

Thermodynamic and dynamical predictions for bifurcations and non-equilibrium phase transitions

Han Yan^a, Feng Zhang^a, and Jin Wang^{b,1}

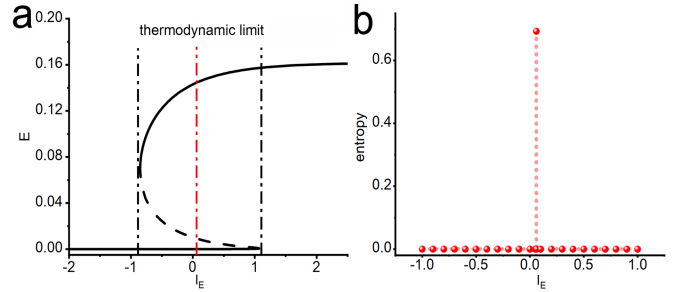
^aState Key Laboratory of Electroanalytical Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, Jilin, 130022, P.R. China; ^bDepartment of Chemistry and Physics, State University of New York at Stony Brook, Stony Brook, NY 11790, USA; ¹E-mail: jin.wang.1@stonybrook.edu.

Supplementary Note 1: Non-equilibrium phase transitions in the thermodynamic limit

The theoretical results in the main text suggest that the specific behaviors in the vicinities of the corresponding transition points in discontinuous and continuous phase transitions share certain analogies to the corresponding equilibrium cases. There are significant differences, however, between the phase transitions in equilibrium and non-equilibrium systems. For a non-equilibrium system under finite fluctuations, the stochastic dynamics may exhibit multi-attractor behaviors and the underlying non-equilibrium steady-state (NESS) probability distribution is an emergence of the underlying stochastic dynamics. In other words, such NESS probability distribution P_{ss} is derived from the corresponding dynamical driving force which is irreversible. Therefore, the non-equilibrium entropy and the heat capacity defined based on the NESS probability distribution P_{ss} can reflect the irreversible dynamical nature of the non-equilibrium systems and they can be used for characterizing the non-equilibrium phase transitions in addition to EPR(1–4). Moreover, such non-equilibrium phase transitions correspond to bifurcations in nonlinear dynamics(5–7), and they can be termed as "non-equilibrium dynamical phase transitions". The equilibrium phase transitions are usually explored in the regime of the thermodynamic limit. Once the thermodynamic limit is introduced for the non-equilibrium systems, the underlying NESS probability distribution can be quite different. The thermodynamic limit means that one has to wait sufficiently long to allow the jumps back and forth between the attractors with sufficiently low but non-neglectable fluctuations. Even though the intrinsic potential landscape ϕ_0 from the weak fluctuation limit can exhibit multi-minima, only one of them with the smaller value of ϕ_0 is singled out under the diminishing fluctuations in the thermodynamic limit. This can result in different critical behaviors in phase transitions. When exploring the phase transitions in the non-equilibrium systems, one needs to differentiate the scenarios under the thermodynamic limit and the finite fluctuations.

As shown in the main text, the discontinuous phase transition emerges at the location where the dynamical saddle-node/fold bifurcation occurs, rather than the location where the two attractors coexist with the same weight in the equilibrium phase transitions. In the thermodynamic limit, only one fixed point is present with

the probability one even through the intrinsic potential ϕ_0 can exhibit double-minimum. The only exception is when both fixed points coexist with the same probability 0.5 as the two minima are equal. Therefore, the entropy defined as $S = -\int P(\mathbf{x}) \ln P(\mathbf{x}) d\mathbf{x}$ is discontinuous at such critical parameter value (see the vertical red lines in Supplementary Fig. 1(a-b)).



Supplementary Figure 1. Non-equilibrium phase transitions occur at different locations when the system is under finite fluctuations or in the thermodynamic limit. (a) The phase diagram of the Wilson-Cowan model varying the parameter I_E . (b) The nonequilibrium entropy versus the control parameter I_E with finite fluctuations and in the thermodynamic limit, respectively. The vertical black dashed lines indicate the transition points with finite fluctuations, while the vertical red dashed lines indicate the transition points in the thermodynamic limit.

The non-equilibrium phase transition with finite fluctuations has a specific entropy production signature(1–4). However, in the zero-noise limit, the specific behavior in the entropy production at the first-order phase transition regime is different from that under the finite fluctuations. The entropy production rate in the zero-noise limit can be approximately computed through Taylor series expansion near the corresponding fixed points. The driving force of a non-equilibrium system can be written as: $\mathbf{F}(\mathbf{x}) = -\mathbf{D}(\mathbf{x}) \cdot \nabla \phi_0(\mathbf{x}) + \mathbf{v}$ in the zero-fluctuation limit(8–10). The intrinsic flux velocity $\mathbf{v} = \mathbf{J}_{SS}/P_{SS}|_{D \rightarrow 0}$ satisfies $\mathbf{v} \cdot \nabla \phi_0 = 0$, which implies that the gradient of the non-equilibrium intrinsic potential ϕ_0 is orthogonal to the intrinsic flux (or intrinsic flux velocity) in the zero-fluctuation limit. Therefore, both the intrinsic flux velocity $\mathbf{v}$ and $\mathbf{D}(\mathbf{x}) \cdot \nabla \phi_0(\mathbf{x})$ should be zero at the fixed point where the driving force is zero. For simplicity, we show here the entropy production rate in a one-dimensional system for the non-equilibrium first order phase transition in the thermodynamic limit as:

$$\begin{aligned}
EPR &= \int_{-\infty}^{+\infty} \mathbf{v} \cdot (D)^{-1} \cdot \mathbf{v} \cdot P_{SS} \cdot dx \\
&\approx \int_{x^*-\epsilon}^{x^*+\epsilon} \mathbf{v} \cdot (D)^{-1} \cdot \mathbf{v} \cdot \frac{e^{-\frac{\phi_0(x-x^*)}{D}}}{Z} \cdot d(x-x^*) \\
&\approx \frac{\int_{x^*-\epsilon}^{x^*+\epsilon} a(x-x^*) \cdot (D)^{-1} \cdot a(x-x^*) \cdot e^{-\frac{b(x-x^*)^2}{D}} \cdot d(x-x^*)}{\int_{x^*-\epsilon}^{x^*+\epsilon} e^{-\frac{b(x-x^*)^2}{D}} \cdot d(x-x^*)} \\
&\approx 1/2 * a^2 * (D^{-1}) \sqrt{\pi D^3/b^3} / \sqrt{\pi D/b} \\
&\approx a^2/(2b)
\end{aligned}$$

Here x^* is the fixed point, $a = \partial \mathbf{v} / \partial x|_{x=x^*}$ and $b = \partial^2 \phi_0 / \partial x^2|_{x=x^*}$. In the zero-fluctuation or thermodynamic limit, only one fixed point is left with the probability one even through the intrinsic potential ϕ_0 can exhibit double-minimum ($x = x_1^*, x_2^*$). Therefore, the EPR tends to be $a_1^2/(2b_1)$ if $\phi_0(x_1^*) < \phi_0(x_2^*)$, and tends to be $a_2^2/(2b_2)$ if $\phi_0(x_2^*) < \phi_0(x_1^*)$. The EPR is discontinuous at the critical point when $\phi_0(x_1^*) = \phi_0(x_2^*)$ (11). It is not difficult to prove that this result is general for systems with high dimensions.

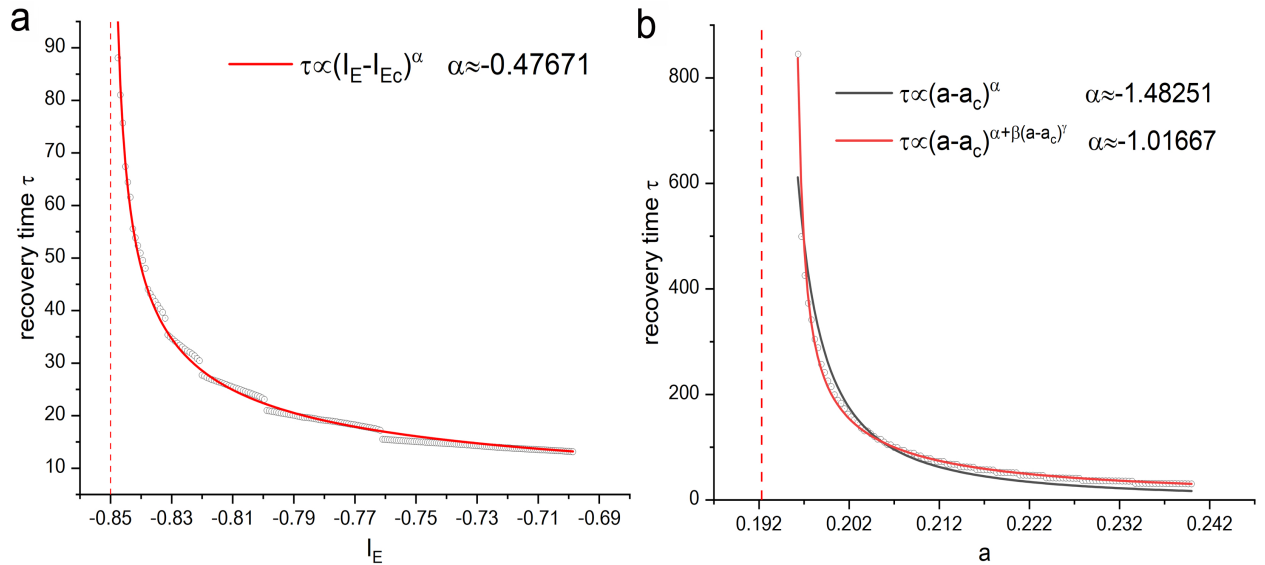
In the thermodynamic limit, the discontinuous/first-order phase transitions are more analogous to the cases in equilibrium systems, and they can be termed as "non-equilibrium thermodynamic phase transitions".

Supplementary Note 2: The divergence of the recovery time as the temporal signature of a phase transition

As discussed in previous works (12), the recovery time after perturbations diverges according to the power law as the

tipping point is approached. We calculated how the recovery time diverges as the system approaches to the tipping point in both the two models in our manuscript. As shown in the following Supplementary Fig.2(a), the recovery time diverges according to the power law $\tau \propto (I_E - I_{E,crit})^\alpha$ shown by the fitted red line. The critical exponent $\alpha \approx -0.47671$, which is consistent with previous work on first-order phase transitions (12). However, for the model with the continuous transition from the mono-stable state to oscillations, it seems that the behavior of the recovery time with respect to the control parameter doesn't display the simple power-law relation. Our result suggests that it diverges faster than the fitted power-law function indicated by the black line (Supplementary Fig.2(b)). The function with the exponent that is dependent on the difference between the value of the control parameter and the critical value fits better (the red line).

The concepts such as scaling, critical exponents and universality classes, which are originally used to describe the critical phenomena in equilibrium systems, are also very important for understanding the non-equilibrium phase transitions. In the main text, we didn't explicitly discuss the critical exponents. This is because that the main purpose of the present work is to provide a practical way for predicting critical transitions in complex systems. For some non-equilibrium systems, we can define the order parameter and further quantify critical exponents. The concepts and methods which were developed for equilibrium critical phenomena can also be applied to these non-equilibrium phase transitions. However, in many non-equilibrium systems, it is not easy to define an explicit order parameter and quantify the corresponding critical exponents. Moreover, critical systems are often character-



Supplementary Figure 2. The divergence of the recovery time as the temporal signature of a phase transition. (a) In the Wilson-Cowan model, the recovery time diverges according to the power law $\tau \propto (I_E - I_{E,crit})^\alpha$. (b) In the model with the continuous transition from the mono-stable state to oscillations, the recovery time diverges faster than the fitted power-law function indicated by the black line.

ized by power-laws sufficiently close to the critical point. As we have discussed in the main text, the warning signals based on the phenomenon of “critical slowing down” are not early enough for predicting the impending critical transitions, since they can only be detected very close to the tipping point. Therefore, quantifying the critical exponents may not be much helpful for providing practical early warning signals for critical transitions.

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