Hydrodynamics of Equilibrium Systems

Theory of dynamic critical phenomena

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An introductory review of the central ideas in the modern theory of dynamic critical phenomena is followed by a more detailed account of recent developments in the field. The concepts of the conventional theory, mode-coupling, scaling, universality, and the renormalization group are introduced and are illustrated in the context of a simple example—the phase separation of a symmetric binary fluid. The renormalization group is then developed in some detail, and applied to a variety of systems. The main dynamic universality classes are identified and characterized. It is found that the mode-coupling and renormalization group theories successfully explain available experimental data at the critical point of pure fluids, and binary mixtures, and at many magnetic phase transitions, but that a number of discrepancies exist with data at the superfluid transition of ^{4}He.

Classified different types of dynamics (models A-J) based on the following:

1. whether the order parameter is conserved or not,
2. whether there are the other conserved charges,
3. whether there exists couplings between these modes.

Equilibrium versus Non-equilibrium hydrodynamics

Equilibrium hydrodynamics: The deterministic part can be written as a gradient descend, i.e., the dynamics is trying to minimize some global functional, e.g., the free energy $\mathcal{F}(\vec{v})$. The noise has no feature, i.e., it is white in space and time. --- "Model A" in Hohenberg and Halperin (RMP, 1977)

$$\frac{\partial \vec{v}}{\partial t} = -\kappa \frac{\delta \mathcal{F}(\vec{v})}{\delta \vec{v}} + \vec{\eta} \quad \Rightarrow \quad P(\vec{v}) \sim e^{-\mathcal{F}/\Delta}$$

Boltzmann Distribution

$$< \eta_i(x,t)\, \eta_j(x',t') >= 2\Delta\kappa\delta_{ij}\delta(x-x')\delta(t-t')$$

e.g., the vector ϕ^4 –theory for XY model: $\mathcal{F}(\vec{v}) = \int [-\frac{\alpha}{2}|\vec{v}|^2 + \frac{\beta}{4}|\vec{v}|^4 + \frac{D}{2}|\nabla\vec{v}|^2]\mathrm{d}\vec{x}$

$$\frac{\partial \vec{v}}{\partial t} = \alpha\vec{v} - \beta|\vec{v}|^2\vec{v} + D\nabla^2\vec{v} + \vec{\eta}$$

Non-equilibrium hydrodynamics: there is NO global functional the dynamics is trying to minimize

$$\frac{\partial \vec{v}}{\partial t} \neq -\frac{\delta \mathcal{F}(\vec{v})}{\delta \vec{v}} + \vec{\eta}$$

$$\frac{\partial \vec{v}}{\partial t} + \lambda_1(\vec{v}\cdot\nabla)\vec{v} + \cdots = \alpha\vec{v} - \beta|\vec{v}|^2\vec{v} + D\nabla^2\vec{v} + \cdots + \vec{\eta}$$

One common consequence of Non-equilibrium systems:

It needs continuous dissipation of energy (cost) to maintain the non-equilibrium steady state

What is the cost-performance tradeoff in biological systems?

Lecture 3 (Boulder Summer School 2022)

Energetics of collective phenomena in strongly interacting nonequilibrium systems:

From synchronization of molecular clocks to flocking of active spins

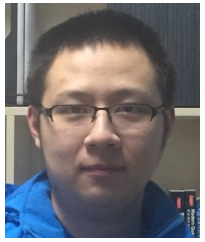
Yuhai Tu

IBM T. J. Watson Research Center, YKT

Acknowledgements

Biochemical Oscillations and Synchronization

Yuansheng Cao
(UCSD)



Dongliang Zhang
(PKU)

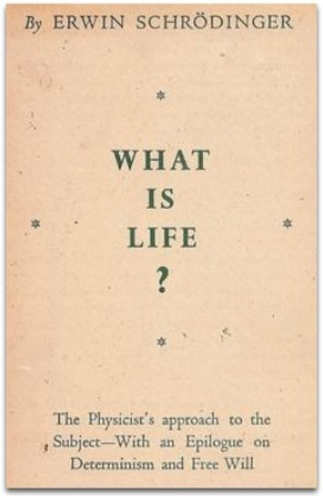
Qi Ouyang
(PKU)

Nonequilibrium Thermodynamics of Flocking

Qiwei Yu
(Princeton U.)

Schrödinger's Question

How are living (biological) systems different from non-living (physical) systems?

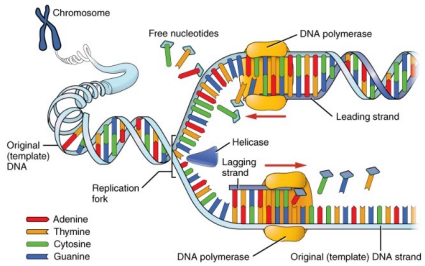


(1944)

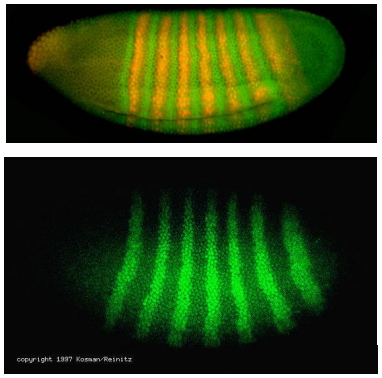
"…life feeds on negative entropy…" – Erwin Schrodinger

Life costs free energy

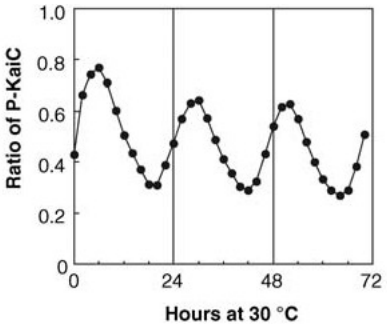
Central Question: How do living systems process information accurately with noisy components and stochastic interactions?



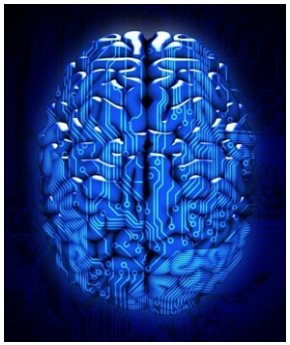
DNA Replication



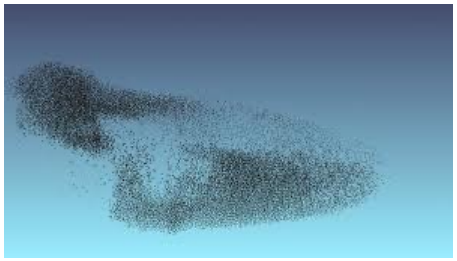
Pattern Formation
(drosophila (fruit fly) embryo)



Circadian rhythm
(Cyanobacteria)



Learning/memory



Flocking

- **Biological systems are noisy – small # of molecules, stochastic interactions, ….**

(1) How? → Mechanisms and Design Principles for Achieving the Biological Functions (Behaviors)

(2) How much? → Free Energy Cost for Biological Functions

The energy cost for creating and maintaining order in noisy nonequilibrium systems

Equilibrium versus Non-equilibrium systems

FEBRUARY 15, 1931 *PHYSICAL REVIEW* *VOLUME 37*

RECIPROCAL RELATIONS IN IRREVERSIBLE PROCESSES. I.

By Lars Onsager

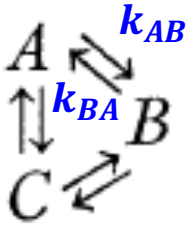
$$J_1 = L_{11}X_1 + L_{12}X_2 + L_{13}X_3$$
$$J_2 = L_{21}X_1 + L_{22}X_2 + L_{23}X_3 \qquad (2.3)$$
$$J_3 = L_{31}X_1 + L_{32}X_2 + L_{33}X_3$$

The Onsager reciprocal relations $L_{12} = L_{21}\ ;\ L_{13} = L_{31}\ ;\ L_{23} = L_{32}.$ (2.4)

(Lars Onsager)

3. Analogy with Chemical Reactions

We shall compare (2.3) with the equations for a chemical monomolecular triangle reaction. Suppose that a certain substance may exist in a homogene-



(3.1)

Detailed balance (DB)

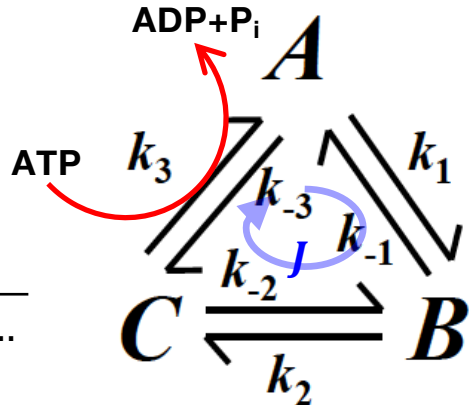
$$k_{BA}\bar{n}_A = k_{AB}\bar{n}_B$$
$$k_{CB}\bar{n}_B = k_{BC}\bar{n}_C \qquad (3.5)$$
$$k_{AC}\bar{n}_C = k_{CA}\bar{n}_A.$$

The cycle rule

$$k_{AC}k_{CB}k_{BA} = k_{AB}k_{BC}k_{CA}.$$

Biochemical systems are far from equilibrium

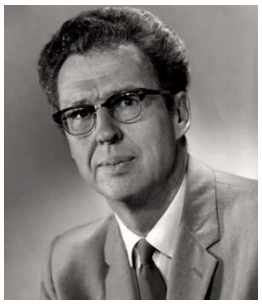
The cycle rule (or DB) is broken: $k_1 k_2 k_3 \neq k_{-1} k_{-2} k_{-3}$



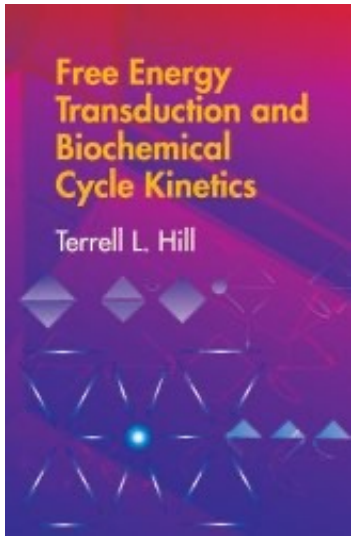
Persistent current J in steady state: $\mathbf{J}=k_2 P_B - k_{-2} P_C = \frac{k_1 k_2 k_3 - k_{-1} k_{-2} k_{-3}}{\ldots sum\ of\ 9\ (>0)\ terms\ \ldots}$

Thermodynamic force: $\Delta\mu = k_B T \ln \frac{k_1 k_2 k_3}{k_{-1} k_{-2} k_{-3}}$

Free energy dissipation rate: $\dot{W} = J \times \Delta\mu \geq 0$



Terrell Hill



Continuous energy dissipation (power consumption) is needed to maintain a non-equilibrium steady state (NESS)

Cost-Performance relation in biological systems

- **Ultrasensitive Biological Switch**

The nonequilibrium mechanism for ultrasensitivity in a biological switch: Sensing by Maxwell's demons

Yuhai Tu*

PNAS | August 19, 2008 | vol. 105 | no. 33 | 11739

- **Sensory Adaptation**

PRL 115, 118102 (2015) PHYSICAL REVIEW LETTERS week ending 11 SEPTEMBER 2015

Free Energy Cost of Reducing Noise while Maintaining a High Sensitivity

Pablo Sartori[1,*] and Yuhai Tu[2]

nature physics ARTICLES

PUBLISHED ONLINE: 25 MARCH 2012 | DOI: 10.1038/NPHYS2276

The energy–speed–accuracy trade-off in sensory adaptation

Ganhui Lan[1†‡], Pablo Sartori[2‡], Silke Neumann[3], Victor Sourjik[3] and Yuhai Tu[1]*

- **Biochemical Oscillation**

nature physics ARTICLES

PUBLISHED ONLINE: 27 JULY 2015 | DOI: 10.1038/NPHYS3412

The free-energy cost of accurate biochemical oscillations

Yuansheng Cao[1], Hongli Wang[1], Qi Ouyang[1,2]* and Yuhai Tu[3]*

nature COMMUNICATIONS

ARTICLE

OPEN

Design principles for enhancing phase sensitivity and suppressing phase fluctuations simultaneously in biochemical oscillatory systems

Chenyi Fei[1], Yuansheng Cao[2], Qi Ouyang[2] & Yuhai Tu[3]

nature physics ARTICLES

https://doi.org/10.1038/s41567-019-0701-7

The energy cost and optimal design for synchronization of coupled molecular oscillators

Dongliang Zhang[1], Yuansheng Cao[2], Qi Ouyang[1,3] and Yuhai Tu[4]*

- **Inverse Power-Law Scaling of Dissipation Rate during coarse-graining**

PHYSICAL REVIEW LETTERS 126, 080601 (2021)

Inverse Power Law Scaling of Energy Dissipation Rate in Nonequilibrium Reaction Networks

Qiwei Yu,[1] Dongliang Zhang,[1] and Yuhai Tu[2]

Strongly interacting systems

Most of the systems studied so far are spatially homogeneous, i.e., well mixed biochemical reaction networks

What about systems that consist of strong-interacting subsystems, which exhibit collective behaviors?

1) Synchronization of molecular clocks

Zhang et al, Nature Phys., 2020

2) Flocking of active spins

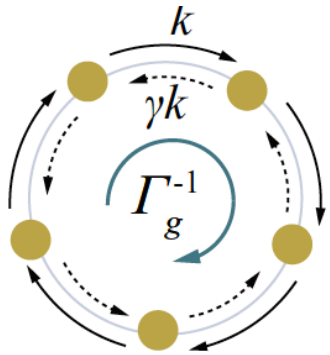
"The energy cost for flocking of active spins", Qiwei Yu, YT, 2022

https://arxiv.org/abs/2205.13149

3) Reaction-diffusion system (not covered in this talk)

Synchronization of Coupled Molecular Clocks

A finite-state Poisson clock

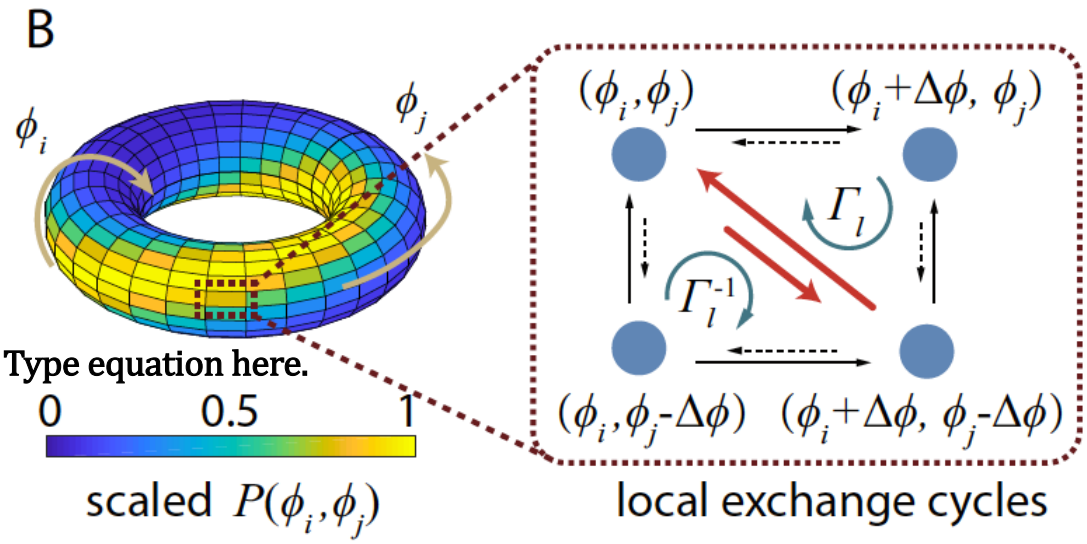


global clock cycle

$$\Gamma_g \equiv \prod_n k_n^- / \prod_n k_n^+ = \gamma^N \neq 1,$$

$$\Gamma_l = e^{-\Delta E_{ij}} \times \gamma^{-1} \times \gamma = e^{-\Delta E_{ij}} \neq 1,$$

Coupled clocks -- exchange interactions



$$\boldsymbol{k_{ex}((\phi_i+\Delta\phi,\ \phi_j-\Delta\phi)\rightarrow(\phi_i,\ \phi_j))=\frac{\Omega}{m}e^{-\frac{\Delta E_{ij}}{2}}}$$

$$\boldsymbol{k_{ex}((\phi_i,\ \phi_j)\rightarrow(\phi_i+\Delta\phi,\ \phi_j-\Delta\phi))=\frac{\Omega}{m}e^{\frac{\Delta E_{ij}}{2}}}$$

$$\boldsymbol{\Delta E_{ij}=-\frac{E_0}{2}\cos(\phi_i-\phi_j)}$$

An analytical solution for the many-oscillator phase distribution

The phase distribution function of *m* interacting oscillators $P(\phi_1, \phi_2, \ldots, \phi_m, t)$ **satisfies the Fokker-Planck equation:**

$$\frac{\partial P}{\partial t} = k \sum_i \frac{\partial}{\partial \phi_i} \left(-e_g + \frac{\partial}{\partial \phi_i} \right) P + \frac{\Omega}{m} \sum_{i<j} \frac{\partial}{\partial \varphi_{ij}} \left(2E'(\varphi_{ij}) + \frac{\partial}{\partial \varphi_{ij}} \right) P,$$

The processive speed: $v = ke_g = -k \ln \Gamma_g / 2\pi$ **Interaction "energy"** $E(\varphi_{ij})$ $with$ $\varphi_{ij} = \phi_i - \phi_j$

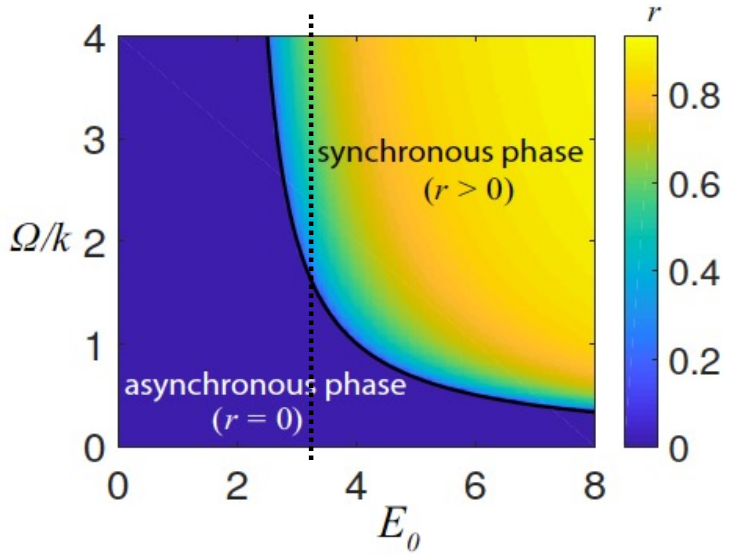
Exact steady-state solution: $P_s(\vec{\phi}) = Z^{-1} \exp(-\beta E_t(\vec{\phi}))$, $E_t = \frac{2}{m} \sum_{(i<j)} E(\phi_i - \phi_j)$

An effective temperature: $T_{eff} = \beta^{-1} = 1 + k/\Omega$ **decreases with exchange frequency** Ω

The nonequilibrium phase transition and energy cost of synchronization

Synchronization order parameter $r \in [0,1]$

$$re^{i\psi} \equiv \frac{1}{m}\sum_{j=1}^{m} e^{i\phi_j}, \qquad \psi = vt$$



Critical line: $\frac{\Omega}{\Omega + k} E_0 = 2$

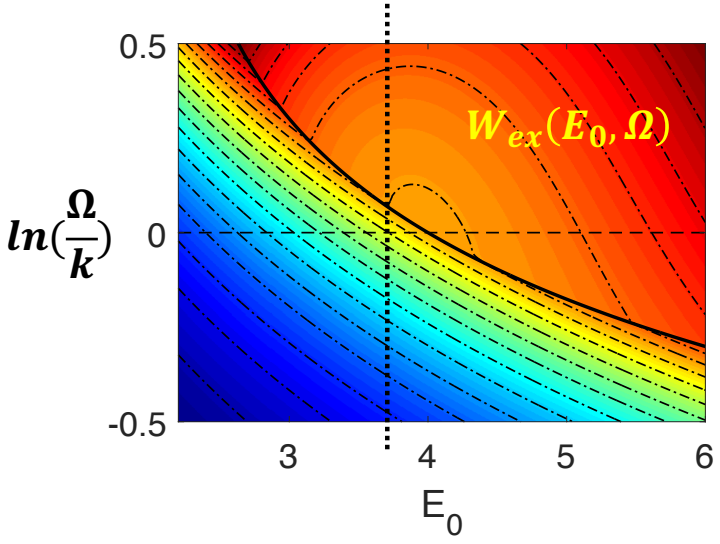
$r > 0$ **when** $\frac{\Omega}{\Omega + k} E_0 > 2$; $r = 0$ **when** $\frac{\Omega}{\Omega + k} E_0 \leq 2$

Energy dissipation rate

$$\dot{W} = \frac{1}{m}\int [\sum_i \frac{J_i^2}{kP_s} + \sum_{i<j} \frac{J_{ij}^2}{\frac{\Omega}{m}P_s}] d\vec{\phi},$$

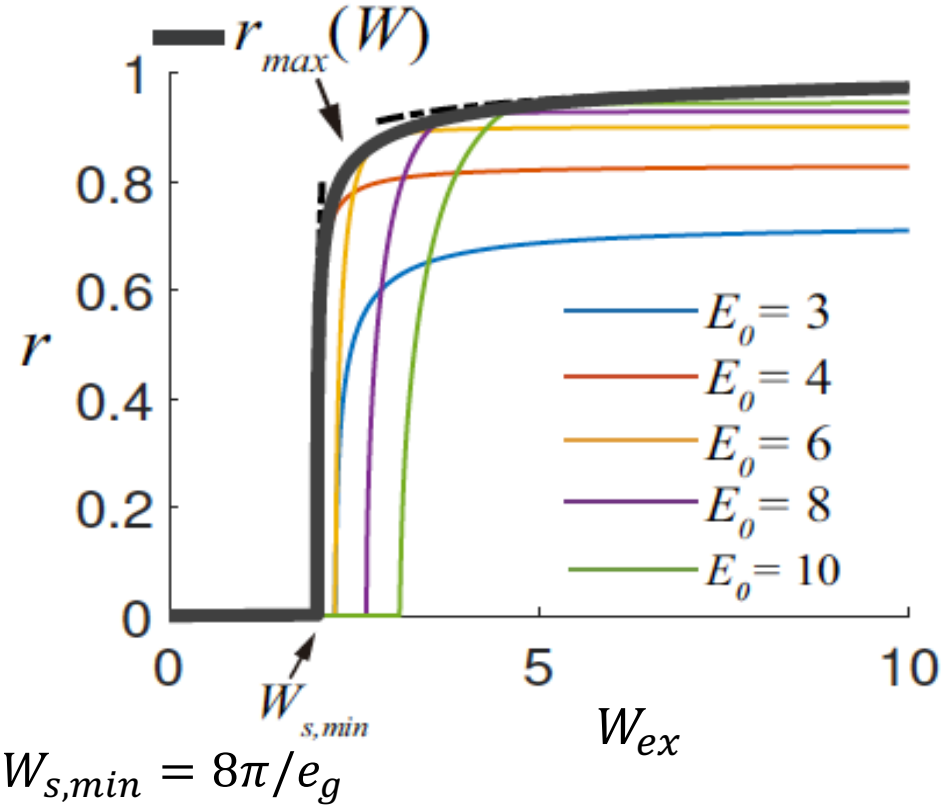
procession energy **exchange energy**

$$W = \dot{W} \times T = W_0 + W_{ex} \qquad W_0 = 2\pi e_g = -\ln \Gamma_g$$



Synchronization transition driven by exchange energy dissipation

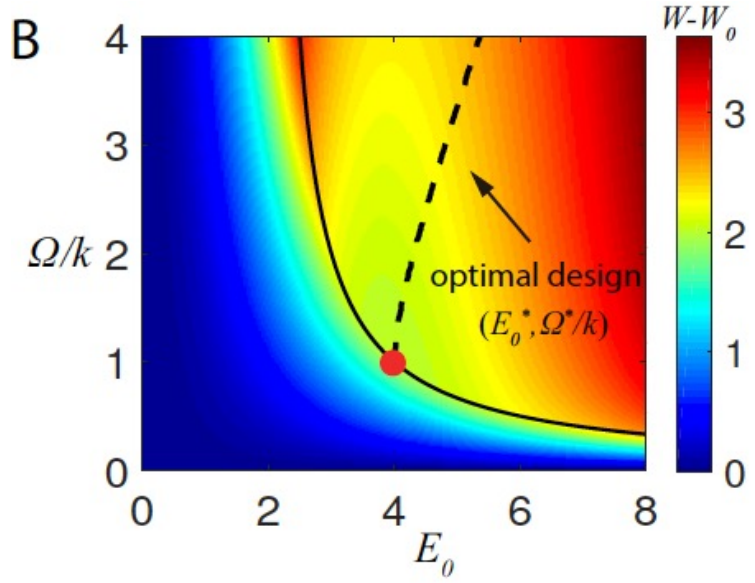
$$r_{max}(W) = \max(r(E_0, \Omega|W))$$



$$W_{s,min} = 8\pi/e_g$$

Optimal design

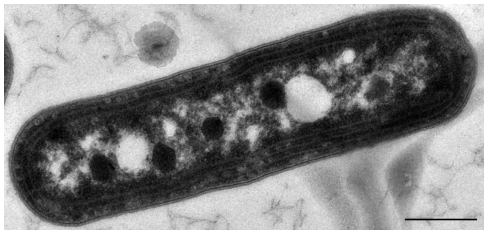
$$(E_0^*, \Omega^*) = \underset{\Omega, E_0}{\operatorname{argmax}}\, r(E_0, \Omega|W)$$



(Zhang et al, Nature Physics, 2020)

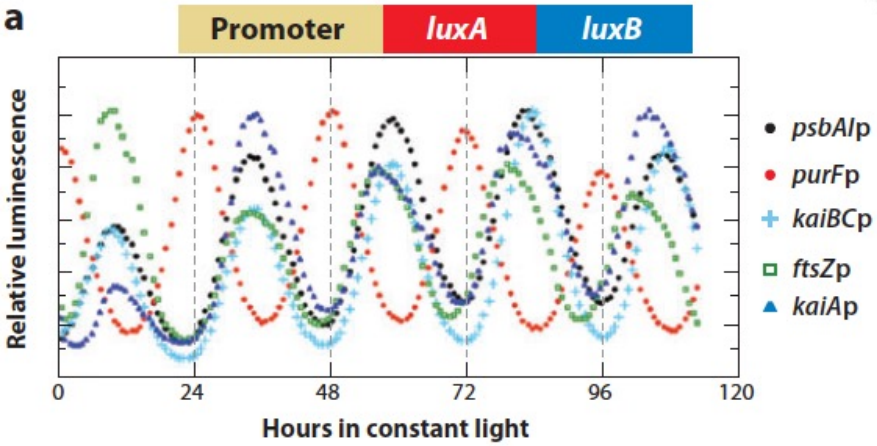
Cyanobacterial circadian clock and the Kai system

Cyanobacteria is the simplest organism that exhibits circadian rhythm (24 hrs)



Synechococcus elongatus

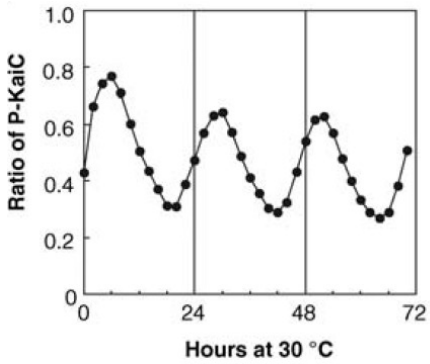
robust 24-hr oscillation in vivo



(Johnson et al, *Ann. Rev. Biophys.* 2011)

A breakthrough!

KaiA, KaiB, KaiC, +ATP

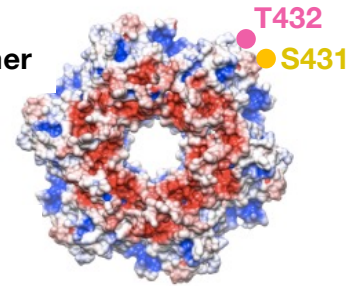


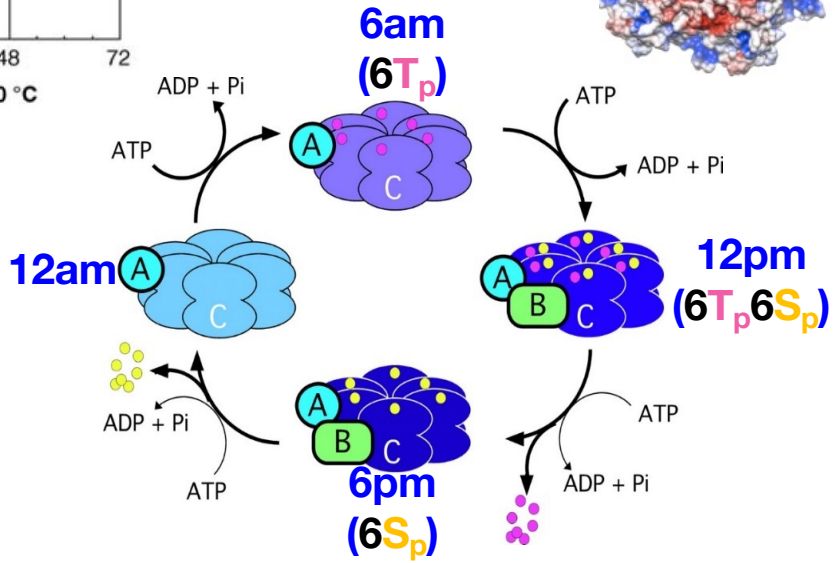
Reconstitution of Circadian Oscillation of Cyanobacterial KaiC Phosphorylation in Vitro

(Nakajima, …, T. Kondo, Science, 2005)

(Takao Kondō)

KaiC hexamer

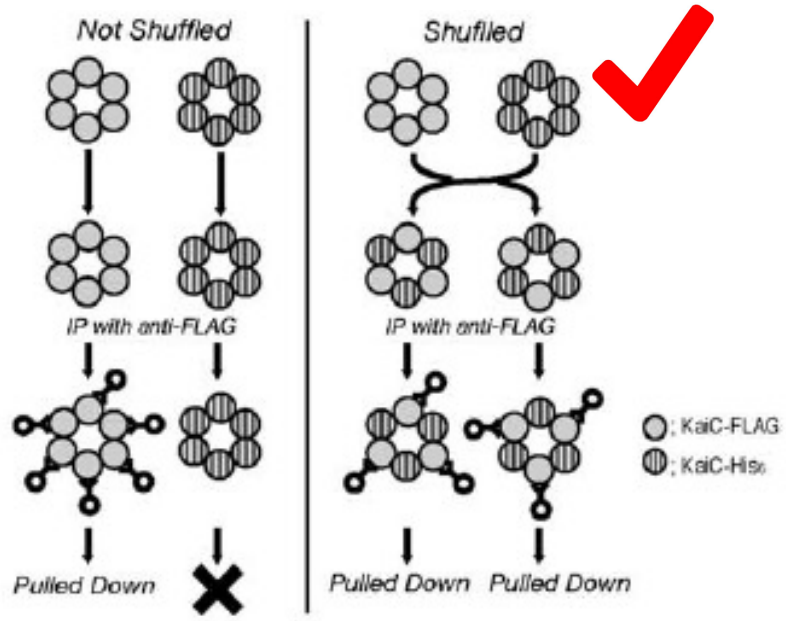




How do individual KaiC hexamers synchronize with each other?

KaiC hexamers exchange monomers

(Kageyama et al, …, T. Kondo, Mol. Cell, 2006)

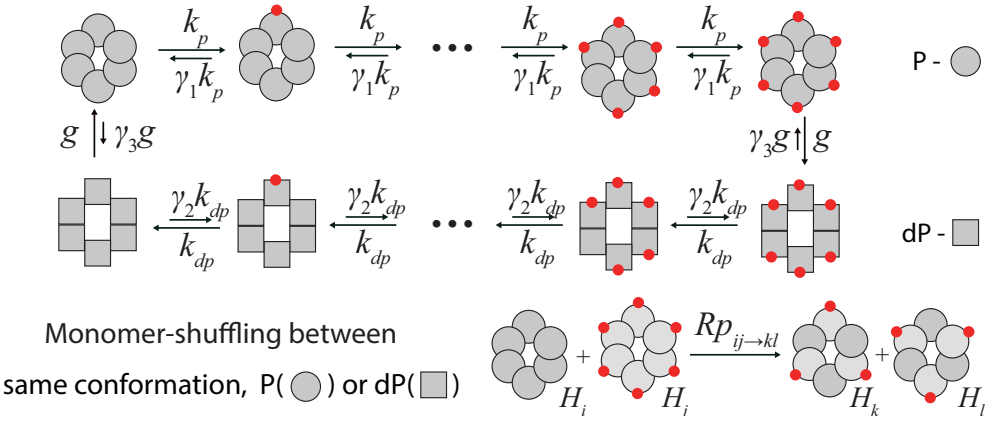


The energy cost of synchronization in the Kai system

An Interesting Puzzle: Only 2 ATP are needed for the P-dP cycle , 16 ATP are hydrolyzed per KaiC per day (Terauchi et al, …, T. Kondo, PNAS 2007)

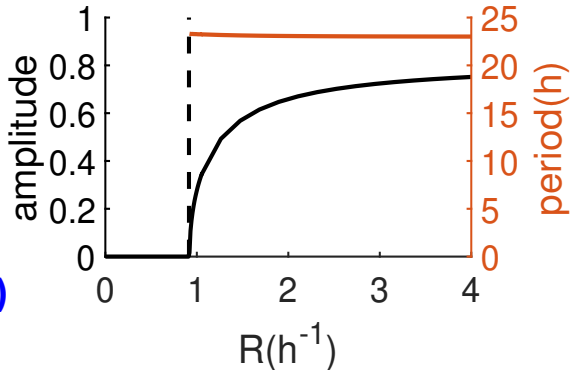
Our model

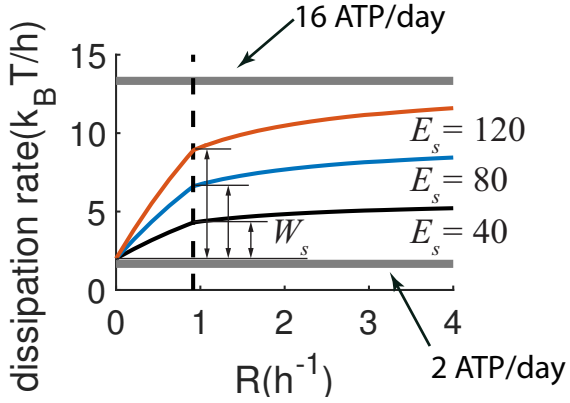
- **(1) Dynamics of individual KaiC hexamer -- PdP cycle**
- **(2) Exchange coupling between two KaiC hexamers**



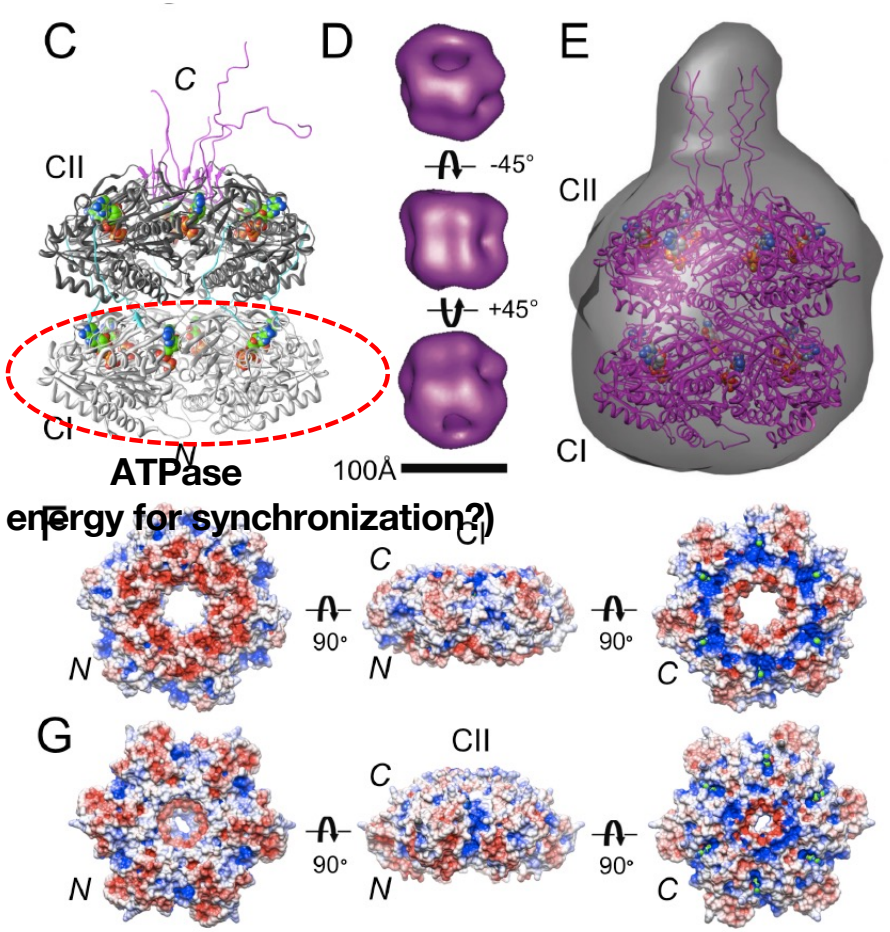
Varying
R– exchange (shuffling) rate

(Zhang et al, Nature Physics, 2020)



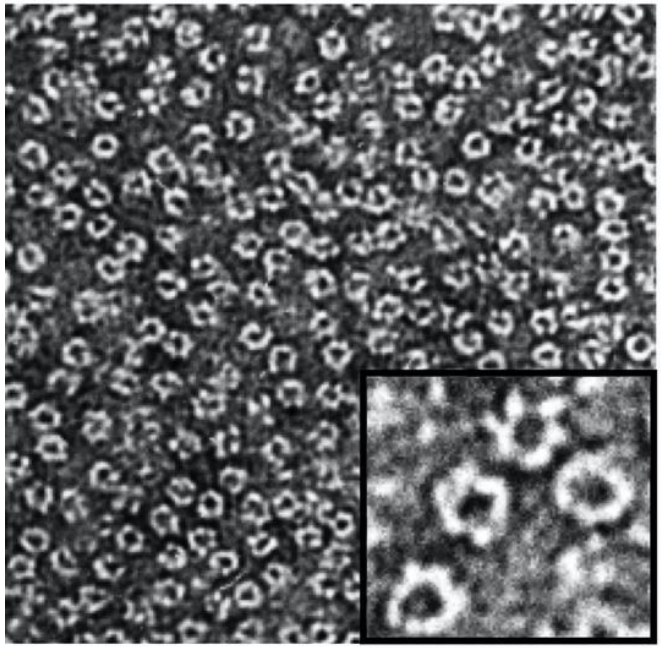


The rings of time: KaiC hexamer consists of two rings (KaiCI and KaiCII)



ATPase

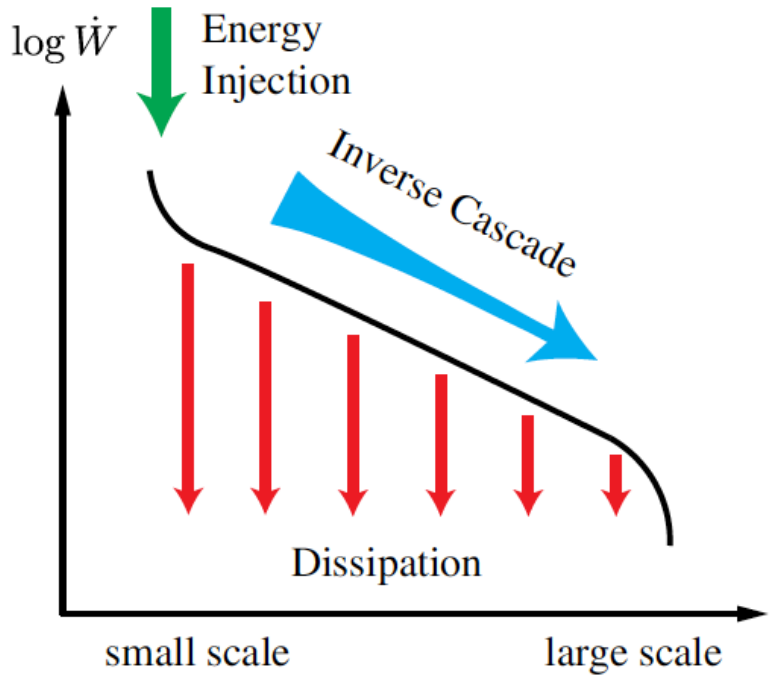
(provide energy for synchronization?)



What about the energy cost for flocking?

The dissipation rate depends inversely on the coarse-graining scale

Coarse-graining can reduce the apparent dissipation rate dramatically

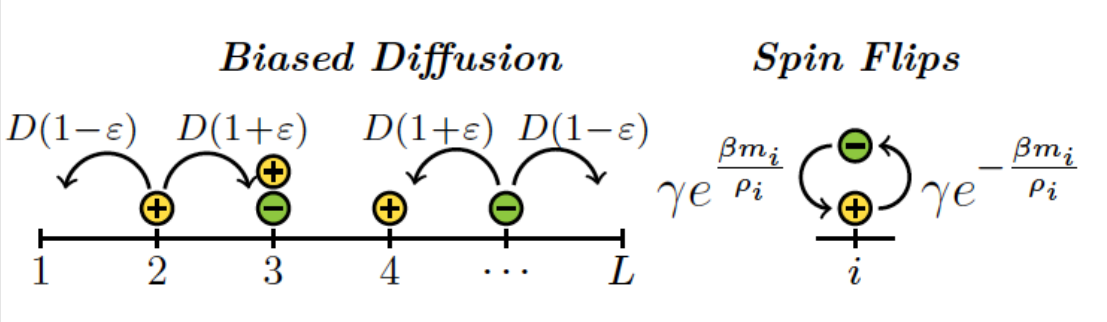


(Qiwei Yu, DL Zhang, YT, PRL, 126 (8), 2021)

To determine the true dissipation rate, we need to compute it at the microscopic level.

Thermodynamic cost for flocking of active spins

The Active Ising Model (AIM)



$$m_i = n_i^+ - n_i^- \qquad \rho_i = n_i^+ + n_i^-$$

n_i^s -- number of spin s(=+, -) at site *i*

$(2\times L)^N$ degrees of freedom

"Flocking with discrete symmetry: The two-dimensional active Ising model"
PRE 2015

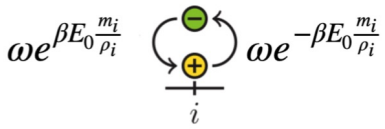
"Revisiting the flocking transition using active spins"
PRL 2013

A. P. Solon and J. Tailleur

The Active Ising Model (AIM): a lattice flocking model

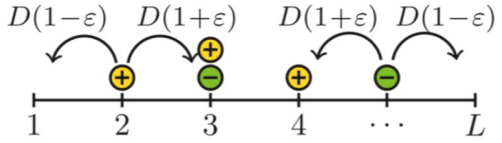
- N **particles (Ising spins),** $L_x \times L_y$ **lattice, no volume exclusion, continuous-time Markov process.**
  - **State variables: local occupation number** $\left(n_{i,j}^{+}, n_{i,j}^{-}\right), i = 1,2,\ldots,L_x, j = 1,2,\ldots,L_y.$
    - **Local density and magnetization:** $\rho_{i,j} = n_{i,j}^{+} + n_{i,j}^{-}, m_{i,j} = n_{i,j}^{+} - n_{i,j}^{-}.$
      - **Dynamics (reactions): local alignment + active transport**

Flipping



$$k_{s\to(-s)} = \omega \exp\left(-s\beta E_0 \frac{m_{\mathbf{r}}}{\rho_{\mathbf{r}}}\right) = \omega e^{-s\beta E_0 \lambda_{\mathbf{r}}}.$$

Hopping



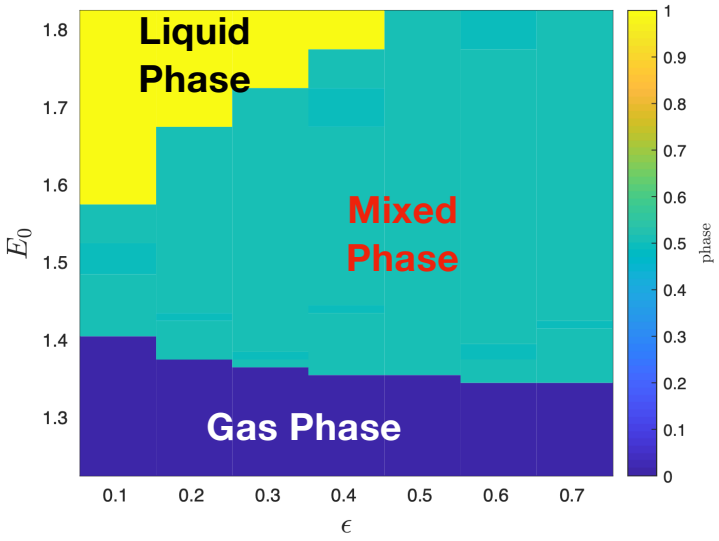
$$k_{(x,y)\to(x+1,y)} = D(1+s\epsilon)$$
$$k_{(x,y)\to(x-1,y)} = D(1-s\epsilon)$$
$$k_{(x,y)\to(x,y+1)} = D$$
$$k_{(x,y)\to(x,y-1)} = D,$$

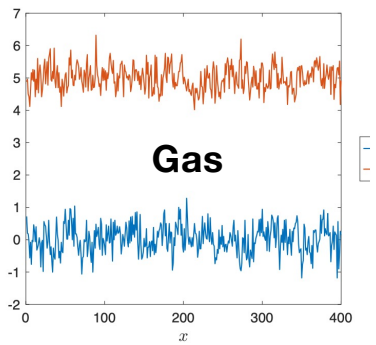
Key control parameters: $\left(\frac{\omega}{D}, E_0, \epsilon\right)$

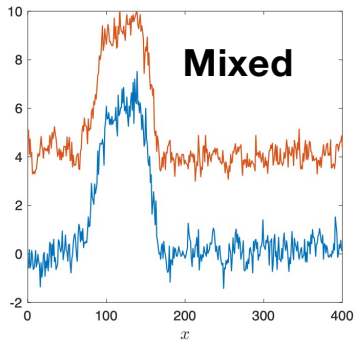
time scale | **coupling energy scale** | **bias**

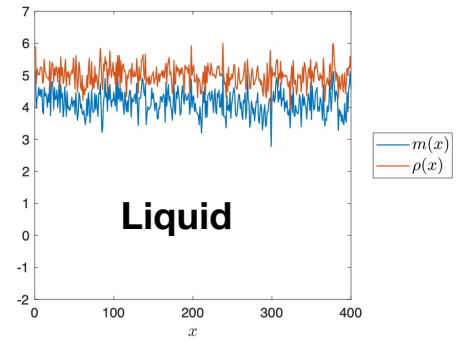
A. P. Solon and J. Tailleur, PRL 2013; PRE 2015

Phase diagram in parameter space (E_0, ϵ)









The three phases in AIM: Simulation results:

Gas Phase

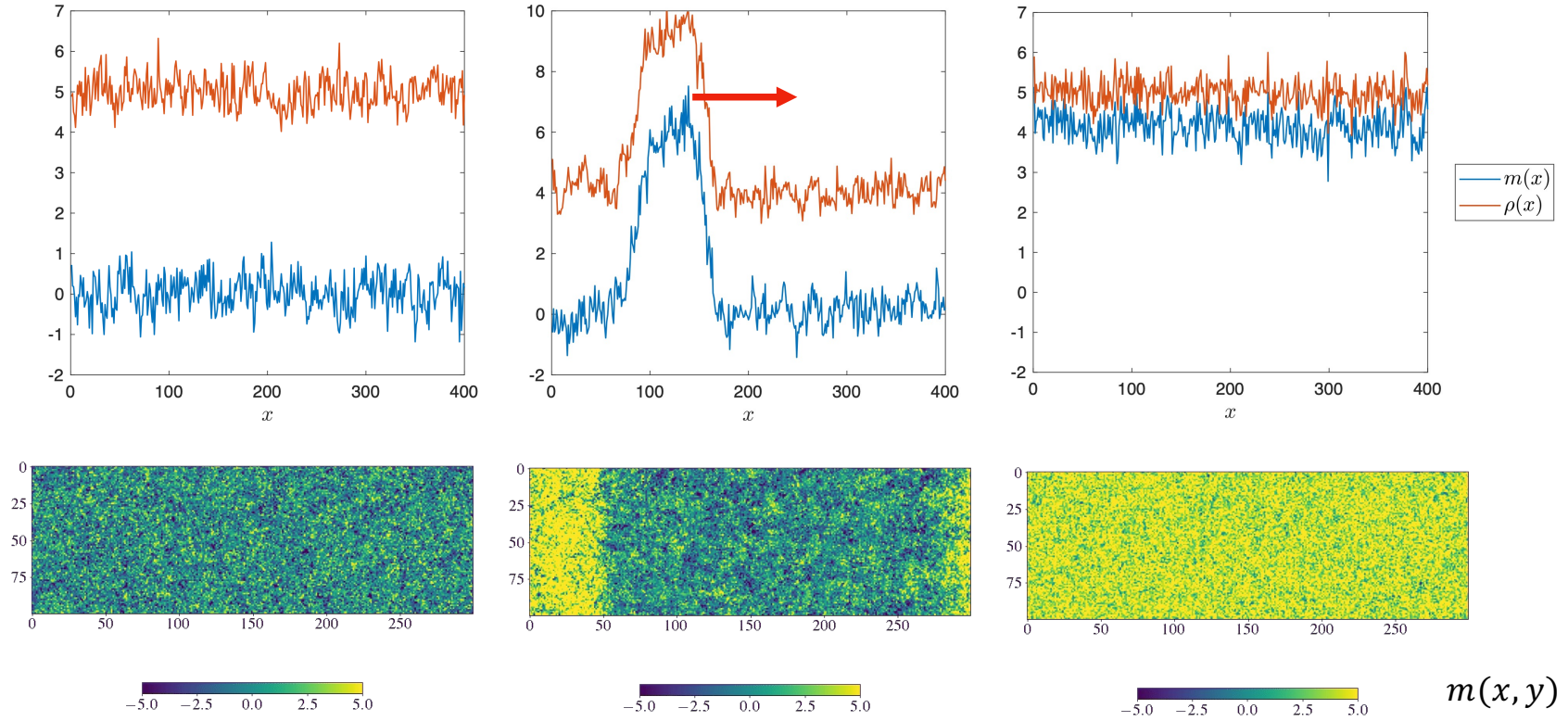
(No flocking)

Mixed Phase

(flocking)

Liquid Phase

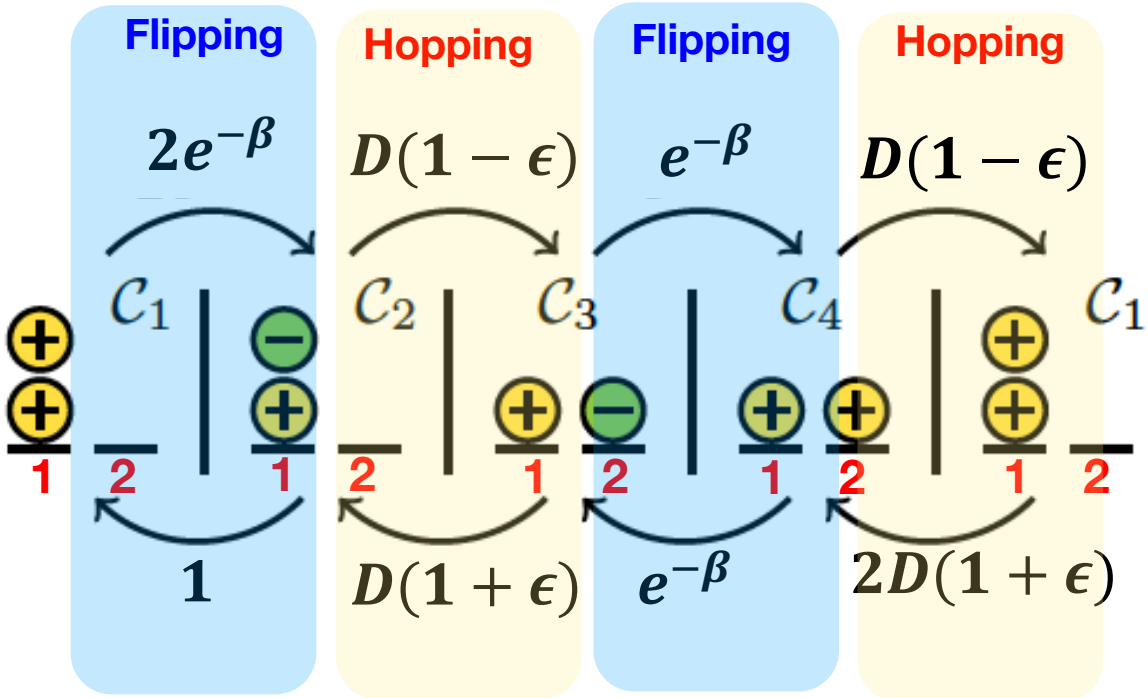
(flocking)



AIM breaks the cycle rule (or Detailed Balance)

The mixed flipping-hopping cycle

Two-site AIM with $N = 2$



$$\Gamma = \frac{2e^{-\beta}\times D(1-\epsilon)\times e^{-\beta}\times D(1-\epsilon)}{2D(1+\epsilon)\times e^{-\beta}\times D(1+\epsilon)\times 1} = e^{-\beta}\left(\frac{1-\epsilon}{1+\epsilon}\right)^2 \neq 1$$

Energy is continuously dissipated to maintain the (non-equilibrium) steady state.

The active Ising model: thermodynamics

General Theoretical Framework

$$\dot{W} = \lim_{t\to+\infty} \frac{1}{t} \left\langle \ln \frac{\mathcal{P}}{\mathcal{P}^R} \right\rangle$$

State variable $\mathbf{n} = (n^+_{1,1}, n^-_{1,1}, n^+_{1,2}, n^-_{1,2}, \ldots, n^+_{L_x,L_y}, n^-_{L_x,L_y})$. Trajectory $\mathbf{n}(t_0), \mathbf{n}(t_1), \mathbf{n}(t_2), \ldots, \mathbf{n}(t_m), \quad t_0 < t_1 < t_2 < \cdots < t_m.$

Forward Probability

$$\begin{aligned}\mathcal{P} &= P(\mathbf{n}_0) e^{-(t_1-t_0)k^{\text{out}}_{\mathbf{n}_0}} k_{\mathbf{n}_0\to\mathbf{n}_1} e^{-(t_2-t_1)k^{\text{out}}_{\mathbf{n}_1}} k_{\mathbf{n}_1\to\mathbf{n}_2} \cdots e^{-(t_m-t_{m-1})k^{\text{out}}_{\mathbf{n}_{m-1}}} k_{\mathbf{n}_{m-1}\to\mathbf{n}_m} \\ &= P(\mathbf{n}_0) e^{-\sum_{i=0}^{m-1}(t_{i+1}-t_i)k^{\text{out}}_{\mathbf{n}_i}} \prod_{i=0}^{m-1} k_{\mathbf{n}_i\to\mathbf{n}_{i+1}}\end{aligned}$$

Backward Probability

$$\begin{aligned}\mathcal{P}^R &= P(\mathbf{n}_m) k_{\mathbf{n}_m\to\mathbf{n}_{m-1}} e^{-(t_m-t_{m-1})k^{\text{out}}_{\mathbf{n}_{m-1}}} \cdots k_{\mathbf{n}_1\to\mathbf{n}_0} e^{-(t_1-t_0)k^{\text{out}}_{\mathbf{n}_0}} \\ &= P(\mathbf{n}_m) e^{-\sum_{i=0}^{m-1}(t_{i+1}-t_i)k^{\text{out}}_{\mathbf{n}_i}} \prod_{i=0}^{m-1} k_{\mathbf{n}_{i+1}\to\mathbf{n}_i}\end{aligned}$$

$$\ln \frac{\mathcal{P}}{\mathcal{P}^R} = \ln \frac{P(\mathbf{n}_0)}{P(\mathbf{n}_m)} + \sum_{i=0}^{m-1} \ln \frac{k_{\mathbf{n}_i\to\mathbf{n}_{i+1}}}{k_{\mathbf{n}_{i+1}\to\mathbf{n}_i}}$$

Finite, vanishes for infinite t

Count all transitions

$$\dot{W} = \lim_{t\to+\infty} \frac{1}{t} \sum_{i=0}^{m-1} \ln \frac{k_{\mathbf{n}_i\to\mathbf{n}_{i+1}}}{k_{\mathbf{n}_{i+1}\to\mathbf{n}_i}}$$

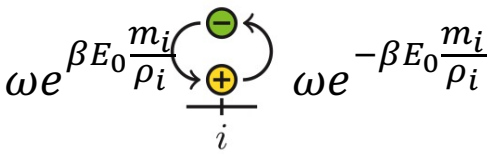
*see book by Peliti & Pigolotti for a comprehensive introduction to stochastic thermodynamics.

The active Ising model: thermodynamics

General Theoretical Framework

$$\dot{W} = \lim_{t\to+\infty} \frac{1}{t} \sum_{i=0}^{m-1} \ln \frac{k_{\mathbf{n}_i \to \mathbf{n}_{i+1}}}{k_{\mathbf{n}_{i+1} \to \mathbf{n}_i}}$$

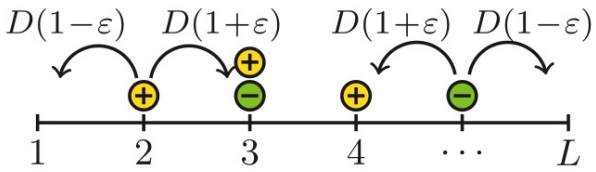
Flipping



$$\left(\frac{k_{\mathbf{n}\to\mathbf{n}'}}{k_{\mathbf{n}'\to\mathbf{n}}}\right)_{+s\to-s} = \frac{\rho_{i,j} + s m_{i,j}}{\rho_{i,j} - s m_{i,j} + 2} \exp\left(-2s \frac{m_{i,j} - s}{\rho_{i,j}} E_0\right)$$

$$= \frac{\rho_{i,j} + s m_{i,j}}{\rho_{i,j} - s m_{i,j} + 2} \exp\left(2E_0 \frac{1 - m_{i,j} s}{\rho_{i,j}}\right)$$

Hopping



$$\left(\frac{k_{\mathbf{n}\to\mathbf{n}'}}{k_{\mathbf{n}'\to\mathbf{n}}}\right)_{(s,i,j)\to(s,i+\Delta x,j)} = \frac{\rho_{i,j} + s m_{i,j}}{\rho_{i+\Delta x,j} + s m_{i+\Delta x,j} + 2} \cdot \frac{1 + \Delta x s \epsilon}{1 - \Delta x s \epsilon}$$

$$\left(\frac{k_{\mathbf{n}\to\mathbf{n}'}}{k_{\mathbf{n}'\to\mathbf{n}}}\right)_{(s,i,j)\to(s,i,j+\Delta y)} = \frac{\rho_{i,j} + s m_{i,j}}{\rho_{i,j+\Delta y} + s m_{i,j+\Delta y} + 2}$$

sum of the energy terms

$$\dot{W} = \lim_{t\to+\infty} \frac{W_1(t) + W_2(t)}{t} = \lim_{t\to+\infty} \frac{W_1(t)}{t} = \dot{W}_a + \dot{W}_m$$

sum of the entropy terms
vanishes in the steady state

$$\dot{W}_a = 2E_0 \lim_{t\to+\infty} \frac{1}{t} \sum_{\text{flip } s} \frac{1 - m_{i,j} s}{\rho_{i,j}}$$

alignment dissipation

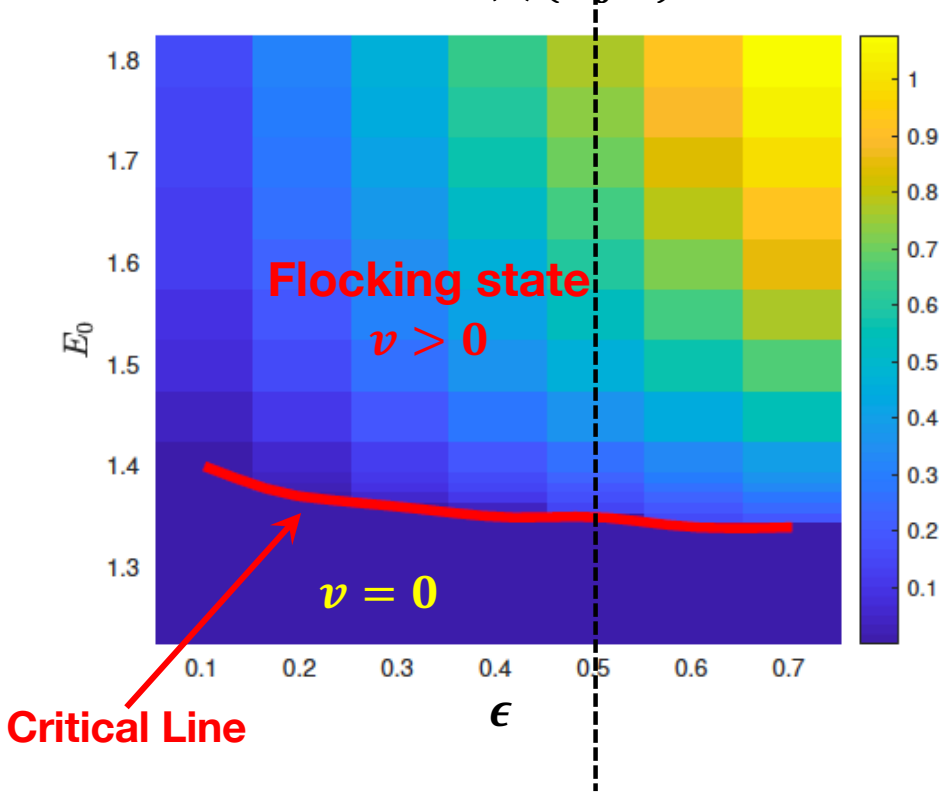
$$\dot{W}_m = \lim_{t\to+\infty} \frac{1}{t} \sum_{\text{hop } (s,\Delta x)} \Delta x s \ln\left(\frac{1+\epsilon}{1-\epsilon}\right) = 2D\epsilon N \ln\left(\frac{1+\epsilon}{1-\epsilon}\right)$$

motion dissipation

The average speed (order parameter) and energy dissipation rate in AIM

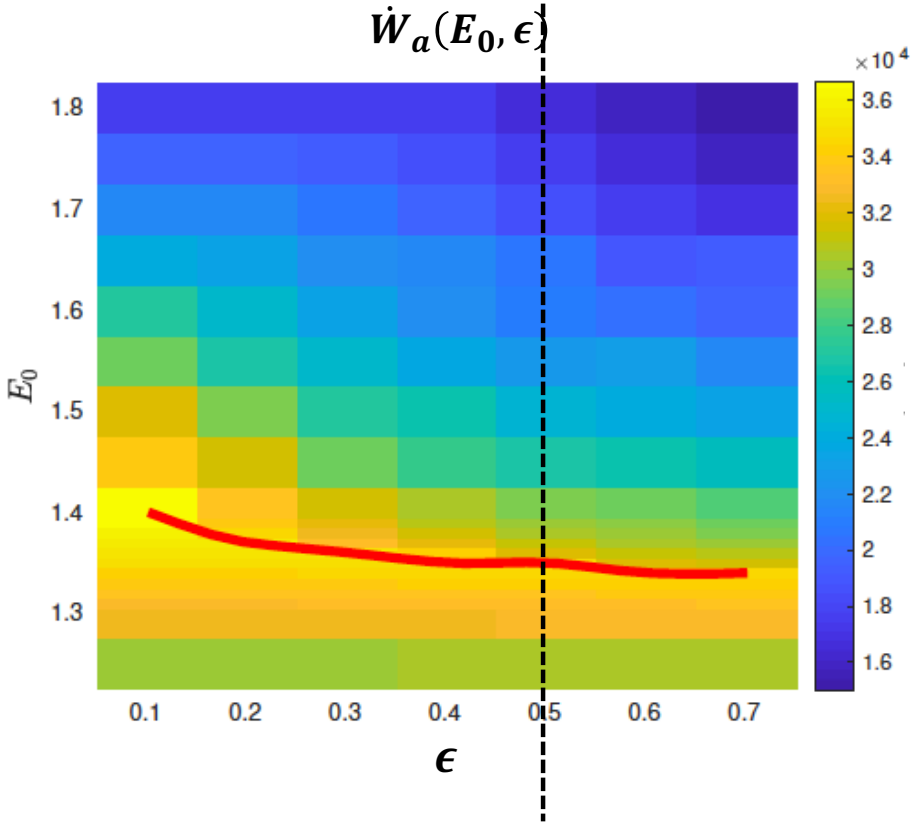
Order parameter

$v \equiv \langle s \rangle (E_0, \epsilon)$

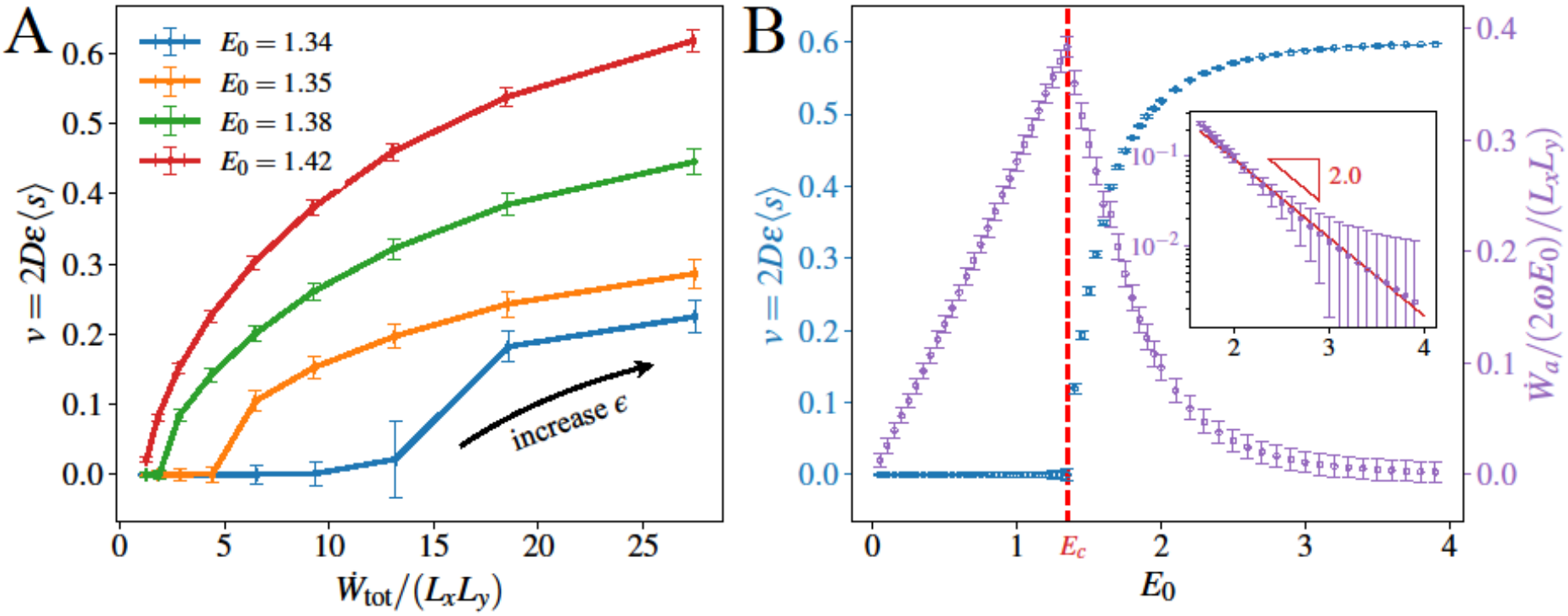


Alignment energy dissipation rate

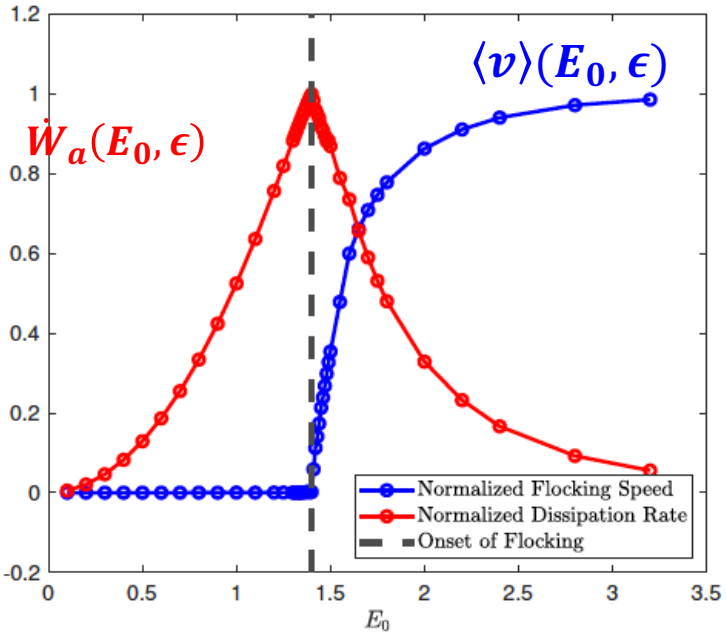
$\dot{W}_a(E_0, \epsilon)$



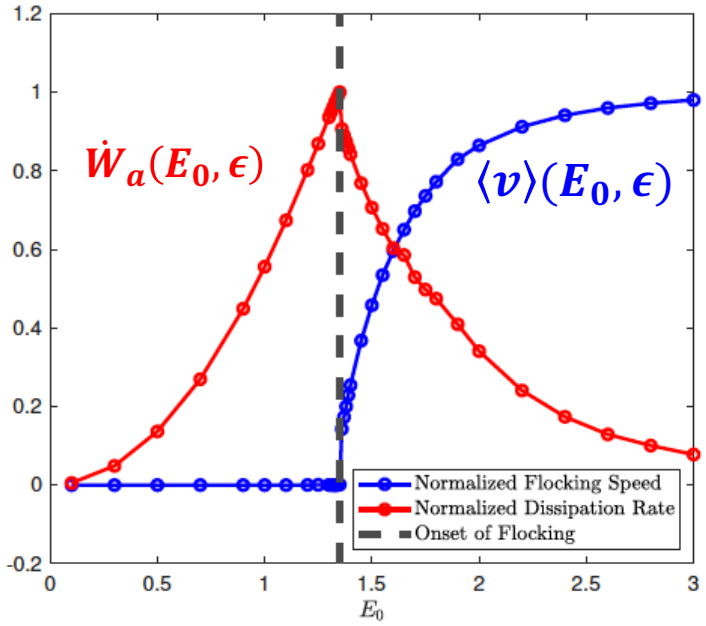
Th alignment energy dissipation peaks at the flocking transition with a cusp



The alignment energy cost peaks at the flocking transition point with a cusp (discontinuity in first derivative)



$\epsilon = 0.1$



$\epsilon = 0.5$

Understanding energy dissipation using a reduced model

General Theoretical Framework

$$\dot{W} = \lim_{t\to+\infty} \frac{1}{t} \left\langle \ln \frac{\mathcal{P}}{\mathcal{P}^R} \right\rangle$$

State variable $\mathbf{n} = (n^+_{1,1}, n^-_{1,1}, n^+_{1,2}, n^-_{1,2}, \ldots, n^+_{L_x,L_y}, n^-_{L_x,L_y})$.

Number of states $\sim (L_x L_y)^N$

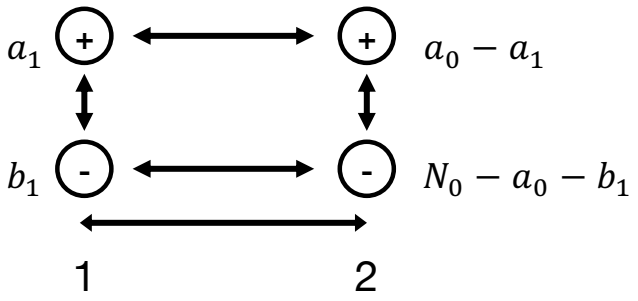
In a small (finite) lattice, we can enumerate all possible states and make analytical progress

Steady-state distribution $$\frac{\mathrm{d}P_{\mathbf{n}}(t)}{\mathrm{d}t} = \sum_{\mathbf{n}'} (k_{\mathbf{n}'\to\mathbf{n}} P_{\mathbf{n}'} - k_{\mathbf{n}\to\mathbf{n}'} P_{\mathbf{n}}) = 0.$$

Energy dissipation rate $$\dot{W} = \sum_{\mathbf{n}<\mathbf{n}'} (J_{\mathbf{n}\to\mathbf{n}'} - J_{\mathbf{n}'\to\mathbf{n}}) \ln \frac{J_{\mathbf{n}}}{J_{\mathbf{n}'}}.$$

Baby step: two sites (minimum system that breaks detailed balance)

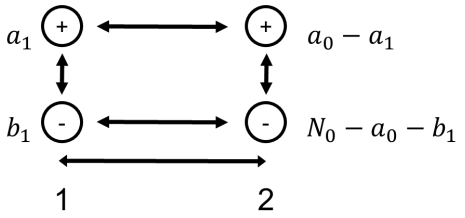
Two-site solution



- Two sites: $L_x = 2$, $L_y = 1$, $N_0 = \rho_0 L_x L_y$ particles.
  - total: a_0 spins up, $(N_0 - a_0)$ spins down.
  - site 1: a_1 spins up, b_1 spins down.
  - site 2: $(a_0 - a_1)$ up, $(N_0 - a_0 - b_1)$ down.
- From infinite DOF (field) to 3 DOF (a_0, a_1, b_1).
- Governed by the Master Equation
- Solution:
  - Numerical: $O(N_0^6)$ complexity, so ~50 particles.
  - Analytical: the limit of infinite particles $(\rho_0 \to \infty)$

$$
\begin{aligned}
\frac{\mathrm{d}P(a_0,a_1,b_1)}{\mathrm{d}t} &= (a_1+1)\cdot 2D\cdot P(a_0,a_1+1,b_1) + (b_1+1)\cdot 2D\cdot P(a_0,a_1,b_1+1) \\
&+ (a_0-a_1+1)\cdot 2D\cdot P(a_0,a_1-1,b_1) + (N_0-a_0-b_1+1)\cdot 2D\cdot P(a_0,a_1,b_1-1) \\
&+ (a_1+1)\cdot \omega e^{-E_0\frac{a_1-b_1+2}{a_1+b_1}}\cdot P(a_0+1,a_1+1,b_1-1) \\
&+ (b_1+1)\cdot \omega e^{E_0\frac{a_1-b_1-2}{a_1+b_1}}\cdot P(a_0-1,a_1-1,b_1+1) \\
&+ (a_0-a_1+1)\cdot \omega e^{-E_0\frac{2a_0-N-a_1+b_1+2}{N_0-a_1-b_1}}\cdot P(a_0+1,a_1,b_1) \\
&+ (N_0-a_0-b_1+1)\cdot \omega e^{E_0\frac{2a_0-N-a_1+b_1-2}{N_0-a_1-b_1}}\cdot P(a_0-1,a_1,b_1) \\
&- \Big[2N_0D + a_1\omega e^{-E_0\frac{a_1-b_1}{a_1+b_1}} + b_1\omega e^{E_0\frac{a_1-b_1}{a_1+b_1}} + (a_0-a_1)\omega e^{-E_0\frac{2a_0-N-a_1+b_1}{N_0-a_1-b_1}} \\
&\quad + (N_0-a_0-b_1)\omega e^{E_0\frac{2a_0-N-a_1+b_1}{N_0-a_1-b_1}}\Big] P(a_0,a_1,b_1).
\end{aligned}
$$

Solving the master equation



$$\frac{\mathrm{d}P}{\mathrm{d}t} = \mathcal{L} \cdot P$$

linear operator containing all the terms on the last slide

Marginal distribution $$Q(a_0) = \sum_{a_1=0}^{a_0} \sum_{b_1=0}^{N-a_0} P(a_0, a_1, b_1), \quad 1 = \sum_{a_0=0}^{N} Q(a_0) = \sum_{a_0=0}^{N} \sum_{a_1=0}^{a_0} \sum_{b_1=0}^{N-a_0} P(a_0, a_1, b_1).$$

Fast distribution $D \gg \omega$ ⇒ the distribution can be factorized $$P(a_0, a_1, b_1) = Q(a_0) \binom{a_0}{a_1} \binom{N - a_0}{b_1}$$

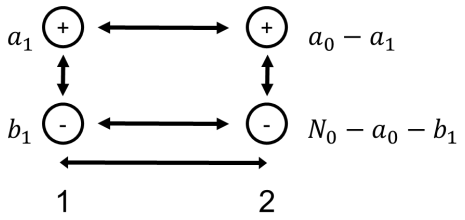
Master equation for $Q(a_0)$ $$\frac{\mathrm{d}Q(a_0)}{\mathrm{d}t} = Q(a_0 - 1)k_+(a_0 - 1) + Q(a_0 + 1)k_-(a_0 + 1) - [k_+(a_0) + k_-(a_0)]Q(a_0),$$

$$k_+(a_0) = \sum_{a_1=0}^{a_0} \sum_{b_1=0}^{N-a_0} \binom{a_0}{a_1} \binom{N - a_0}{b_1} \left[b_1 \omega e^{E_0 \frac{a_1 - b_1}{a_1 + b_1}} + (N - a_0 - b_1)\omega e^{E_0 \frac{2a_0 - N - a_1 + b_1}{N - a_1 - b_1}} \right],$$

$$k_-(a_0) = \sum_{a_1=0}^{a_0} \sum_{b_1=0}^{N-a_0} \binom{a_0}{a_1} \binom{N - a_0}{b_1} \left[a_1 \omega e^{-E_0 \frac{a_1 - b_1}{a_1 + b_1}} + (a_0 - a_1)\omega e^{-E_0 \frac{2a_0 - N - a_1 + b_1}{N - a_1 - b_1}} \right].$$

$$Q(a_0) = \frac{k_+(0)Q(0)}{k_-(a_0)} \prod_{n=1}^{a_0 - 1} \frac{k_+(n)}{k_-(n)}.$$

Solving the master equation

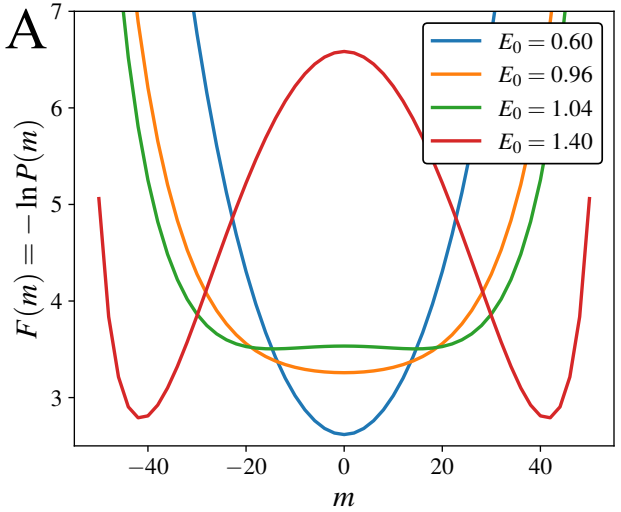


$$\frac{\mathrm{d}P}{\mathrm{d}t} = \mathcal{L} \cdot P \qquad P(a_0, a_1, b_1) = Q(a_0)\binom{a_0}{a_1}\binom{N-a_0}{b_1}$$

$$Q(a_0) = \frac{k_+(0)Q(0)}{k_-(a_0)} \prod_{n=1}^{a_0-1} \frac{k_+(n)}{k_-(n)}. \qquad z = \frac{a_0}{N}, \quad x = \frac{a_1}{a_0}, \quad y = \frac{b_1}{N-a_0}. \qquad N \to \infty$$

$$Q(z) = \frac{C}{k_-(z)} \exp\left(N \int_{\frac{1}{2N}}^{z-\frac{1}{2N}} \ln\left(\frac{k_+(t)}{k_-(t)}\right) \mathrm{d}t \right) = C \cdot \frac{e^{2E_0 z(1-z)}}{\sqrt{z(1-z)}} e^{-N(g(z)+2E_0 z(1-z))},$$

$$g(x) = x\ln x + (1-x)\ln(1-x) = -\ln 2 + 2\left(x-\frac{1}{2}\right)^2 + O\left[\left(x-\frac{1}{2}\right)^4\right],$$

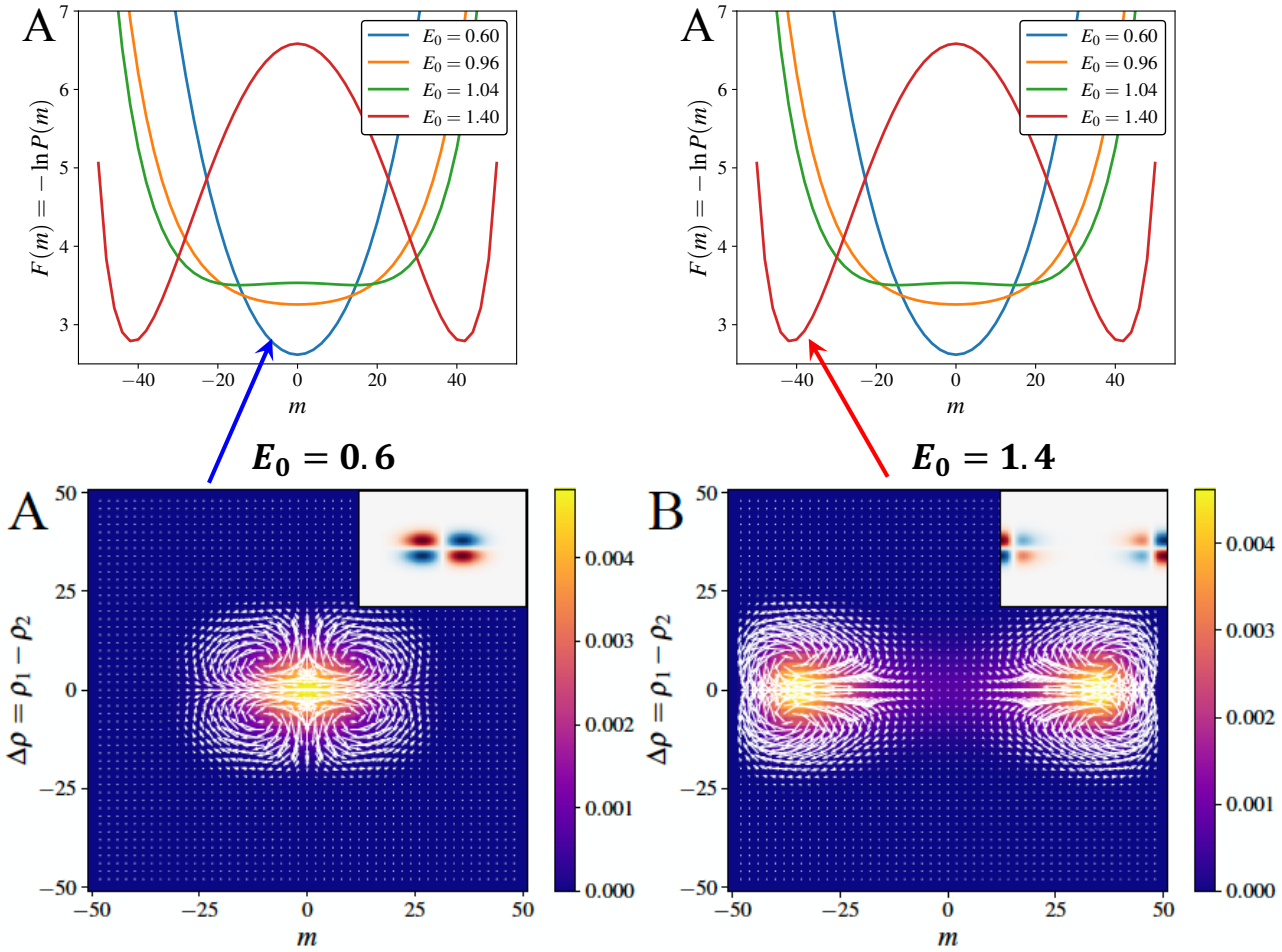


The free energy landscape

$$\frac{F(z)}{N} = -\frac{\ln Q(z)}{N} = [g(z) + 2E_0 z(1-z)] + O(N^{-1}).$$

magnetization: $m = N(2z-1)$

The system is non-equilibrium in both the ordered and disordered states



The energy dissipation (entropy production) rate in AIM

$$H = \sum_r H_r, H_r = -\frac{E_0}{2\rho_r} \sum_{r_i=r} \sum_{r_j=r}^{i\neq j} S_i S_j = -E_0 \left(\frac{m_r^2}{2\rho_r} - \frac{1}{2} \right). \qquad (\boldsymbol{\beta \to E_0})$$

$$\Delta W(t) = \begin{cases} -\Delta H, & \text{for flipping,} \\ \ln\left(\frac{1+\epsilon}{1-\epsilon}\right)\Delta r, & \text{for x-directional hopping,} \\ 0, & \text{for y-directional hopping,} \end{cases}$$

$$\dot{W}(E_0, \epsilon) = \lim_{T\to\infty} \frac{1}{T} \int_0^T \Delta W(t) dt$$

Energy cost for motion ($E_0 = 0$): $\dot{W}_m = \dot{W}(0, \epsilon) = 2ND\epsilon ln\left(\frac{1+\epsilon}{1-\epsilon}\right)$

Energy cost for alignment: $\dot{W}_a(E_0, \epsilon) = \dot{W}(E_0, \epsilon) - \dot{W}(0, \epsilon)$

Computing the free energy cost in 2-site model

Physical observables $$\langle A\rangle = \sum_{a_0,a_1,b_1} A(a_0,a_1,b_1)P(a_0,a_1,b_1) = \frac{\iiint A(x,y,z)w(x,y,z)e^{-NG(x,y,z)}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}{\iiint w(x,y,z)e^{-NG(x,y,z)}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}$$

$$w(x,y,z) = \frac{e^{2E_0 z(1-z)}}{\sqrt{x(1-x)y(1-y)}}, \quad G(x,y,z) = g(z) + zg(x) + (1-z)g(y) + 2E_0 z(1-z).$$

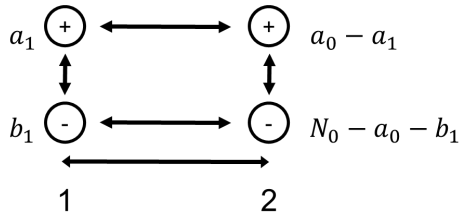
Alignment dissipation $$\frac{\dot{W}_a}{2} = \underbrace{\sum_{a_0,a_1,b_1} (J_+ - J_-)\ln\frac{J_+}{J_-}}_{\text{only count flipping on site 1}} = \sum_{a_0,a_1,b_1} P(a_0,a_1,b_1) b_1 \omega e^{E_0\lambda}\left(1-\frac{J_-}{J_+}\right)\ln\frac{J_+}{J_-} = \left\langle b_1\omega e^{E_0\lambda}\left(1-\frac{J_-}{J_+}\right)\ln\frac{J_+}{J_-}\right\rangle$$

$$\ln\frac{J_+}{J_-} = \underbrace{4E_0\frac{z(1-z)(x-y)}{zx+(1-z)y}}_{O(1)} + \underbrace{\frac{1}{N}\left[\frac{2E_0}{zx+(1-z)y} + 4E_0(z-1)\right]}_{O(N^{-1})} + \cdots = J_0 + J_1 N^{-1} + O(N^{-2})$$

(nondimensionlized) $$\dot{w}_a = \frac{1}{2\omega E_0}\sum_{\text{flip}}(J_+ - J_-)\ln\frac{J_+}{J_-} = N\langle w_1\rangle + \langle w_0\rangle + O(N^{-1})$$

evaluate using the saddle point method
(expansion near the saddle point)

Computing the free energy cost in 2-site model



$$z = \frac{a_0}{N}, \quad x = \frac{a_1}{a_0}, \quad y = \frac{b_1}{N - a_0}.$$

Alignment dissipation $\dot{w}_a = \frac{1}{2\omega E_0} \sum_{\text{flip}} (J_+ - J_-) \ln \frac{J_+}{J_-} = N \langle w_1 \rangle + \langle w_0 \rangle + O(N^{-1})$

evaluate using the saddle point method
(expansion near the saddle point)

$O(1)$ order: no number fluctuation, no dissipation

$$\text{Disordered phase: } \langle w_0 \rangle = w_0\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = 0,$$
$$\text{Flocking phase: } \langle w_0 \rangle = w_0\left(\frac{1}{2}, \frac{1}{2}, z^\star\right) = 0.$$

$$\frac{1}{2(1-2z^\star)} \ln \frac{1-z^\star}{z^\star} = E_0, \quad (E_0 > 1)$$

$O(N^{-1})$ order: expansion near the saddle point captures number fluctuation

$$\begin{aligned}
\langle w_1 \rangle &= \frac{1}{2} \sum_{\xi=x,y,z} \frac{\partial^2 w_1}{\partial \xi^2} \cdot \left(\frac{\partial^2 G}{\partial \xi^2}\right)^{-1} + \sum_{\xi=x,y,z} \frac{\partial w_1}{\partial \xi} \frac{\partial \ln w}{\partial \xi} \cdot \left(\frac{\partial^2 G}{\partial \xi^2}\right)^{-1} \\
&= \frac{1}{2} \sum_{\xi=x,y,z} \frac{\partial^2 w_1}{\partial \xi^2} \cdot \left(\frac{\partial^2 G}{\partial \xi^2}\right)^{-1} + 2E_0(1-2z) \frac{\partial w_1}{\partial z} \left(\frac{\partial^2 G}{\partial z^2}\right)^{-1} \\
&= \frac{1}{2} \left[\frac{\partial^2 w_1}{\partial x^2} \left(\frac{\partial^2 G}{\partial x^2}\right)^{-1} + \frac{\partial^2 w_1}{\partial y^2} \left(\frac{\partial^2 G}{\partial y^2}\right)^{-1} \right]
\end{aligned}$$

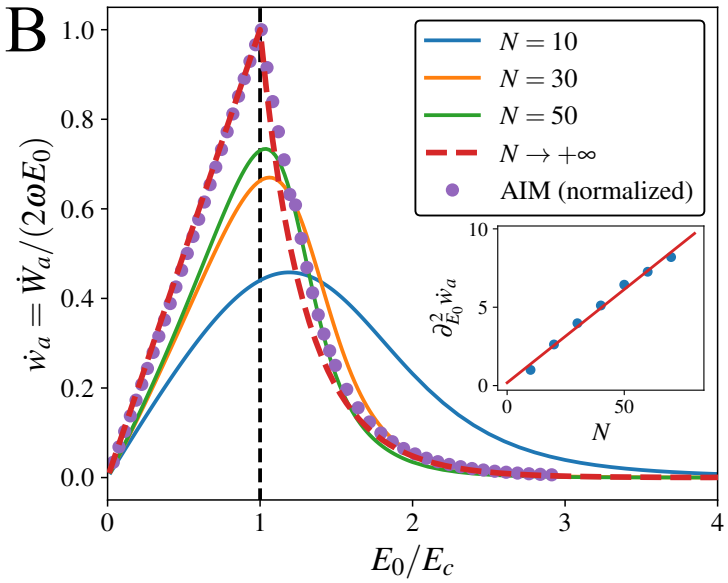
$$\dot{w}_a = \frac{\dot{W}_a}{2\omega E_0} = \langle w_1 \rangle = \begin{cases} E_0, & 0 < E_0 < 1 \\ 8E_0[z^\star(1-z^\star)]^{3/2}, & E_0 > 1 \end{cases},$$

Energy dissipation in the 2-site and full AIM

$$\dot{w}_a = \frac{\dot{W}_a}{2\omega E_0} = \langle w_1 \rangle = \begin{cases} E_0, & 0 < E_0 < 1 \\ 8E_0[z^\star(1-z^\star)]^{3/2}, & E_0 > 1 \end{cases}, \quad \frac{1}{2(1-2z^\star)} \ln \frac{1-z^\star}{z^\star} = E_0, \quad (E_0 > 1)$$

Cusped maximum at the critical point!

Linear increase in the disordered phase



Exponential decay in the highly ordered phase

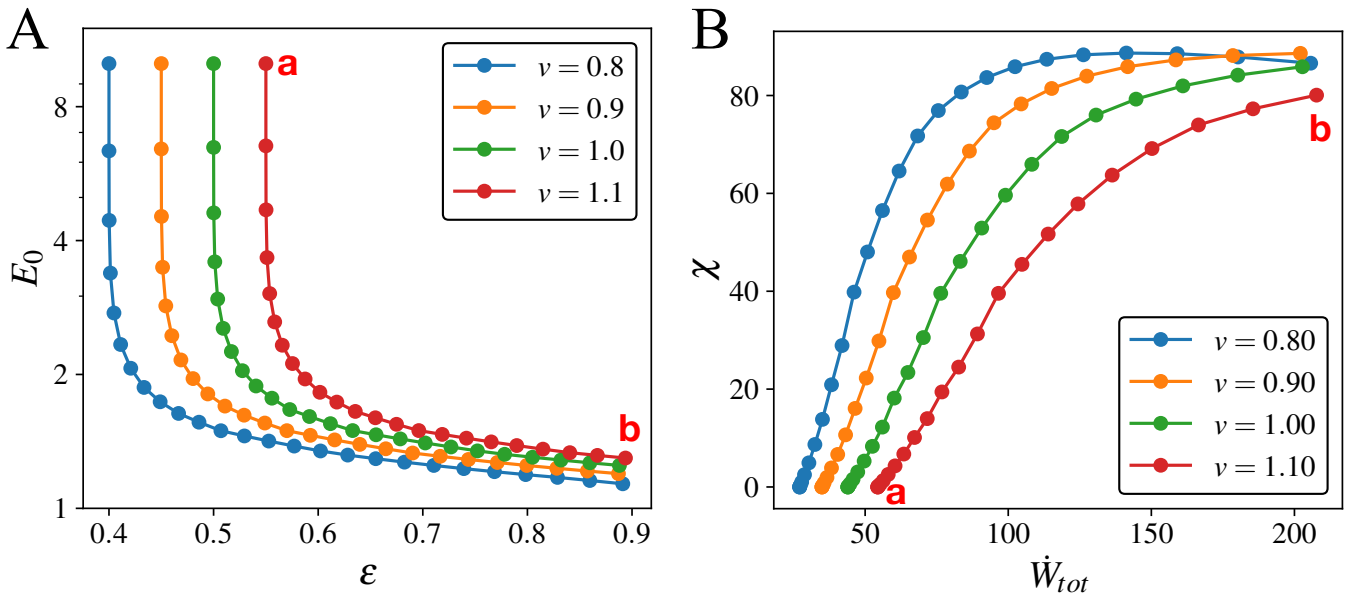
The energy-speed-sensitivity tradeoff in flocking

external field

$$H_r(m_r, \rho_r) - hm_r \qquad k_{s\to(-s)} = \omega \exp\left[-s\left(E_0 \frac{m}{\rho} + h\right)\right]$$

Equal-speed lines

sensitivity $\chi = \frac{\partial m}{\partial h}|_{h=0}$



Some general take-home messages

A continuous energy dissipation (cost) is needed for creating and maintaining order (generally defined) in nonequilibrium systems.

The cost directly constrains the functional performance of the system.

The cost-performance tradeoff relation provides a new perspective for investigating the mechanism and/or design principle of the underlying systems (natural or artificial).

Thank you!