Supporting Information

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SI Text

Numerical Methods. The softened Fredrickson–Andersen (sFA) model is simulated by a continuous-time Monte Carlo method (1). To efficiently sample trajectories within the s ensemble, we use transition path sampling (TPS) (2). Starting from an equilibrated initial condition, we simulate a trajectory of length t_{obs}, storing the configuration of the system at a set of equally spaced times. We then generate new trajectories using "half-shooting" and "shifting" TPS moves (2), starting from the stored configurations.

To sample the equilibrium ensemble of trajectories, we accept all trajectories generated in this way: This corresponds to an unbiased random walk in trajectory space. To sample the symmetrized s ensemble, we use a Metropolis-like criterion for acceptance or rejection of the trial TPS move. For each trajectory, we calculate the quantity

$$\mathscr{E} = sK - g[\mathcal{N}(0) + \mathcal{N}(t_{\mathrm{obs}})], \quad \textbf{[S1]}$$

where K is the number of configuration changes in the trajectory, $\mathcal{N}(t) = \sum_{i=1}^{N} n_i(t)$ is the number of excited sites in the system at time t, and the fields s and g depend on the ensemble being sampled, as described in the main text. (An expression for g is given in Eq. **S22** below.) We then compare the value of $\mathscr{E}$ for the original (old) trajectory and for the new trajectory generated by TPS. We accept the new (trial) trajectory with a probability $P^0_{\mathrm{acc}} = \min\{1, \exp[\mathscr{E}_{\mathrm{old}} - \mathscr{E}_{\mathrm{trial}}]\}$. Generalizing the results of refs. 2 and 3, it can be shown that these rules respect detailed balance in the space of trajectories, according to the distribution $P_s[x(t)]$. Thus, after repeating many such moves, the algorithm generates trajectories according to this distribution.

Theoretical Analysis. In this section, we outline the theoretical analysis that underlies the work presented in the main article. We state only the main results, referring to textbooks and reviews for standard results and deferring a more detailed physical discussion of the various mappings to a later work.

Definitions of operators. The master equation of the sFA model takes the standard form

$$\partial_t P(\mathscr{C},t) = -r(\mathscr{C})P(\mathscr{C},t) + \sum_{\mathscr{C}'} W(\mathscr{C}' \to \mathscr{C})P(\mathscr{C}',t), \quad \textbf{[S2]}$$

where $P(\mathscr{C},t)$ is the probability that the system is in some configuration $\mathscr{C}$ at time t, the $W(\mathscr{C}' \to \mathscr{C})$ are the rates for transitions between configurations, and $r(\mathscr{C}) = \sum_{\mathscr{C}'} W(\mathscr{C} \to \mathscr{C}')$.

We use a spin-half representation of the master equation of the sFA model (4). A configuration of the system is specified by the spin variables n_i with $i = 1,\ldots,N$. We represent the $\{n_i\}$ by N quantum spins, and we denote the state with all spins down ($n_i = 0$) by $|\Omega\rangle$. Then, if $\sigma_i^{x,y,z}$ are Pauli matrices associated with the sites, and $\sigma_i^{\pm} = \frac{1}{2}(\sigma_i^x \pm \sigma_i^y)$ as usual, then $\sigma_i^-|\Omega\rangle = 0$ by construction of $|\Omega\rangle$, whereas a configuration of the sFA model is represented by

$$|\{n_i\}\rangle = \prod_{i=1}^{N} (\sigma_i^+)^{n_i}|\Omega\rangle. \quad \textbf{[S3]}$$

We construct a ket state

$$|P(t)\rangle = \sum_{\mathscr{C}} P(\mathscr{C},t)|\mathscr{C}\rangle, \quad \textbf{[S4]}$$

where the sum runs over all configurations of the system. Then, the master equation is

$$\frac{\partial}{\partial t}|P(t)\rangle = \mathbb{W}|P(t)\rangle \quad \textbf{[S5]}$$

with

$$\mathbb{W} = \sum_{\langle ij\rangle}\{(\hat{n}_j + \epsilon/2)[(1-\sigma_i^+)\sigma_i^- + \gamma(1-\sigma_i^-)\sigma_i^+] + D[\sigma_i^+\sigma_j^- - (1-\hat{n}_i)\hat{n}_j]\} + (i \leftrightarrow j), \quad \textbf{[S6]}$$

where the sum is over (distinct) pairs of nearest neighbors. We define $\hat{n}_j \equiv \sigma_j^+\sigma_j^-$, and the notation $(i \leftrightarrow j)$ indicates that the entire summand is to be symmetrized between sites i and j.

Operator representations of biased ensembles. To investigate the model within the s ensemble, we follow ref. 5 in writing $P(\mathscr{C},K,t)$ for the probability of being in configuration $\mathscr{C}$ at time t, having accumulated K configuration changes between times 0 and t. Then, we write $P(\mathscr{C},s,t) = \sum_K P(\mathscr{C},K,t)\mathrm{e}^{-sK}$ and consider the equation of motion for $|P(s,t)\rangle = \sum_{\mathscr{C}} P(\mathscr{C},s,t)|\mathscr{C}\rangle$, which is

$$\frac{\partial}{\partial t}|P(s,t)\rangle = \mathbb{W}(s)|P(s,t)\rangle \quad \textbf{[S7]}$$

with

$$\mathbb{W}(s) = \sum_{\langle ij\rangle}\{(\hat{n}_j + \epsilon/2)[(\mathrm{e}^{-s}-\sigma_i^+)\sigma_i^- + \gamma(\mathrm{e}^{-s}-\sigma_i^-)\sigma_i^+] + D[\mathrm{e}^{-s}\sigma_i^+\sigma_j^- - (1-\hat{n}_i)\hat{n}_j]\} + (i \leftrightarrow j). \quad \textbf{[S8]}$$

The dynamics of the sFA model respect detailed balance, with an energy function $E = J\sum_i n_i$ and $\gamma = \mathrm{e}^{-J/T}$, so we define an energy operator $\mathbb{E} = J\sum_i \hat{n}_i$. Then, it can be verified that

$$\mathbb{H}(s) \equiv \mathrm{e}^{\mathbb{E}/2T}\mathbb{W}(s)\mathrm{e}^{-\mathbb{E}/2T} = \sum_{\langle ij\rangle}\{(\hat{n}_j + \epsilon/2)[(\sqrt{\gamma}\mathrm{e}^{-s}-\sigma_i^+)\sigma_i^- + (\sqrt{\gamma}\mathrm{e}^{-s}-\gamma\sigma_i^-)\sigma_i^+] + D[\mathrm{e}^{-s}\sigma_i^+\sigma_j^- - (1-\hat{n}_i)\hat{n}_j]\} + (i \leftrightarrow j) \quad \textbf{[S9]}$$

is a Hermitian (symmetric) operator, i.e., $\langle\mathscr{C}|\mathbb{H}(s)|\mathscr{C}'\rangle = \langle\mathscr{C}'|\mathbb{H}(s)|\mathscr{C}\rangle$.

Writing $\mathbb{H}(s)$ in terms of the $\sigma^{x,y,z}$, we recover

$$\mathbb{H}(s) = -NC + \sum_i (h_x\sigma_i^x - h_z\sigma_i^z) + \sum_{\langle ij\rangle}\sum_{\mu\nu}\sigma_i^{\mu}M^{\mu\nu}\sigma_j^{\mu}, \quad \textbf{[S10]}$$

with

$$h_x = dz(1+\epsilon)\sqrt{\lambda}, \qquad h_z = d[2+\epsilon-\gamma\epsilon]/2, \quad \textbf{[S11]}$$

and

$$M = \frac{1}{2}\begin{pmatrix} zD & 0 & z\sqrt{\gamma} \\ 0 & zD & 0 \\ z\sqrt{\gamma} & 0 & D+\lambda-1 \end{pmatrix}. \quad \textbf{[S12]}$$

We use the shorthand notation $z = \mathrm{e}^{-s}$ for convenience.

Finally, we make a rotation of the spins, letting $R(\alpha) = \mathrm{e}^{\mathrm{i}\,\alpha\sum_j \sigma_j^y/2}$, so that

$$R(-\alpha)\begin{pmatrix}\sigma_i^x\\ \sigma_i^y\\ \sigma_i^z\end{pmatrix}R(\alpha) = \begin{pmatrix}\sigma_i^x\cos\alpha - \sigma_i^z\sin\alpha\\ \sigma_i^y\\ \sigma_i^z\cos\alpha + \sigma_i^x\sin\alpha\end{pmatrix}. \qquad \textbf{[S13]}$$

We choose

$$\tan 2\alpha = \frac{2z\sqrt{\gamma}}{1-\lambda-D(1-z)}, \qquad \textbf{[S14]}$$

so as to diagonalize M. That is

$$\mathbb{H}'(s) \equiv R(-\alpha)\mathbb{H}(s)R(\alpha) = -NC + \sum_i (B\sigma_i^x - h\sigma_i^z) + \sum_{\langle ij\rangle}\sum_\mu J_\mu \sigma_i^\mu \sigma_j^\mu, \qquad \textbf{[S15]}$$

where

$$B = h_x\cos\alpha - h_z\sin\alpha, \qquad h = h_z\cos\alpha + h_x\sin\alpha, \qquad \textbf{[S16]}$$

and $J_{x,y,z}$ are the eigenvalues of the matrix M.

Interpretation of $\mathbb{H}(s)$ and $\mathbb{H}'(s)$ as transfer matrices, and ensembles S and S'. In the main text, we discussed how singularities in the ground-state energy of $[-\mathbb{H}'(s)]$ may be interpreted as quantum phase transitions. Alternatively, one may interpret $\mathbb{H}(s)$ as a transfer matrix for a classical spin system in $(d+1)$ dimensions. This mapping between quantum and classical systems is now standard (S6), the only subtlety being that the classical system has discrete coordinates along the spatial axes of the relevant quantum system, but the extra $(d+1)$th dimension in the classical system is a continuous coordinate. This leads to a direct analogy between trajectories of the sFA model and configurations of the classical spin system in $(d+1)$ dimensions, on this slightly unusual anisotropic lattice.

The most natural approach is to discretize the time axis using a small time δt. Then, one may interpret the sequence of d-dimensional configurations at time $0, \delta t, 2\delta t, \ldots$ in the sFA model as "planes" in a $(d+1)$-dimensional classical spin model. This may be achieved by taking $\mathrm{e}^{\mathbb{H}(s)\delta t}$ as a classical transfer matrix. That is, $\langle \mathscr{C}|\mathrm{e}^{\mathbb{H}(s)\delta t}|\mathscr{C}'\rangle$ is proportional to the probability that the final plane of a system is in configuration $\mathscr{C}$, given that its penultimate plane is in configuration $\mathscr{C}'$. For constructing the ensemble S, one uses the σ^z components of the spins in $\mathscr{C}$ to give the states of the classical Ising spins, as in the sFA model.

However, for the ensemble S' formed from $\mathrm{e}^{\mathbb{H}'(s)\delta t}$, we make a different choice. We associate up (down) spins in S' with spins in $|\mathscr{C}\rangle$ that are aligned along the positive (negative) σ^x direction. This ensures that S' has the appropriate symmetries when the σ^x component of the spins in $\mathbb{H}'(s)$ are inverted. This means that the configurations of S' do not have a straightforward relation with the trajectories of the sFA model. However, one may always relate expectation values in the two ensembles by writing them as Dirac brackets, as discussed in *Construction of symmetrized s ensemble* below.

Finally, it is also important to consider the boundary conditions associated with ensemble S'. For the d spatial dimensions of the sFA model, we take periodic boundaries, corresponding to periodic boundaries in S'. However, for the $(d+1)$th dimension in S', the boundary conditions depend on the initial and final conditions for the s ensemble. These conditions are specified in turn by the initial condition of the unbiased ($s=0$, equilibrium) average $\langle\cdot\rangle_0$ used in the definition of the s ensemble. Consequences of these boundary conditions are discussed in *Construction of symmetrized s ensemble*, below

Order of limits of N and t_{obs}. As discussed in the main text, we consider trajectories where t_{obs} is very long, and we also consider systems where N is large. For example, the sFA model in one dimension maps to the two-dimensional Ising model, and in that case we must take a limit of large system size both parallel and perpendicular to the transfer direction in order to observe any phase transition.

When considering systems evolving in time, it is usual to take the limit of large system size N before any limit of large time t_{obs}. However, our theoretical analyses based on the space–time free energy $\psi(s)$ implicitly assume a limit of large t_{obs} before large N. Based on physical considerations, we expect these limits to commute but we have not verified this in our analysis.

Symmetries. Necessary condition for phase coexistence. An important special case for the sFA model occurs when $B=0$, since $\mathbb{H}'(s)$ is then invariant under $\sigma_i^x \to -\sigma_i^x$. As in the main text, we interpret $[-\mathbb{H}'(s)]$ as the Hamiltonian for a quantum spin system, and this symmetry may be spontaneously broken in the ground state, if J_x/h is sufficiently large. The condition $B=0$ occurs for $\tan\alpha = 2\sqrt{\lambda}z(1+\epsilon)/(2+\epsilon-\epsilon\gamma)$. Combining this condition for α with Eq. **S14**, one arrives at the condition for $B=0$:

$$\frac{1+\gamma}{1+\epsilon} = \sqrt{[1-\lambda-D(1-z)]^2 + 4z^2\gamma} - D(1-z). \qquad \textbf{[S17]}$$

This is consistent with Eq. **3** of the main text.

Construction of symmetrized s ensemble. We now motivate our definition of the symmetrized s ensemble as a tool for accurate characterization of space–time phase coexistence. For convenience, we consider the behavior of a one-time observable $F(t)$ in the s ensemble. If $F(t)$ has different expectation values in the two phases, one expects it to cross over sharply between these two values, as s is tuned through its coexistence value s^*. By casting the expectation of $F(t)$ as an observable in the thermodynamic ensemble S', we now explain why the symmetrized s ensemble is superior to the s ensemble for characterizing the behavior of $F(t)$ near space–time phase coexistence.

In the main text, we define s ensembles through their expectation values. The expectation value of $F(t)$ may be written in terms of Dirac brackets

$$\langle F(t)\rangle_s = \frac{\langle -|\mathrm{e}^{\mathbb{W}(s)(t_{\mathrm{obs}}-t)}\hat{F}\mathrm{e}^{\mathbb{W}(s)t}|\mathrm{eq}\rangle}{\langle -|\mathrm{e}^{\mathbb{W}(s)t_{\mathrm{obs}}}|\mathrm{eq}\rangle} \qquad \textbf{[S18]}$$

where $\hat{F}$ is the operator corresponding to the observable F, $\langle -| = \langle\Omega|R(-\pi/2)$ is a projection state, and $|\mathrm{eq}\rangle = R(2\chi)|\Omega\rangle$ is the equilibrium state, with $\tan\chi = \lambda$.

If we then use the similarity transform $\mathbb{H}'(s) = R(-\alpha)\,\mathrm{e}^{\mathbb{E}/2T}\mathbb{W}(s)\mathrm{e}^{-\mathbb{E}/2T}R(\alpha)$, we have

$$\langle F(t)\rangle_s = \frac{\langle\Psi|\mathrm{e}^{\mathbb{H}'(s)(t_{\mathrm{obs}}-t)}\hat{F}'\mathrm{e}^{\mathbb{H}'(s)t}|\Psi\rangle}{\langle\Psi|\mathrm{e}^{\mathbb{H}'(s)t_{\mathrm{obs}}}|\Psi\rangle} \qquad \textbf{[S19]}$$

with $|\Psi\rangle = R(2\theta-\alpha)|\Omega\rangle$ and $\langle\Psi|$ its Hermitian conjugate, with $\tan\theta = \sqrt{\gamma}$.

This equation may also be interpreted as a transfer matrix representation of an expectation value in ensemble S', which may be seen by writing the numerator of Eq. **S19** as

$$\sum_{\mathscr{C}_0\cdots\mathscr{C}_M} h(\mathscr{C}_M)\left[\prod_{i=m+1}^{M-1} U(\mathscr{C}_{i+1},\mathscr{C}_i)\right]U(\mathscr{C}_{m+1},\mathscr{C}_m)F'(\mathscr{C}_{m+1},\mathscr{C}_m) \times \left[\prod_{i=0}^{m-1} U(\mathscr{C}_{i+1},\mathscr{C}_i)\right]h(\mathscr{C}_0), \qquad \textbf{[S20]}$$

where the $\mathscr{C}_i$ are configurations of the planes of the system, which are to be summed over, with $M = t_{\mathrm{obs}}/\delta t$ and $m = t/\delta t$. Here, $h(\mathscr{C})$, $U(\mathscr{C},\mathscr{C}')$, and $\hat{F}'(\mathscr{C},\mathscr{C}')$ are matrix elements of $|\Psi\rangle$, $\mathrm{e}^{\mathbb{H}'(s)\delta t}$, and $\hat{F}'$, where $\hat{F}' = R(-\alpha)\mathrm{e}^{\mathbb{E}/2T}\hat{F}\mathrm{e}^{-\mathbb{E}/2T}R(\alpha)$ corresponds to a new observable to be measured in ensemble S'.

If space–time phase coexistence occurs in the sFA model, then the ensemble S' is also at phase coexistence. For this to occur, $\mathbb{H}'(s)$ should be invariant under inversion of σ^x. However, for ensemble S' to be invariant under a global spin flip, one requires not just that the transfer matrix be invariant, but also that the boundary conditions along the transfer direction are unbiased between the coexisting phases. Within the s ensemble, there is a finite boundary bias. This is apparent from Eq. **S19** because the state $|\Psi\rangle$ is not invariant under inversion of σ^x (in general, $\theta \neq 2\alpha$). This leads to a predominance of one phase over the other near the boundaries in S'.

To accurately characterize phase coexistence in the classical system, one may replace $|\Psi\rangle$ in Eq. **S19** by a new state vector that is symmetric between the two phases: The natural choice is to replace $|\Psi\rangle$ with $|\Omega\rangle$ (and similarly $\langle\Psi|$ by $\langle\Omega|$). Making this replacement, and transforming back to the sFA representation, this symmetrized matrix element takes the form

$$\langle F(t)\rangle_{s,\mathrm{sym}} = \frac{\langle -|\mathrm{e}^{g\sum_i \hat{n}_i}\,\mathrm{e}^{\mathbb{W}(s)(t_{\mathrm{obs}}-t)}\hat{F}\mathrm{e}^{\mathbb{W}(s)\,t}\mathrm{e}^{g\sum_i \hat{n}_i}|\mathrm{eq}\rangle}{\langle -|\mathrm{e}^{g\sum_i \hat{n}_i}\,\mathrm{e}^{\mathbb{W}(s)\,t_{\mathrm{obs}}}\,\mathrm{e}^{g\sum_i \hat{n}_i}|\mathrm{eq}\rangle} \qquad \textbf{[S21]}$$

with

$$\mathrm{e}^{g} = \tan(\alpha/2)/\sqrt{\lambda}, \qquad \textbf{[S22]}$$

which defines g.

It may be verified that this result is equivalent to Eq. **5** of the main text, for the expectation value of $F(t)$ in the symmetrized s ensemble. The generalization to more complex observables A is trivial, requiring only a slightly heavier notation. Thus, the symmetrized s ensemble allows accurate characterization of phase coexistence, which may be verified by showing that it corresponds to removal of boundary biases in expectation values of an equivalent magnetic system.

Conditions for free fermion solution and analytic calculation of phase diagram. A further special case occurs in $d = 1$, when $B = 0$ and $J_z = 0$ together. In this case, the only couplings in $\mathbb{H}'(s)$ are $(h, J_x$, and $J_y)$ and the model may be diagonalized by a Jordan–Wigner transformation (4, 6). Using these standard methods, one finds that spontaneous symmetry breaking occurs for $h < J_x + J_y$, with criticality occurring for $h = J_x + J_y$.

By calculating the determinant of M, it can be seen that $J_z = 0$ if

$$D(D + \lambda - 1) = z\lambda. \qquad \textbf{[S23]}$$

Solving for D gives Eq. **4** of the main text.

Mean-field approximation and construction of field theory. As discussed in the main text, the space–time phase transitions of the sFA model in d dimensions are closely related to symmetry breaking in Ising-like models in $(d+1)$ dimensions. There are several ways to demonstrate this. One option is to generalize the sFA model to allow sites to contain more than one excitation. This allows the master equation to be written in a bosonic representation due to Doi and Peliti (7). For small λ, it may be shown that the behavior of this generalized ('bosonic') sFA model approaches that of the original model, via a large-S expansion [see, for example, the analysis of the FA model (with $\epsilon = 0$) in ref. 8]. Further, even if λ is not small, the universal (critical) behavior of generalized and original sFA models are the same.

Following the Doi–Peliti procedure for this generalized sFA model, the master operator within the s ensemble is

$$\mathbb{W}_b(s) = \sum_{\langle ij\rangle}\{(a_i^\dagger a_i + \epsilon/2)[(z - a_j^\dagger)a_j + \gamma(a_j^\dagger - z)] + (i \leftrightarrow j)\} + D[z(a_i^\dagger a_j + a_j^\dagger a_i) - (a_i^\dagger a_i + a_j^\dagger a_j)], \qquad \textbf{[S24]}$$

where a_i and $a_i^\dagger$ are bosonic operators, so $[a_i, a_j^\dagger] = \delta_{ij}$ as usual. In treating this generalized model as an approximate representation of the sFA model, the parameters D, γ, and ϵ play the same role as in the original model. Within this new representation, the density of excitations in the sFA model corresponds to the density of bosons through the number operators $a_i^\dagger a_i$.

One may then use coherent state path integrals to represent Dirac brackets such as those of Eq. **S18**. This is discussed, for example, in ref. S8. One arrives at

$$Z(s, t_{\mathrm{obs}}) = \int \mathscr{D}(\phi,\bar{\phi})\exp\left(-\int d^d x\, dt L[\phi,\bar{\phi}]\right), \qquad \textbf{[S25]}$$

where $\phi(x,t)$ and $\bar{\phi}(x,t)$ are complex conjugate fields, and

$$L[\phi,\bar{\phi}] = \bar{\phi}\frac{\partial\phi}{\partial t} - zD\ell_0^2\bar{\phi}\nabla^2\phi + 2dD(1-z)\bar{\phi}\phi - d(2\bar{\phi}\phi + \epsilon\ell_0^{-d})[z(\phi + \gamma\bar{\phi})\ell_0^{d/2} - (\gamma + \bar{\phi}\phi\ell_0^d)]. \qquad \textbf{[S26]}$$

Here, ℓ_0 is the lattice spacing of the sFA model and we recall that the units of time have been set by taking $\gamma = 1$ in the original definition of the model. The operators a_i and $a_i^\dagger$ have become fields ϕ and $\bar{\phi}$, with the combination $\phi\bar{\phi}$ corresponding to the density of excitations in the sFA model.

As discussed in refs. 9 and 10, one may either analyze the resulting field theory through the saddle points of $L[\phi,\bar{\phi}]$ or by using a variational analysis that leads to a free energy $\mathscr{F}(\phi)$, as in the main text. The saddle points of $L[\phi,\bar{\phi}]$ give the properties of space–time phases: Free energies are obtained from the values of L, whereas surface tensions between phases may be estimated from inhomogeneous saddle points of the action. The free energy $\mathscr{F}(\phi)$ may also be used to obtain spinodal conditions on the properties of metastable phases (9, 10).

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