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

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Buča *et al.* [Phys. Rev. E **100**, 020103(R) (2019)] study the dynamical large deviations of a boundary-driven cellular automaton. They take a double limit in which first time and then space is made infinite, and interpret the resulting large-deviation singularity as evidence of a first-order phase transition and the accompanying coexistence of two distinct dynamical phases. This view is characteristic of an approach to dynamical large deviations in which time is interpreted as if it were a spatial coordinate of a thermodynamic system [Jack, Eur. Phys. J. B **93**, 74 (2020)]. Here, I argue that the large-deviation function produced in this double limit is not consistent with the basic features of the model of Buča *et al.* I show that a modified limiting procedure results in a nonsingular large-deviation function consistent with those features, and that neither supports the idea of coexisting dynamical phases.

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The authors of Ref. [1] study the dynamical trajectories of a boundary-driven cellular automaton on a lattice of size N. They obtain the scaled cumulant-generating function (SCGF) $\theta_N(s)$ for a particular time-integrated observable, by invoking the limit of long time T and extracting $\theta(s)$ from the largest eigenvalue of a tilted rate matrix (s is the tilting- or Legendre-transform parameter). They then take the limit of large system size N, the result being a kinked function $\lim_{N\to\infty} N^{-1}\theta_N(s)$ [Eq. (10) of the paper]. The authors state that this kinked function signals a first-order dynamical phase transition with an accompanying dynamical phase coexistence. However, while Eq. (10) is reminiscent of the singular large-deviation function of the Ising model below its critical temperature, which does display phase coexistence [2,3], a similar interpretation is not consistent with the basic phenomenology of the model of Ref. [1].

Principally, the model has a well-defined mean or typical value of the chosen observable, even in the limit $N \to \infty$, given by Eq. (8) of the paper. If the function $\lim_{N\to\infty} N^{-1}\theta_N(s)$ is the cumulant-generating function then it should be able to generate this mean value, but it cannot: It is not differentiable at $s = 0$, and contains none of the model parameters α to δ that appear in Eq. (8). Thus Eq. (10) is not the SCGF, and Eqs. (8) and (10) of the paper are not consistent in the limit of large N, the latter containing less information than the former [4]. Equivalently, the large-deviation rate function associated with Eq. (10) possesses a line of zeros. If a large deviation principle applies, we would expect a rate function with a unique zero that corresponds to the model's typical behavior [3,5].

A singularity that emerges in the limit $N \to \infty$ does not necessarily imply the presence of coexisting phases [6]. The emergence of a singularity means only that the large-deviation principle (LDP) has broken down. I argue that the cause of the singularity for the present model is not the emergence of distinct phases but the divergence of the model's basic timescale. The large-deviation formalism assumes the long-time limit, in order to associate the SCGF with the largest eigenvalue of the tilted rate matrix, but this assumption breaks down when the $N \to \infty$ limit is taken in the manner done in the paper.

However, there is a way to take the limit $N \to \infty$ that preserves the long-time assumption. Under this modified procedure, an LDP exists, and the resulting large-deviation functions are consistent with the basic physics of the model, including Eq. (8) of the paper. Neither these large-deviation functions nor the physics of the model support the idea of phase coexistence.

To proceed, we can look for an LDP with a large parameter (or speed) $\tilde{T} \equiv T/\tau(N)$, where $\tau(N)$ is the dominant model timescale, by writing $P_T(x) \sim \exp[-T\varphi_N(x)] \equiv \exp[-\tilde{T}\tilde{\varphi}_N(x)]$. Here, $P_T(x)$ is the probability of observing a particular value x of the observable, and the rate functions on speed T and $\tilde{T}$ are respectively $\varphi_N(x)$ and $\tilde{\varphi}_N(x) = \tau(N)\varphi_N(x)$. The SCGF corresponding to $\varphi_N(x)$ is $\theta_N(s)$, while the SCGF corresponding to $\tilde{\varphi}_N(x)$ is obtained by sending $s \to s/\tau(N)$, giving the function $\theta_N(s/\tau(N))$.

Given that the model's dynamics is ballistic, I assume that the dominant timescale is linear in system size, i.e., $\tau(N) = N$, and plot in Fig. 1 the large-deviation functions on speed $\tilde{T} = T/N$. As N becomes large, these functions tend to a limiting, nonsingular form, validating the assumption of an LDP on speed $\tilde{T}$. The colored lines were produced by numerically evaluating Eq. (4) of Ref. [1]. The black dashed line was produced by taking the limit $N \to \infty$ analytically (having first sent $s \to s/N$) and evaluating the resulting equation numerically. The resulting function is the limiting form to which the SCGF tends. The inset of Fig. 1 shows the corresponding limiting rate function, $\lim_{N\to\infty} \tilde{\varphi}_N(x)$, which quantifies the logarithmic probability of observing certain values x of the time-integrated observable. As expected from a well-defined LDP, this has a unique zero corresponding to the typical value of the observable [Eq. (8) of the paper]. That is, the limiting

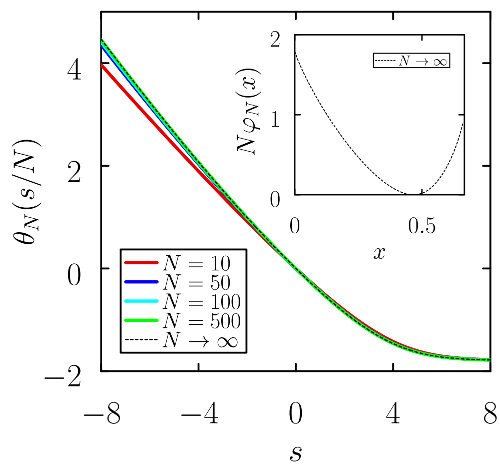

FIG. 1. Large-deviation functions of the boundary-driven cellular automaton of Ref. [1] on speed T/N (compare Fig. 2 of that paper). Functions tend to a nonsingular form in the large-N limit, indicating the existence of a well-defined LDP. Inset: Limiting form of the corresponding rate function, which quantifies the logarithmic probability of observing a value x of the dynamical observable. This function describes the fluctuations of the observable in the large-N limit. It is consistent with Eq. (8) of the paper, the unique zero corresponding to the model's typical behavior.

procedure consistent with a well-defined LDP is to assume that T is large, in order to associate the SCGF with the largest eigenvalue of the tilted generator, then rescale the Legendre-transform parameter s by the system's dominant timescale, in this case N, and then take $N \to \infty$.

The functions of Fig. 1 do not support the idea of coexisting dynamical phases at the level of the time-integrated observable (coexistence of this nature can be seen in, e.g., the right-hand panel of Fig. 6 of Ref. [6]). The logarithmic probability of observing trajectories of the model of Ref. [1] having values x of the time-integrated observable is $-T/N$ multiplied by the function shown in the inset of Fig. 1. This function resembles the Gibbs free energy of the Ising model *above* its critical temperature, where there is a single phase [2,3]. The rate function shows dynamical fluctuations to occur about a well-defined mean value (the rate function has a unique zero), to be Gaussian about the mean (the rate function is quadratic about its zero), and to have non-Gaussian tails.

Another way a system could be said to exhibit coexistence is if the trajectories that realize particular values of the time-integrated observable are intermittent, switching back and forth between distinct values of the instantaneous counterpart of the time-integrated observable (coexistence of this nature can be seen in, e.g., the middle panel of Fig. 6 of Ref. [6]). Whether or not this is the case cannot be deduced directly from the rate function [7], and must be assessed by direct calculation of rare trajectories. The authors of Ref. [1] rule out this scenario in the text, and show in Fig. 3 some rare trajectories of the model. Those trajectories display fluctuations, because the model is stochastic, but they are not intermittent in the sense of exhibiting switches between two distinct states.

Kinked large-deviation functions that emerge in a double-limit procedure, in which first time and then space are taken infinite, are usually described as dynamical phase transitions, accompanied by dynamical phase coexistence [8]. However, for some models, such as that of Ref. [1], singularities can arise in this limit in the absence of phase-transition-like phenomenology. Therefore the automatic use of the terminology is not appropriate, and the implication for how the system behaves in the large-size limit may be inaccurate.

For instance, for large system size and below its critical temperature, the Ising model's Helmholtz free energy is kinked and its Gibbs free energy possesses a line of zeros. Such features have become synonymous with the idea of a phase transition. However, these singular large-deviation functions tell us only that the LDP on the bulk speed has broken down, and do not give us all the necessary information about the system: The flat-bottomed Gibbs free energy of the Ising model cannot tell us even its typical magnetization [2]. Information about phase coexistence in the Ising model comes instead from consideration of the spin-up–spin-down symmetry of its energy function, the microscopic cooperativity of the energy function that induces nonzero surface tension, and the resulting surface free energy that reveals the existence of two typical behaviors, the coexisting phases [2]. A literal interpretation of Fig. 2 of Ref. [1] suggests something similar: In the limit of large N, dynamical phases with large and small values of x "coexist" at the point $s = 0$, meaning that the natural (i.e., unbiased) dynamics of the model should support those (and only those) two phases. However, this interpretation is problematic when set against the physics of the model: Its dynamical rules are not cooperative, and there is no obvious physical reason it would support two phases, however large is the lattice. Consistent with this expectation, Eq. (8) shows that the typical behavior of the unbiased model in the limit $N \to \infty$ corresponds to a single, intermediate value of x.

I argue that the resolution of this inconsistency is to note that the space and time dimensions of a dynamical model are not equivalent: We must take the large-N limit so that the scaled observation time $T/\tau(N)$ remains large, or else we have made an ergodic system nonergodic in an artificial way. For the model of Ref. [1], the modified procedure described in this Comment results in the large-deviation functions shown in Fig. 1. These functions are well defined, validating the assumption of an LDP on the scale $T/\tau(N)$, and are consistent with the idea that the model does not exhibit phase coexistence.

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