice this when I read it a while back, so will need to go back and re-read

Fluctuation-Dissipation Theorem

- Generalizing the fluctuation-dissipation theorem to out-of-equilibrium conditions [13], citation 15 in [13]

Tracer particles

- “Temperature should be measurable with a thermometer. A tracer particle with a long internal time scale proportional to the square root of its mass acts as a thermometer that couples to the long-time-delay structural rearrangements and not to the fast vibrations $t \sim 0$ which yield the ambient temperature” [12]

- Using a free tracer particle with mass much larger than one of the polymer beads, whose kinetic energy can be related to the system’s effective temperature via an equipartition theorem [13], yield an expression where the T_{eff} is a function of the activity

Tracer particles + active stress

- Apparent temperature can be probed from the motion of a tracer particle and “can be estimated by the zero-frequency, zero-wave number variance of the active stress”
- These experiments are put into some more context in the always-helpful Ref [15]

Configurational entropy

- If we assume entropy is a continuous function of internal (or potential) energy, we can define a potential energy and configurational entropy for the system and use that to find an effective temperature
- Preisler et al use a density of states argument to find the configurational entropy to then derive a temperature [9]

Fitting activity/comparing to [a] Boltzmann distribution at T_{eff}

- Included for attempted completeness

Comparison with glass transition

- Berthier and Kurchan argue that “dynamic arrest in driven and active materials shares important similarities with the equilibrium glass transition, in particular... the behaviour of time-correlation functions and the emergence of an effective thermal behaviour”
- Ref [13] citations 18-23 are examples of measuring T_{eff} in glassy systems; the argument that the active matter community makes is that very dense systems can be treated like glasses, and therefor similar approaches to develop the effective temperature can be used

4 Side note: Granular materials

Granular materials are another non-equilibrium system with a wealth of literature attempting to define an “effective temperature”. These materials are athermal and composed of cohesionless particles. They are “nonergodic in the extreme sense, as they stay in a single configuration unless driven externally.” We can think of these as the extreme case of our systems in which we set $T = 0$, resulting in a non-Brownian system. Not unlike in an active system without Brownian noise, collective behavior emerges solely as a response to

driving forces. In contrast with the types of active systems commonly studied, in which each particle converts its internal energy to a driving force whose direction is often fixed relative to the particle, granular matter is often driven by an *external* force whose direction is fixed relative to the *frame*. [19]

The review cited above is an excellent 2015 overview of this field by Karen Daniels of NC State (who spoke in the Physics department back in the fall). A key topic of her talk was the effective temperature often used in the granular matter community, called the “compactivity,” X.

$$\frac{1}{X} = \frac{\partial S(V)}{\partial V} \quad (3)$$

Daniels’ talk discussed why this might not be a great temperature stand-in, which is not something I’m going to get into here.

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