Reply to "Comment on 'Exact large deviation statistics and trajectory phase transition of a deterministic boundary driven cellular automaton' "

Berislav Buča,[1,2] Juan P. Garrahan,[3] Tomaž Prosen,[4] and Matthieu Vanicat[4]

[1]*Niels Bohr International Academy, Niels Bohr Institute, Copenhagen University, Universitetsparken 5, 2100 Copenhagen, Denmark*
[2]*Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom*
[3]*School of Physics and Astronomy and Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems, University of Nottingham, Nottingham NG7 2RD, United Kingdom*
[4]*Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia*

(Received 30 May 2023; accepted 4 August 2023; published 25 September 2023)

We reply to Whitelam's Comment [Phys. Rev. E **108**, 036105 (2023)] on our paper [Phys. Rev. E **100**, 020103(R) (2019)] where we compute the exact large deviation (LD) statistics of a wide class of observables in the rule 54 cellular automaton. Using some heuristic arguments, Whitelam states that despite the fact that the LD functions we compute display singular behavior, this is not indicative of a LD phase transition or of dynamical phase coexistence. Here, we refute this observation and confirm that the (standard) interpretation of our exact results stands.

DOI: 10.1103/PhysRevE.108.036106

In our paper [1], we computed exactly the large deviation (LD) statistics of a class of trajectory observables of the boundary driven and bulk deterministic rule 54 cellular automaton (CA). We did this by obtaining via matrix product states (MPS) the exact scaled cumulant generating function (SCGF), i.e., the largest eigenvalue of the corresponding tilted evolution operator. As is customary in LD studies of stochastic systems, we solved the problem for finite size N and for long times where the LD regime is applicable (times larger than the inverse of the dynamical gap). The SCGF so obtained displays an increasingly pronounced crossover with increasing size, indicative of a LD phase transition between active and inactive dynamical phases, as occurs in several other constrained systems [2–4]. We also showed explicitly the distinct phases by generating trajectories using the exact Doob or optimal sampling dynamics.

While the results from our exact calculations above are not in dispute, in Ref. [5] Whitelam raises an interesting question about the interpretation of these results. This is based on an observation in an earlier work by Whitelam and Jacobson [6] about apparent yet nonexistent LD phase transitions in single-particle systems, apparently resolved (see our remarks below on that paper) by a rescaling of timescales with system size. Whitelam applies a similar logic to our (many-body rather than single-particle) system, concluding that the singular SCGF that we obtain cannot be interpreted as one due to a dynamical LD transition and coexistence of phases. We now explain how this interpretation is not applicable in our case.

Reference [6], on which Whitelam's comment is based, considers the case of single-particle systems, such as a random walker (RW) in a segment. Since genuine phase transitions only occur in many-body systems in the large size limit, it is evident that no LD transition is possible in that case. Nevertheless, Whitelam and Jacobson show in Ref. [6] that if one tilts the evolution operator by certain dynamical observables, the corresponding SCGF appears singular [7]. This occurs when there is a mismatch in scales: While the untilted evolution operator is $O(1)$ (as there is a single particle), the tilting perturbation scales exponentially with N in the RW example; this introduces an artificially large N singularity in the otherwise regular RW problem. Whitelam and Jacobson [6] resolve this problem by rescaling the counting field in the SCGF with size, arguing that this is a necessary time rescaling—a simpler explanation is that this just restores the correct size scaling in the tilted operator.

In contrast to the single-particle models of [6], the rule 54 CA is a many-body interacting system [1]. Furthermore, we tilt with respect to extensive operators, that is, with the appropriate $O(N)$ scaling. The model is made stochastic through the boundary, and for all finite N the dynamical gap is nonvanishing. This leads to a LD principle for both the SCGF and the LD rate function (the scaled logarithm of the probability of the observable) that is linear in time T. In the Comment, Whitelam states that we need to look at a different timescale than the customary T. More specifically, the suggestion is that one takes instead T/N, in analogy with the single-body problems of Ref. [6], on the grounds that the model is ballistic (due to the bulk conservation of quasiparticles). The argument is that if this N-dependent speed is taken then in the large size limit both the SCGF and rate function acquire a general form that is nonsingular.

The problem with this argument is the following. The rescaling of time above is equivalent to a rescaling of the Legendre-transform parameter (or counting field) s in the SCGF $\theta(s)$. For clarity it is convenient to change notation, writing $s = \lambda/N$, where λ is the abscissa of the figure in the Comment. In this way we distinguish between the original counting field s and the rescaled one λ. This rescaling corresponds to focusing on a small window around $s = 0$, one that shrinks with increasing N. At any finite N there is no transition but a crossover which remains smooth in the limit $N \to \infty$. This means that in a vicinity of $s = 0$, explored in terms of the rescaled field λ, we necessarily have smooth behavior for the SCGF. This, as expected, is what Fig. 1 of the Comment is showing, not the absence of a transition: In terms of λ only the vanishing regime around $s = 0$ is accessible and not the full range of the SCGF (and therefore the full range of dynamical fluctuations). For more detailed discussions on the transition region, see Ref. [4] for the simple exclusion process (SEP), and Refs. [8–10] for kinetically constrained models.

The model we study in Ref. [1] is deterministic in the bulk and the stochasticity comes only from the boundary sites. One could ask whether this system is actually a few-body problem in disguise, for which a LD transition would not be possible: After all, the characteristic equation that defines the SCGF is given by a quartic polynomial, as would occur in a four-level system. This is not the case. First, one cannot simply integrate out the bulk leaving a four-state boundary system, since, given the delay in propagating the signal between the boundaries, such tracing out would produce a non-Markovian dynamics, where nontrivial spatial correlations would convert into a nontrivial memory kernel. Second, the SCGF equation reducing to a quartic one is connected to the fact that the "metastable manifold" is formed by the four leading eigenvalues (represented as rank-3 MPS) of the many-body evolution operator [11]. Intuitively, these four eigenstates are the relevant ones for the finite- (but long-) time dynamics of the model and hence they are reflected in the computation of the LDs.

A final observation in the Comment against the LD transition relates to the rare trajectories of the model. This is somewhat surprising: In Fig. 3 of Ref. [1] we show explicitly trajectories in both phases (constructed from the exact, or Doob, optimal dynamics for the rare events). The Comment also states that the dynamics is not intermittent. Again, we refer back to Ref. [1]: In Fig. 1(c) we show a typical trajectory, displaying fluctuating patterns of activity and inactivity, a clear sign of intermittency in the dynamics (termed "dynamic heterogeneity" in the context of glassy dynamics). Furthermore, using the methods applied to a different but related model in Ref. [12], it should be possible to prove that the dynamical free energy for the inactive "bubbles" in Fig. 1(c) scales with their (space-time) perimeter rather than their area, a clear indication of an underlying first-order phase transition (cf. Ref. [12]).

In summary, none of our exact calculations or results are brought into question by the Comment. The disagreement is only on the interpretation of the results in relation to the existence of competing dynamical phases. As we explain above, we object to the time-scaling procedure proposed in the Comment which is (i) not the standard in the field of dynamical large deviations, and more importantly (ii) could always be adapted to remove the signature of a true trajectory phase transition by impeding access to the relevant fluctuation regime.

B.B. was supported by a research Grant No. (42085) from VILLUM FONDEN.

[1] B. Buča, J. P. Garrahan, T. Prosen, and M. Vanicat, Exact large deviation statistics and trajectory phase transition of a deterministic boundary driven cellular automaton, Phys. Rev. E **100**, 020103(R) (2019).

[2] T. Bodineau and B. Derrida, Distribution of current in nonequilibrium diffusive systems and phase transitions, Phys. Rev. E **72**, 066110 (2005).

[3] J. P. Garrahan, R. L. Jack, V. Lecomte, E. Pitard, K. van Duijvendijk, and F. van Wijland, Dynamical First-Order Phase Transition in Kinetically Constrained Models of Glasses, Phys. Rev. Lett. **98**, 195702 (2007).

[4] C. Appert-Rolland, B. Derrida, V. Lecomte, and F. van Wijland, Universal cumulants of the current in diffusive systems on a ring, Phys. Rev. E **78**, 021122 (2008).

[5] S. Whitelam, Comment on "Exact large deviation statistics and trajectory phase transition of a deterministic boundary driven cellular automaton", Phys. Rev. E **108**, 036105 (2023).

[6] S. Whitelam and D. Jacobson, Varied phenomenology of models displaying dynamical large-deviation singularities, Phys. Rev. E **103**, 032152 (2021).

[7] There are particular instances of singularities in large deviation functions for few-body problems. An example is that of Ref. [13], where for a large enough counting field and for a nonlinear function of position as observable, the tilted generator changes from one with a bounded potential to one with an unbounded potential, giving rise to a singularity at long times (which remains the only large "size" in that problem). The class considered in Ref. [6] is not of this kind.

[8] T. Bodineau, V. Lecomte, and C. Toninelli, Finite size scaling of the dynamical free-energy in a kinetically constrained model, J. Stat. Phys. **147**, 1 (2012).

[9] T. Nemoto, R. L. Jack, and V. Lecomte, Finite-Size Scaling of a First-Order Dynamical Phase Transition: Adaptive Population Dynamics and an Effective Model, Phys. Rev. Lett. **118**, 115702 (2017).

[10] M. C. Bañuls and J. P. Garrahan, Using Matrix Product States to Study the Dynamical Large Deviations of Kinetically Constrained Models, Phys. Rev. Lett. **123**, 200601 (2019).

[11] T. Prosen and B. Buča, Exact matrix product decay modes of a boundary driven cellular automaton, J. Phys. A: Math. Theor. **50**, 395002 (2017).

[12] K. Klobas, C. D. Fazio, and J. P. Garrahan, Exact hydrophobicity in deterministic circuits: Dynamical fluctuations in the Floquet-East model, arXiv:2305.07423.

[13] P. T. Nyawo and H. Touchette, A minimal model of dynamical phase transition, Europhys. Lett. **116**, 50009 (2016).