

## Effective Temperatures in Driven Systems: Static Versus Time-Dependent Relations

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Using simulations of glassy systems under steady-state shear, we compare effective temperatures obtained from static linear response with those from time-dependent fluctuation-dissipation relations. Although these two definitions are not expected to agree, we show that they yield the same answer over two and a half decades of effective temperature. This suggests that a more complete conceptual framework is necessary for effective temperatures in steady-state driven systems.

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Temperature is one of the fundamental variables in an equilibrium system that determines not only the system's average properties, but also fluctuations around those averages. Temperature also relates, via linear response, fluctuations in a thermodynamic quantity to that quantity's response to a small perturbation in its conjugate variable. When a system is far from equilibrium, temperature is no longer well defined. Nevertheless, in many cases fluctuations occur, though they are not thermal in origin. An example is a steady-state driven system such as a sheared material where shear introduces fluctuations that are not described by a thermal bath temperature. Can one define an appropriate "effective temperature" to characterize these fluctuations?

For the idea of an effective temperature to be useful, a clear prescription for defining it should exist and this prescription should apply generally in different contexts. Various groups have defined and measured different effective temperatures in systems far from equilibrium [1–4]. We will show here that two prescriptions based on linear response that have seemed to be fundamentally incompatible do, surprisingly, give the same value for the effective temperature. For this to occur, neither prescription can work infallibly in all cases. Thus, our results pose the conceptual question: under which conditions should either linear response prescription be applied?

Linear response provides a large number of possible definitions for the effective temperature, each based on a different pair of conjugate variables, which all reduce to the true temperature in thermal equilibrium. Effective temperatures based on these different relations have been used to model simulations of particulate systems driven out of equilibrium by steady-state shear [5–7]. There are two ways in which such relations have been implemented with significant success. One way uses static linear response, which relates equal-time fluctuations to the response at *infinite times* to yield an effective temperature  $T_I$ . The other way, argued to be more fundamental [8,9], measures the autocorrelation function and relates it to the response *as a function of time*. In equilibrium,

there is a strict proportionality between correlation and response at all times and therefore a single well-defined temperature, but in driven systems, the situation is more subtle. The conceptual picture behind this is that there can be two widely separated time scales in the presence of shear. Degrees of freedom that decay on a short-time scale are characterized by one effective temperature,  $T_S$ , while those that take a longer time to decay are characterized by a different (higher) value,  $T_L$ . It has been predicted that  $T_S$  is the bath temperature because fast degrees of freedom decay before shear has any effect, while  $T_L$ , which can only be obtained from the long-time behavior of correlation and response, corresponds to a well-defined effective temperature characterizing structural rearrangements driven by shear [8].

As will be made clear below, an effective temperature based on infinite time, or static linear response,  $T_I$ , should generally not agree with  $T_L$  obtained from time-dependent linear response in nonequilibrium systems. Indeed, for the same pair of conjugate variables, we always find in our simulations that  $T_I \neq T_L$ . However, for a wide variety of simulations, we find that  $T_I$  for one conjugate pair can be equal to  $T_L$  for a different pair. Therefore, it appears that under different conditions, both definitions of effective temperature must be equally valid. The conceptual framework [4,10] that has been used to argue for the validity of  $T_L$  would imply that  $T_I$  should never be valid, in contradiction to our findings. That scenario must therefore be incomplete.

In order to demonstrate these results, we have performed numerical simulations of systems undergoing linear shear flow in both two and three spatial dimensions (2D and 3D) under conditions of fixed volume, fixed number of particles, and fixed shear rate. The systems are composed of 50-50 bidisperse mixtures with diameter ratio 1.4, which prevents crystallization and segregation. The system is enclosed in a cubic simulation cell with Lees-Edwards periodic boundary conditions to impose shear in the  $x$  direction and a shear gradient in the  $y$  direction. Particles interact via one of the following pair-

wise, finite-range, purely repulsive potentials:

$$\begin{aligned} V^{hs}(r_{ij}) &\equiv \frac{\epsilon}{2}(1 - r_{ij}/\sigma_{ij})^2 \\ V^H(r_{ij}) &\equiv \frac{2\epsilon}{5}(1 - r_{ij}/\sigma_{ij})^{5/2} \\ V^{RLJ}(r_{ij}) &\equiv \frac{\epsilon}{72}[(\sigma_{ij}/r_{ij})^{12} - 2(\sigma_{ij}/r_{ij})^6 + 1], \end{aligned} \quad (1)$$

where  $\epsilon$  is the characteristic energy scale of the interaction,  $\sigma_{ij} = (\sigma_i + \sigma_j)/2$  is the average diameter of particles  $i$  and  $j$ , and  $r_{ij}$  is their separation. All potentials (harmonic spring, Hertzian nonlinear spring, and repulsive Lennard-Jones) are zero when  $r_{ij} \geq \sigma_{ij}$ . Our results have been obtained with packing fractions ranging from  $\phi = [0.70, 0.84]$  in 3D and  $\phi = [0.85, 1.20]$  in 2D, which are all above random close-packing [11]. We varied the number of particles in the range  $N = [256, 1024]$  and found no appreciable finite-size effects for the results reported here. The units of length, energy, and time are  $\sigma$ ,  $\epsilon$ , and  $\sigma\sqrt{m/\epsilon}$ , respectively, where  $m$  is the particle mass and  $\sigma$  is the small-particle diameter.

We have studied both thermal and athermal (or dissipative) systems to show that our results are *not* specific to any particular dynamics. Thermal systems under shear can be described by the Sllod equations of motion for the position  $\vec{r}_i$  and velocity fluctuation  $\vec{v}_i$  of each particle around the average linear velocity profile [12]:

$$\frac{d\vec{r}_i}{dt} = \vec{v}_i + \dot{\gamma}y_i\hat{x}, \quad \frac{d\vec{v}_i}{dt} = \vec{F}_i^r/m - \dot{\gamma}v_{y_i}\hat{x} - \alpha\vec{v}_i, \quad (2)$$

where  $\vec{F}_i^r = -\sum_j dV(r_{ij})/dr_{ij}\hat{r}_{ij}$  is the repulsive force on particle  $i$  due to neighboring particles  $j$ ,  $\dot{\gamma}$  is the shear rate, and  $\alpha$  is chosen to fix the kinetic energy per degree of freedom,  $T_{KE}$ , associated with velocity fluctuations. We set  $T_{KE}$  to be below the glass transition temperature of the unsheared system.

Athermal dissipative systems can be described by [13]:

$$m\frac{d^2\vec{r}_i}{dt^2} = \vec{F}_i^r - b\sum_j(\vec{v}_i^t - \vec{v}_j^t), \quad (3)$$

where  $\vec{v}_i^t$  is the total velocity (including shear) of particle  $i$ ,  $b > 0$  is the damping coefficient, and the sum over  $j$  only includes particles that overlap particle  $i$ . At finite shear rate, these systems reach a steady state where the power put in by the shear flow balances the power dissipated. In this study, we focused on underdamped dissipative dynamics and therefore fixed the dimensionless damping coefficient  $b^* = b\sigma/\sqrt{\epsilon m} \ll 1$ .

We now describe how to calculate the effective temperature from a set of conjugate variables and then show explicitly the incompatibility of the static and the time-dependent definitions for the same conjugate pair of variables. Since we are concerned with systems in

steady-state shear, we assume a final steady state in which averaged quantities become time independent. Consider an observable,  $A(t)$ , that fluctuates in time  $t$ , such as the number density or the total pressure of the system. Then one can define the autocorrelation function:

$$\tilde{C}_A(t) = \langle A(t)A(0) \rangle - \langle A \rangle^2, \quad (4)$$

where  $\langle A \rangle$  represents an average of  $A$  over time and configurations. If  $B$  is the thermodynamic field conjugate to  $A$ , then one can also define an integrated response function which measures the response to a small constant perturbation,  $\delta B$ , applied from time  $t = 0$  onward:

$$\tilde{R}_A(t) = \frac{\langle A(t) \rangle - \langle A(0) \rangle}{\delta B}. \quad (5)$$

If we now introduce the rescaled variables

$$R_A(t) = \frac{\tilde{R}_A(t)}{\tilde{C}_A(t=0)} \quad \text{and} \quad C_A(t) = \frac{\tilde{C}_A(t)}{\tilde{C}_A(t=0)}, \quad (6)$$

the fluctuation-dissipation relation states that

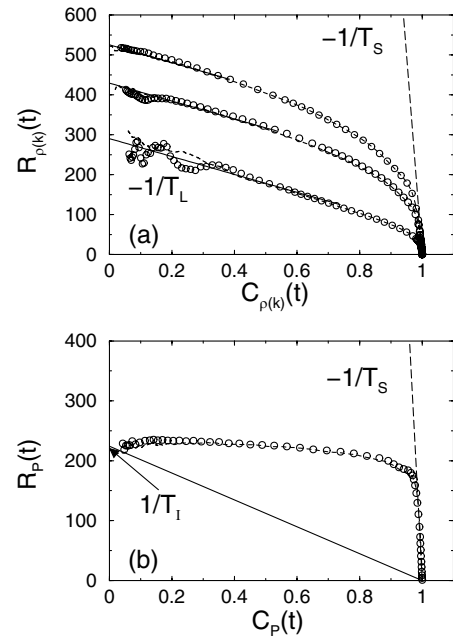


FIG. 1. (a)  $R_{\rho(k)}(t)$  vs  $C_{\rho(k)}(t)$  in a 2D system with repulsive harmonic interactions at  $T_{KE} = 10^{-4}$ ,  $\dot{\gamma} = 0.01$ , and  $\phi = 0.90$  for  $N = 256$  particles.  $\vec{k}$  lies in the shear gradient direction;  $k = 4.5, 9$ , and  $11$  are shown decreasing from top to bottom. The solid lines are guides to the eye and have slopes equal to  $-1/T_L$ . (b)  $R_p(t)$  vs  $C_p(t)$  in the same system as (a). The solid line was drawn for reference and has negative slope and  $R$ -intercept  $1/T_I$ , where  $T_L$  was obtained from (a). Note that  $T_I$  from (b) is equal to  $T_L$  from (a). The results are in the linear response regime, as shown by the open circles and dashed lines in each panel, which are for two values of the perturbing field that differ by a factor of 5.

$$R_A(t) = \frac{1}{T} [1 - C_A(t)]. \quad (7)$$

This implies that if  $R_A$  is plotted parametrically against  $C_A$ , the result should be a straight line with slope  $-1/T$  for an equilibrium system. Moreover, the infinite-time limit, which is the intercept of such a plot on the  $R$  axis, has the value  $1/T$ . According to Eqs. (6) and (7), the intercept satisfies

$$\tilde{R}_A(t = \infty) = \tilde{C}_A(t = 0)/T. \quad (8)$$

Thus, the intercept, which defines a temperature  $T_I$ , corresponds to the static linear response relation whereby the infinite-time response,  $\tilde{R}_A(t = \infty)$  [Eq. (5)], is related to the equal-time correlation function,  $\tilde{C}_A(t = 0)$  [Eq. (4)].

As indicated earlier, Kurchan [8] has predicted that for driven steady-state systems, such a parametric plot has two regimes [5,8]. Berthier and Barrat have conducted simulations of sheared Lennard-Jones glasses and shown that at short times ( $C_A$  close to one and  $R_A$  close to zero), the slope of the line,  $-1/T_S$ , defines a temperature characterizing the fast modes in the system and corresponds to the bath temperature,  $T_{KE}$ . At long times, the slope,  $-1/T_L$ , is a good measure of the effective temperature produced by shear for the slow modes. We show a similar plot for a 2D sheared thermal system in Fig. 1(a) using as the variable the Fourier component of the number density of the large particles at various values of the wave vector  $\vec{k}$ :  $\rho(\vec{k}, t) = \sum_{i=1}^{N/2} e^{i\vec{k}\cdot\vec{r}_i(t)}$ . For this variable, we calculate the incoherent part of the scattering function for the large particles,  $C_{\rho(k)}(t)$  [5]. In Fig. 1(a), there is a well-defined slope at short times and a smaller slope at long times (i.e., at smaller values of  $C_A(t)$ ). It is quite obvious that the long-time slopes are all the same so that there is a common effective temperature that describes the fluctuation and response for all of these variables. These results are consistent with those found by Berthier and Barrat [5] for a three-dimensional system. Note that for each  $k$ , the value at which each of these curves intercepts the  $R_{\rho(k)}$  axis cannot have the value  $1/T_L$ . This could only be the case if  $T_S = T_L$  (as in equilibrium), or if the regime corresponding to  $T_S$  shrinks to zero [14]. If the curve is not a straight line, then  $T_I$  (determined from the intercept) must be different from *either*  $T_S$  or  $T_L$ .

In Fig. 1(b), we show the parametric plot for the identical system as in Fig. 1(a) but for a different variable, namely, the total pressure,  $P$ . We calculate the pressure  $P = P_{\alpha\alpha}/d$  in  $d$  spatial dimensions, using the following expression for the pressure tensor

$$L^d P_{\alpha\beta} = \sum_{i=1}^N m v_{\alpha i} v_{\beta i} + \sum_{i=1}^{N-1} \sum_{j=i+1}^N r_{\alpha ij} F_{\beta ij}^r, \quad (9)$$

where  $\alpha, \beta = x, y, \text{ or } z$  and  $L$  is the edge length of the simulation box. The shape of this curve is very different from those shown in Fig. 1(a). In this case, the response

rises rapidly at short times and then turns over and becomes horizontal at long times [4,15]. The striking result is that, although this curve is manifestly different from those shown earlier, it has an intercept temperature,  $T_I$ , with the same value,  $T_I = T_L$ , obtained from the late-time slopes of the curves in Fig. 1(a).

We stress here that this is not a coincidence. In Fig. 2, we show for an athermal system the response versus correlation plots for the same sets of variables as shown for thermal systems in Fig. 1. Again we see that  $T_I$  obtained from  $P$  has the same value as  $T_L$  obtained from  $\rho(k)$ . To indicate the full extent of agreement, we plot in Fig. 3 the ratio  $T_L/T_I$  versus  $\log_{10} T_L$  for all systems studied. This figure shows that within error  $T_L = T_I$  over two and half decades of effective temperature. These data are collected from thermal and athermal simulations at different values of the shear rate and density in 2D and 3D for systems with different particle interactions. For the thermal simulations, we also varied the bath temperature.

We have shown that both static linear response and time-dependent fluctuation-dissipation relations can yield consistent values of effective temperature. However, it is unclear when one should use static relations and when one should use time-dependent ones. Pressure is not the only observable for which the static relation is appropriate. Previously, we showed that static relations yield a con-

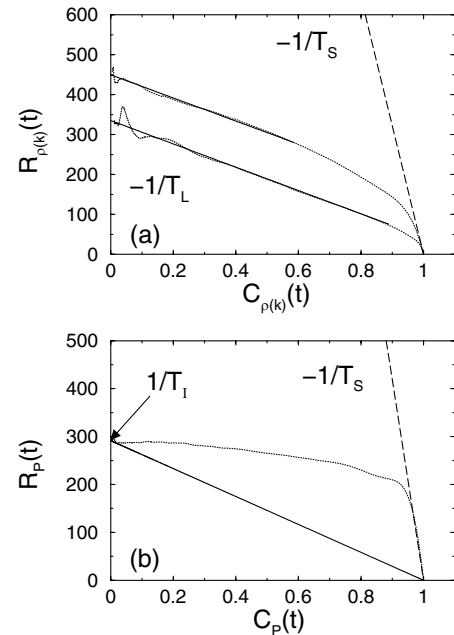


FIG. 2. (a)  $R_{\rho(k)}(t)$  vs  $C_{\rho(k)}(t)$  in a 2D sheared, *athermal* system with repulsive harmonic interactions at  $\phi = 0.90$  and  $\dot{\gamma} = 0.01$ .  $\vec{k}$  lies in the shear gradient direction and  $k = 4.5$  and  $9$  are shown with  $k$  decreasing from top to bottom. The solid lines have slope equal to  $-1/T_L$ . (b)  $R_P(t)$  vs  $C_P(t)$  in the same system as (a). The solid straight line has negative slope and  $R$ -intercept  $1/T_I$ , where  $T_L$  was obtained from (a).

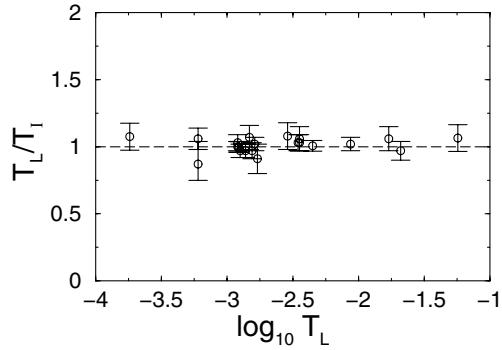


FIG. 3.  $T_L/T_I$  vs  $T_L$ , where  $T_I$  is obtained from the  $R$ -intercept of integrated response ( $R$ ) vs correlation ( $C$ ) for pressure and  $T_L$  is obtained from the long-time slope of  $R$  vs  $C$  for  $\rho(k)$ . The largest error comes from estimating the long-time slope of  $R$  vs  $C$  for  $\rho(k)$ .

sistent effective temperature for shear stress and potential energy as well [7]. It is also not true that one should invariably use the static relation for quantities involving pressure. We have calculated response vs correlation for pressure at different values of  $\vec{k}$  in 2D sheared systems. At large  $k$ ,  $T_L$  yields the correct effective temperature whereas at  $k = 0$ ,  $T_I$  does.

It is not true that the effective temperature for all  $k = 0$  observables should be given by static linear response. While static linear response appears appropriate for  $k = 0$  pressure, energy, and shear stress, we find other examples for which this does not hold, including  $P_{zz}$  [5] and the deviatoric pressure  $P_{\text{dev}} = (2P_{11} - P_{22} - P_{33})/3$  where 1, 2, 3 =  $x, y, z$  [16]. We find that the  $R(C)$  curves for each of these  $k = 0$  variables are not flat as in Fig. 1(b), but have nonzero long-time slopes. However, the corresponding effective temperatures can differ by factors of 5–10 from those in Fig. 1(a) even when other effective temperatures agree.

There are regimes where the idea of an effective temperature is valid and others where it breaks down [17]. For example, at high densities (e.g.,  $\phi \approx 1.1$ , typical of liquids) and high bath temperatures ( $T_{KE} > 0.1T_g$ ), we find that the various effective temperatures are the same. However, these begin to deviate as  $T_{KE}$  is lowered. Previous studies [8,9] have suggested that the concept of effective temperature should be valid when there is a clear separation between the short-time regime and the long-time, shear-rate-dependent regime. This criterion cannot be sufficient because as  $T_{KE}$  is lowered, the separation between these two time scales does not decrease.

We have shown that  $T_I$  for the zero-wave vector pressure is equal to  $T_L$  for  $\rho(k)$  over a range of two and a half decades in effective temperature. This remarkable result suggests that static as well as time-dependent linear

response relations can be used to define a consistent effective temperature, in contradiction to expectations based on spin models subjected to nonconserved fields [8,9]. These results also leave us with a puzzle: when should one use static linear response and when should one use a time-dependent relation? For a given pair of conjugate variables, there is no obvious criterion for which of these two kinds of relations should be used.

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