Informatic vs Thermodynamic Entropy Production in Active Systems

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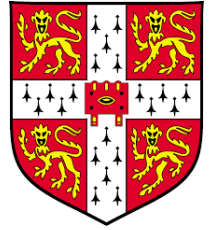
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Informatic vs Thermodynamic Entropy Production in Active Systems

- Stochastic Thermodynamics for particles and fields

- When $F \neq E - TS$:

  - Coarse-grained active matter

  - Informatic EPR $\neq$ Thermodynamic

- When $F = E - TS$:

  - Restoring Thermodynamics when appropriate

- Ambiguities under $t \rightarrow -t$

- Conclusions

Stochastic Thermodynamics

overdamped particle
$$\dot{x} = -M\frac{dV}{dx} + \sqrt{2D}\Lambda$$

$D = Mk_BT,$
$$\mathbb{P}[\Lambda(t)] = \mathcal{N}\exp\left[-\frac{1}{2}\int |\Lambda|^2 dt\right]$$

$$\exp[\Delta S/k_B] = \frac{\mathbb{P}_F}{\mathbb{P}_B} = \frac{\exp\left[-\frac{1}{4D}\int |\dot{x} + MV'|^2 dt\right]}{\exp\left[-\frac{1}{4D}\int |-\dot{x} + MV'|^2 dt\right]}$$

second law

$$T\Delta S = -\frac{k_BT}{4D}\int 4M\dot{x}V'\, dt = -\int_{t_1}^{t_2} \dot{x}\frac{dV}{dx}dt = -[V_2 - V_1]$$

Stochastic Thermodynamics

nonconservative force

$$\dot{x} = -M(V' + f) + \sqrt{2D}\Lambda$$

steady state EPR

$$T\dot{S}_{ss} = \lim_{t_2 - t_1 \to \infty} \frac{k_B T}{t_2 - t_1} \langle \ln \frac{\mathbb{P}_F}{\mathbb{P}_B} \rangle$$

$$= -\frac{\Delta V}{\infty} + \langle \dot{x}f \rangle_t$$

= rate of work by f

$\dot{S}_{ss}$ = Thermodynamic EPR

- measure of irreversibility
- quantifies heat flow

Stochastic Thermodynamics of Fields

e.g. scalar field for mixture of A, B molecules $\phi = \dfrac{n_A - n_B}{n_A + n_B}$

$$\dot{\phi} = -\nabla \cdot \mathbf{J}$$

$$\mathbf{J} = -M\nabla \frac{\delta F}{\delta \phi} + \sqrt{2D}\, \mathbf{\Lambda}(\mathbf{r}, t) \qquad\qquad D = Mk_B T$$

$$\mathbb{P}_{F,B} \propto \exp\left[-\frac{1}{4D} \int \left| \pm\mathbf{J} + M\nabla \frac{\delta F}{\delta \phi} \right|^2 \, d\mathbf{r}\, dt \right]$$

second law

$$T\Delta S = k_B T \ln \frac{\mathbb{P}_F}{\mathbb{P}_B} = -\int_{t_1}^{t_2} \mathbf{J} \cdot \nabla \frac{\delta F}{\delta \phi}\, d\mathbf{r}\, dt = -[F_2 - F_1]$$

Stochastic Thermodynamics of Fields

e.g. scalar field for mixture of A, B molecules $\quad \phi = \dfrac{n_A - n_B}{n_A + n_B}$

$$\dot{\phi} = -\nabla \cdot \mathbf{J}$$

$$\mathbf{J} = -M\nabla\frac{\delta F}{\delta \phi} + \sqrt{2D}\,\boldsymbol{\Lambda}(\mathbf{r}, t) + \mathbf{Y} \qquad \textbf{\textcolor{magenta}{Forcing Term}}$$

$$\mathbb{P}_{F,B} \propto \exp\left[-\frac{1}{4D}\int \left|\pm\mathbf{J} + M\nabla\frac{\delta F}{\delta\phi} - \mathbf{Y}\right|^2 d\mathbf{r}\,dt\right]$$
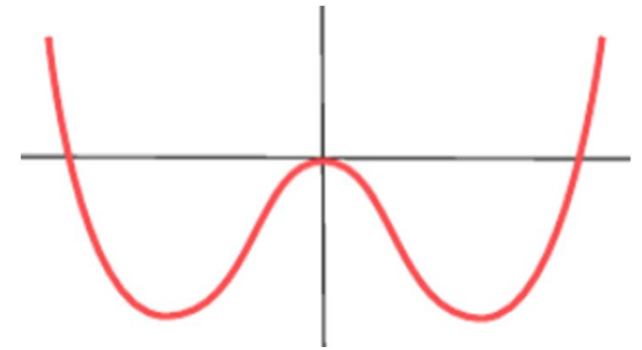
steady state EPR

$$T\dot{S}_{ss} = \lim_{t_2 - t_1 \to \infty} \frac{k_B T}{t_2 - t_1}\langle \ln\frac{\mathbb{P}_F}{\mathbb{P}_B}\rangle = -\frac{\Delta\!\!\!/F}{\infty}\!\!\!\Big/ + \int \frac{\langle \mathbf{J}\cdot\mathbf{Y}\rangle_t}{M}\,d\mathbf{r}$$

Minimal Models of Active Phase Separation

Dynamics of above form with

$$F = \int \left[\frac{a}{2}\phi^2 + \frac{b}{4}\phi^4 + \frac{\kappa}{2}(\nabla\phi)^2 \right] d\mathbf{r}$$

a < 0 gives phase separation: **Model B**

lowest order local TRS-breaking terms:

$$\mathbf{Y} = -\lambda\nabla(\nabla\phi)^2 + \zeta(\nabla^2\phi)\nabla\phi$$

Active Model B   B+

steady state EPR

$$T\dot{S}_{ss} = \lim_{t_2-t_1\to\infty} \frac{k_B T}{t_2 - t_1}\langle \ln \frac{\mathbb{P}_F}{\mathbb{P}_B} \rangle = -\cancel{\frac{\Delta F}{\infty}} + \int \frac{\langle \mathbf{J}\cdot\mathbf{Y}\rangle_t}{M}\, d\mathbf{r}$$

Active Model B/B+: No Thermodynamics in General

e.g. $\phi = \dfrac{n_A - n_B}{n_A + n_B}$ A = sheep, B = goats

$$\mathbf{J} = -M\nabla\frac{\delta F}{\delta\phi} + \mathbf{Y} + \sqrt{2D}\,\mathbf{\Lambda}$$

integrable + not + noise

Informatic EPR

$$\mathcal{S} = \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \langle \ln \frac{\mathbb{P}_F}{\mathbb{P}_B} \rangle = \int \frac{\langle \mathbf{J}\cdot\mathbf{Y}\rangle_t}{D} d\mathbf{r} \equiv \int \sigma(\mathbf{r}) d\mathbf{r}$$
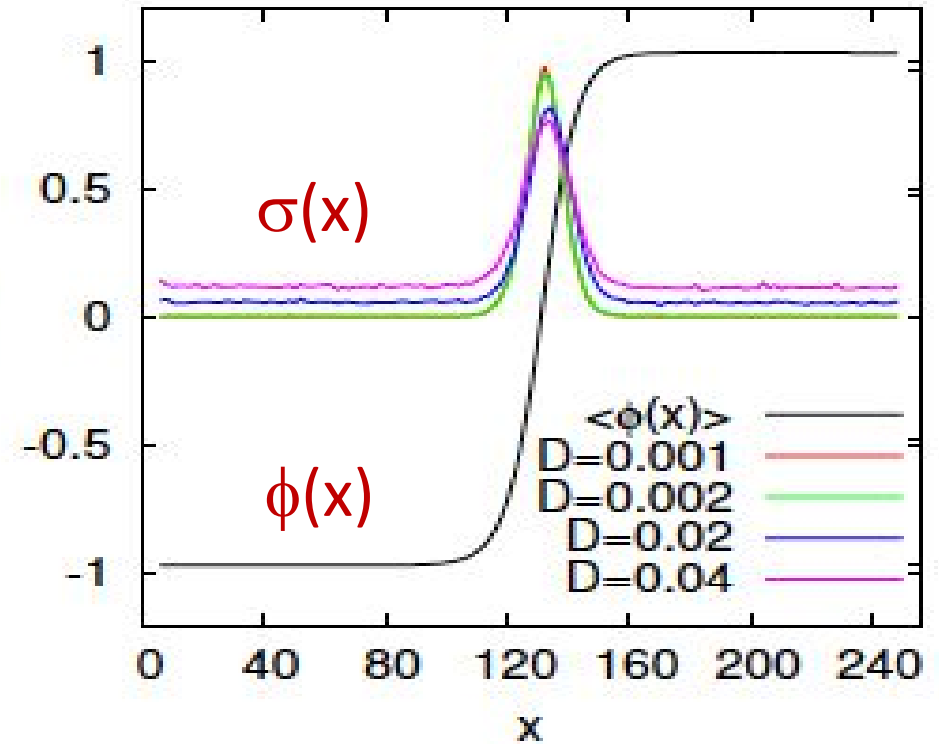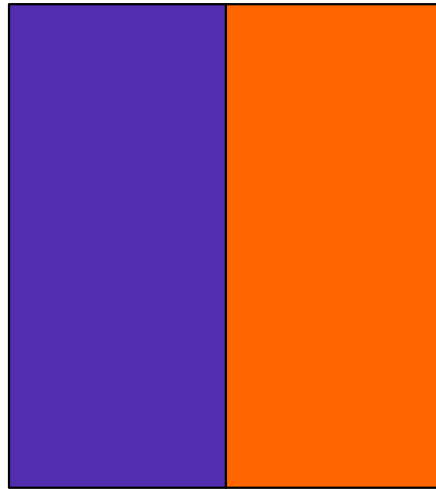
$$\neq \frac{\dot{S}_{ss}}{k_B}$$

unless $F = E - TS$
$D = Mk_BT$
Y = forces (not psychology)

IEPR as Irreversibility Measure

e.g. AMB

$\sigma \propto D^1$ bulk phases, $\propto D^0$ at interface

Generic scalings of IEPR density σ for coarse-grained fields:

D^{-1}: dynamics breaks TRS/DB at deterministic level

D^0: TRS/DB broken by leading-order fluctuations

$D^{1,2...}$: only broken at higher order

Thermodynamic vs Informatic EPR

Sheep-Goat phase separation: $\dot{S}_{ss} >>>>>> k_B \mathcal{S}$

Full EPR:

    dominated by microscopics, no insight into macro dynamics

    backward path must reverse metabolism as well as motion

IEPR:

    self-contained probe of macro dynamics

    depends on our definition of backward path [later]

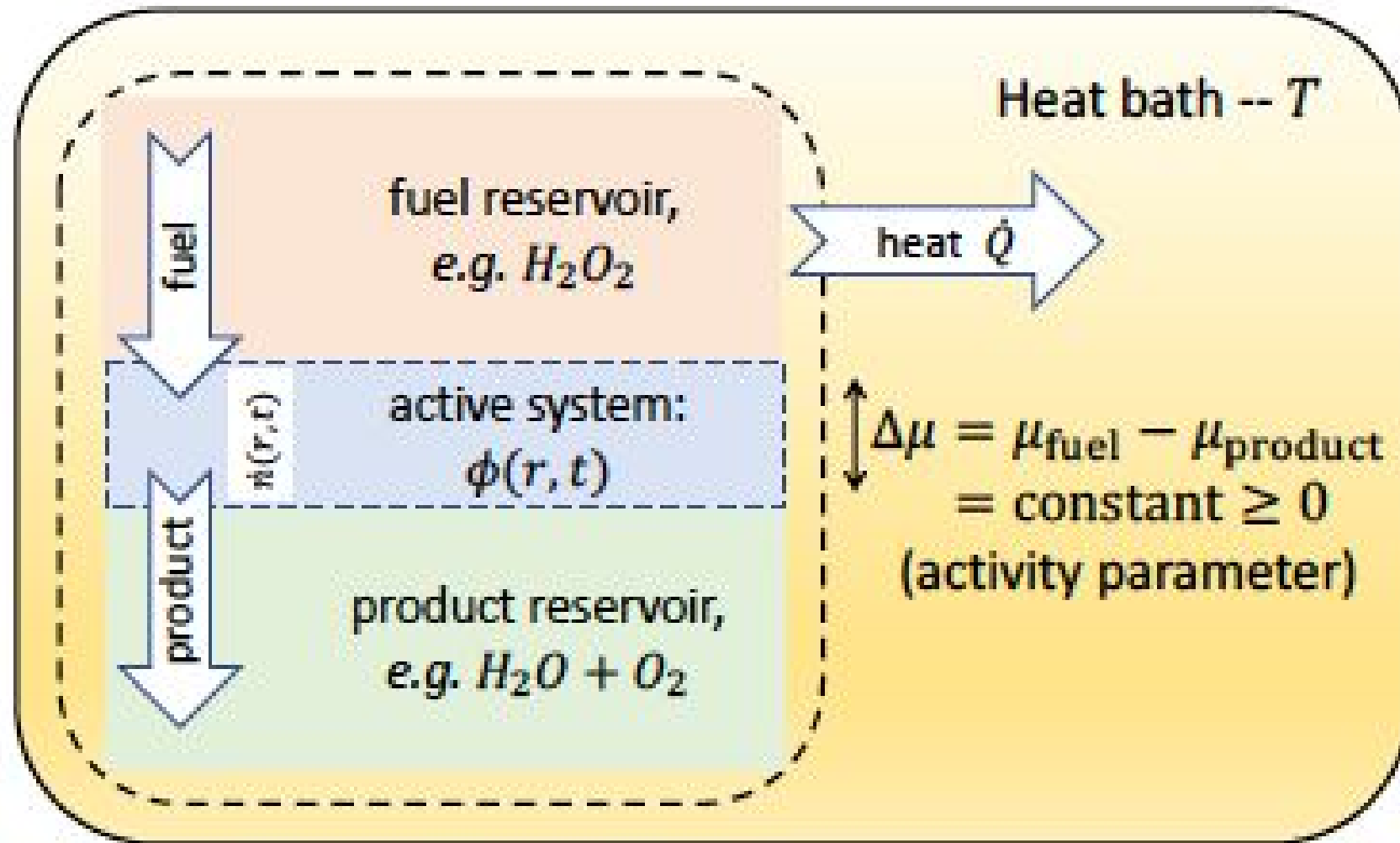**Subcellular active phase separation:** $F = E - TS \dots, \quad \dot{S}_{ss} \geq k_B \mathcal{S}$

IEPR: coarse-grained dynamics with active terms **Y**

EPR: must includes chemical processes giving rise to **Y**

) IEPR and EPR distinct but relatable in principle: How?

Thermal Active Matter

Near-equilibrium system, T well defined, $F = E - TS \dots, D = Mk_BT$

Markovich et al, arXiv:2008.06735 = PRX in press

Thermal Active Matter

Near-equilibrium system, T well defined, $F = E - TS \ldots, D = Mk_BT$

Chemical drive: $\Delta\mu = \mu_{\mathrm{ATP}} - \mu_{\mathrm{ADP}} > 0$

Simplest illustration (for more see PRX):

$\phi(\mathbf{r},t)$ = composition variable for binary mixture

$n(\mathbf{r},t) = (n_{\mathrm{ATP}} - n_{\mathrm{ADP}})/2$ = local reaction coordinate

Linear Irreversible Thermodynamics:

$$(\mathbf{J} , \dot{n}) = \mathbb{L} \cdot \begin{pmatrix} -\nabla \delta F/\delta\phi \\ \Delta\mu \end{pmatrix} \qquad + \text{ noise terms}$$

$\mathbb{L}$ = Onsager matrix

Markovich et al, arXiv:2008.06735 = PRX in press

Thermal Active Matter

Onsager reciprocity:

if
$$\mathbf{J} = -M\nabla\frac{\delta F}{\delta\phi} + \mathbf{Y} + \sqrt{2D}\,\mathbf{\Lambda}$$

active term $\mathbf{Y} = \Delta\mu\,\mathbf{g}$

[**g** = $\mathbb{L}_{12}$ = off-diagonal Onsager coupling]

then
$$\dot{n} = \gamma\,\Delta\mu - \mathbf{g}\cdot\nabla\frac{\delta F}{\delta\phi} + \sqrt{2\gamma k_B T}\Lambda'$$

Note: nonzero $\mathbb{L}_{12}$)
- noise terms for **J**, n are correlated
- the off-diagonal noise is multiplicative
- spurious drift terms require attention

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Thermal Active Matter

Full EPR: $\quad T\dot{S}_{ss} = \lim_{\Delta t \to \infty} \frac{k_B T}{\Delta t} \langle \ln \frac{\mathbb{P}_F}{\mathbb{P}_B} \rangle = \int \langle \dot{n}\, \Delta\mu \rangle_t \, d\mathbf{r}$

= rate of chemical work $\qquad$ [compare $\langle \dot{x} f \rangle_t$ for single particle]

$\dot{n}$ equation: $\quad \dot{n}\, \Delta\mu = \gamma(\Delta\mu)^2 - \mathbf{Y} \cdot \nabla \frac{\delta F}{\delta \phi} + \text{noise}$

sub **J** equation: $\qquad \nabla \frac{\delta F}{\delta \phi} = \frac{1}{M}\left(\mathbf{Y} - \mathbf{J} + \text{noise} \right)$

then $\quad \dfrac{\dot{S}_{ss}^{\text{TOT}}}{k_B} = \displaystyle\int \left[\underbrace{\frac{\langle \mathbf{J} \cdot \mathbf{Y} \rangle_t}{D}} + \frac{\gamma(\Delta\mu)^2}{T} - \frac{\langle \mathbf{Y} \cdot \mathbf{Y} \rangle_t}{D} \right] d\mathbf{r}$
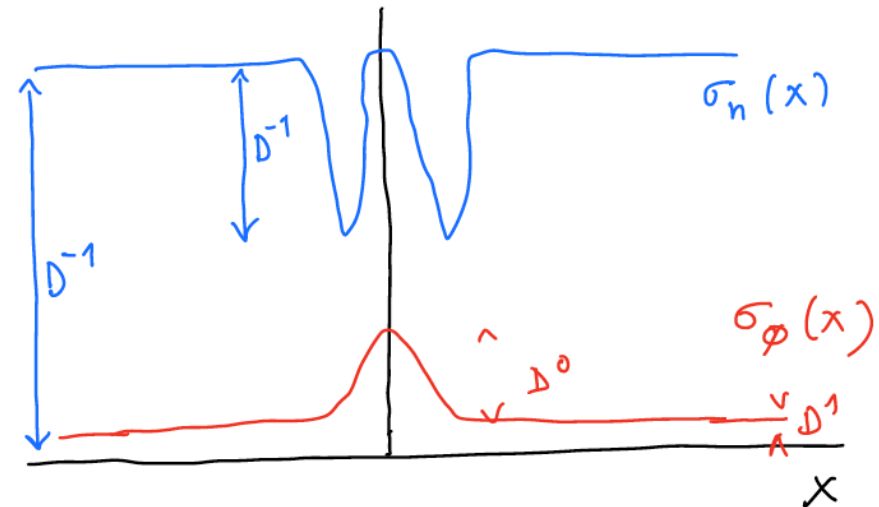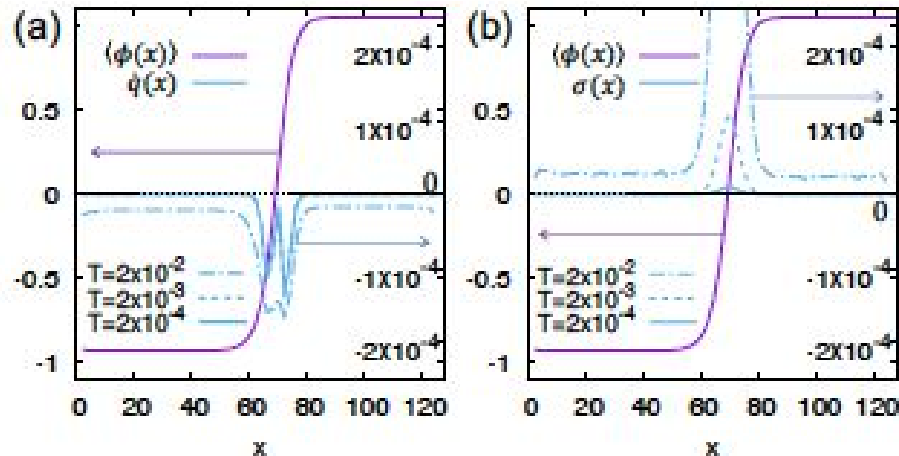
IEPR S[φ] + chemical part ≥ 0 via $\mathbb{L} \geq 0$

Markovich et al, arXiv:2008.06735 = PRX in press

IEPR vs Full EPR: Active Model B

Active term $\quad\quad \mathbf{Y} = -\lambda\nabla(\nabla\phi)^2$

local IEPR density: $\quad\quad \sigma_\phi \propto D^{0,1}$ for interface, bulk

chemical EPR density: $\quad \sigma_n \propto D^{-1}$ everywhere (ϕ-dependent)

- reduced $\dot{n}\,\Delta\mu$ where $|r^2\phi|$ large (interfaces)
- chemistry works locally against F to maintain $\dfrac{\delta F}{\delta\phi} \propto \lambda$
- similar results for other models

Markovich et al, arXiv:2008.06735 = PRX in press

What is a Backward Path?

Thermal active matter: $Q = T\dot{S}_{ss}$ is measurable in principle
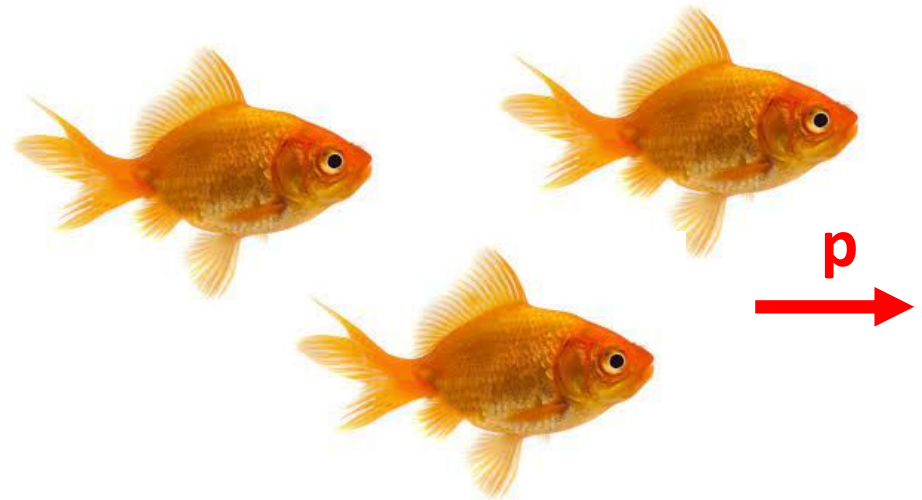
$)$ only one correct definition of $\mathbb{P}_B$

Toner-Tu Dilemma

Toner-Tu: **p** is a current
$)$ $TR_1(\mathbf{p}) = -\mathbf{p}$

Polar LC models: **p** is structural
$)$ $TR_2(\mathbf{p}) = +\mathbf{p}$

p

Forward path: **p** is both structural and a current
Backward path: we can choose TR_1 or TR_2
S_1 and S_2 separately interesting

Shankar & Marchetti PRE (2018), Dodhichi et al JSTAT (2018)
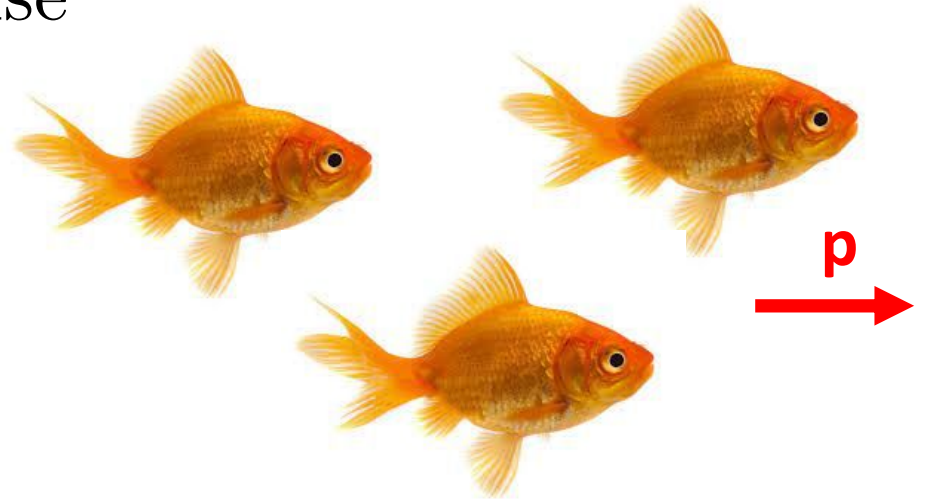*Borthne et al, arXiv:2008.06735, NJP **22,** 123012 (2020)*

Diffusive Flocking Model

$$\partial_t \rho = -\nabla \cdot \mathbf{J}$$

$$\mathbf{J} = w\mathbf{p} - M\nabla \frac{\delta F}{\delta \phi} + \text{noise}$$

$$\partial_t \mathbf{p} + \lambda \mathbf{p} \cdot \nabla \mathbf{p} = -\Gamma \frac{\delta F}{\delta \mathbf{p}} + \text{noise}$$

$$F[\rho, \mathbf{p}] = \dots$$

p

Results for various phases:

Polar liquid (uniform **p**): $S_{1,2} \sim D^0$

Polar liquid in field, TR(**h**) = -**h** (e.g. flow): $S_{1,2} \sim D^{0,-1}$

Polar liquid in field, TR(**h**) = +**h** (e.g. food): $S_{1,2} \sim D^{-1,0}$

*Borthne et al, arXiv:2008.06735, NJP **22**, 123012 (2020)*

Diffusive Flocking Model

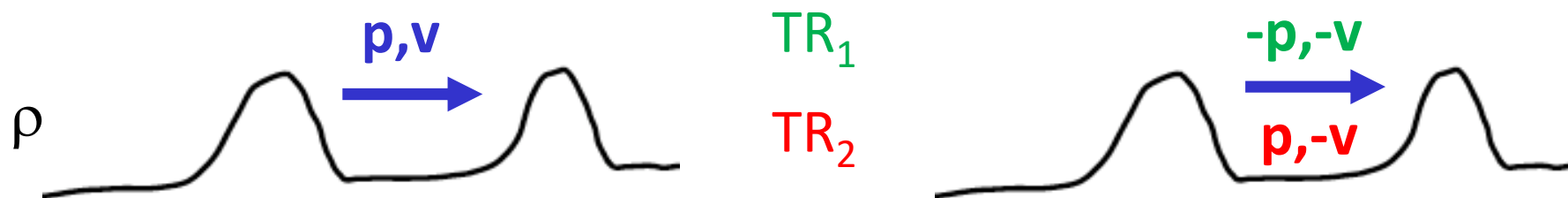$$\partial_t \rho = -\nabla \cdot \mathbf{J}$$

$$\mathbf{J} = w\mathbf{p} - M\nabla \frac{\delta F}{\delta \phi} + \text{noise}$$

$$\partial_t \mathbf{p} + \lambda \mathbf{p} \cdot \nabla \mathbf{p} = -\Gamma \frac{\delta F}{\delta \mathbf{p}} + \text{noise}$$

$$F[\rho, \mathbf{p}] = \ldots$$

Results for various phases:

Travelling waves/clusters: asymmetric waveform, $S_{1,2} \sim D^{-1}$

p,v   TR$_1$ **-p,-v**

ρ TR$_2$ **p,-v**

[D^0 in polar liquid: same, but for fluctuations]

*Borthne et al, arXiv:2008.06735, NJP **22,** 123012 (2020)*
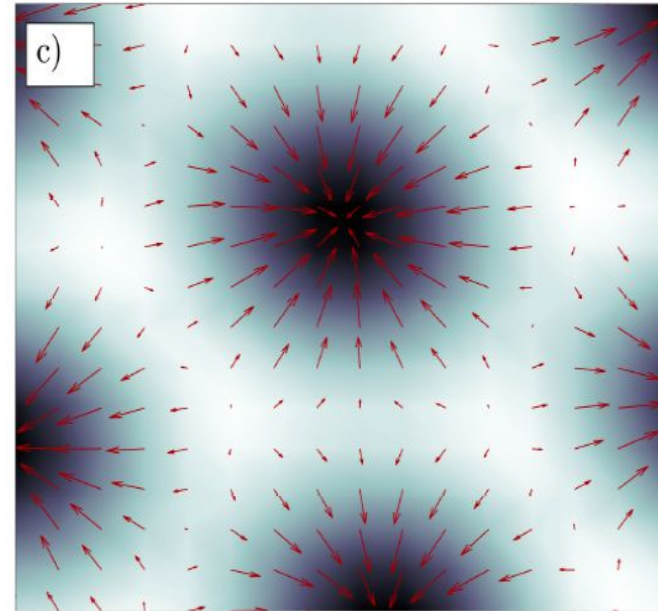
Diffusive Flocking Model

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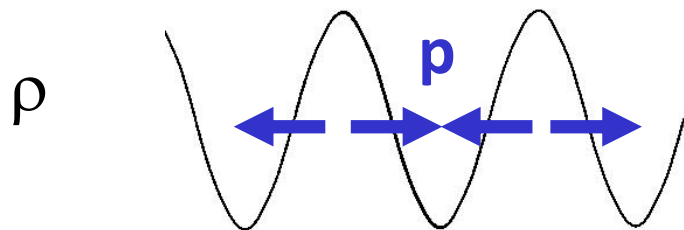
$$\partial_t \mathbf{p} + \lambda \mathbf{p} \cdot \nabla \mathbf{p} = -\Gamma \frac{\delta F}{\delta \mathbf{p}} + \text{noise}$$
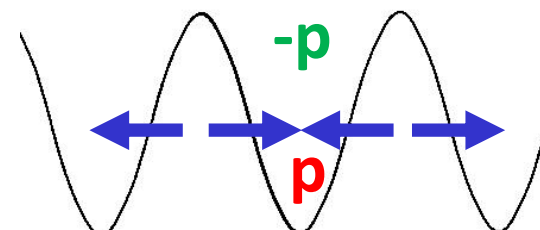
$$F[\rho, \mathbf{p}] = ...$$

Results for various phases:

Static crystal $S_{1.2} \sim D^{-1,0}$

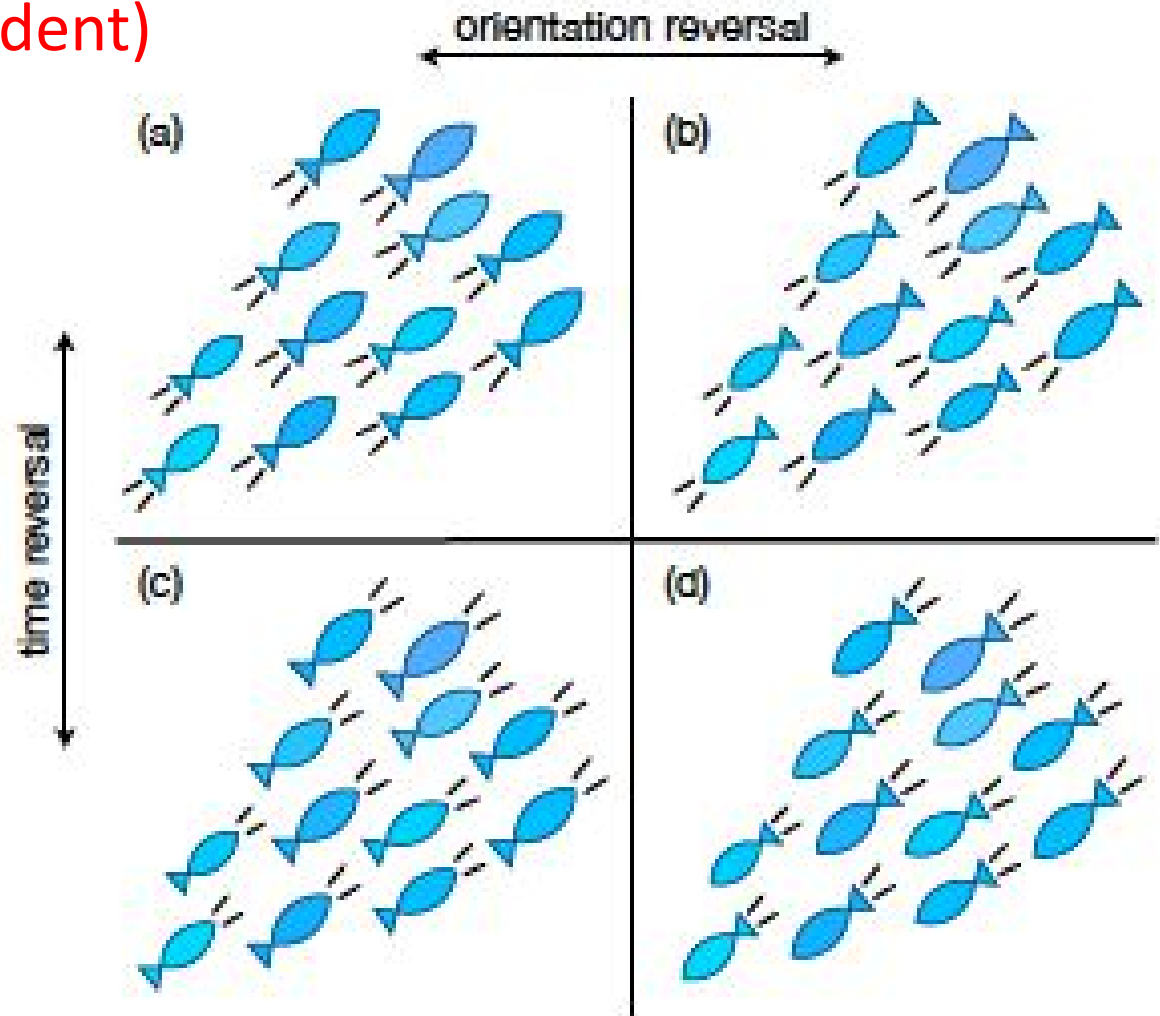ρ **p**   TR$_1$ TR$_2$ **-p**   **p**

*Borthne et al, arXiv:2008.06735, NJP **22,** 123012 (2020)*

Strategy far from Equilibrium

- Choose TR operation to minimize IEPR (choice is phase-dependent)

- See what remains

Review:
E. Fodor, R. Jack + MEC
arXiv:2104.06634

Shankar & Marchetti PRE (2018), Dodhichi et al JSTAT (2018)
*Borthne et al, arXiv:2008.06735, NJP **22,** 123012 (2020)*

Conclusions

Micro active matter, close to equilibrium (e.g. subcellular)

$$TÅ\dot{S}_{ss} = \int \langle \dot{n}\,\Delta\mu \rangle_t d\mathbf{r}$$ is true but not the whole story!

- IEPR is lower bound on full EPR
- Each identifies different aspects of local irreversibility

Markovich et al, arXiv:2008.06735 = PRX in press

Macro active matter, far from equilibrium (animals, bacteria)

- IEPR: useful and calculable for coarse-grained models
- Full EPR: neither ($\approx \infty$)

- Time-reversal operation is user-defined
- Differently interesting IEPR for each choice

*Borthne et al, arXiv:2008.06735, NJP **22,** 123012 (2020)*