Effective Temperatures in Driven Systems near Jamming

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Modern Challenge

- We understand a lot about the collective properties of many-particle systems in thermal equilibrium

- But flowing glassy systems are far from equilibrium

microscopic \[\left\{\begin{array}{c}
\text{systems near thermal equilibrium} \\
\text{statistical mechanics}
\end{array}\right\} \rightarrow \text{macroscopic}
\]

\[\left\{\begin{array}{c}
\text{systems far from equilibrium} \\
??
\end{array}\right\}
\]
Can fluctuations be described by effective temperature?

If so, so what?
Testing Effective Temperature

• We and others conducted numerical simulations of simple models under steady-state shear

• Calculate $T_{\text{eff}}$ in several independent ways

• In an equilibrium system, all calculations must yield same result

• Are they the same in a driven system?

Model: Equations of Motion

\[ m \frac{d^2 \vec{r}_i}{dt^2} = \vec{F}_i^e + \alpha \vec{F}_i^v - \beta \Delta \vec{v}_i \]

\[ \Delta \vec{v}_i = \vec{v}_i - \dot{\gamma} y_i \hat{x} \]

Constant Shear-rate \( \dot{\gamma} \) b.c.’s

Types of simulations:

1. Sheared; massless; athermal \( \dot{\gamma} > 0; m = 0; \beta = 0 \)
2. Sheared; massive; athermal \( \dot{\gamma} > 0; m \neq 0; \beta = 0 \)
3. Sheared; massive; thermal \( \dot{\gamma} > 0; m \neq 0; \alpha = 0; T > 0 \)
4. Equilibrium \( \dot{\gamma} = 0; m \neq 0; \alpha = 0; T > T_g \)
Temperatures from Linear Response

• Thermal diffusion

\[ \langle (\Delta r(t))^2 \rangle = 6Dt \]

\[ D = \frac{T}{S} \]

- Temperature
- Drag

• Response to Force F

Particles move at speed \( F / \zeta \) where \( \zeta = 6\pi \eta a \) is drag

\[ T_{eff} = \left\{ \frac{D}{v/F}, \frac{\langle (\Delta V)^2 \rangle}{V \kappa_T}, \ldots \right\} \]

- Size of fluctuations (correlation)
- Ease of creating fluctuation (response)
Other Linear Response Relations

Adiabatic compressibility ↔ Pressure Fluctuations

\[ \kappa_s^{-1} = \frac{A}{T} \left\langle (p - \langle p \rangle)^2 \right\rangle \]


Viscosity ↔ Shear Stress Fluctuations

\[ \eta = \frac{A}{T} \int_0^\infty dt \left\langle \sigma_{xy}(t) \sigma_{xy}(0) \right\rangle \]

Heat Capacity ↔ Energy Fluctuations

\[ \frac{\partial \langle U \rangle}{\partial T} = \frac{1}{T^2} \left\langle (U - \langle U \rangle)^2 \right\rangle \]

\[ \int \frac{d \langle U \rangle}{\left\langle (\delta U)^2 \right\rangle} = \int \frac{dT}{T^2} \]
Results

• 4 indep. def’ns of $T_{\text{eff}}$ yield the same result
• Effective temperature appears to be a useful concept!

• AND there’s more....
Textbook Definition of Temperature

• Monte-Carlo results for $1/T = dS/dU$:

- Shear makes system nearly ergodic!


• Shear makes system nearly ergodic! BUT…….
Two Time-Scale/Two Temperatures


• At short times, system sees $T_{\text{bath}}$

• At long times, system sees $T_{\text{eff}}$

• What happens if harmonic oscillator is inserted into system?

$k_B T_{spr} = k_{spr} < y^2 >$

T. Danino
Time-Dependent Linear Response

e.g. FD relation for density

\[ \rho(\vec{k},t) = \sum_{j=1}^{N} e^{i\vec{k}\cdot\vec{r}_j(t)} \]

\[ C(t) = \langle \rho(\vec{k},t)\rho(-\vec{k},0) \rangle \]

correlation

\[ h_\rho = \text{perturbation} \]

\[ \bar{R}(t) = \frac{\langle \rho(\vec{k},t) - \rho(\vec{k},0) \rangle}{h_\rho} \]

response

\[ \bar{R}(t) = \frac{\bar{C}(0)}{T} \left[ 1 - \frac{\bar{C}(t)}{\bar{C}(0)} \right] \]

\[ C(t) = \frac{\bar{C}(t)}{\bar{C}(0)} \]

Fluctuation-Dissipation Theorem

\[ R(t) = \frac{\bar{R}(t)}{\bar{C}(0)} \]

\[ R(t) = \frac{[1 - C(t)]}{T} \]
Intercept vs. Long-Time Slope

• Previous definitions based on static linear response
  \[ R(t) = \frac{1 - C(t)}{T} \]
  \[ R(t = \infty) = \frac{1}{T} \]

• Definitions based on time-dependent linear response

System in thermal equilibrium
Sheared Glassy Systems

The response-correlation curve is not a straight line!

• short-time slope: \( T_S \) is bath temperature
• long-time slope: \( T_L \) depends on shear rate

Because curve is not straight, \( T_L \neq T_I \)


Cugliandolo and Kurchan, PRL 71, 173 (1993)
Density fluctuations: Def. 4


\[ \rho(\vec{k}, t) = \sum_{j=1}^{N} e^{i\vec{k} \cdot \vec{r}_j(t)} \]

\( m > 0; \) athermal
\( \dot{\gamma} = 0.01 \)

\[ R_{\rho(k)}(t) \]

\[ C_{\rho(k)}(t) \]

\( T_L \) from density fluctuations matches Defs. 1-3 based on static linear response!
Pressure fluctuations

\[ P = \sum_{j=1}^{N} P_j \]

k=0 quantity

\[ m>0; \text{thermal} \]

\[ \dot{\gamma} = 0.01 \]

\[ R_P(t) \]

\[ C_P(t) \]

\[ \frac{1}{T_L} \]

\[ \frac{1}{T_S} \]

\[ \frac{-1}{T_S} \]

\[ \frac{1}{T_I} \]

\[ 0 \]

\[ 0.2 \]

\[ 0.4 \]

\[ 0.6 \]

\[ 0.8 \]

\[ 1 \]

• Intercept, not slope, corresponds to consistent \( T_{\text{eff}} \)
This result is robust. We have varied

- **System** (athermal with dissipation, thermal with no dissipation)
- **Potential**
- **Density**
- **Shear rate**
- **Bath temperature**

\[ T_I(p) = T_L(\rho_k) \]


- Static and dynamic linear response give consistent \( T_{\text{eff}} \)
- Cugliandolo-Kurchan picture is conceptually incomplete
The Complications

For most observables, can choose consistent set

<table>
<thead>
<tr>
<th>Quantity</th>
<th>$T_I$</th>
<th>$T_L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p(k=0)$</td>
<td>✓</td>
<td>X</td>
</tr>
<tr>
<td>$\sigma(k=0)$</td>
<td>✓</td>
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<tr>
<td>$p(k_y)$</td>
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</tr>
<tr>
<td>$\rho(k_y)$</td>
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<td>✓</td>
</tr>
</tbody>
</table>

But how to know which definition to use???

- $k=0$ quantities: $T_I$
- $k>0$ or local quantities: $T_L$

Others don’t agree

$p_{zz}, (2p_{xx}-p_{yy}-p_{zz})/3,$ config. temps, force temp. (Shokef)
Altogether, 8 indep. def'ns of $T_{\text{eff}}$ yield same value

- $T_p, T_\sigma, T_{pk}, T_U, T_\rho, T_E, T_{spr}, T_K$

$T_S$ is consistent

Effective temp. appears to be reasonable concept
Why should we care?

• If I tell you the temperature of a material, you don’t get very excited.

• What does $T_{\text{eff}}$ tell us about the system (other than the relation between correlation and response)?

• Does $T_{\text{eff}}$ tell us anything about the dynamics of the system near jamming?
• But this is a weird phase diagram
  - Shear stress is nonequilibrium axis
  - Can we replace shear stress with $T_{\text{eff}}$?
Glass Transition

\[ \log \tau(s) \]

\[ T_g / T \]

Super-Arrhenius dependence of relaxation time

Viscosity vs. T

T. Haxton

\[ \eta = \eta_0 e^{A/(T-T_0)} \]

\[ T_0 \approx 0.0013 \]

Super-Arrhenius dependence of viscosity on T
System has apparent yield stress for $T < T_0$.

Apparent yield stress increases with decreasing $T$.

Power-law rheology for $T \equiv T_0$ (SGR)
Behavior of $T_{\text{eff}}$

- For $T>T_0$, $T_{\text{eff}} \rightarrow T$ as $\dot{\gamma} \rightarrow 0$
- For $T<T_0$, $T_{\text{eff}} \rightarrow T_{\text{eff},g}$ as $\dot{\gamma} \rightarrow 0$
- $\eta$ vs. $T_{\text{eff}}$ is super-Arrhenius
- $T_{\text{eff},g} < T_0$
What do shear-induced fluctuations do?

Let $V_r =$ typical size of rearrangement events

Suppose that between rearrangements, local strain can build up to $\gamma_{\text{max}} \approx \exp\left(\Delta E / T_{\text{eff}}\right)$ due to activated crossing of energy barriers $\Delta E$ with $T_{\text{eff}}$.

But $\Delta E \approx \sigma_{xy} \gamma_{\text{max}} V_r$

This yields $\sigma_{xy} \approx \sigma_0 \exp(-\Delta E / T_{\text{eff}})$

Data collapse for $T \ll T_0$ or large $\sigma_{xy}$

Limiting behavior:

$$1/T_{\text{eff}} \approx -\frac{1}{\Delta E} \log\left[\sigma_{xy} / \sigma_0\right]$$
Summary

• Steady shear appears to have two effects
  - It lowers typical energy barriers
  - But it also gives rise to fluctuations, which allow activated crossing of the barriers

• The typical energy barrier should depend on shear rate (Ashwin, Brumer, Reichman, Sastry, J Phys Chem B 108, 19703 (2004)).
• Still ahead: analysis of inherent structures
Second law of thermodynamics

• Do 2 systems in “thermal” contact equilibrate to same $T_{\text{eff}}$?

• Recall earlier results:
  - Small and large particles in binary sheared glass have same $T_{\text{eff}}$ (Berthier & Barrat, J Chem Phys, 116, 6228 (2002))
  - Massive particle has same $T_{\text{eff}}$ as small particles (Berthier & Barrat, PRL 89, 095702 (2002)).
  - Harmonic oscillator has same $T_{\text{eff}}$ as system

• Requires matching of time scales
  - Massive particle
  - Low-frequency oscillator

• What about two large systems? How can we place them in contact?
Preliminary studies of 2nd law

- Separate by flexible chain with $k_{\text{chain}}$
- This allows
  - No particle exchange
  - Propagation of rearrangement events
  - Equilibration of shear stress if average horizontal position is not fixed
  - Equilibration of pressure if average vertical position is not fixed
Preliminary results

<table>
<thead>
<tr>
<th>Pressure allowed to equilibrate?</th>
<th>Shear stress allowed to equilibrate?</th>
<th>$T_{\text{eff}}$ equilibrates?</th>
</tr>
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<tbody>
<tr>
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• Final effective temps of both systems are equal if final pressures are equal.

• Does $T_{\text{eff}}$ depend only on pressure? (N. Xu & C. S. O’Hern)
If $T_{\text{eff}}$ were just a function of $p$, then all data for different $T$ would collapse on single curve.

No, $T_{\text{eff}}$ does not just depend on pressure.

So why does equilibration of $p$ allow equilibration of $T_{\text{eff}}$?
Conclusions

• $T_{\text{eff}}$ seems to be reasonable for sheared glassy systems
• Experiments need to measure as many $T_{\text{eff}}$ as possible (Durian)
  • Einstein relation
  • Harmonic oscillator (optical or magnetic trap)
• $T_{\text{eff}}$ seems to control barrier hopping w/ Boltzmann prob.
• When is $T_{\text{eff}}$ useful? (2 time-scale/2 temp?)
• Second law?
  • How is “effective heat” exchanged?
  • Is configurational entropy conjugate to $T_{\text{eff}}$ even when particles have inertia?

Song, et al. (PNAS 05)
Acknowledgements

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