

is strongly recommended to extract meaningful statistics by simulation.

B. Definition of Coordinate Bins for Shear-Ising Calculation

The coordinate over configurations was defined simply as the total number of up spins present, $\lambda = N_{up}$. The source bin, A , was defined as $\lambda < 25$ and the sink bin B was defined as $\lambda > 2005$ (as in the FFS calculation [18]). The intervening space on λ was divided into 990 equal increments. It might have been possible to make a more sympathetic definition of the intervening bins, such as by spacing them more closely together for smaller values of λ where the dynamics on λ is expected to be slow, however this crude binning was found to be effective.

The sampling parameters $\gamma = 0.5$, $\tau = 10$ and $N = 100$ were used. Occasional ‘dead-end’ configurations manifested, where λ was large due to multiple isolated clusters of spins rather than due to a single nucleus: a maximum n_i threshold of 2000 was therefore set, in order to prevent eqn. 1 from diverging due to these instances.

C. Results for Shear-Ising Calculation

It was necessary to run the calculation for 2500 MC sweeps at the initial shear rate $\dot{\gamma} = 0.04$ before all bins of the coordinate λ were populated, allowing meaningful statistics to be collected. Fig. 2 shows the flux against time as the shear rates were changed ($\dot{\gamma} = 0.04, 0.02$, and 0.0). Horizontal lines (black) indicate steady state FFS data from a separate research group [10]; the trace (red online) is the S-PRES results. After each change of shear rate the time-dependent flux relaxes to the known steady state value (actually the quasi-equilibrium value in the case $\dot{\gamma} = 0.0$), validating the method. The trace is an average over 100 independent runs.

IV. APPLICATION TO RARE EVENTS IN THE ISING MODEL - KAWASAKI-ISING AFTER A QUENCH

A. Introduction to System

Phase separation in the 2D Ising model after a quench into the temperature region between the nucleation-dominated and spinodal decomposition-dominated regimes is a quintessential problem in non-equilibrium dynamics. Under Kawasaki dynamics (sometimes called a ‘lattice gas’) the total magnetisation is conserved and time-evolution is controlled by diffusion of spins. The base timescale of the system is set by one MC sweep, equal to N_{up} attempts to move a random up-spin. Because the diffusive and evaporative behaviour of spin clusters is determined by both their size and shape

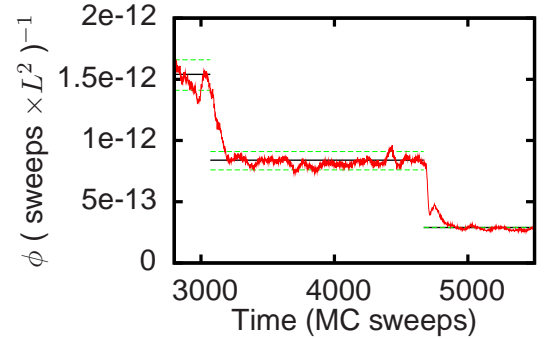


FIG. 2. **Example use of S-PRES: Nucleation in the 2D Ising model under shear.** Solid horizontal lines: reference steady state nucleation rates for each value of imposed shear [10] (dashed lines show the reported errorbars). Fluctuating trace (red online): S-PRES time-series as the shear is changed.

it is difficult to predict their rates of collision and growth or shrinkage and the evolution of the size distribution of clusters over time. Despite these difficulties a theory based on the iterative evolution of a population vector of clusters of different sizes, $p_n(t)$ is available from the literature [22], which has not until now received direct validation from simulation studies (although a closely related approach has had the benefit of such scrutiny [23]). The existence of an untested theory for such a simple but important model system is an ideal opportunity to further demonstrate the S-PRES method while at the same time making a small contribution to the basic study of phase-change dynamics.

The equilibrium thermodynamics of this model are well understood, as are the phase-change dynamics in both the nucleation-dominated (surface-energy limited) and spinodal decomposition-dominated (diffusion limited) regimes [24]. We carried out an instantaneous quench from $T = \infty$ to $T = 0.6T_c$, which lies between these two regimes, for a system of 100×100 spins with a 0.1 concentration of up-spins. The coupling constant J was set to $1k_B T$. $T = 0.6T_c$ was set to 1.36151, using the Onsager result of $T_c = 2/\ln(1 + \sqrt{2})$ [25].

B. Definition of Coordinate Bins for Kawasaki-Ising after a Quench

As the coordinate we chose $\lambda = \sum_c (n_c - 1)$, where n_c is the number of spins in cluster c and a cluster is defined as a connected group of up spins. This coordinate was chosen because it is simple to calculate and has a value of zero when all up spins are isolated, increasing after any collision between spins or clusters. The lowest bin was defined as $\lambda \leq 9$ and the highest bin was defined as $\lambda \geq 91$, with the intervening integer values assigned to a