

Numerical comparison of a constrained path ensemble and a driven quasisteady state

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We investigate the correspondence between a nonequilibrium ensemble defined via the distribution of phase-space paths of a Hamiltonian system and a system driven into a steady state by nonequilibrium boundary conditions. To discover whether the nonequilibrium path ensemble adequately describes the physics of a driven system, we measure transition rates in a simple one-dimensional model of rotors with Newtonian dynamics and purely conservative interactions. We compare those rates with known properties of the nonequilibrium path ensemble. In doing so, we establish effective protocols for the analysis of transition rates in nonequilibrium quasisteady states. Transition rates between potential wells and also between phase-space elements are studied and found to exhibit distinct properties, the more coarse-grained potential wells being effectively further from equilibrium. In all cases the results from the boundary-driven system are close to the path-ensemble predictions, but the question of equivalence of the two remains open.

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I. INTRODUCTION

Equilibrium thermal systems obey the principle of detailed balance [1], a physical law concerning the rates of a system's microscopic dynamical processes, which can ultimately be traced to the statistics of the heat bath that supplies noise to the system. A class of far-from-equilibrium system, which shares the Hamiltonian of an equilibrium system, can be defined by a subset of the equilibrium ensemble of phase-space trajectories, conditioned by a finite flux [2–5]. That is to say, those members of the equilibrium ensemble of systems, which exhibit a given flux during some time interval, are defined as belonging to the nonequilibrium constrained-flux ensemble. For such a constrained-flux ensemble, the rates of microscopic processes have been shown [2,3,6,7] to respect physical laws equivalent to (but different from) equilibrium detailed balance, which can ultimately be traced to the statistics of a nonequilibrium reservoir that supplies biased noise to the system [8].

Such an ensemble is appealing in that it shares many features of an equilibrium ensemble and admits elegant techniques for investigation of its properties, both in the case where the constrained dynamical quantity is antisymmetric under time reversal (a flux) [4,5,9] and where it is symmetric (a “dynamical activity”) [4,5,10–16]. However, it remains unclear whether such ensembles are realized in practice, i.e., whether a nonequilibrium ensemble defined via the distribution of its phase-space trajectories in this way corresponds to a physically realistic system driven away from equilibrium.

Here, we test whether such an ensemble is a good description of a system subjected to torsional shear flow, by investigating relationships between its transition rates ω_{ij} , defined as the probability per unit time that the system occupying microstate i transforms to microstate j within a vanishingly small time interval. For the steady state of an ensemble of trajectories conditioned by a finite mean shear flux, the values of such transition rates are related to the rates ω_{ij}^{eq} measured in the same fluid (i.e., with the same

Hamiltonian) at equilibrium (in contact with an equilibrium heat bath and not constrained to flow). The relationships [6] are as follows.

(i) The product of forward and reverse transition rates between any two microstates is the same in the equilibrium and sheared ensembles, i.e.,

$$\omega_{ij} \omega_{ji} = \omega_{ij}^{\text{eq}} \omega_{ji}^{\text{eq}} \quad \forall i, j. \quad (1)$$

(ii) The exit rate (i.e., the sum of all outward transition rates) from any given microstate differs from its equilibrium value by a shear-rate-dependent constant that is the same for all microstates, i.e.,

$$\sum_j (\omega_{ij} - \omega_{ij}^{\text{eq}}) = Q \quad \forall i. \quad (2)$$

If, in addition to the mean flux, the mean potential energy $\langle U \rangle$ (a time-reversal symmetric quantity) is also constrained, further conditioning the nonequilibrium ensemble of trajectories, then Eq. (2) no longer holds for all microstates i but continues to hold for all microstates of equal potential energy [5].

Testing the applicability of this nonequilibrium counterpart to detailed balance requires the rates of transitions between microstates to be measured, in a suitably driven system that has physically valid equations of motion (rather than one in which nonequilibrium transition rates are specified *a priori*). Such a model system—a line of angular-momentum-conserving rotors with nearest-neighbor interactions—was simulated in Ref. [17], in the Brownian limit, where frictional and stochastic forces between neighbors dominate over momentum degrees of freedom. In the present study, we test the proposed statistical laws in a deterministic Hamiltonian system with nontrivial interactions and with no friction or stochastic forces (other than the emergent quasirandom motion of the many deterministic degrees of freedom). This model allows us to investigate a phase space with nontrivial momenta as well as positional coordinates.

Because the model has continuous degrees of freedom, the “microstates” that we analyze are, by necessity, not strictly

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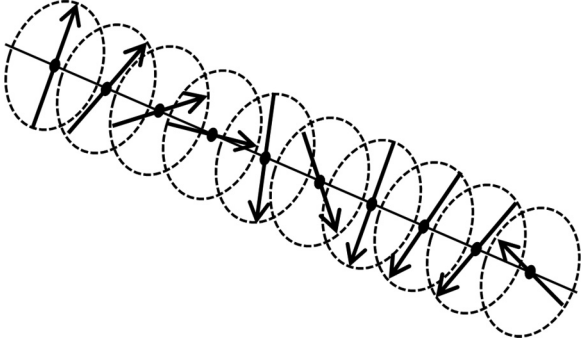


FIG. 1. The model system under investigation: a one-dimensional chain of simple rotors with conservative nearest-neighbor interactions. The chain may be allowed to equilibrate, or can be driven by continuously twisting the boundary rotors. This many-body system is a simple model for a complex fluid in shear flow.

single states, but finite regions of phase space, which we define in two different ways. In the first test (Sec. IV A), we assume that momentum degrees of freedom are well thermalized and therefore irrelevant, while positional degrees of freedom make distinct transitions between minima of a potential that play the role of microstates. In the second test (Sec. IV B), we divide phase space into a grid of coarse-grained “microstates” characterized by both positional and momentum coordinates and study transitions between the cells of that grid. Comparing the two characterizations of the same system—with and without regard of momenta—reveals some important issues concerning the statistical mechanics of deterministic systems in nonequilibrium environments.

II. THE MODEL

The model, in which we measure transition rates for comparison with the predictions for constrained ensembles, is depicted in Fig. 1. It consists of a one-dimensional chain of simple rotors. The dynamical variables are the angles θ_i of the rotors (each labeled by its index i), relative to some overall reference direction, and their angular momenta $I\dot{\theta}_i$, where the moment of inertia I will henceforth be set to unity without loss of generality. Nearest neighbors in the chain apply equal and opposite torques to each other, thus exactly conserving angular momentum.

Unlike Ref. [17], in which only the zero-mass, overdamped regime with added noise was studied, here we investigate the deterministic model in which the torques are purely conservative, being the negative gradient of the potential $U(\Delta\theta) = -\cos(\Delta\theta) - \cos(4\Delta\theta)$ shown in Fig. 2. This symmetric function of the angular difference between the rotors, $\Delta\theta_i \equiv \theta_{i+1} - \theta_i$, has four wells, allowing us to measure and compare the transition rates between various states, approximating microstates.

The equations of motion are

$$\frac{\partial^2 \theta_i}{\partial t^2} = U'(\Delta\theta_i) - U'(\Delta\theta_{i-1}), \quad (3)$$

with U' being the derivative of the function U . The boundary conditions are periodic, and the equations of motion are numerically time-stepped using the velocity Verlet algorithm

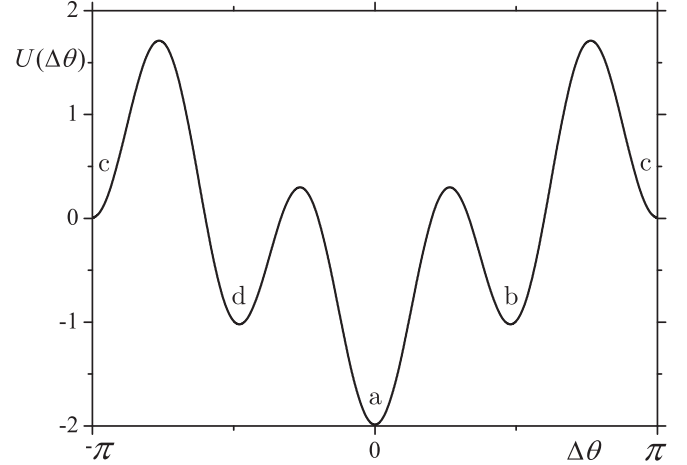


FIG. 2. The interaction potential between neighboring rotors, $U(\Delta\theta) = -\cos(\Delta\theta) - \cos(4\Delta\theta)$, in terms of the angular difference $\Delta\theta$ between the neighbors.

[18], which approximately conserves energy in the absence of external work. The time step used was 10^{-3} , as this was found to be sufficiently small to obtain data that were independent of time step. We use a system of $N = 300$ rotors, as this is found to be sufficiently large to avoid any system-size dependence of the results.

As described thus far, this is an equilibrium model. Once initial transients have died away, the time-averaged distribution of relative angles $\Delta\theta$ between neighbors was measured and plotted logarithmically in Fig. 3, together with the function $-U(\Delta\theta)$ for comparison. Despite having deterministic dynamics, this steady-state system exhibits Boltzmann statistics

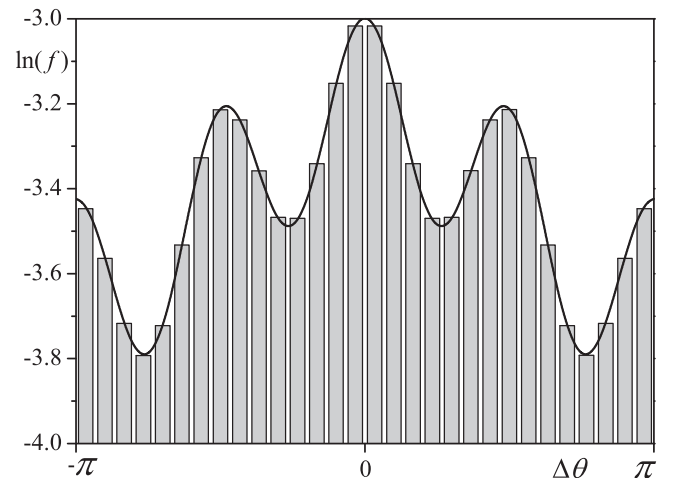


FIG. 3. The steady-state distribution of relative angles $\Delta\theta$ between neighbors in the chain without driving. The vertical axis shows $\ln(f)$, where f is the probability per unit angle of finding a given relative angle between neighbors. Also plotted as a continuous curve is $-\beta U(\Delta\theta) + c$ for the function U defined in the legend of Fig. 2, where β and c are fitting parameters. Agreement between the curve and the data confirms that the deterministic system is at thermodynamic equilibrium, respecting Boltzmann’s law: $f \propto \exp(-\beta U)$.

in the absence of driving. At low temperature (i.e., evolved from an initial condition with low energy per rotor) the relative angles between neighbors are then mostly confined close to the local potential minima, with only occasional transitions between potential wells.

The rates of those transitions (without driving) have also been measured and were found to respect detailed balance, thus suggesting that this 1D deterministic system is ergodic, at least in the absence of driving. Note that detailed balance is not imposed *a priori*; it emerges from the dynamics at equilibrium.

To drive the system, in a way reminiscent of shearing a fluid, we modify the boundary condition, which is a simple periodic boundary condition for the equilibrium case. We could simply control the motion of the first and last rotors ($i = 1$ and $i = N$), to impose a torsional shear rate, but this might introduce nontrivial edge effects by breaking the translational symmetry. Instead, we impose an angular version of Lees-Edwards boundary conditions [19], in which rotor N is coupled to rotor 1 with an angular offset that increases linearly with time, by defining

$$\Delta\theta_N = \Delta\theta_0 = \theta_1 - \theta_N + N\dot{\gamma}t, \quad (4)$$

where the parameter $\dot{\gamma}$ is the shear rate. So the N th rotor interacts with the first rotor via a potential that has a minimum, not at $\theta_1 - \theta_N = 0$ (i.e., parallel alignment), but at $\theta_1 - \theta_N = -N\dot{\gamma}t$ (an increasing angle). Nevertheless, these boundary rotors could feel a constant interaction force if one of them spins relative to other rotors in the chain. Hence, the effect of the boundary condition is nonlocal, imposing an overall torsional shear flow with average relative velocity between neighbors $\langle \dot{\theta}_{i+1} - \dot{\theta}_i \rangle = \dot{\gamma}$, while treating all rotors equally.

III. DATA ACQUISITION FROM QUASISTEADY STATES

We repeated the deterministic simulations 250 times at each shear rate, with randomly varying initial conditions. The initial angles were set to $\theta_i = 0 \forall i$ in each case (to keep the initial energy low) and the velocities randomly scattered about an affinely sheared state, so that the values of $\Delta\theta_i$ have a mean of $\dot{\gamma}$ and a Gaussian distribution whose variance determines the initial energy density. This initial condition is sometimes called a “water bomb” initialization, because when a child’s water bomb (a balloon filled with water) hits the ground, all of the water is initially in the same location, but with a scatter of velocities that soon cause the water to spread out. We found it convenient to set the variance of the initial Gaussian equal to $\dot{\gamma}/2$, to allow a statistically significant number of the rarest transitions to be observed within a reasonable time, for a range of shear rates. Starting transients were allowed to decay before any data were taken.

Since no dissipation is present, the driven system “heats up,” i.e., its energy density on average increases with time, since the nonequilibrium boundary condition applies work to the system. This is true also of an adiabatic experimental system. The quasisteady-state statistics of such a system remain well defined and reproducible so long as it does not heat up too quickly on the timescale of the measurements.

To measure transition rates at a well-defined energy density (corresponding to a constant temperature in the case of an equilibrium simulation), and in a quasistationary state, we

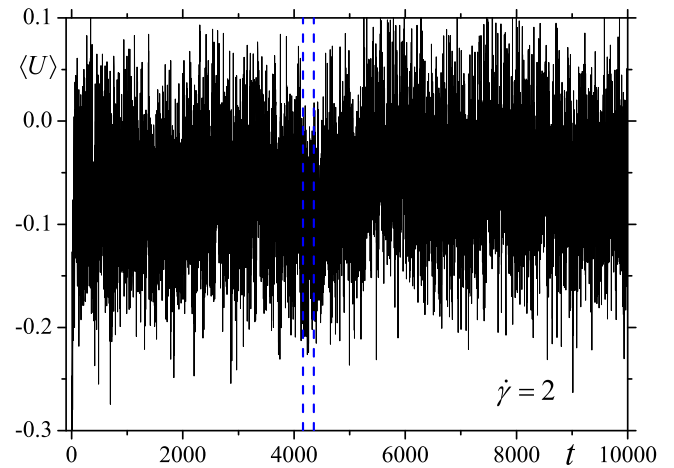


FIG. 4. (Color online) Mean potential energy per rotor as a function of time, for one of the many simulations performed at a shear rate $\dot{\gamma} = 2$. Vertical dashed lines delineate the interval during which data were obtained with the appropriate mean potential energy per rotor. Note the slow systematic energy increase, only apparent on the longest timescale. Note also the rapid noisy variation on a timescale much shorter than the measurement interval.

took data over only short intervals Δt , within each of the much longer simulations, during which there was negligible systematic rise in the energy density compared with its noisy variation (see Fig. 4).

It is important to choose a value of Δt longer than the timescale of the noise but shorter than the timescale on which the internal energy significantly increases in a systematic manner. The data in Fig. 5 were used to assess the most suitable choice of Δt . The figure shows a graph of the standard deviation in mean potential energy per rotor (averaged over many simulations) as a function of the measurement interval Δt . The data shown are for simulations at a shear rate $\dot{\gamma} = 1$. For other values of $\dot{\gamma}$, the corresponding graphs are qualitatively (and in most cases quantitatively) the same. The graph shows a shoulder, at a timescale required to

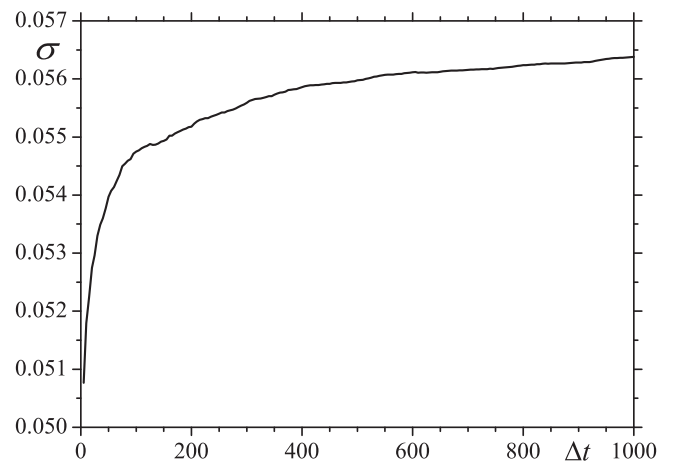


FIG. 5. Graph of the standard deviation in mean potential energy per rotor (averaged over many simulations) as a function of the measurement interval Δt . The data shown are for simulations at a shear rate $\dot{\gamma} = 1$.

representatively sample the noisy variations in energy. Further increasing the measurement interval beyond this shoulder value increases the standard deviation only slowly, as it encompasses a systematically increasing range of temperatures (a range of different quasisteady states). From the figure, a value of Δt in the interval (150, 200) is judged to be the most suitable quasisteady timescale. In practice, for each of the investigations presented below, data were collected until the rarest transition, in each case, was observed a given number of times. That number was chosen, for each investigation, to yield values of Δt in the interval (150, 200).

The total duration of each simulation was 10^4 natural time units, chosen to provide a useful amount of data following starting transients. Within each of the 250 simulated trajectories for each shear rate, several distinct measurements of duration Δt were taken.

At the end of each of these measurement intervals, counting began again for a new measurement interval. The mean potential energy per rotor was recorded during each interval. Hence, from the many simulations, we obtained a large set of quasistatic measurements with a range of different energy densities.

To obtain statistically significant data at a well-defined energy density, we combined only those measurements for which the mean potential energy per rotor was in the interval $(-0.11, -0.09)$. One of the intervals from which data were used is indicated by the vertical lines in the example of Fig. 4. As discussed below Eq. (2), this extra constraint on the (time-reversal-symmetric) potential energy density only has the effect of confining Eq. (2) to a set of microstates of equal potential energy density [5].

It was difficult to obtain statistically significant results above a shear rate of $\dot{\gamma} = 2$ because the system heated up more quickly at higher shear rate, therefore spending less time in the chosen energy interval.

We choose to characterize the macrostates by their potential energy density because it is well defined, whereas kinetic energy density in the sheared periodic system depends on system size and rest frame. We chose as low an energy as possible, whilst still achieving statistically significant counting, in order to observe nontrivial variations in transition rates, controlled by an interplay between interactions and driving (rather than just a shear-dominated high-temperature regime).

To check that our protocol truly yielded quasisteady-state results that are independent of initial conditions, we performed detailed comparisons at $\dot{\gamma} = 0.4, 1, 1.6,$ and 2 . For each of these shear rates, we performed a further set of 250 simulations with the initial peculiar velocities drawn from a Gaussian with a smaller variance: a quarter of that in our standard protocol. For these simulations, we reperformed all measurements. In each case, we found that the two sets of results differed by only small amounts, consistent with our quoted uncertainties. We therefore interpret the driven system as reaching an ergodic quasisteady state, independent of the initial conditions, although the time taken to reach a given value of the internal energy must depend on the initial energy.

The equilibrium state $\dot{\gamma} = 0$ is an exception. Because the velocity-Verlet dynamics are approximately conservative, the internal energy of the system remains equal to its initial value, in the absence of driving. Hence, the results never become

independent of the initial variance of the velocity distribution in this case. For this reason results are given, below, for nonzero values of $\dot{\gamma}$ only.

IV. RESULTS AND DISCUSSION

The potential, shown in Fig. 2, acts on the variables $\Delta\theta_i$, which are the angular differences between neighboring rotors. These variables are associated with the gaps, or spaces between rotors. It is the gaps, then, that occupy the potential and make occasional transitions between its wells, under the influence of the erratic forces from the rest of the system. The rest of the system, then, acts as a nonequilibrium reservoir that supplies biased noise to a rotor gap, with an average tendency to make $\Delta\theta$ increase with time. If the motion of neighboring gaps is not strongly correlated, then each gap can be treated as an independent system, weakly coupled to the noisy nonequilibrium reservoir, and driven by it. This situation is directly analogous to an equilibrium system, for which the *microstate* (rather than the motion) must be uncorrelated with its surroundings in order for Boltzmann's law to hold and the reservoir to be regarded as weakly coupled. Subject to the assumption of uncorrelated dynamics, then, we regard each gap as an independent system, with phase-space coordinates $(\Delta\theta, \Delta\dot{\theta})$, for which we can test the statistical laws stated in Sec. I.

A. Test 1: Transition rates between potential wells

If transitions between potential wells are rare on the timescale of temporal correlations in $\Delta\dot{\theta}$ (i.e., the gap “forgets” its value of $\Delta\dot{\theta}$ between transitions in $\Delta\theta$), then momenta can be neglected, and potential wells can be regarded as effective microstates, labeled $a, b, c,$ and d in Fig. 2.

A transition is deemed to have occurred when a gap-angle $\Delta\theta$ is found crossing the *bottom* of a potential well, having previously crossed the bottom of another well. This criterion prevents multiple counting due to erratic motion at the threshold of a well. These transition counts are divided by the occupancies of the potential wells, to obtain all eight transition rates between the wells. Note that many transitions were observed, in both the forward and reverse directions, across all four potential barriers. This provides further confidence that the system is in an ergodic state.

Equation (2) relates transition rates for the driven system to those at equilibrium. Rather than comparing our driven system with an equilibrium one, for which the temperature would be an unknown fitting parameter, we instead exploit the symmetry of the potential $U(\Delta\theta)$ and notice that the *equilibrium* exit rates from wells b and d must be equal, due to the symmetry $\Delta\theta \leftrightarrow -\Delta\theta$ of the equilibrium ensemble. Hence, although that symmetry is broken in the driven ensemble by the shear flux in the positive $\Delta\theta$ direction, substitution into Eq. (2) nonetheless predicts equal exit rates from wells b and d in the nonequilibrium ensemble. That prediction is tested, in regimes of varying shear rate and internal energy, by the data in Fig. 6.

While the four transition rates involved individually behave quite distinctly as shear rate varies, the predicted invariant combination remains almost constant up to large shear rates. So Eq. (2), which applies to a nonequilibrium ensemble

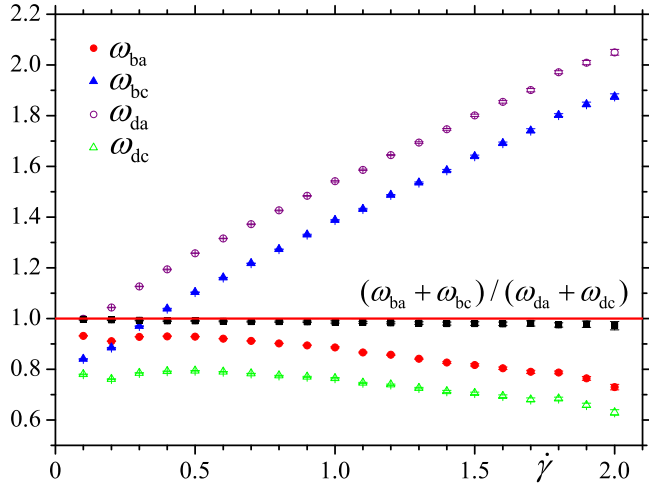


FIG. 6. (Color online) The measured rates ω_{ba} , ω_{bc} , ω_{da} , and ω_{dc} for a wide range of shear rates $\dot{\gamma}$, both in natural time units. Also plotted is the combination $(\omega_{ba} + \omega_{bc})/(\omega_{da} + \omega_{dc})$, which is the ratio of exit rates from wells b and d, predicted to remain constant at unity in a constrained ensemble, subject to the assumptions that momentum variables can be neglected, and that potential wells represent distinct microstates of a system weakly coupled to the nonequilibrium reservoir embodied by the other rotors. The red line is the theoretical prediction of this ratio (unity), while results of simulations are depicted by black squares. The mean potential energy per rotor is selected in the range -0.1 ± 0.01 .

conditioned by flux, appears to be consistent with an ensemble of systems driven by a nonequilibrium shearing reservoir.

Again appealing to the symmetry of an equilibrium system with the potential $U(\Delta\theta)$, we test Eq. (1) for the transition from well a to b , which must be identical to the transition from a to d at equilibrium, but not when driven. Nevertheless, substitution into Eq. (1) determines that the products of forward and reverse transition rates between these pairs of states remain equal in the constrained nonequilibrium ensemble. That is, $\omega_{ab}\omega_{ba} = \omega_{ad}\omega_{da}$ irrespective of the constrained flux. This relation is tested in our driven system by the data in Fig. 7, and the relation $\omega_{cd}\omega_{dc} = \omega_{cb}\omega_{bc}$, based on symmetry about well c , is tested in

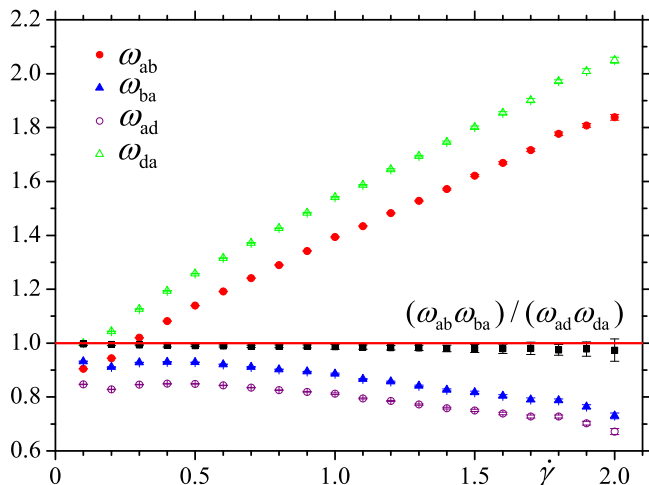


FIG. 7. (Color online) As described in the legend of Fig. 6, for the rates ω_{ab} , ω_{ba} , ω_{ad} , ω_{da} , and their combination $(\omega_{ab}\omega_{ba})/(\omega_{ad}\omega_{da})$.

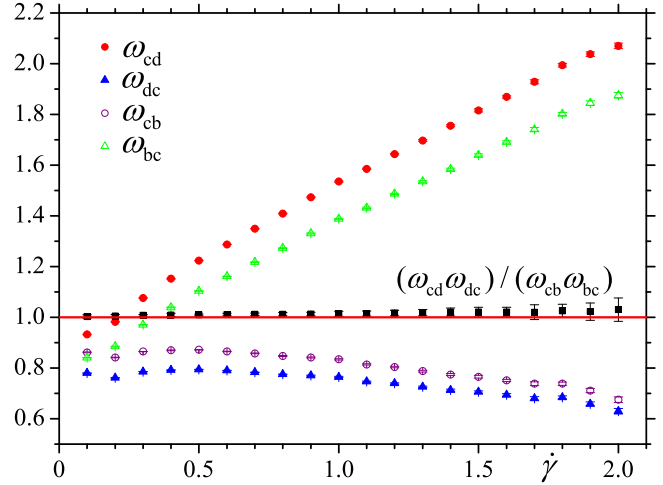


FIG. 8. (Color online) As described in the legend of Fig. 6, for the rates ω_{cd} , ω_{dc} , ω_{cb} , ω_{bc} , and their combination $(\omega_{cd}\omega_{dc})/(\omega_{cb}\omega_{bc})$.

Fig. 8. Again, we see that the nonequilibrium invariants remain almost constant while the relevant individual transition rates vary distinctly and by large amounts.

B. Test 2: Phase-space transition rates

As discussed in Sec. I, the predicted relations strictly concern the rates of transitions between discrete microstates, and we wish to test them in the continuum limit for a phase space with nontrivial momentum as well as positional degrees of freedom. To that end, we again treat each interrotor gap as a system weakly coupled to a nonequilibrium reservoir but, in contrast to Sec. IV A, we monitor both its “positional” coordinate $\Delta\theta$ and its “momentum” degree of freedom $\Delta\dot{\theta}$. To determine the phase-space occupancies and transition rates, the two-dimensional phase space spanned by these coordinates is discretized as shown in Fig. 9. At each time step during

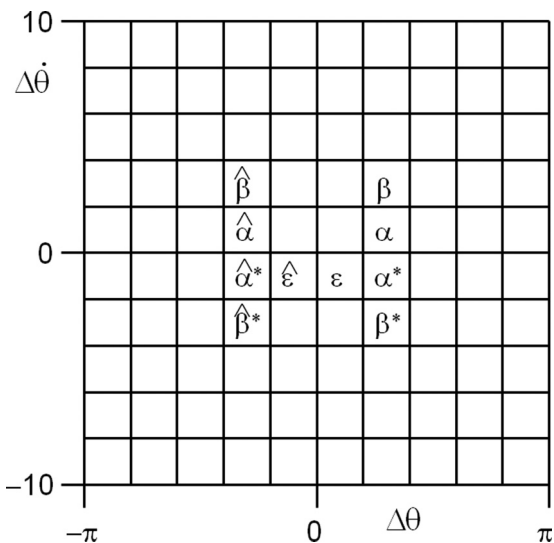


FIG. 9. Discretization of the phase space occupied by the gaps between neighboring rotors, with coordinates $\Delta\theta$ (the relative angle between the pair) and $\Delta\dot{\theta}$ (their relative angular velocity). The states α , β , and ε are identified for analysis, as well as states reversed in $\Delta\theta$ only, denoted by $\hat{\cdot}$, and time-reversed states denoted by $*$.

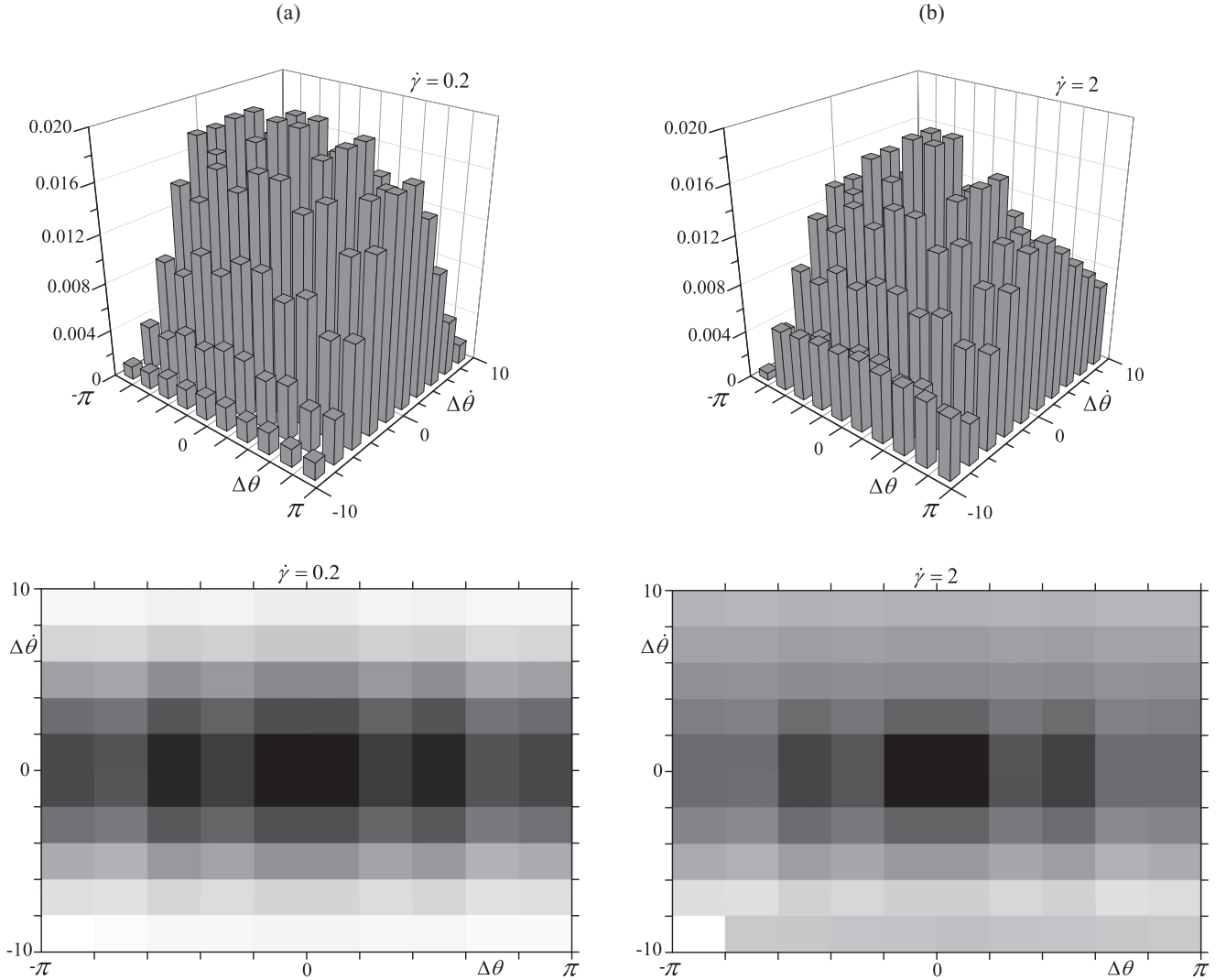


FIG. 10. Histograms and density plots of occupancies of the phase-space bins defined in Fig. 9, measured in quasisteady states with mean potential energy density -0.1 ± -0.01 and shear rate (a) $\dot{\gamma} = 0.2$, (b) $\dot{\gamma} = 2$.

the measuring interval, the values measured in a quasisteady state are binned into 100 cells (ten columns across a full turn of the periodic coordinate $\Delta\theta$, and ten rows spanning a limited domain of $\Delta\dot{\theta}$ values). A transition is recorded whenever a gap's coordinates cross a line between two such cells.

The measured quasisteady-state occupancies at two different shear rates, but the same mean potential energy density -0.1 ± -0.01 , are shown in Fig. 10. At low shear rate [Fig. 10(a)], $\dot{\gamma} = 0.2$, the ensemble of rotors is not far from equilibrium, with the angular ($\Delta\theta$) distribution similar to the Boltzmann distribution of Fig. 3 and the velocity ($\Delta\dot{\theta}$) distribution independent of $\Delta\theta$ and approximately Gaussian with a mean value of 0.2. At shear rate $\dot{\gamma} = 2$ [Fig. 10(b)], the velocity distribution has more nontrivial structure, no longer resembling the equilibrium Gaussian form, while the angular distribution is also significantly altered, particularly at the most negative velocity.

The measured transition rates are compared with the relationships that hold for a conditioned ensemble of

trajectories, Eqs. (1) and (2). As in Sec. IV A, to test the relation between exit rates, Eq. (2), we appeal to the symmetry of the equivalent equilibrium ensemble. In particular, we concentrate on the cell labeled ε in Fig. 9, and its inverted image $\hat{\varepsilon}$. Note that these two states are related by the transformation $(\Delta\theta, \Delta\dot{\theta}) \leftrightarrow (-\Delta\theta, \Delta\dot{\theta})$, equivalent to parity *and* time reversal, “PT” (since $\Delta\dot{\theta}$ is not reversed). The equilibrium ensemble is invariant under that transformation, so Eq. (2) implies $\sum_i \omega_{\varepsilon i} = \sum_i \omega_{\hat{\varepsilon} i}$, an equation involving eight transition rates in the driven ensemble (transitions into the four neighbors of ε and the four neighbors of $\hat{\varepsilon}$). Two of those rates are for forbidden transitions and therefore vanish both at equilibrium and with driving. They involve escape, in the direction of increasing $\Delta\theta$, from a state with negative velocity, which would require an improbably large stochastic impulse from the reservoir. The remaining six finite rates are plotted in Fig. 11 for various shear rates, for quasisteady states selected with mean potential energy density -0.1 ± 0.01 , as in Sec. IV A. The ratio of the two exit rates (the combination predicted to be invariant at unity) is also plotted.

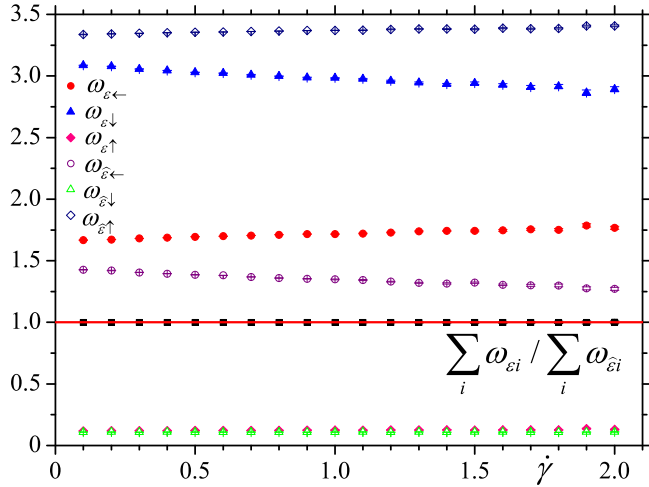


FIG. 11. (Color online) Test of the relationship $\sum_i \omega_{\varepsilon_i} = \sum_i \omega_{\widehat{\varepsilon}_i}$ between exit rates from states ε and $\widehat{\varepsilon}$, defined in Fig. 9, in quasisteady states with mean potential energy per rotor -0.1 ± 0.01 as for Fig. 6. The key gives symbols representing the individual rates $\omega_{\varepsilon \leftarrow}$ etc. where the arrow indicates the direction (relating to Fig. 9) of the transition out of the initial state. Black symbols: $\sum_i \omega_{\varepsilon_i} / \sum_i \omega_{\widehat{\varepsilon}_i}$ are in very close agreement with the theoretical value (red line) of unity.

Similarly, in Figs. 12–14, the product relations in Eq. (1) are compared with data for transitions between “microstates” α and β (see Fig. 9) and their symmetry-related microstates, which have equal statistical properties at equilibrium. The symmetries in question are PT, discussed above, and denoted by a hat ($\widehat{}$) and T, simple time reversal, $(\Delta\theta, \Delta\dot{\theta}) \leftrightarrow (\Delta\theta, -\Delta\dot{\theta})$ denoted by an asterisk (*). Some small deviations from unity are observed in some cases.

Notice that the transition rates vary much less, across the range of shear rates, than the transition rates measured in Sec. IV A. Nevertheless, their small changes are sufficient

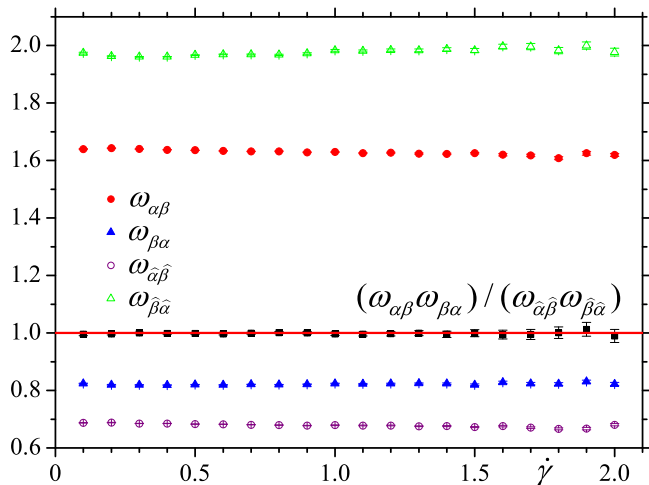


FIG. 12. (Color online) Test of the relationship $\omega_{\alpha\beta}\omega_{\beta\alpha} = \omega_{\widehat{\alpha}\widehat{\beta}}\omega_{\widehat{\beta}\widehat{\alpha}}$ for states α and β defined in Fig. 9, in quasisteady states with mean potential energy per rotor -0.1 ± 0.01 as for Fig. 6. Black symbols: $\omega_{\alpha\beta}\omega_{\beta\alpha} / \omega_{\widehat{\alpha}\widehat{\beta}}\omega_{\widehat{\beta}\widehat{\alpha}}$ are in very close agreement with the theoretical value (red line) of unity.

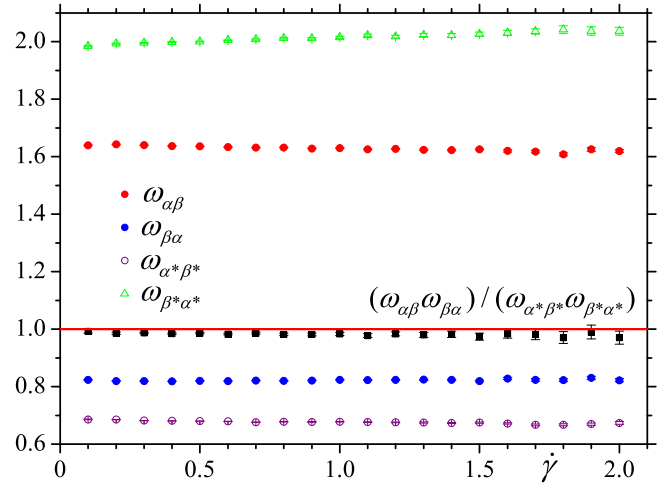


FIG. 13. (Color online) As described in the legend of Fig. 12, for the relationship $\omega_{\alpha\beta}\omega_{\beta\alpha} = \omega_{\alpha^*\beta^*}\omega_{\beta^*\alpha^*}$.

to result in significantly altered occupancies [Figs. 10(a) and 10(b)]. This is because phase space is now being examined in finer detail (Fig. 9). The occupancies are the result of many microscopic transition rates, so that tiny changes in each of those many rates, leading to tiny changes in the relative occupancies of neighboring cells, can have a large effect on the large-scale shape of the distribution.

One might ask whether the ensemble under investigation is near or far from equilibrium. The answer depends on the level of detail at which its properties are interrogated. In terms of transitions between the potential wells, the ensemble at $\dot{\gamma} = 2$ is far from equilibrium, as witnessed by the rates in Figs. 6–8, which are grossly altered from their equilibrium values (which can be inferred from the graphs by extrapolating to $\dot{\gamma} = 0$). The relationships in Eqs. (1) and (2) are tested far from equilibrium in that case. However, at a more microscopic level the transitions between “microstates” in Fig. 9 have rates that are barely perturbed from their equilibrium values by an imposed shear rate $\dot{\gamma} = 2$, as shown in Figs. 11–14, so that the

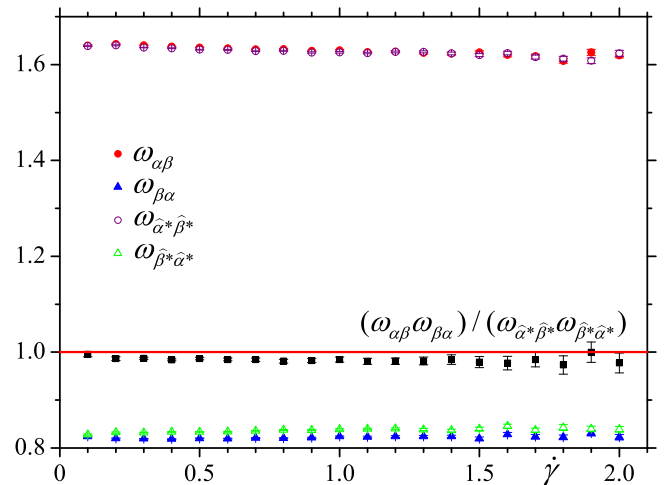


FIG. 14. (Color online) As described in the legend of Fig. 12, for the relationship $\omega_{\alpha\beta}\omega_{\beta\alpha} = \omega_{\widehat{\alpha}^*\widehat{\beta}^*}\omega_{\widehat{\beta}^*\widehat{\alpha}^*}$.

relationships [Eqs. (1) and (2)], between the equilibrium and driven rates trivially hold (approximately) in this case.

This scale-dependence of the distance from equilibrium is a very general phenomenon. For instance, when polymeric fluids flow, the constituent polymer-chains become stretched into highly nonequilibrium conformations on the large scale. But more detailed measurements of their small-scale conformations remain equilibrium-like up to much higher flow rates. The system exists both near to and far from equilibrium, depending on the scale of the properties being measured [20].

V. CONCLUSION

It remains the case that all of the quantities tested, that are invariant in a constrained ensemble, are found to lie very close to unity in all of the cases that we have measured in the quasisteady states of our sheared deterministic system. This is a nontrivial observation but not sufficient in itself to conclude that the boundary-driven set of coupled systems are in every way consistent with the hypothetical conditioned

ensemble of trajectories. It is unclear whether the very small deviations from unity observed in Figs. 13 and 14 arise from a discrepancy between the two types of ensembles, or only from the nonideality of the microstates approximated by finite bins in Fig. 9.

We speculate that this one-dimensional model captures some of the essential physics of real complex fluids in steady shear flow. In such fluids, one of the three dimensions is assigned a special role by the imposition of a velocity gradient, while the other two dimensions contribute only to the complexity of the interactions. Nevertheless, it would be interesting, in future work, to study our driven rotor model on a higher-dimensional lattice, to observe the effects of added dimensions perpendicular to the gradient.

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