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Unveiling the Phase Diagram and Reaction Paths of the Active Model B with the Deep Minimum Action Method

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Nonequilibrium phase transitions are notably difficult to analyze because their mechanisms depend on the system's dynamics in a complex way due to the lack of time-reversal symmetry. To complicate matters, the system's steady-state distribution is unknown in general. Here, the phase diagram of the active Model B is computed with a deep neural network implementation of the geometric minimum action method (gMAM). This approach unveils the unconventional reaction paths and nucleation mechanism by which the system switches between the homogeneous and inhomogeneous phases in the binodal region. Our main findings are: (i) the mean time to escape the phase-separated state is (exponentially) extensive in the system size L , but it increases *non-monotonically* with L ; (ii) the mean time to escape the homogeneous state is always finite, in line with the recent work of Cates and Nardini [1]; (iii) at fixed L , the active term increases the stability of the homogeneous phase, eventually destroying the phase separation in the binodal for large but finite systems. Our results are particularly relevant for active matter systems in which the number of constituents hardly goes beyond 10^7 and where finite-size effects matter.

Introduction— Activated processes are ubiquitous in nature but intrinsically difficult to probe in simulations since they require the sampling of rare events [2–5]. When a first-order phase transition occurs, a nucleation event is usually required for the system to reach its stable phase [1, 6–8]. In equilibrium systems, we can exploit the property of time-reversal symmetry (TRS) and the knowledge of their equilibrium distribution to derive a free energy from which we can infer both the thermodynamic stability of each phase, and the reaction paths that are followed by the system during activation [9–11]. In contrast, the breakdown of TRS in nonequilibrium systems means that we no longer have access to their free energy, and the mechanism of activated processes must be understood from their dynamics rather than their unknown steady-state distribution [12–19]. Mapping their phase diagram therefore poses a persistent challenge.

In this letter, we consider this problem in the context of the active Model B, a natural nonequilibrium extension of the Cahn-Hilliard dynamics with a nonlinear growth term [20, 21] that breaks TRS. This generic model has attracted a lot of attention in the last decade [22–25], and can be used, for instance, as an effective description of the dynamics of active particles that are known to undergo a motility-induced phase separation (MIPS) [26–28]. Here, we map the phase diagram of the active Model B and calculate the pathways by which first-order phase transitions occur in this system. Our results indicate that these transitions involve nucleation events that are markedly different from their equilibrium counterpart, and are shaped by the interplay between the noise and nongradient terms in the stochastic dynamics of the system. In large but finite systems, we also show that the active term can decrease the probability to observe the nucleation of the phase-separated state and help the reverse transition from the phase-separated phase to the homogeneous state. To obtain these results, we compute reaction paths using an implementation of the geometric Minimum Action Method

(gMAM) [29–31] that relies on Physics-Informed Neural Networks (PINNs) [32, 33]; this neural implementation, referred to as *deep gMAM* [34], is interesting in its own right as it is transferable to study first-order phase transitions in other nonequilibrium systems. Here we also cross-check some of the results of the deep gMAM algorithm using the traditional gMAM method as benchmark.

Problem setting— The active Model B (AMB) describes the stochastic dynamics of a conserved scalar field $\phi(x, t)$, typically interpreted as the local (relative) density of particles or the local composition of a mixture, and can be written as the divergence of a noisy flux [1, 22, 23, 35]

$$\partial_t \phi = \nabla \cdot (M \nabla \mu + \xi), \quad (1)$$

$$\mu([\phi], x) = \frac{\delta \mathcal{F}[\phi]}{\delta \phi(x)} + \lambda |\nabla \phi(x)|^2, \quad (2)$$

where $\mathcal{F}[\phi]$ is a Ginzburg-Landau free energy, M is the mobility operator, and ξ is a spatio-temporal white-noise, i.e. a Gaussian process with mean zero and covariance $\langle \xi(x, t) \xi(x', t') \rangle = 2\epsilon M \delta(x - x') \delta(t - t')$ with ϵ controlling the amplitude of the fluctuations. We will investigate Eq. (1) in $d = 1$ and $d = 2$ dimensions, assuming periodic boundary condition of the domain $\Omega = [0, L]^d$ with lateral size L . For simplicity, we will focus on the situations where $M = \mathbb{1}$ and $\mathcal{F}[\phi] = \int_{\Omega} [\frac{1}{2} \nu (\nabla \phi)^2 + f(\phi)] dx$, where $\nu > 0$ and $f(\phi)$ is a double-well potential. With this choice of free energy there exists a region in the phase diagram where a homogeneous state, denoted ϕ_H , will coexist with a phase-separated state (or inhomogeneous state), denoted ϕ_I , see Fig. 1(a). These states correspond to the two (locally) stable fixed points of the noiseless version of Eq. (1), i.e. the solution to $\nabla \cdot (M \nabla \mu) = 0$ with a prescribed value of the spatial average ϕ_0 of ϕ in the domain.

When $\lambda = 0$ the chemical potential μ is the functional derivative of a free energy $\mathcal{F}[\phi]$, and the dynamics is in detailed balance with respect to the Gibbs-Boltzmann measure,

and the stationary probability of observing a configuration $\phi(x)$ is thus given by $P_s[\phi] \propto \exp(-\mathcal{F}[\phi]/\epsilon)$. In this case, the relative stability of the phases associated with ϕ_H and ϕ_I can be inferred from the values of $\mathcal{F}[\phi_H]$ and $\mathcal{F}[\phi_I]$, and transitions between these states involve a reaction path that goes through a saddle point configuration on $\mathcal{F}[\phi]$.

In contrast, when $\lambda \neq 0$, TRS is broken because μ does not satisfy the Schwarz condition on its functional derivative [25, 36, 37], and the stationary distribution of the system is no longer available. As a consequence, the functional $\mathcal{F}[\phi]$ brings no information on the relative stability of the phases associated with ϕ_H and ϕ_I . Rather, a characterization of the relative stability of these phases must rely on the dynamics.

Phase transitions and quasipotential– We will resort to Freidlin-Wentzell large-deviation theory (LDT) to calculate the rates of the transitions from ϕ_H to ϕ_I and vice-versa, as well as their most likely paths [12], in the limit as $\epsilon \rightarrow 0$ (i.e. when the system is either in ϕ_H or in ϕ_I with probability one, and proper phases can be defined). Denoting by $k_{I,H}$ the rate to go from ϕ_I to ϕ_H , it is asymptotically given by $k_{I,H} \asymp \exp(-V_{\phi_I}(\phi_H)/\epsilon)$, where $V_{\phi_I}(\phi_H)$ is the so-called quasipotential of ϕ_H relative to ϕ_I that plays a role similar to a potential barrier in Arrhenius' law; a similar expression holds for $k_{H,I}$, the rate to go from ϕ_H to ϕ_I . The relative stability of the two phases can then be assessed by the difference of the logarithm of ratio of these escape rates

$$\epsilon \log k_{I,H} - \epsilon \log k_{H,I} \asymp -V_{\phi_I}(\phi_H) + V_{\phi_H}(\phi_I), \quad (3)$$

which is positive when ϕ_H is the preferred phase, and negative when ϕ_I is. Note that the values of the quasipotential $V_{\phi_I}(\phi_H)$ and $V_{\phi_H}(\phi_I)$ depend on the control parameters in the system, such as λ and ϕ_0 , and so the sign of their difference can switch: when this happens, it is the signature of a first-order phase transition. This offers us a route to analyze these transitions, as advocated in [38], by computing these quasipotentials for various values of λ and ϕ_0 , using the fact that they are the minima of the action functional $S_T[\phi]$ defined as

$$S_T[\phi] = \int_0^T \int_{\Omega} |\nabla^{-1}(\partial_t \phi - \nabla^2 \mu)|^2 dx dt \quad (4)$$

where Ω denotes the domain. The action (4) must be minimized with respect to both T and ϕ , subject to $\phi(t=0, x) = \phi_H$ and $\phi(t=T, x) = \phi_I$ to get $V_{\phi_H}(\phi_I)$, and $\phi(t=0, x) = \phi_I$ and $\phi(t=T, x) = \phi_H$ to get $V_{\phi_I}(\phi_H)$.

Deep gMAM– To minimize (4) we use the PINN scheme introduced in [34]. In a nutshell, this approach amounts to approximating the field $\phi(x, t)$ within a rich parametric class, such as a deep neural network, and viewing (4) as an objective (or loss, in the terminology of machine learning) for the parameters in the representation. The boundary conditions in space and time are accounted for by adding suitable pieces to (4), and the parameter optimization is performed using a standard stochastic gradient descent (SGD) algorithm such as ADAM on this compounded loss. This requires evaluating the loss, which is done using space-time collocation points that are drawn randomly at each step of SGD (which amounts to

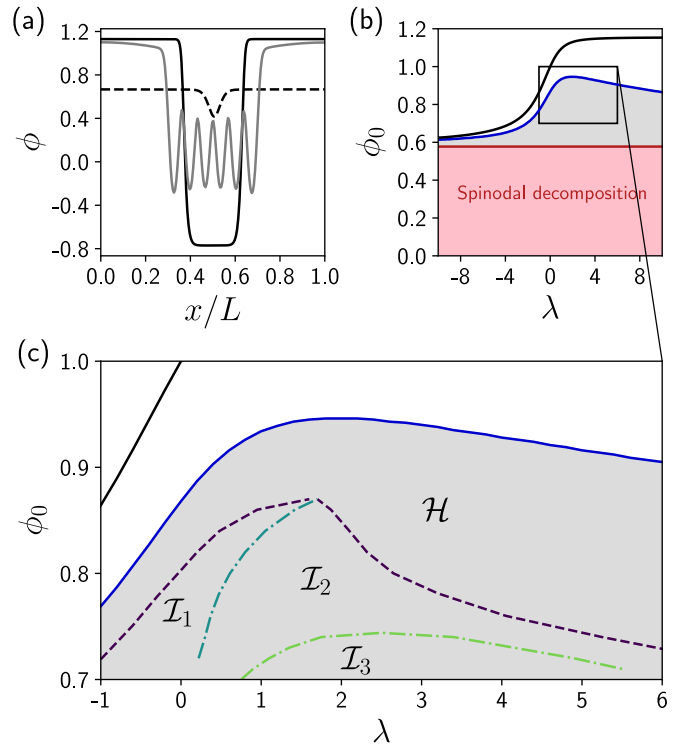


FIG. 1. (a) Three remarkable configurations in dimension $d = 1$. The solid line is the inhomogeneous state ϕ_I (stable). The dashed line indicates the (unstable) critical state $\phi_{c,1}$. The grey line is a configuration of the field on the nonequilibrium reaction path from ϕ_I to the homogeneous state ϕ_H (not shown). Parameters: $\phi_0 = 0.65$, $\lambda = 2$, and $L = 120$. (b) Phase diagram of active Model B in parameter space (λ, ϕ_0) in $d = 1$ dimension. Panel (b) shows the binodal (black line) and the spinodal (red line) that were already computed in [22]. In finite size systems, the bistable region does not fully span between the spinodal and the binodal but stops at the blue line (here plotted for $L = 60$). The states ϕ_H and ϕ_I are both stable in the shaded region. Panel (c) focuses on the bistable region. The purple dashed line pinpoints the first-order (f.-o.) transition between ϕ_H and ϕ_I . On this line, one has $V_{\phi_H}(\phi_I) = V_{\phi_I}(\phi_H)$. In region \mathcal{H} , above the f.-o. transition, ϕ_H is thermodynamically preferred, while below the f.-o. transition, in regions $\mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3$, the inhomogeneous state ϕ_I is preferred. The index q in \mathcal{I}_q refers to the number of bumps that appear along the reaction path from ϕ_I to ϕ_H . Note that the region \mathcal{I}_3 may display asymmetric paths with an action slightly smaller than their symmetric versions.

performing online learning). The deep gMAM algorithm is simple to implement, does not require any gridding of space or time, and gives an analytical approximation of $\phi(t, x)$ everywhere in the spatio-temporal domain. Here the results of the deep gMAM algorithm in $d = 1$ were cross-checked against those obtained using a classical implementation of gMAM, which requires discretizing the field in space and time, and is somewhat more delicate to implement. For more details on both the deep and the classic gMAM algorithms, in particular how to handle the optimization on T by reparameterizing the solution using arc-length instead of physical time, see the Supplemental Material (SM).

Phase diagram in 1d– We focus first on the one-

dimensional system, whose dynamics reads

$$\partial_t \phi = -\partial_x^2 [\partial_x^2 \phi + \phi - \phi^3 - \lambda(\partial_x \phi)^2] + \partial_x \xi, \quad (5)$$

with $\langle \xi(x, t) \xi(x', t') \rangle = 2\epsilon \delta(t - t') \delta(x - x')$. Space has been rescaled such that all lengths are given in units of $\sqrt{\nu}$. We consider a system of size L and we take periodic boundary conditions. The relevant parameters are thus L , the total mass $\phi_0 \equiv L^{-1} \int_0^L \phi dx$, and the activity level λ . The constant density solution of Eq. (5) is the homogeneous state ϕ_H , and since the mass ϕ_0 is conserved, we have $\phi_H = \phi_0$. In the following, using the fact Eq. (5) is invariant under $(\lambda, \phi) \rightarrow (-\lambda, -\phi)$, we restrain the study to the region $\phi_0 > 0$. The homogeneous state ϕ_H is always a stable fixed point of the noiseless dynamics for $\phi_0 > \phi_{\text{sp}+}^\lambda$, where $\phi_{\text{sp}+}^\lambda = 1/\sqrt{3}$ is the frontier of the spinodal in the space (λ, ϕ_0) for $\phi_0 > 0$. We are interested in the region where ϕ_H competes with the inhomogeneous state ϕ_I . In the infinite system size limit, this region lies between the spinodal $\phi_{\text{sp}+}^\lambda$ (red line in Fig. 1(b)) and the binodal curve $\phi_{\text{bi}+}^\lambda$ (black line in Fig. 1(b-c)) that yields the bulk densities of each phase when the system undergoes a phase separation. The binodal curve $\phi_{\text{bi}+}^\lambda$ has been obtained in a series of works [22, 27], in which it was also shown that the (active) term $\lambda(\partial_x \phi)^2$, though seemingly being dynamically relevant only close to interfaces where strong gradients exist, has in fact a deep and non-local impact on the bulk of each phase. However, the stationary measure associated to the stochastic dynamics is still unknown. In particular, in the binodal region, where both the homogeneous state and the phase-separated state are metastable, the thermodynamically preferred phase is not necessarily the phase-separated state. We will denote by $\phi_{\text{f.o.}}^\lambda$ the transition density indicating the change of thermodynamic stability of the two competing phases. Naturally we have $\phi_{\text{sp}+}^\lambda \leq \phi_{\text{f.o.}}^\lambda \leq \phi_{\text{bi}+}^\lambda$. The gMAM algorithm will eventually allow for inferring $\phi_{\text{f.o.}}^\lambda$, by providing insights on the nucleation paths between the two states.

First, let us recall that for large but finite systems, the phase-separated state cannot be the preferred phase if ϕ_0 is taken too close to the binodal density $\phi_{\text{bi}+}^\lambda$. For instance, in equilibrium, (i.e. $\lambda = 0$) the binodal densities are $\phi_{\text{bi}\pm}^{\lambda=0} = \pm 1$ but a free energy argument that compares interfaces and bulk contributions shows that $\phi_{\text{f.o.}}^{\lambda=0}$ converges to 1 as $\phi_{\text{f.o.}}^{\lambda=0} \sim 1 - (1/L)^{1/2}$. More than that, due to finite-size effects, the phase-separated state may not exist at all when there is not enough space in the domain to nucleate the phase separation. Hence, one should keep in mind that in a finite system, say of size L , bistability can only be observed below some threshold density $\phi_{\text{m}L}^{\lambda=0} \leq \phi_{\text{bi}+}^{\lambda=0}$, represented as the blue curve in Fig. 1. Nonetheless, we have $\phi_{\text{m}L}^{\lambda} \rightarrow \phi_{\text{bi}\pm}^{\lambda}$ as $L \rightarrow \infty$. To pinpoint the first-order phase transition (FOPT), we run the gMAM algorithm for $\phi_0 \in [\phi_{\text{sp}+}^\lambda, \phi_{\text{m}L}^\lambda]$ and $\lambda \in [-10, 10]$. Solving $V_{\phi_H}(\phi_I) = V_{\phi_I}(\phi_H)$ identifies the FOPT line $\phi_{\text{f.o.}}^\lambda$, the purple dashed line in Fig. 1(c), which splits the diagram into two regions: for $\phi_0 < \phi_{\text{f.o.}}^\lambda$ the thermodynamically stable state is the inhomogeneous one, ϕ_I , while for $\phi_0 > \phi_{\text{f.o.}}^\lambda$ the homogeneous state $\phi_H = \phi_0$ is preferred. Interestingly, we also find that the binodal and the FOPT have a reentrance direction

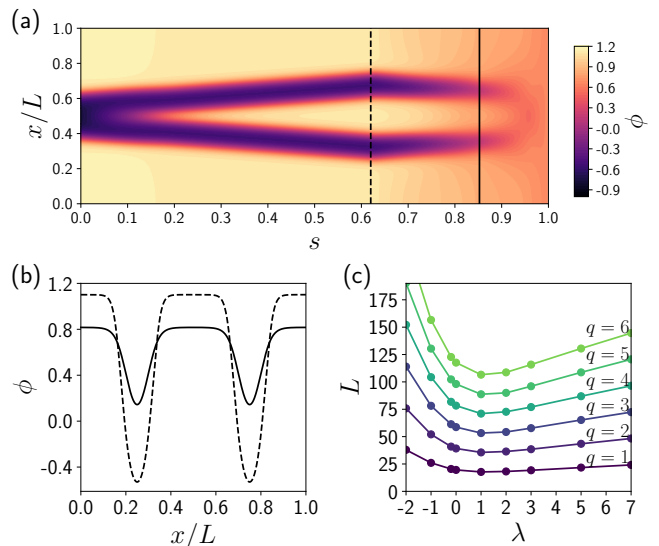


FIG. 2. (a) Minimum action path joining ϕ_I (at $s = 0$) to ϕ_H (at $s = 1$) for $\lambda = 2$, $\phi_0 = 0.65$ and $L = 44.7$ in $d = 1$ dimension. The vertical lines pinpoint the states where the norm of the flow is minimal (and almost zero), corresponding to the states close to the critical points. The corresponding critical points are displayed in panel (b). The state at the dashed line lies in the basin of attraction of the inhomogeneous state, while the state at the solid line lies on the separatrix between the ϕ_I and ϕ_H . The action from the dashed line to the solid line is strictly positive, while the action from the solid line to ϕ_H is zero. (b) Pair of critical states displaying two bumps, for same parameters as panel (a). If $L = L_2^*$, these two states merge in a saddle-node bifurcation. (c) Threshold lengths $L_q^*(\lambda)$ indicating the apparition of critical states with a given number q of bumps as a function of the system activity λ . Above the critical q -line, pairs of critical states with q bumps are dynamically accessible.

along λ that does not exist in the system of infinite size (see Fig. 1(c)).

Reaction paths in 1d– We consider first the reaction path starting from the homogeneous state ϕ_H and reaching ϕ_I , and we compute $V_{\phi_H}(\phi_I)$ for different values of λ and system size L . Interestingly this path is very close to the heteroclinic orbit joining ϕ_H to ϕ_I , and going through the critical (saddle) state $\phi_{c,1}(x)$ that displays one density bump (see Fig. 1(a)) and possesses only one unstable direction. This behavior is very similar to the equilibrium nucleation scenario occurring in the Cahn-Hilliard dynamics, as already noted in [1]: to escape ϕ_H , the system only needs to nucleate a finite size droplet of the opposite phase. The cost for the action associated to this event is always finite, and the value of the action does not differ much from the one computed using the time-reversed relaxational path (a few percent difference, not shown).

In contrast, the transition from ϕ_I to ϕ_H is more complex, and its analysis had never been explored so far. For $\phi_0 > 0$, as λ increases, the reaction path no longer follows the time-reverse relaxation path that goes through the saddle $\phi_{c,1}$, but rather passes close to critical points with a large number of unstable directions, see Fig. 2(a) and 2(b), as it may sometimes be observed in nonequilibrium systems [34, 38]. In ad-

dition, nothing prevents the reaction paths to cross the separatrix at non-critical points, a feature that cannot be observed in equilibrium, where reaction paths necessarily go through saddles of the potential. The critical points of higher Morse index can be obtained by solving the noiseless and stationary version of Eq. (5). Since the system is one-dimensional with periodic boundary conditions, the critical point solves $\partial_x^2 \phi_c = -\phi_c + \phi_c^3 + \lambda(\partial_x \phi_c)^2 + \mu_0$, with μ_0 a constant, subject to the constraints of periodicity and $L^{-1} \int_0^L \phi_c(x) dx = \phi_0$. A Newton mapping similar to the one introduced in [22] enables us to compute precisely the critical points using a symplectic scheme (see SM). For given λ and ϕ_0 , pairs of critical points with q bumps ($q \in \mathbb{N}^*$) appear at critical values of the system size denoted L_q^* , reported in Fig. 2(c). The saddle-node bifurcation at L_q^* occurs when the system size L is large enough to fit an additional bump on the density profile. At precisely the bifurcation length L_q^* , one degenerate critical state $\phi_{c,q}$ becomes accessible to the dynamics. As $L > L_q^*$, the degeneracy is lifted and two distinct critical states of q bumps appear. Any of the states $\phi_{c,q}$ can be decomposed into q identical bumps of size L/q . Notably, the state with bumps of largest amplitude strictly lies in the basin of attraction of ϕ_I , while the other state lies on the separatrix between ϕ_I and ϕ_H . We display an example of such a pair of critical states for $q = 2$ in Fig. 2(b). For all $q \geq 2$, the critical states are of Morse index $q \geq 2$. The case $q = 1$ is special as it corresponds to the apparition of the inhomogeneous metastable state ϕ_I , jointly with the critical state of Morse index 1, $\phi_{c,1}(x)$. A sketch of the structure of the deterministic flow between critical points is given in the SM. In summary, while the path from ϕ_H to ϕ_I indeed resembles the equilibrium one, the path from ϕ_I to ϕ_H displays spatial microstructures which are not present in equilibrium. Notably, the number q of bumps along the instanton changes with parameters L , ϕ_0 and λ , which is indicated by the \mathcal{I}_q -labeled regions in Fig. 1.

The roles of ϕ_0 , λ and L —Even with the ability to compute the critical states, it remains a hard task to gain analytical insights on the complete reaction paths. Our extensive numerical computations eventually show several non-trivial features, gathered in Fig. 3. First, for fixed ϕ_0 and λ , we notice that the action $V_{\phi_I}(\phi_H)$ non-monotonically increases as the system size L increases, a behavior that is triggered by the apparition of new bumps along the reaction path. Second, the scaling of the action remains extensive in the system size: we find that $V_{\phi_I}(\phi_H) \propto c(\phi_0, \lambda)L$ asymptotically. Our study suggests that c is a *decreasing* function of ϕ_0 and λ : for given system size L , increasing ϕ_0 or λ drives the system in the homogeneous phase, see Fig. 1. Third, above some critical value of λ , we find that the reaction path from ϕ_I to ϕ_H goes through the critical states with the *highest number* of unstable directions. More precisely, when the critical states with q bumps fit into the system, then, *either* (i) the reaction path goes through the critical states $\phi_{c,q}(x)$ (and displays also q bumps), *or* (ii) the reaction path displays $q + 1$ bumps, does not converge to $\phi_{c,q}(x)$ and crosses the separatrix elsewhere. Situation (i) corresponds to the parts of the curves in Fig. 3 where the action is locally increasing, while situation (ii) corresponds to the locally decreasing parts of the curves on the same plot.

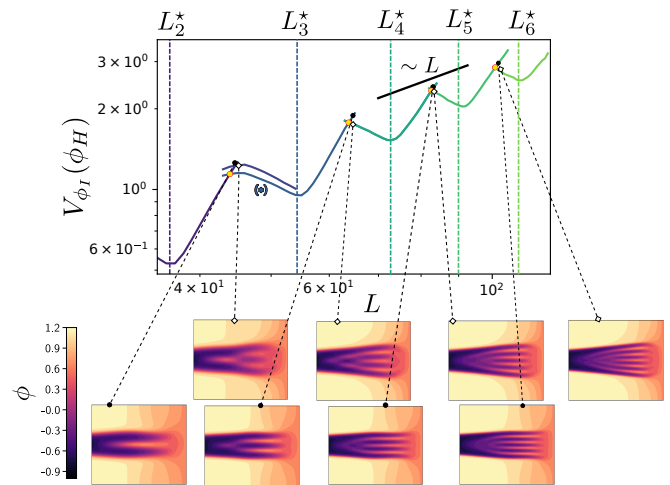


FIG. 3. Minimum action $V_{\phi_I}(\phi_H)$ as a function of the system size L (top panel), for paths starting at ϕ_I and reaching ϕ_H . Here $\lambda = 2$ and $\phi_0 = 0.65$. The action non-monotonically increases because increasing the system size L allows for qualitatively different reaction paths. The successive portions of the curve correspond to different types of paths displaying an increasing number of bumps, see bottom panels. The vertical dashed lines indicate the L_q^* , the critical lengths where pairs of critical states with q bumps appear. The values L_q^* are also given in Fig. 2(c). The yellow dots indicate where branches cross each other. The (*) symbol indicates a branch on which the path is no longer axisymmetric (see SM).

In other words, Fig. 3 shows that the reaction paths can display q bumps *before* the corresponding critical states $\phi_{c,q}(x)$ emerges. The fact that the reaction paths go through the highest Morse index states is not observed for values of $\lambda < 0$ (when $\phi_0 > 0$). To gain insights on the selected reaction paths, we have performed a spectrum analysis of the operator acting on the perturbations around ϕ_I (see SM). The analysis confirms that ϕ_I possesses stable direction only, and two marginally stable directions (Goldstone modes) corresponding to the mass conservation and to space translation invariance (due to the periodic boundary condition). Interestingly, the eigenvectors may display an oscillating profile reminiscent of the states along the instanton. However, the less stable eigenvector (corresponding to the less negative eigenvalue) does not correlate to the number of bumps selected along the instanton, as one could have expected.

Finally, our numerical results seem to indicate that more than one reaction path can be accessible. The yellow dots in Fig. 3 pinpoint the crossing of the branches where reaction paths display q and $q + 1$ bumps. There is thus a region close to these points where the action $S[\phi]$ is multivalued, and convergence seems to depend on the path initialization.

Phase transitions in 2d—The reaction paths can also be calculated in dimension $d = 2$ using the deep gMAM algorithm. We found that the path from ϕ_H to ϕ_I (not shown) follows what is predicted by classical nucleation theory [1]. Also, as expected, the path from ϕ_I to ϕ_H for $\lambda = 0$ follows the reverse relaxation path since the dynamics is in equilibrium (not shown). As with $d = 1$, the action path from ϕ_I to ϕ_H

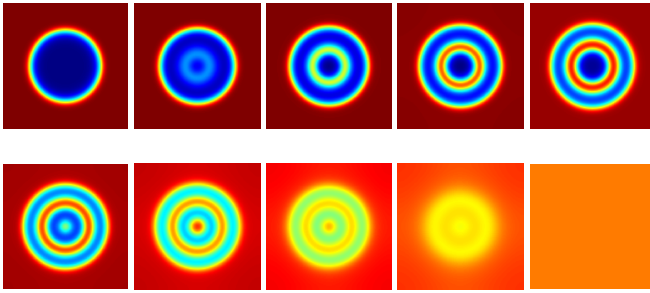


FIG. 4. Successive states along the Minimum Action Path joining ϕ_I (top left) to ϕ_H (bottom right) in a 2d system with periodic boundary conditions. Similarly to the 1d path, the instanton in 2d also displays a microstructure. Parameters: $L = 44.7$, $\lambda = 2$, $\phi_0 = 0.65$. The path has been obtained with the deep gMAM algorithm, whose details are given in the SM.

is however more complicated, displaying microstructure patterns, now with radial symmetry. There is some evidence that the instantons do not go through multi-spike profiles that are found (numerically) to be the critical states of the AMB (see SM and Ref. [39]), since the action values for such instantons are always larger than the one of the radially symmetric path. We emphasize that in $d = 2$ the critical states in Cahn-Hilliard are much more difficult to characterize [39] than in $d = 1$ [40], and this question remains open for the active Model B. All in all, a comparison to the Arrhenius law for $\lambda = 0$ shows that the active term significantly reduces the action needed to escape the inhomogeneous state.

Conclusion— We have computed the phase diagram of the AMB in $d = 1$, identified the various nucleation scenarii

in the binodal, and showed that the instanton phenomenology is similar in $d = 2$. By computing the reaction paths, we were able to identify the regions where the homogeneous state is thermodynamically preferred. The fact that the action $V_{\phi_I}(\phi_H)$ remains extensive in the system size, while $V_{\phi_H}(\phi_I)$ remains finite, confirms that eventually, the system should phase-separate as $L \rightarrow \infty$, when lying in the binodal region. Our results are consistent with the ones of Cates and Nardini [1], who show that nucleation from homogeneous state in AMB for $d \geq 2$ is qualitatively similar to classical nucleation theory in equilibrium. Our numerical results were obtained using deep gMAM [34] and cross-checked in $d = 1$ by running the classical gMAM [30]. While the latter algorithm is more accurate, the discretization scheme adopted for the Cahn-Hilliard equation is very hard to treat in $d \geq 2$, where the stability conditions of the scheme are very constraining. The deep gMAM suffers less from the increase of dimensionality. These features make the method proposed here relevant for numerous active matter systems which may undergo phase separation.

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Supplemental Material: Unveiling the Phase Diagram and Reaction Paths of the Active Model B with the Deep Minimum Action Method

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I. COMPUTING THE CRITICAL STATES

To compute the critical states we must calculate the fixed points of the noiseless equation:

$$\partial_t \phi = -\partial_x^2 [\nu \partial_x^2 \phi + \phi - \phi^3 - \lambda (\partial_x \phi)^2]. \quad (1)$$

Since space can be rescaled, here we work on a domain of size $L = 1$ where ν can vary (in the main text, we rather chose to work with $\nu = 1$ and varying L). Using stationarity and the periodic boundary conditions, a critical points ϕ_c must satisfy

$$\nu \partial_x^2 \phi_c + \phi_c - \phi_c^3 - \lambda (\partial_x \phi_c)^2 - \mu_0 = 0, \quad (2)$$

with μ_0 a constant, and ϕ_c subject to constraints of periodicity and $\int_0^1 \phi_c(x) dx = \phi_0$. The Newton mapping rephrases the stationary equation into an equation of motion, see e.g. [1]. With the correspondence $x \leftrightarrow t$ and $\phi_c \leftrightarrow z$, one gets

$$\nu \ddot{z}(t) = -z(t) + z^3(t) + \lambda (\dot{z}(t))^2 + \mu_0, \quad (3)$$

where the $\dot{z} \equiv dz/dt$.

It turns out that this system is integrable, whether $\lambda = 0$ or not. Indeed, one can set $v(z(t)) \equiv \dot{z}$, such that $\ddot{z} = \frac{dv}{dz} \frac{dz}{dt} = \frac{dv}{dz} v$, which enables us to write

$$\begin{cases} \dot{z} = v \\ \frac{d}{dz}(v^2) - \frac{2\lambda}{\nu} v^2 = \frac{2(\mu_0 - z + z^3)}{\nu}, \end{cases} \quad (4)$$

whose solution takes the form

$$v^2(z) = e^{2\alpha z} (K + \int^z h(z') e^{-2\alpha z'} dz'), \quad (5)$$

with $\alpha = \lambda/\nu$, $h(z) = 2(\mu_0 - z + z^3)/\nu$, and K some constant. For $\alpha = 0$, eq. (5) simplifies into

$$v^2 = K - \frac{2}{\nu} V(z), \quad (6)$$

with $V(z) = z^2/2 - z^4/4 - \mu_0 z$. For $\alpha \neq 0$, one computes explicitly

$$e^{2\alpha z} \int^z h(z') e^{-2\alpha z'} dz' \quad (7)$$

$$= -\frac{3 + 6\alpha z + 2(3z^2 - 1)\alpha^2 + 4(\mu_0 - z + z^3)\alpha^3}{4\alpha^4 \nu} \quad (8)$$

$$\equiv g(z), \quad (9)$$

such that we have

$$v^2 = e^{2\alpha z} K + g(z). \quad (10)$$

Since a conserved quantity exists whether $\lambda = 0$ or not, one should resort to a symplectic scheme [2] to find the periodic orbits that need to be computed with high accuracy. We use the high-order symplectic scheme proposed by Forest and Ruth [3]. For $\lambda = 0$, the equation of motion is simply

$$\nu \ddot{z} = -z + z^3 + \mu_0, \quad (11)$$

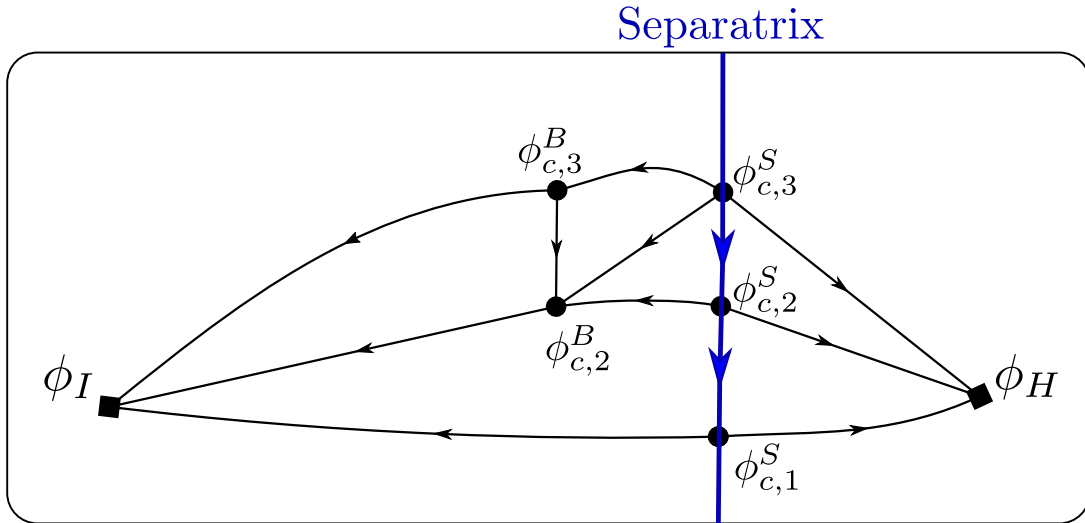


FIG. 1. Sketch of the relaxation flow lines joining different critical points with number of bumps $q < 4$. A directed link corresponds to an existing relaxation path between two critical points (the arrow indicates the noiseless flow). Critical states $\phi_{c,q}^{S,B}$ appear as pairs in a saddle-node bifurcation. States $\phi_{c,q}^S$ lie on the separatrix, states $\phi_{c,q}^B$ lie in the basin of attraction of ϕ_I . The separatrix is a high-dimensional manifold that cannot be easily represented. The path is obtained with the string method, and the action is computed along each path to check that it is indeed 0 along a relaxation path.

and for $\lambda \neq 0$ we instead solve:

$$\ddot{z} = \alpha e^{2\alpha z} K + \frac{g'(z)}{2} \quad (12)$$

$$= \alpha e^{2\alpha z} K - \frac{3 + 6\alpha z + \alpha^2(6z^2 - 2)}{4\alpha^3\nu}, \quad (13)$$

where $K = -g(z_0)e^{-2\alpha z_0}$ is obtained from (10) considering the initial conditions $(z(0), \dot{z}(0)) = (z_0, 0)$.

The orbits are closed and $z(t)$ evolves between the maximum and the minimum root of $-V'(X) = X^3 - X + \mu_0$. This notably constrains $|\mu_0| < 2\sqrt{3}/9$ for $V'(X)$ to display 3 real roots. Denoting r_1, r_2, r_3 (with $r_1 < r_2 < r_3$) the roots of $V'(X)$, we initialize the dynamics close r_3 , for instance $(z(0), \dot{z}(0)) = (r_3 - \delta, 0)$, with $\delta \ll 1$. We run the symplectic scheme and compute the distance between the position at time 1 and the position at time 0, $|z(1) - z(0)| \equiv \xi$. The parameter δ is varied until we obtain $\xi < 10^{-8}$, which is our criterion to obtain periodic orbits. Note that for given (ν, α, μ_0) , there may be several values $\delta_1 < \delta_2 < \dots < \delta_q$ each leading to different periodic orbits $\phi_{c,1}, \phi_{c,2}, \dots, \phi_{c,q}$, that each display a different number q of bumps. The symplectic scheme is implemented with $\Delta t = 10^{-4}$, such that the number of points on the orbit is 10^4 . For each acceptable periodic orbit, we compute $\int_0^1 z(t) dt \equiv \bar{z}_q(\nu, \alpha, \mu_0)$ where the index q indicates the number of periods on the domain $[0, 1]$. The equation

$$\phi_0 - \bar{z}_q(\nu, \alpha, \mu_0) = 0, \quad (14)$$

where μ_0 is the unknown, has always 0, 1 or 2 solutions. When no solution exists, it means that no critical states with a given number q of bumps are accessible. When two solutions exist for μ_0 , it means that two periodic orbits of mass ϕ_0 can be found for given (ν, α) . These two orbits correspond to two critical states (see e.g. Fig. 2 in main text), one state sitting on the separatrix between ϕ_I and ϕ_H , and the other lying strictly in the basin of attraction of ϕ_I (see Fig. 1 in Appendix, and see main text). When (14) has one solution only, then there is a unique critical orbit of q bumps and mass ϕ_0 accessible. This critical state is denoted $\phi_{c,q}^*$ in the main text. Going from zero to two solutions in (14) corresponds to a saddle-node bifurcation. For fixed density ϕ_0 , the manifolds on which the saddle-node bifurcations occur for a given q are displayed in Fig. 2c in the main text.

II. DETAILS ON THE GMAM IMPLEMENTATION

In this section we detail the numerical algorithm based on the classic gMAM [4] that we run to obtain the minimum action path. Before running the gMAM, we first run the string method detailed in [5]. The starting point of the string method is to consider a path $\{\varphi_i\}$ made of N successive states interpolating between ϕ_H and ϕ_I . We set $\varphi_1 = \phi_H(x) \equiv \phi_0$ and $\varphi_N = \phi_I(x)$,

but since $\phi_I(x)$ is not known analytically, it is obtained from the noiseless evolution of ϕ , starting from any state in the basin of attraction of ϕ_I . To solve the evolution equation of $\phi(x, t)$, space is discretized on a 1-d domain with periodic boundary conditions. We use a semi-implicit and pseudo-spectral scheme: the $\partial_x^4 \phi$ term is treated implicitly in time in Fourier space and all the other terms are treated explicitly in time in real space.

Now, at each iteration of the string method, we perform two steps: (i) for all $i \in \{1, \dots, N\}$, the states φ_i along the path perform a relaxation step using our semi-implicit scheme; (ii) after the relaxation step, a new path with regularly spaced states replaces the former path. The states along the new path are obtained by interpolation and arclength renormalization. This step prevents the states to collapse onto ϕ_I or ϕ_H , as they would do if only the relaxation was implemented. The endpoints of the string, φ_1 and φ_N , are left free and keep undergoing pure relaxation evolution to ensure that the two fixed points ϕ_I and ϕ_H are indeed dynamically stable. At the end of the string algorithm, one obtains the heteroclinic orbit joining ϕ_I to ϕ_H and going through an unstable fixed point of Morse index 1. The heteroclinic orbit (or relaxation path) is then a good candidate for the instanton (since it is indeed the instanton in equilibrium).

We then run the gMAM algorithm with the string as a starting point. The geometric implementation allows for reaching reaction paths of infinite duration. We follow a hybrid implementation of the gMAM, using both the Lagrangian formulation [4, 6] and the Hamiltonian formulation to update the Lagrange multiplier [7]. We recall that in the presence of a conserved Gaussian white noise, the action we consider reads

$$S_T = \int_0^T \|\partial_t \phi - F_{\text{AMB}}(\phi)\|_{-1}^2 dt, \quad (15)$$

with the flow of the active Model B given by $F_{\text{AMB}}(\phi) = \partial_x^2(-\nu \partial_x^2 \phi + \phi^3 - \phi + \lambda(\partial_x \phi)^2)$, and where the norm $\|\cdot\|_{-1}$ is defined from a scalar product $\langle \cdot, \cdot \rangle_{-1}$ on any spatial domain Ω :

$$\langle u, v \rangle_{-1} = \int_{\Omega} u(-\Delta^{-1}v), \quad (16)$$

with $\Delta^{-1} \equiv \partial_x^{-2}$ the inverse Laplacian. The minimum action method performs a gradient descent on the action S_T to obtain the instantons. Introducing an artificial time τ to evolve the path $\{\phi(t, x)\}_{t \in [0, T]}$, one solves numerically (see Ref. [6])

$$\partial_{\tau} \phi(t, x; \tau) = -\frac{\delta S_T}{\delta \phi(t, x)}. \quad (17)$$

When ϕ eventually solves $\frac{\delta S_T}{\delta \phi} = 0$, the Euler-Lagrange equation is satisfied and $\{\phi(t, x)\}_{t \in [0, T]}$ is the instanton. For convenience, we work with θ , the conjugate field of ϕ in the Hamiltonian formulation, which solves the Hamilton equations of motion for the instanton. Here the Hamiltonian explicitly reads

$$H(\phi, \theta) = \int_{\Omega} \left[F_{\text{AMB}}(\phi)\theta + \frac{1}{2}(\partial_x \theta)^2 \right] dx, \quad (18)$$

and the instanton solves (in addition to the boundary conditions at $t = 0, T$)

$$\begin{cases} \partial_t \theta = -\partial_{\phi} H(\phi, \theta) \\ \partial_t \phi = \partial_{\theta} H(\phi, \theta). \end{cases} \quad (19)$$

or, explicitly for the second equation,

$$\partial_t \phi = F_{\text{AMB}}(\phi) - \partial_x^2 \theta. \quad (20)$$

The gradient descent (17) amounts to solving

$$\partial_{\tau} \phi = \partial_t \theta + \frac{\delta H}{\delta \phi}. \quad (21)$$

Using the explicit formula for θ from (20), namely

$$\theta = -\Delta^{-1}(\partial_t \phi - F_{\text{AMB}}(\phi)), \quad (22)$$

and using

$$\frac{\delta H}{\delta \phi} = \left\langle \frac{\delta F_{\text{AMB}}(\phi)}{\delta \phi}, \partial_t \phi - F_{\text{AMB}}(\phi) \right\rangle_{-1}, \quad (23)$$

Algorithm 1 : Geometric Minimum Action Method, pseudo-spectral and semi-implicit scheme

- 1: **Inputs:** $N \in \mathbb{N}$; two stable fixed points ϕ_a and ϕ_b of the noiseless dynamics; a path $\{\hat{\phi}_i^0\}_{i \in I}$ and $I = \{1, \dots, N\}$, with $\hat{\phi}_0^0 = \phi_a$ and $\hat{\phi}_M^0 = \phi_b$, such that $|\hat{\phi}_{i+1}^0 - \hat{\phi}_i^0|$ is constant in i ; the functions $F_{\text{AMB}}(\phi)$, $\gamma(\phi, \theta)$; $\Delta\tau > 0$,
- 2: **Initialization:** For every $i \in I$, take $\hat{\theta}_i^0 = 0$; set $\Delta s = 1/N$.
- 3: **for** $n \geq 0$ **do**
- 4: Compute $F_{\text{AMB}}(\phi^n)$ in real space.
- 5: Compute $\gamma^n = \gamma(\hat{\phi}^n, \hat{\theta}^n)$.
- 6: Compute the Fourier transform $\mathcal{F}_k(F_{\text{AMB}})$.
- 7: Compute in Fourier space $\bar{\theta}_{i,k}^n$:

$$\bar{\theta}_{i,k}^n = k^{-2} \mathcal{F}_k \left(\gamma^n \frac{\hat{\phi}_{i+1}^n - \hat{\phi}_i^n}{\Delta\tau} - F_{\text{AMB}}(\phi^n) \right)$$

- 8: Update ϕ with the semi-implicit Thomas algorithm, namely, solve $\bar{\phi}^{n+1}$

$$\begin{aligned} \frac{\bar{\phi}_{i,k}^{n+1} - \bar{\phi}_{i,k}^n}{\Delta\tau} = & k^{-2} (\gamma_i^n)^2 \frac{\bar{\phi}_{i+1,k}^{n+1} + \bar{\phi}_{i-1,k}^{n+1} - 2\bar{\phi}_{i,k}^{n+1}}{(\Delta\tau)^2} + k^{-2} \gamma_i^n \gamma_i^{n'} \bar{\phi}_i^{n'} + k^{-2} \gamma_i^n \mathcal{F}_k [F_{\text{AMB}}(\phi^n)]'_i \\ & + \mathcal{F}_k \left(\left\langle \frac{\delta F_{\text{AMB}}(\hat{\phi}^n)}{\delta \hat{\phi}^n}, \gamma_i^n \hat{\phi}_i^{n'} \right\rangle_{-1} \right) - \mathcal{F}_k \left(\left[\left\langle \frac{\delta F_{\text{AMB}}(\hat{\phi}^n)}{\delta \hat{\phi}^n}, F_{\text{AMB}}(\hat{\phi}^n) \right\rangle_{-1} \right]_i \right). \end{aligned}$$

For the arclength derivative of a function g , we take $g'_i = (g_{i+1} - g_i)/(\Delta s)$ for $i \in [1, N-1]$, and $g'_M = (g_N - g_{N-1})/(\Delta s)$ for the endpoint.

- 9: Compute the inverse Fourier transform of $(\bar{\phi}^{n+1}, \bar{\theta}^n) = (\mathcal{F}_k^{-1} \bar{\phi}_k^n, \mathcal{F}_k^{-1} \bar{\theta}_k^n)$.
 - 10: Interpolate $\{(\bar{\phi}_i^{n+1}, \bar{\theta}_i^{n+1})\}_{i \in I}$ onto a path $\{(\hat{\phi}_i^{n+1}, \hat{\theta}_i^{n+1})\}_{i \in I}$ such that $|\hat{\phi}_{i+1}^{n+1} - \hat{\phi}_i^{n+1}|$ is constant in i , as in the string method.
-

one obtains

$$\begin{aligned} \partial_\tau \phi = & -\Delta^{-1} \partial_t^2 \phi + \partial_t \Delta^{-1} F_{\text{AMB}}(\phi) + \left\langle \frac{\delta F_{\text{AMB}}(\phi)}{\delta \phi}, \partial_t \phi \right\rangle_{-1} \\ & - \left\langle \frac{\delta F_{\text{AMB}}(\phi)}{\delta \phi}, F_{\text{AMB}}(\phi) \right\rangle_{-1}. \end{aligned} \quad (24)$$

This equation can be solved with a pseudo-spectral method since the operator $-\Delta^{-1}$ is diagonal in Fourier space. The relaxation along t contains a diffusion term that can be treated implicitly by means of a Thomas algorithm [4, 6]. In addition, the flow $F_{\text{AMB}}(\phi)$ can further decomposed into the

$$F_{\text{AMB}}(\phi) = -\nu \Delta^2 \phi + \mathcal{K} \phi, \quad (25)$$

with $\mathcal{K} \phi = \partial_x^2 (\phi^3 - \phi + \lambda (\partial_x \phi)^2)$, such that the relaxation of the field in x can also be treated implicitly in τ when diagonalizing the operator Δ^2 . Without this decomposition, the Courant–Friedrichs–Lewy condition for the scheme to be stable is extremely restrictive.

Finally, we use arclength parametrization of the path such that time t is a function of arclength $s \in [0, 1]$, and instantons between fixed points that require $t \rightarrow \infty$ can then be computed. In particular, we now have $\partial_t \phi(t) = (dt/ds)^{-1} \partial_s \hat{\phi}(s) \equiv \gamma(s) \hat{\phi}'$, and $\partial_t \theta(t) = (dt/ds)^{-1} \partial_s \hat{\theta}(s) \equiv \gamma(s) \hat{\theta}'$, where the $'$ denotes the derivative w.r.t arclength s . The function $\gamma(s)$ is also a Lagrange multiplier enforcing $H = 0$ along the instanton [4]. The geometric minimization now reads

$$\begin{aligned} \partial_\tau \hat{\phi} = & -\Delta^{-1} \gamma^2 \partial_s^2 \hat{\phi} - \Delta^{-1} \gamma \gamma' \partial_s \hat{\phi} + \gamma \partial_s \Delta^{-1} F_{\text{AMB}}(\hat{\phi}) \\ & + \left\langle \frac{\delta F_{\text{AMB}}(\hat{\phi})}{\delta \hat{\phi}}, \gamma \partial_s \hat{\phi} \right\rangle_{-1} - \left\langle \frac{\delta F_{\text{AMB}}(\hat{\phi})}{\delta \hat{\phi}}, F_{\text{AMB}}(\hat{\phi}) \right\rangle_{-1}. \end{aligned} \quad (26)$$

Note that $\gamma(s)$ is numerically computed using [7]:

$$\gamma = \frac{|\langle \partial_\theta H, \partial_s \hat{\phi} \rangle| + \sqrt{\max(0, \langle \partial_\theta H, \partial_s \hat{\phi} \rangle^2 - 4H |\partial_s \hat{\phi}|^2)}}{2|\partial_s \hat{\phi}|^2}. \quad (27)$$

The complete algorithm is summarized in Algorithm 1. It is worth mentioning that the equation, already in 1d, is very ill-conditioned, and forces us to take a fine grid, which in turn leads to very long computation times. Typically, for physical parameters $L = 1$, $\nu = 5 \times 10^{-4}$, $\alpha = 2$, $\phi_0 = 0.65$, one must take $N_x = 256$ space grid points, $N_s = 400$ arclength grid, and $\Delta\tau = 10^{-6}$ to reach the minimum action path in a typical computation time of $\simeq 3$ weeks on a 2.8GHz machine.

III. DEEP GMAM METHOD: COMPUTING REACTION PATHS USING NEURAL NETWORKS

Here we detail the deep gMAM algorithm [8]. This method differs from the classical gMAM algorithm in two significant ways. Firstly, instead of decomposing the path into ad-hoc space-time bases (e.g., pseudo-spectral decomposition, finite differences method, etc...), the reaction path is parametrized in both space and time by a neural network. Secondly, it directly tackles the geometric action as the cost functional to minimize, as opposed to finding the zeros of the Euler-Lagrange equation. There are several advantages to this approach. The remarkable expressivity of neural networks and their ability to overcome the curse of dimensionality enable the consideration of higher dimensional problems. Furthermore, the method determines its own parametrization rather than relying on a rigid constant arclength constraint. This method also offers high flexibility, providing multiple approaches to address the minimization problem and construct ad-hoc surrogate/ansatz for the reaction path. However, there are some drawbacks. Tuning of the hyperparameters is often necessary, and the precision may be degraded compared to classical methods, particularly when dealing with ill-conditioned problems.

Below is a detailed description of the algorithm used to obtain the various reaction paths and action values in Figures 1, 3 and 4 in the main text. Let d be the spatial dimension, where $d = 1$ or $d = 2$ for Figure 4. We define $u : (s, \mathbf{x}) \in (0, 1) \times (0, 1)^d \mapsto u(s, \mathbf{x})$ some reaction path such that $u(0, \mathbf{x}) = a(\mathbf{x})$ and $u(1, \mathbf{x}) = b(\mathbf{x})$, where a, b are two given fields, for instance $a = \phi_I$ (inhomogeneous state) and $b = \phi_H$ (homogeneous state).

To minimize the AMB geometric action, four important constraints must be taken into account:

1. It is a boundary-value problem;
2. The mass of the solution ϕ_0 must be conserved along the reaction path, namely $\langle u \rangle \equiv \int_{\Omega} u(s, \mathbf{x}) d\mathbf{x} = \phi_0$ for all $s \in (0, 1)$;
3. The noise conservation (see the term $\partial_x \xi$ in Eq.(5)) implies that one must work with respect to the H^{-1} norm;
4. The periodic boundary conditions must also be satisfied.

As shown below, it is possible to formulate the problem in a way that eliminates three of these constraints, leaving only the noise conservation constraint. This remaining constraint must be explicitly enforced through penalization.

We need to find the minimizers of the geometric action:

$$\mathcal{A}_g[u] = \int_0^1 (\|\dot{u}\|_{-1} \|F(u)\|_{-1} - \langle \dot{u}, F(u) \rangle_{-1}) ds,$$

where $\langle u, v \rangle_{-1} \equiv \langle u, -\Delta^{-1}v \rangle$, $\dot{u} = du/ds$, and $F(u) = -\Delta F_{\text{aGL}}(u)$, with $F_{\text{aGL}}(u) = \nu\Delta u + u - u^3 - \lambda|\nabla u|^2$, the flow of the active Ginzburg-Landau dynamics. The problem can be reformulated as:

$$\mathcal{A}_g[u] = \int_0^1 (\|\nabla v\| \|\nabla F_{\text{aGL}}\| - \langle \nabla v, \nabla F_{\text{aGL}} \rangle) ds$$

with the constraint

$$-\Delta v = \dot{u}.$$

We now consider a neural network parameterization for u . We use the simplest fully connected architecture given by $\mathcal{N}_u(s, \mathbf{x}; \mathcal{T}) = \mathcal{N}_{D+1} \circ \mathcal{N}_D \cdots \mathcal{N}_1 \circ \mathcal{N}_0(s, \mathbf{x})$, where $\mathcal{N}_k(\mathbf{y}) = \sigma_k(W_k \mathbf{y} + \mathbf{b}_k)$ for $k = 0, \dots, D+1$. Here, \mathcal{T} is the set of the NN parameters weights/bias $\{W_k, \mathbf{b}_k\}$, σ_k are the activation functions, and D is often called the depth or number of hidden layers. In our setting, we use swish activation function with $\text{swish}(x) = x/(1 + e^{-x})$ for all $k < D+1$ and a linear output for the last layer $k = D+1$. The matrices W_k have size $c \times c$ for all $k = 1, \dots, D$, W_0 has size $c \times d+1$, and the last output layer has size $1 \times c$, where c is the number of neurons per layer, often called capacity. A naive approach would be to directly substitute u with its neural network representation, denoted as \mathcal{N}_u . However, this would necessitate penalizing the remaining constraints. Instead, we adopt the following ansatz:

$$\begin{aligned} \mathcal{U}(s, \mathbf{x}) = & (1-s)a(\mathbf{x}) + sb(\mathbf{x}) \\ & + s(1-s)(\mathcal{N}_{u,\text{per}}(s, \boldsymbol{\varphi}) - \langle \mathcal{N}_{u,\text{per}} \rangle), \end{aligned} \quad (28)$$

with

$$\boldsymbol{\varphi}(\mathbf{x}) \equiv (\cos 2\pi\mathbf{x}, \sin 2\pi\mathbf{x}). \quad (29)$$

It is easy to check that $\mathcal{U}(0, \mathbf{x}) = a(\mathbf{x})$, $\mathcal{U}(1, \mathbf{x}) = b(\mathbf{x})$. Moreover, we have $\langle \mathcal{U} \rangle = (1-s)\langle a \rangle + s\langle b \rangle + 0 = \phi_0$ since $\langle a \rangle = \langle b \rangle = \phi_0$ by hypothesis. Finally, it is periodic on the domain $(0, 1)^d$. In fact, $\mathcal{N}_{u,\text{per}}$ depends nonlinearly on $\boldsymbol{\varphi}$, so that adding higher harmonics in the input is unnecessary. Note that the input dimension has increased from $1+d$ to $1+2d$. The term $\langle \mathcal{N}_{u,\text{per}} \rangle$ is numerically approximated on a Gauss-Legendre grid $\{\omega_k, \mathbf{x}_k\}$:

$$\langle \mathcal{N}_{u,\text{per}} \rangle \approx \sum_{k=1}^{N_g} \omega_k \mathcal{N}_{u,\text{per}}(s, \boldsymbol{\varphi}).$$

The noise constraint imposes the need for another periodic NN to represent the function v , namely we use the ansatz

$$\mathcal{V}(s, \mathbf{x}) = \mathcal{N}_{v,\text{per}}(s, \boldsymbol{\varphi}),$$

and minimize the residual $\|\Delta\mathcal{V} + \dot{\mathcal{U}}\|$ for all s . Due to the ill-conditioned nature of the problem, it is beneficial to replace both $\mathcal{N}_{u,\text{per}}$ and $\mathcal{N}_{v,\text{per}}$ with more expressive neural network terms. Specifically, each of these periodic NNs is replaced by a sum of K independent NNs with rescaled inputs. For example, the periodic NN for u is given by

$$\mathcal{N}_{u,\text{per}}(s, \boldsymbol{\varphi}) = \sum_{k=0}^{K-1} \mathcal{N}_k(4^k(s, \boldsymbol{\varphi})),$$

where each \mathcal{N}_k represents an independent neural network. This replacement enables the high-frequency terms to be learned more quickly (see e.g. [9]). We set $K = 4$ in practice.

The final cost functional that we aim to minimize is given by

$$\begin{aligned} \mathcal{C}[\mathcal{U}, \mathcal{V}] = & \mathcal{A}_g[\mathcal{U}] + \gamma_v \int_0^1 \|\Delta\mathcal{V} + \dot{\mathcal{U}}\|^2 ds + \\ & \gamma_{\text{arc}} \left(\int_0^1 \|\dot{\mathcal{U}}\|^2 ds - \left(\int_0^1 \|\dot{\mathcal{U}}\| ds \right)^2 \right), \end{aligned}$$

where γ_v and γ_{arc} are penalty coefficients. We use a small penalty coefficient $\gamma_{\text{arc}} \ll 1$ so that constant arclength parametrization is favored but not strictly enforced. On the other hand, γ_v must be chosen to be large enough. In practice, we use $\gamma_v = O(10)$ initially and increase it to $O(100)$ towards the end of the simulations.

Once the cost functional is written, the minimization follows classical machine learning techniques. We use here Monte-Carlo batches by sampling uniformly $(s, \mathbf{x}) \sim U([0, 1]) \times U([0, 1]^d)$. We call N_s the number of points for s and $N_{\mathbf{x}}$ for the variable \mathbf{x} . One must then compute the gradients of the cost functional w.r.t. the NNs parameters $\nabla_{\mathcal{T}_u, \mathcal{T}_v} \mathcal{C}[\mathcal{U}, \mathcal{V}](s_i, x_i), i = 1, \dots, N_s \times N_{\mathbf{x}}$ and use a gradient descent approach (here, ADAM method [10]). The parameters used for Fig. 4 are $c = 15$, $D = 15$, $K = 4$, $N_s = 40$, $N_{\mathbf{x}} = 120$, $N_g = 30^2$ with swish activation function and learning rate $\eta = 10^{-3}$ which is decreased to 10^{-4} at the end of the simulation. The penalization coefficients are $\gamma_v = 10$, $\gamma_{\text{arc}} = 10^{-2}$ and γ_v is increased to 100 at the end of the simulation giving a L^2 residual for the Poisson constraint $\approx 10^{-3}$. The physical parameters are $\phi_0 = 0.65$, $L = 44.7\nu^{1/2}$, and $\lambda = 2\nu$. We also illustrate the efficiency of the method by displaying an asymmetric path located above the (*) symbol in Figure 3 of the main text, it is shown in Fig. 2. Such asymmetric configurations are always observed when the reaction path exhibits an even number of bumps (here, 2 bumps in Fig. 2). They have lower action values than their symmetric versions suggesting that the breaking of the symmetry $x \rightarrow -x$ facilitates transitions.

IV. COMPUTATION OF AMB CRITICAL POINTS BY NEURAL NETWORKS IN DIMENSION $d \geq 2$

The computation of the inhomogeneous state ϕ_I is a prerequisite in the previous section. Additionally, it is often of interest to investigate the reaction paths that connect ϕ_I to some critical points, i.e., the ending state b is a chosen critical point that satisfies

$$\nabla F_{\text{aGL}}(u) = 0. \quad (30)$$

In two dimensions, the one-dimensional techniques discussed above do not hold anymore, and one must solve Eq. (30) directly. One expects to have not just one but many solutions as $\nu \rightarrow 0$. As in the previous section, two constraints are present: the

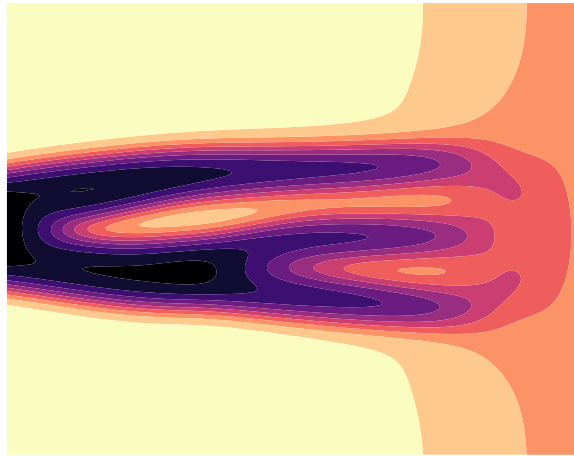


FIG. 2. Asymmetric instanton for $\phi_0 = 0.65$, $L = 50\nu^{1/2}$ and $\alpha = 2$ with lower action value ≈ 0.0215 compared to its symmetric counterpart with action value ≈ 0.0235 ($L = 1$).

periodic constraint and the mass constraint $\langle u \rangle = \phi_0$. A convenient NN ansatz that replaces u and satisfies both constraints is given by

$$\mathcal{U}(\mathbf{x}) = f(\mathbf{x}) - \langle f \rangle + \mathcal{N}_u(\boldsymbol{\varphi}) - \langle \mathcal{N}_u \rangle + \phi_0,$$

where f is chosen to initialize the gradient descent properly since at the beginning of the descent, \mathcal{N}_u is typically small, so that $\mathcal{U} \approx f - \langle f \rangle + \phi_0$. One then minimizes the cost functional

$$\mathcal{C}[\mathcal{U}] = \|\nabla F_{\text{aGL}}\|^2. \quad (31)$$

We show below that the critical points obtained are spikes [11] constrained by C_n (or product of) discrete rotation symmetries. In order to compute these critical points, we choose $f(x)$ as a sum of exponentials: $f(x) = c_0 - c_1 \sum_{k=1}^n e^{-\gamma \|\mathbf{x} - \mathbf{x}_k\|^2}$ where \mathbf{x}_k are chosen arbitrarily and c_0, c_1 are constants so that $\langle f \rangle = \phi_0$. Due to the torus geometry, purely radial solutions cannot

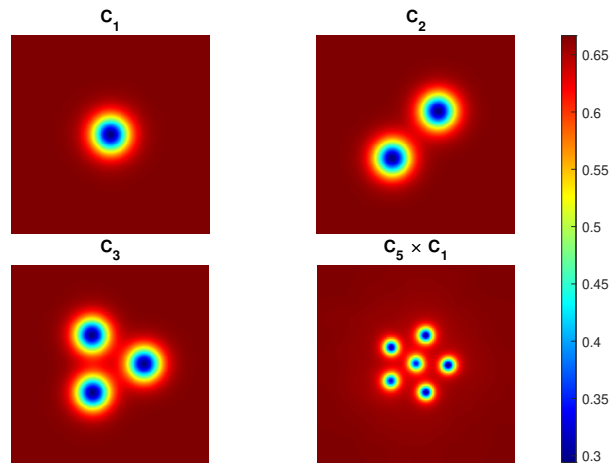


FIG. 3. Various spikes (critical solutions) obtained by minimizing (31) by deep neural networks and for $\phi_0 = 0.65$, $L = 44.7\nu^{1/2}$ and $\lambda = 2\nu$. The last one is for $L = 100\nu^{1/2}$.

exist. However, since solutions are exponentially damped away from the inhomogeneities, radial structures are often observed. An example is the stable inhomogeneous state (see first snapshot of Fig. 4 in the main text). We have checked that this state is always obtained by direct simulations of the deterministic equation starting from various initial conditions (not shown). At this stage, it is unclear whether annular-like critical points with Morse index ≥ 1 do exist or not. We show a typical scenario in Fig. 4 where one is able to identify a pair of radial solutions but which do not seem to be some zeros of ∇F_{aGL} and saturate to a finite but small value of the residual no matter the NN size and hyperparameter changes.

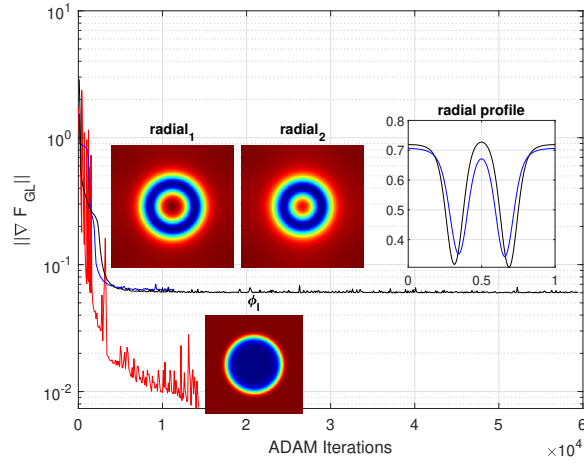


FIG. 4. An example of radial solutions which behave as pseudo-critical points for $\phi_0 = 0.65$, $L = 44.7\nu^{1/2}$ and $\lambda = 2\nu$. The inhomogeneous state is shown for comparison. *to be updated.*

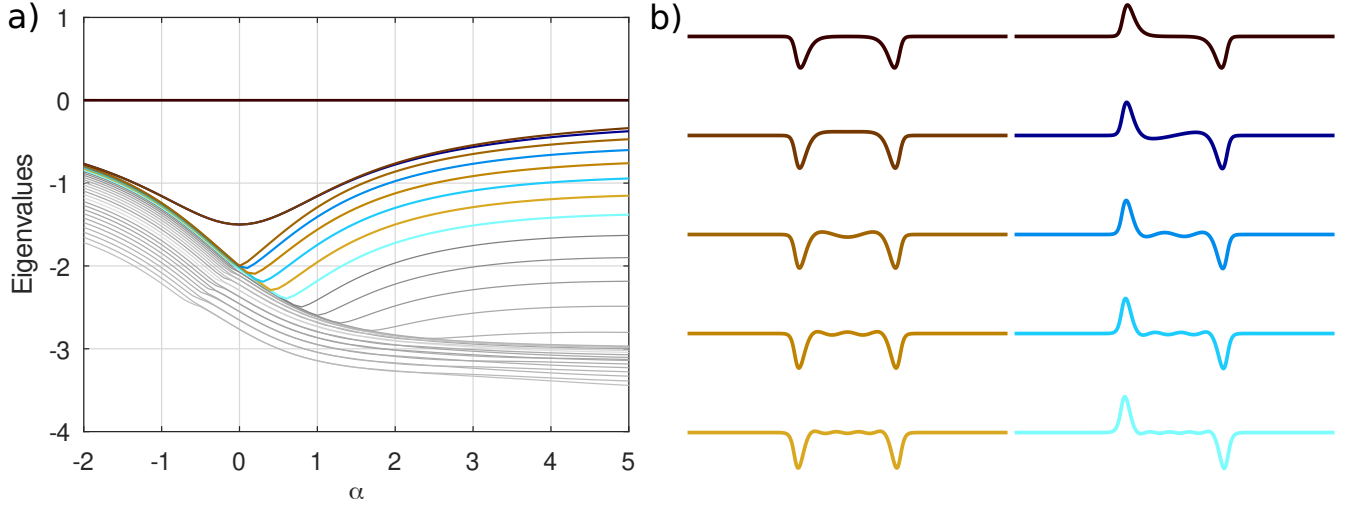


FIG. 5. Leading spectrum of \mathcal{A} as a function of $\alpha \in (-2, 5)$ for $\nu = 10^{-4}$ and $\phi_0 = 0.65$. The 29 first eigenvalues are displayed on the left, the corresponding leading 10 eigenvectors (in color) are displayed on the right. The more the eigenvalue is negative, the more its eigenvector display bumps. The eigenvectors to the right are computed for $\alpha = 5$ with eigenvalues (1, 2) : $\sigma = (0, 0)$, (3, 4) : $\sigma = (-0.33, -0.37)$, (5, 6) : $\sigma = (-0.47, -0.60)$, (7, 8) : $\sigma = (-0.75, -0.94)$, (9, 10) : $\sigma = (-1.15, -1.38)$.

V. LINEAR STABILITY ANALYSIS

We discuss here the stability of the inhomogeneous state ϕ_I in 1-d as a function of the active term intensity. We consider here the spectral stability of ϕ_I giving the following eigenvalue problem:

$$\mathcal{M}\phi \equiv -\mathcal{A}''\phi = \sigma\phi \quad (32)$$

with $\mathcal{A}\phi = \nu\phi'' + (1 - 3\phi_I^2)\phi - 2\lambda\phi_I'\phi'$ and where u' means du/dx . A first remark is that one can show that there is always two neutral modes denoted ϕ_1, ϕ_2 for the operator \mathcal{M} . By remarking that neutral modes for \mathcal{A} are necessary neutral for \mathcal{M} we observe that $\mathcal{A}\phi = 0$ has the nontrivial solution

$$\phi_1 = \phi_I'.$$

This is a direct consequence of ϕ_I solving $\nabla F_{\text{aGL}} = 0$. The other solution can be obtained using e.g. the Wronskian $W = \phi_1\phi_2' - \phi_2\phi_1'$ which gives $W = Ce^{2\alpha\phi_I}$. These neutral modes have a simple interpretation and correspond to Goldstone modes for the mass conservation and invariance by translation.

We proceed to calculate the leading spectrum of \mathcal{L} as a function of the intensity α of the active term. The results are presented in Figure 5a, which shows the eigenvalues, and Figure 5b, which displays the corresponding eigenvectors. Our analysis reveals the emergence of "microstructures" or "bumps" at different wavenumbers, localized on the negative plateau of the ground state ϕ_I . As α increases, higher wavenumber modes begin to activate from the background spectrum at specific values of α . We also note that high wavenumber modes are more stable than small wavenumber modes. There is a well-defined spectral gap visible in Fig. 5a (blue curve) with corresponding eigenmodes 3 and 4 in Fig. 5b. This spectral gap decreases as α approaches infinity.

Our results help to explain why microstructures are observed in the minimum action paths. Although the inhomogeneous state is stable, noise excitations would tend to involve some of these modes. However, it is not clear why higher wavenumber bumps are preferred for the minimum action paths. Direct gMAM computations are necessary to reveal this behavior. Specifically, for this value of ν , we would expect the one-bump regime to be involved in the minimum action paths, but this is not what is observed.

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