Entropy Production Rate in Active Field Theories

Collaborators:

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EPR in Active Field Theories

- Entropy Production: General Formalism
- Field Theories of Active Matter
  - Active Model B/B+
  - Model A+B: microphase separation
  - Hydrodynamic Vicsek / Diffusive flocking model
  - Active B (and Active A) near critical point
- Conclusions

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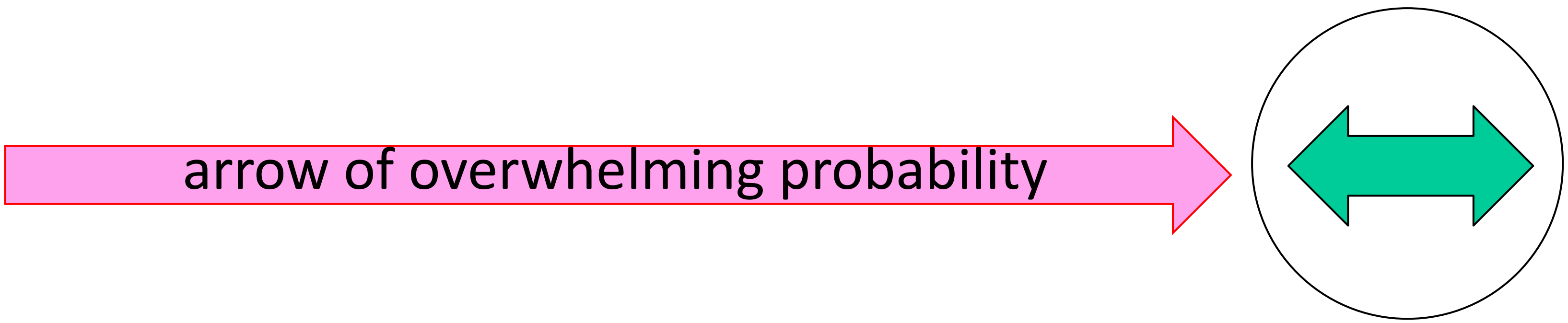
The Arrow of Time

Direction of time's arrow is set by $dS/dt \geq 0$

Once thermal equilibrium is reached, $dS/dt = 0$

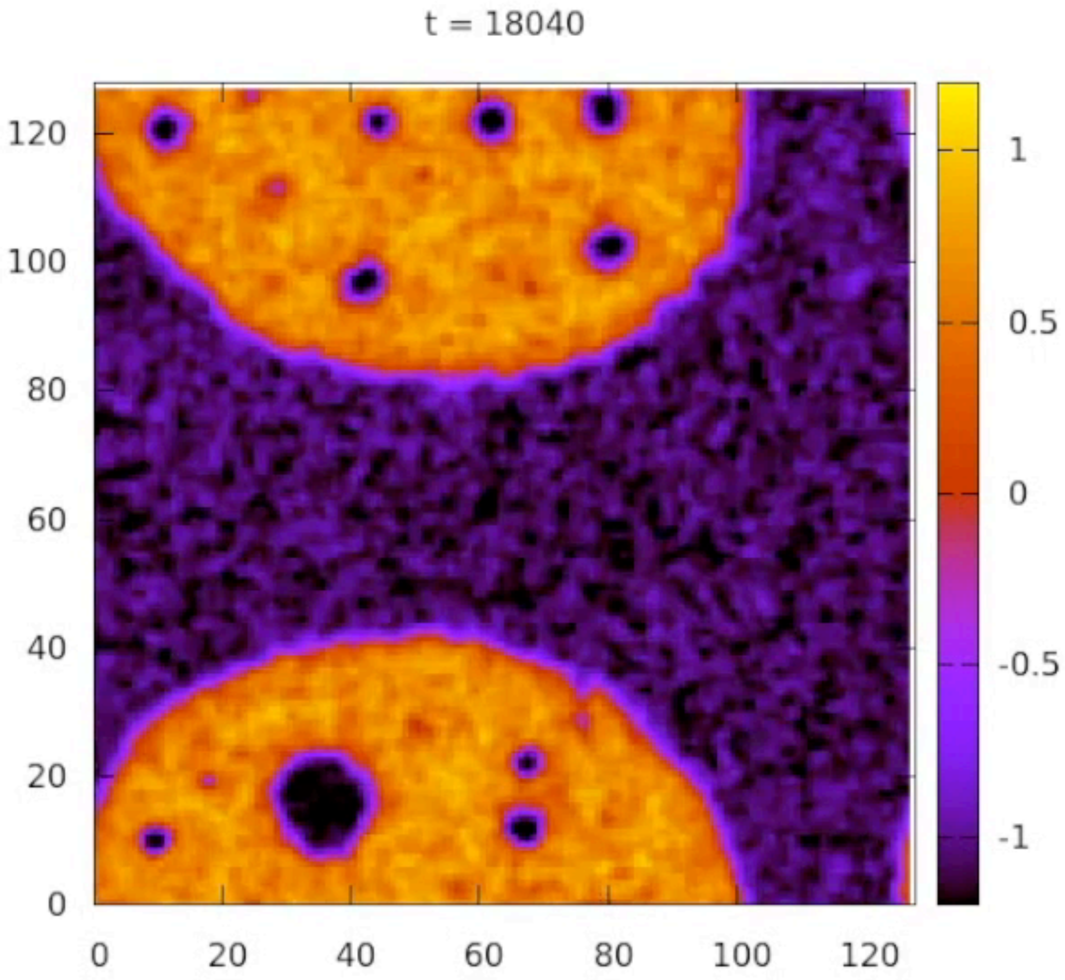
Corollary: In thermal equilibrium, you cannot tell if a movie is running forward or backwards



time-reversal symmetry (TRS)

more fundamentally: CPT symmetry

Active Matter: TRS Broken in Steady State



Time-Reversed Steady State: **not the same**

Active Model B+

Quantification via Stochastic Thermodynamics

In steady state

$$\frac{dS}{dt} = \frac{1}{t_2 - t_1} \log \left(\frac{\text{Prob(forward sequence)}}{\text{Prob(backward sequence)}} \right)$$

dS/dt **directly quantifies** the unlikelihood of reverse processes

review: U Seifert, Rep. Prog. Phys. (2012)

- dS/dt depends on scale of observation
- Field theories are coarse-grained $\Rightarrow$
  our dS/dt quantifies "visible" irreversibility only
- Directly calculable from field theory path integral

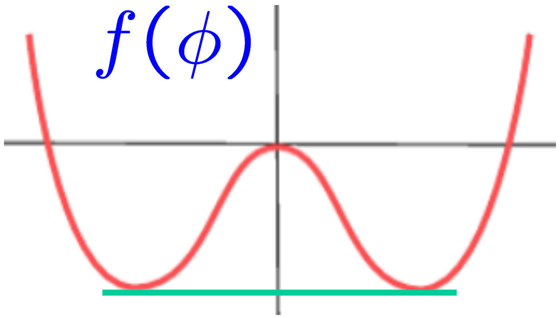
Continuum Theory of Phase Separation

$$\dot{\phi} = -\nabla.\mathbf{J}$$
$$\mathbf{J} = -\nabla\mu + \sqrt{2D}\boldsymbol{\Lambda}$$
$$\mu = a\phi + b\phi^3 - \kappa\nabla^2\phi$$

Λ = unit white noise
$D = k_B T\, M$
$M = 1$ mobility

MODEL B

$$\mu = \delta\mathcal{F}/\delta\phi$$
$$\mathcal{F} = \int dV [f(\phi) + \tfrac{\kappa}{2}(\nabla\phi)^2]$$
$$f(\phi) = \tfrac{a}{2}\phi^2 + \tfrac{b}{4}\phi^4$$



phase equilibria:
common tangent

$$\mu_1 = \mu_2$$
$$P_1 = P_2 \qquad \text{where } P = \mu\phi - f$$

Active Continuum Theory of Phase Separation

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

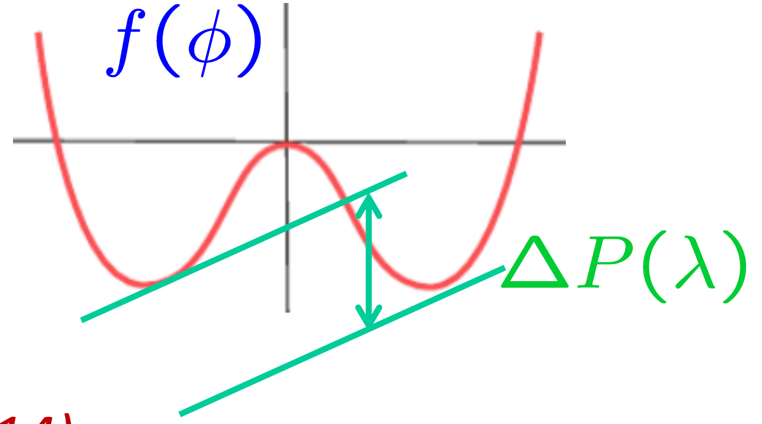
$$\mathbf{J} = -\nabla\hat{\mu} + \sqrt{2D}\mathbf{\Lambda}$$

$$\hat{\mu} = a\phi + b\phi^3 - \kappa\nabla^2\phi \;\; +\lambda(\nabla\phi)^2$$

ACTIVE MODEL B

$\lambda(\nabla\phi)^2 \neq \delta\mathcal{F}/\delta\phi$ for any $\mathcal{F}$

= **minimal** violation of TRS



Active Phase Separation:
uncommon tangent construction

R Wittkowski et al, Nat Comm 5 4351 (2014)
More general method: *A Solon et al, PRE (2018)*

Active Model B+

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

$$\mathbf{J} = -\nabla\hat{\mu} + \sqrt{2D}\mathbf{\Lambda} + \mathbf{J}_\zeta$$

$$\hat{\mu} = a\phi + b\phi^3 - \kappa\nabla^2\phi \ +\lambda(\nabla\phi)^2$$

Dealing with the ζ current:

$$\mathbf{J}_\zeta = -\nabla\mu_\zeta + \nabla \times \mathbf{H}$$

invisible for ϕ dynamics

Leaves nonlocal chemical potential (3D):

$$\mu_\zeta(\mathbf{r}) = -\int d\mathbf{r}' \frac{\nabla \cdot \mathbf{J}_\zeta}{4\pi|\mathbf{r} - \mathbf{r}'|}$$

$\mu = \mu_E + \mu_{NE}$

E. Tjhung et al., PRX 8, 031080 (2018)

Quantifying TRS Violations: Active Model B/B+

$$\nabla^{-1}\dot{\phi} = \mathbf{J} = -\nabla(\mu_{\mathsf{E}} + \mu_{\mathsf{NE}}) + (2D)^{1/2}\boldsymbol{\Lambda}$$

$$P[\phi] = \exp -\frac{1}{4D}\int_0^\tau dV\,dt|\nabla^{-1}\dot{\phi} + \nabla(\mu_{\mathsf{E}} + \mu_{\mathsf{NE}})|^2$$

$$\ln(P_{\mathsf{f}}/P_{\mathsf{b}}) = \frac{1}{D}\int_0^\tau dV\,dt(\nabla^{-1}\dot{\phi}\nabla\mu_{\mathsf{E}} + \nabla^{-1}\dot{\phi}\nabla\mu_{\mathsf{NE}})$$

$$= \frac{\Delta\mathcal{F}}{D} - \frac{1}{D}\int_0^\tau \dot{\phi}\mu_{\mathsf{NE}}\,dV\,dt$$

steady state: $$\frac{dS}{dt} = \lim_{\tau\to\infty}\frac{[\text{this}]}{\tau} = -\frac{1}{D}\int\langle\dot{\phi}\mu_{\mathsf{NE}}\rangle\,dV$$

C. Nardini et al., PRX 7, 021007 (2017)

Quantifying TRS Violations: Active Model B

$$\frac{dS}{dt} = \int \sigma(\mathbf{r})\, dV$$

steady state **local** entropy production rate density

$$\sigma(\mathbf{r}) = \langle \widehat{\sigma}(\mathbf{r}) \rangle$$

$$\widehat{\sigma}(\mathbf{r}) = -\lambda\dot{\phi}(\nabla\phi)^2/D$$

$$\doteq \nabla(a\phi + b\phi^3 - \kappa\nabla^2\phi + \lambda(\nabla\phi)^2).\nabla(\lambda(\nabla\phi)^2)/D$$

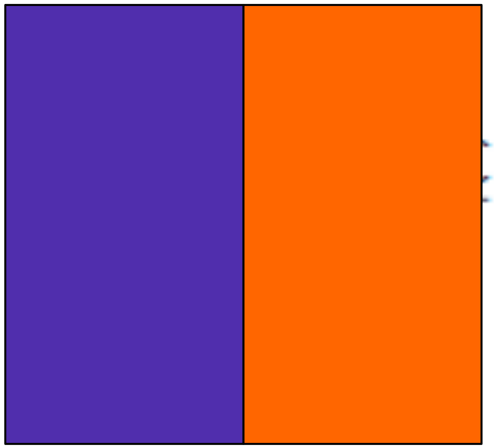
EPR is **local operator** in field theory

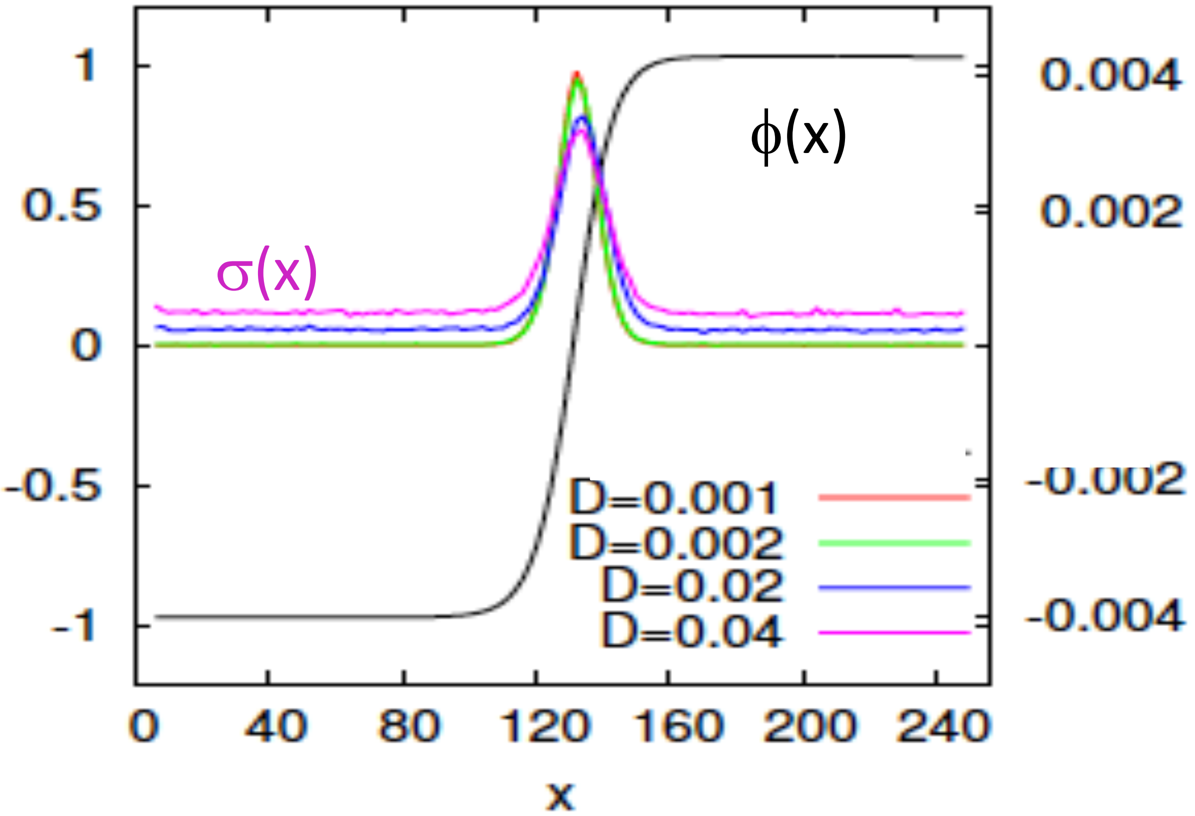
Global EPR calculable from stationary measure P[$\phi(\mathbf{r})$]

C. Nardini et al., PRX 7, 021007 (2017)

Quantifying TRS Violations: Active Model B

Interface between bulk phases





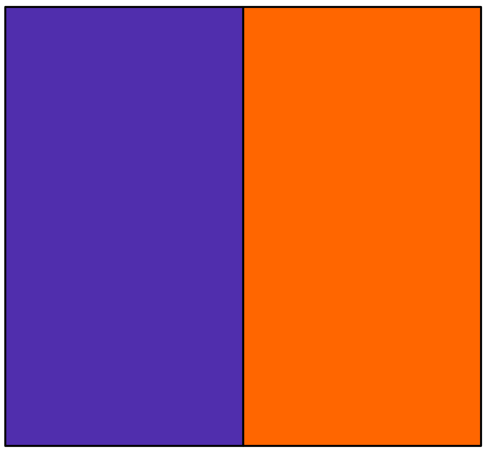
Low noise expansion:

D^0 contribution from interfaces, D^1 from bulk phases

C. Nardini et al., PRX 7, 021007 (2017)

Quantifying TRS Violations: Active Model B+

Interface between bulk phases



$$\hat{\sigma} = \dot{\phi}\mu_{NE}/D$$

$$\mu_{NE} = (\lambda - \zeta/2)(\nabla\phi)^2 - \zeta\nabla^{-2}[(\nabla^2\phi)^2 - (\nabla_\alpha\nabla_\beta\phi)^2]$$

important for curved interfaces

Low noise expansion:

D^0 contribution from interfaces, D^1 from bulk phases **unchanged**

C. Nardini et al., PRX 7, 021007 (2017)

Quantifying TRS Violations

Questions:

How should we understand these scalings?

How does EPR behave close to liquid-vapour critical point?

Preceded by:

(i) can TRS emerge upon coarse-graining?

(ii) what about vector fields?

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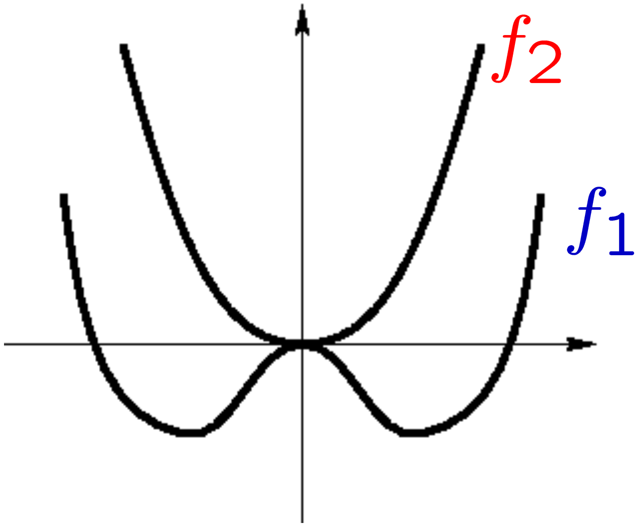
Active Microphase Separation: Model A+B

$$\dot{\phi} = -\nabla.\mathbf{J} \; -\Gamma\mu_2 + \sqrt{2D\Gamma}\Lambda'$$

$$\mathbf{J} = -\nabla\mu_1 + \sqrt{2D}\boldsymbol{\Lambda}$$

$$\mu_1 = a\phi + b\phi^3 - \kappa\nabla^2\phi$$

$$\mu_2 = \mu_1 + \alpha\phi$$



Simplified model of bacterial patterning

Cates et al PNAS 2010; Grafke et al PRL 2018, Li + MEC JSTAT 2000

- diffusive phase separation + population dynamics
- target density inside miscibility gap for B
- steady state: microphase separation

Active Microphase Separation: Model A+B

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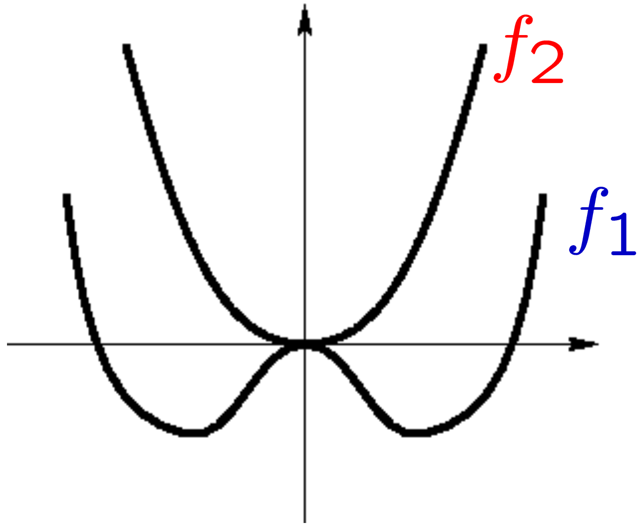


Simplified model of bacterial patterning

Cates et al PNAS 2010; Grafke et al PRL 2018, Li + MEC JSTAT 2000

A, B sectors each passive but with linearly different $\mu_{1,2}$

More generally: can make μ's differ in ϕ^3 term

can add λ, ζ for B and λ' for A

Active Microphase Separation: Model A+B

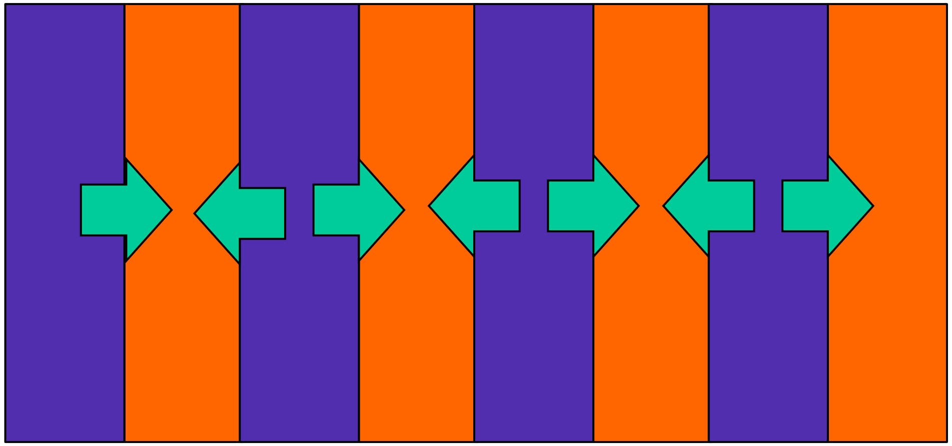
$$\dot{\phi} = -\nabla.\mathbf{J} - \Gamma\mu_2 + \sqrt{2D\Gamma}\Lambda'$$

$$\mathbf{J} = -\nabla\mu_1 + \sqrt{2D}\boldsymbol{\Lambda}$$

$$\mu_1 = a\phi + b\phi^3 - \kappa\nabla^2\phi$$

$$\mu_2 = \mu_1 + \alpha\phi$$

Model shows steady-state fluxes and large EPR:



- birth in dilute zones
- death in dense zones
- current in between

Emergent TRS

$$\dot{\phi} = -\nabla.\mathbf{J} \; -\Gamma\mu_2 + \sqrt{2D\Gamma}\Lambda'$$

$$\mathbf{J} = -\nabla\mu_1 + \sqrt{2D}\boldsymbol{\Lambda}$$

$$\mu_1 = a\phi + b\phi^3 - \kappa\nabla^2\phi$$

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Li + MEC JSTAT 2000

Emergent TRS

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$$\mathbf{J} = -\nabla\mu_1 + \sqrt{2D}\boldsymbol{\Lambda}$$

$$\mu_1 = a\phi + b\phi^3 - \kappa\nabla^2\phi$$

$$\mu_2 = \mu_1 + \alpha\phi$$

$$\frac{dS}{dt}[\phi] = 0$$

$$\frac{dS}{dt}[\phi, \mathbf{J}] \neq 0$$

ϕ dynamics (eliminating **J**) has exact detailed balance with (3D):

$$F = \int \left(f_1(\phi) + \frac{\kappa}{2}(\nabla\phi)^2 \right) d\mathbf{r} + \Gamma\alpha \int \frac{\phi(\mathbf{r})\phi(\mathbf{r}')}{4\pi|\mathbf{r} - \mathbf{r}'|} e^{-|\mathbf{r}-\mathbf{r}'|\Gamma^{1/2}} \, d\mathbf{r}d\mathbf{r}'$$

= a passive smectic

Li + MEC JSTAT 2000

Emergent TRS

$$\dot{\phi} = -\nabla.\mathbf{J} - \Gamma\mu_2 + \sqrt{2D\Gamma}\Lambda'$$

$$\mathbf{J} = -\nabla\mu_1 + \sqrt{2D}\mathbf{\Lambda}$$

$$\mu_1 = a\phi + b\phi^3 - \kappa\nabla^2\phi$$

$$\frac{dS}{dt}[\phi] = 0$$

$$\frac{dS}{dt}[\phi, \mathbf{J}] \neq 0$$

μ

Ye

- TRS can emerge upon eliminating degrees of freedom
- EPR depends on what you choose to watch
- Gives information about TRS breaking for retained variables

$$F = \int \left(f_1(\phi) + \frac{\kappa}{2}(\nabla\phi)^2 \right) d\mathbf{r}$$

$$+\Gamma\alpha \int \frac{\phi(\mathbf{r})\phi(\mathbf{r}')}{4\pi|\mathbf{r}-\mathbf{r}'|} e^{-|\mathbf{r}-\mathbf{r}'|\Gamma^{1/2}} d\mathbf{r}d\mathbf{r}'$$

= a passive smectic

Li + MEC JSTAT 2000

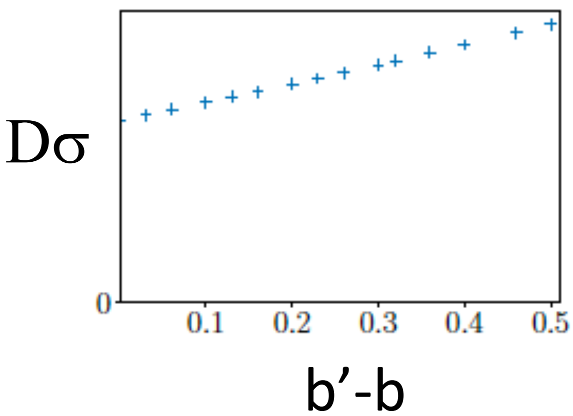
Further Results

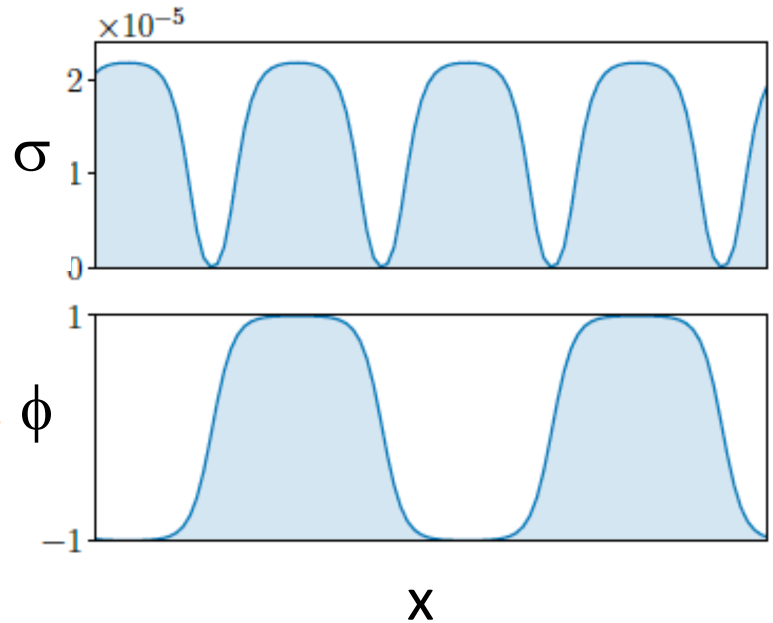
Suppose $\mu_2 = \mu_1 + \alpha\phi + (b'-b)\phi^3$

Emergence of full TRS on **J**-elimination is special to b'-b = 0

Before elimination

$\sigma \propto (cst + b'-b)D^{-1}$





Li + MEC arXiv 2000

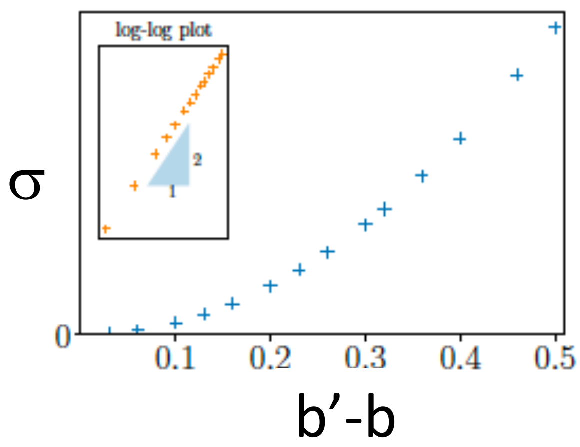
Further Results

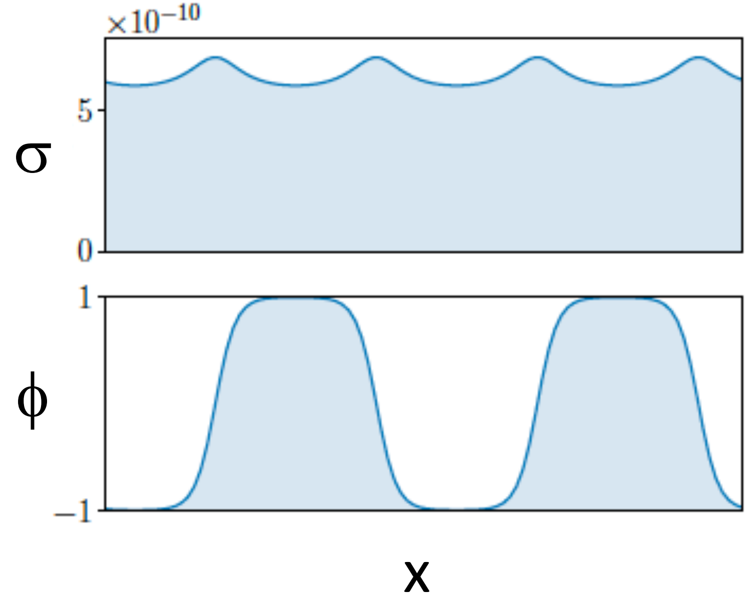
Suppose $\mu_2 = \mu_1 + \alpha\phi + (b'-b)\phi^3$

Emergent TRS on **J**-elimination is special to b'-b = 0

After elimination

$\sigma \propto (b'-b)^2 D^0$





Li + MEC arXiv 2000

Further Results

For local scalar Langevin fields (A, B, A+B type, additive noise)

Can express global EPR[ϕ(x)] in terms of quasipotential $\mathcal{V}$ [ϕ(x)].

Schematically:

$$\dot{\phi} = G(\phi, \nabla\phi \ldots) + \sqrt{2D}\,\zeta\Lambda \qquad \zeta\zeta^{\dagger} = K$$

$$EPR = A^{\dagger}K^{-1}A/D > 0 \text{ where } A = G + K\delta\mathcal{V}/\delta\phi$$

- asymmetric dynamics $A =$ (true dynamics) – (FDT for given K, $\mathcal{V}$)
- small-noise limit requires only mean-field solution for ϕ(x)

Li + MEC arXiv 2000

Quantifying TRS Violations

Questions:

How should we understand these scalings?

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First:

(i) can TRS emerge upon coarse-graining?

(ii) what about vector fields?

Active Vector Fields

Flocking models with scalar density and vector polarity

1. Hydrodynamic Vicsek model ⊂ Toner-Tu

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

$$\boldsymbol{J} = w\boldsymbol{P}$$

$$\partial_t \boldsymbol{P} + \lambda \boldsymbol{P} \cdot \nabla \boldsymbol{P} = -\frac{\delta F}{\delta \boldsymbol{P}} + \boldsymbol{\eta}$$

$$F[\rho, \boldsymbol{P}] = \int_{\mathcal{V}} \mathrm{d}\boldsymbol{x} \left(f(\rho, \boldsymbol{P}) + \frac{\nu_\rho}{2} |\nabla \rho|^2 + \frac{1}{2} (\nabla_\alpha P_\beta)^2 + \boldsymbol{P} \cdot \nabla \Phi(\rho, \boldsymbol{P}) \right)$$

$$f(\rho, \boldsymbol{P}) = \frac{a_\rho}{2} \rho^2 + \frac{1}{2}(1-\rho)|\boldsymbol{P}|^2 + \frac{1}{4}|\boldsymbol{P}|^4 \qquad \Phi(\rho, \boldsymbol{P}) = w_1 \rho - \frac{\kappa}{2}|\boldsymbol{P}|^2$$

$$\langle \eta_\alpha(\boldsymbol{x}, t) \eta_\beta(\boldsymbol{x}', t') \rangle = 2D\, \delta_{\alpha\beta} \delta(\boldsymbol{x} - \boldsymbol{x}') \delta(t - t')$$

Borthne, Fodor + MEC NJP 2000

Active Vector Fields

Flocking models with scalar density and vector polarity

2. Diffusive Flocking Model

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

$$\mu = \frac{\delta F}{\delta \rho}$$

$$\boldsymbol{J} = w\boldsymbol{P} - \gamma^{-1}\nabla\mu + \boldsymbol{\xi}$$

$$\langle \xi_\alpha(\boldsymbol{x}, t)\xi_\beta(\boldsymbol{x}', t')\rangle = 2D_\rho \delta_{\alpha\beta}\delta(\boldsymbol{x} - \boldsymbol{x}')\delta(t - t')$$

$$\partial_t \boldsymbol{P} + \lambda \boldsymbol{P} \cdot \nabla \boldsymbol{P} = -\frac{\delta F}{\delta \boldsymbol{P}} + \boldsymbol{\eta}$$

$$F[\rho, \boldsymbol{P}] = \int_{\mathcal{V}} \mathrm{d}\boldsymbol{x} \left(f(\rho, \boldsymbol{P}) + \frac{\nu_\rho}{2}|\nabla\rho|^2 + \frac{1}{2}(\nabla_\alpha P_\beta)^2 + \boldsymbol{P} \cdot \nabla\Phi(\rho, \boldsymbol{P}) \right)$$

$$f(\rho, \boldsymbol{P}) = \frac{a_\rho}{2}\rho^2 + \frac{1}{2}(1-\rho)|\boldsymbol{P}|^2 + \frac{1}{4}|\boldsymbol{P}|^4 \qquad \Phi(\rho, \boldsymbol{P}) = w_1\rho - \frac{\kappa}{2}|\boldsymbol{P}|^2$$

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Borthne, Fodor + MEC NJP 2000

Active Vector Fields

Key distinction

1. No noise in $\boldsymbol{J} = w\boldsymbol{P}$: polarization **must be odd** under TR

else P[backward path] = 0 : EPR = ∞

Borthne, Fodor + MEC NJP 2000

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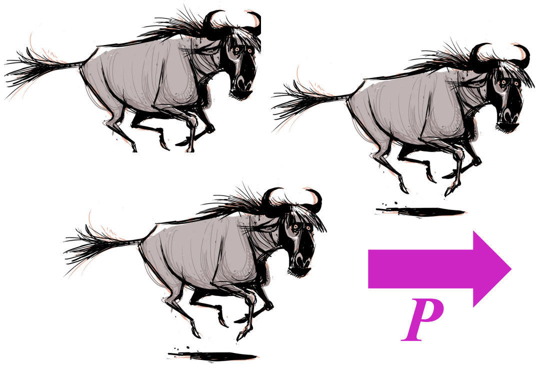
2. With noise in $\boldsymbol{J} = w\boldsymbol{P} + \ldots$ polarization is **even or odd** under TR

until specified, the model is **undefined** for EPR purposes



structural (liquid crystal) or dynamic (Toner-Tu)?

Borthne, Fodor + MEC NJP 2000

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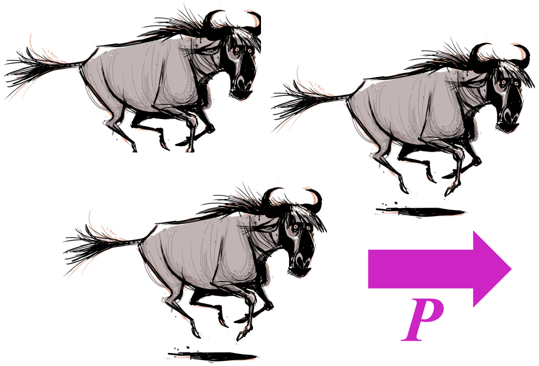

structural (liquid crystal)
or dynamic (Toner-Tu)?

can be both, for forward paths...
but not remain so upon on TR

Borthne, Fodor + MEC NJP 2000

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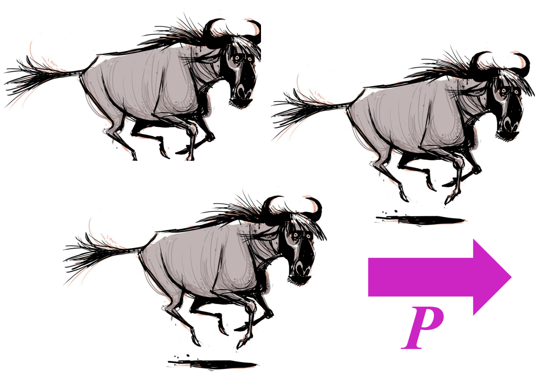
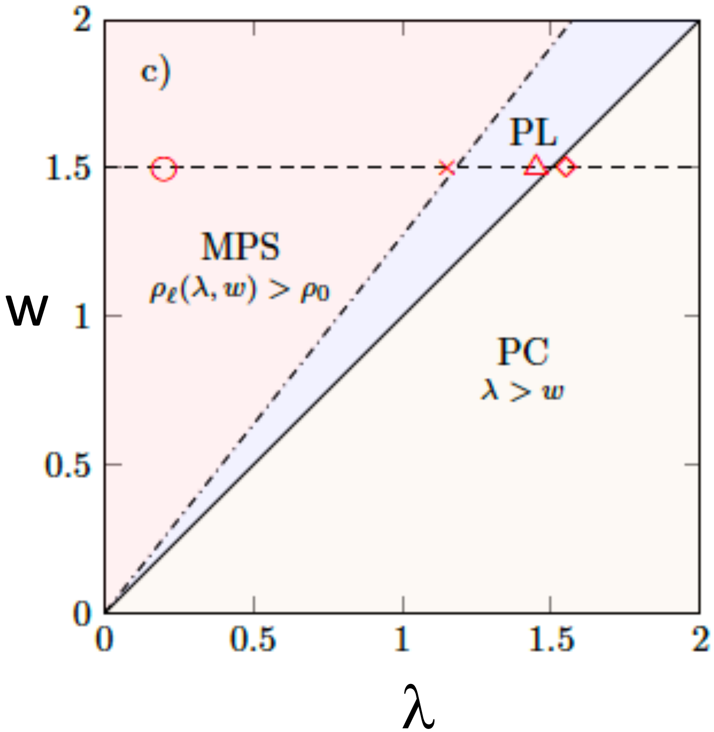


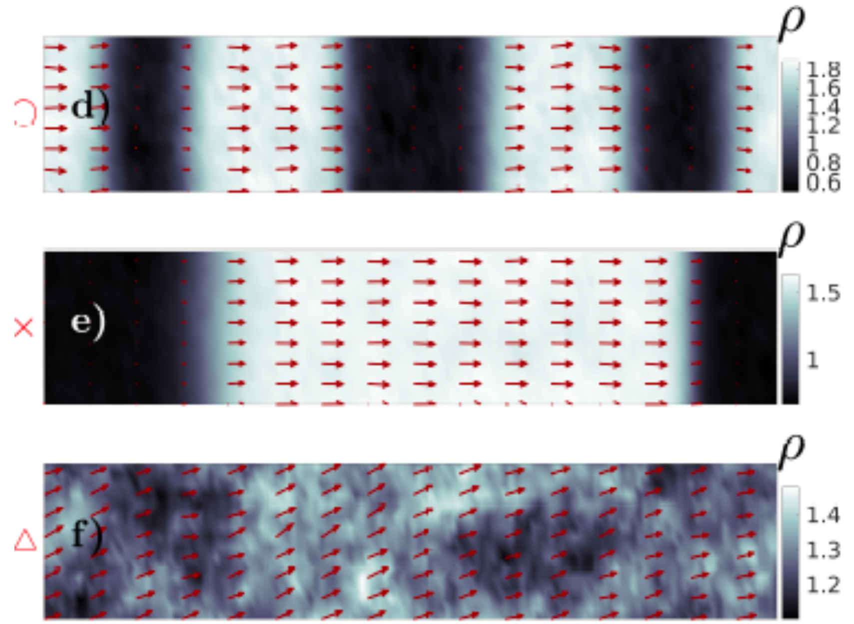
related discussions:
Shankar + Marchetti PRE 2018
Dadhichi et al JSTAT 2018

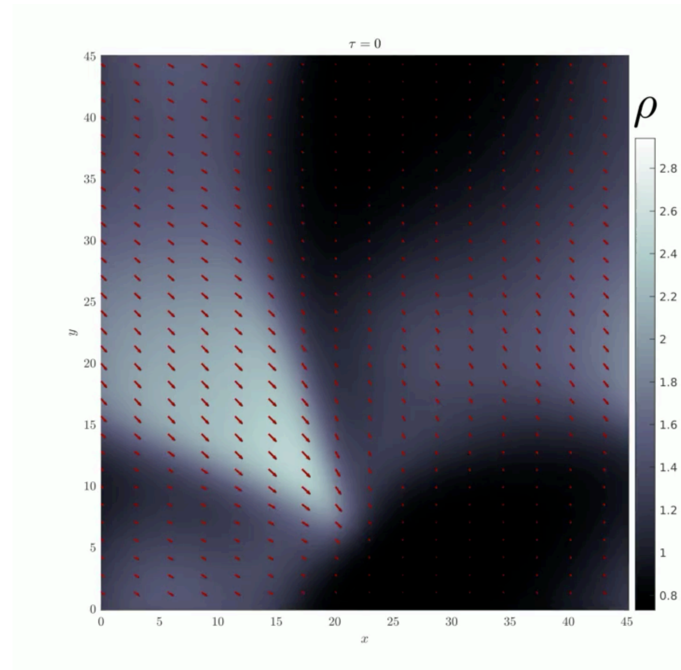
Borthne, Fodor + MEC NJP 2000

Active Vector Fields

Hydrodynamic Vicsek model







Borthne, Fodor + MEC NJP 2000

Active Vector Fields

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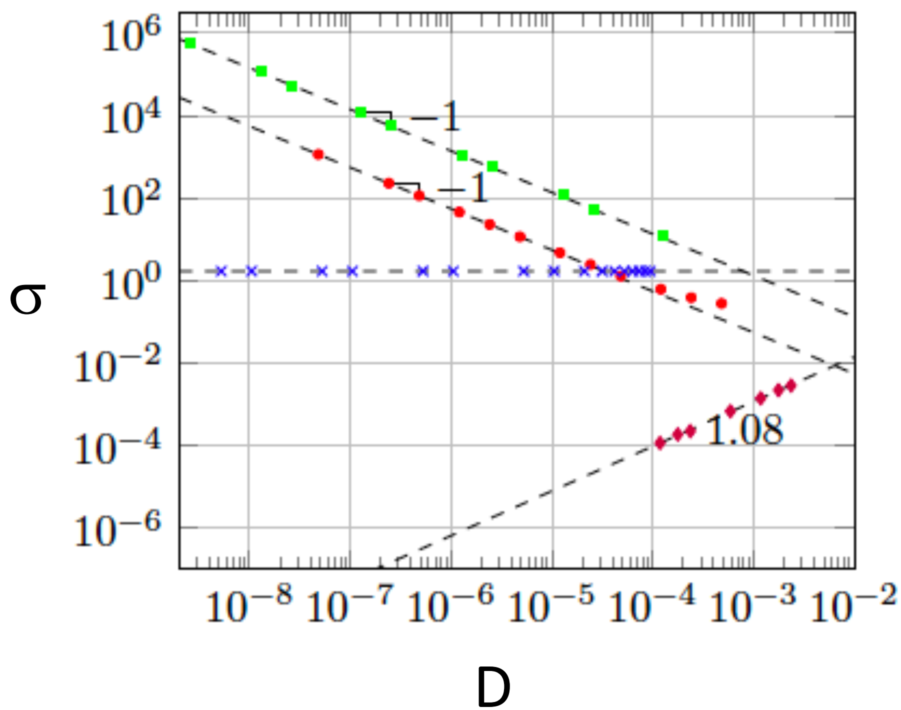


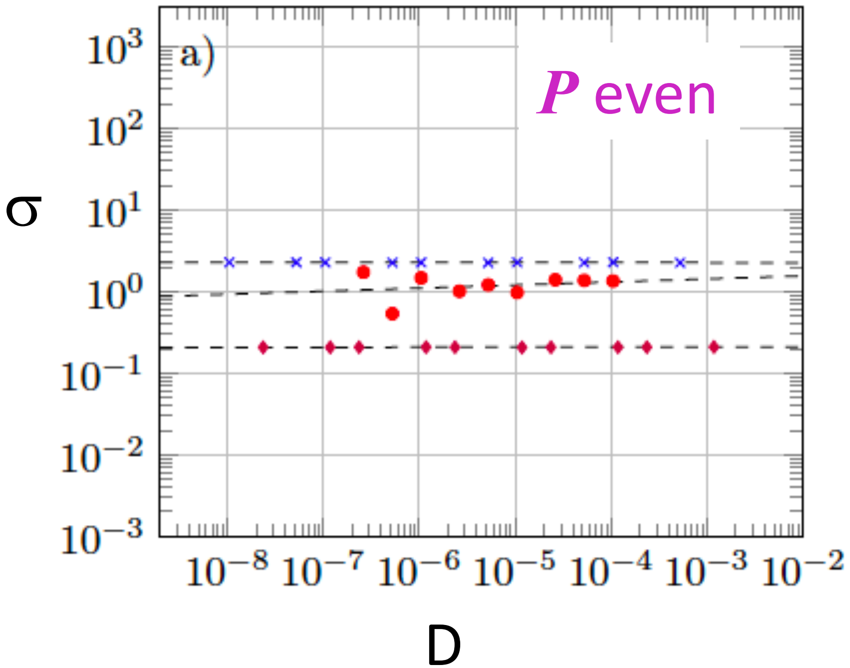
		broken symmetry:	
		GS	flucts
isotropic*:	D^1	∅	(PT)
polar liquid:	D^0	T	PT
microphase:	D^{-1}	**PT**	
polar cluster:	D^{-1}	**PT**	

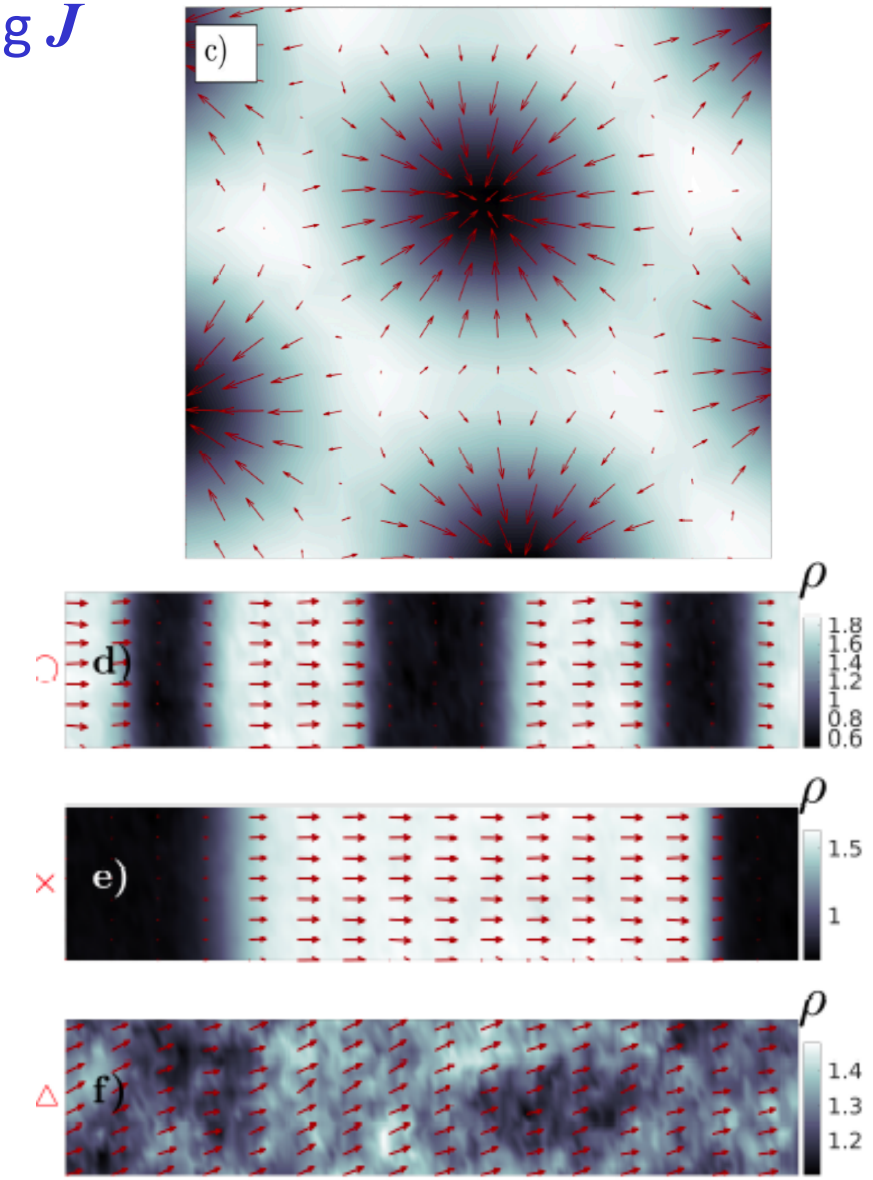
*D^0 term = 0, non-generic

Borthne, Fodor + MEC NJP 2000

Active Vector Fields

Diffusive Flocking Model eliminating $\boldsymbol{J}$



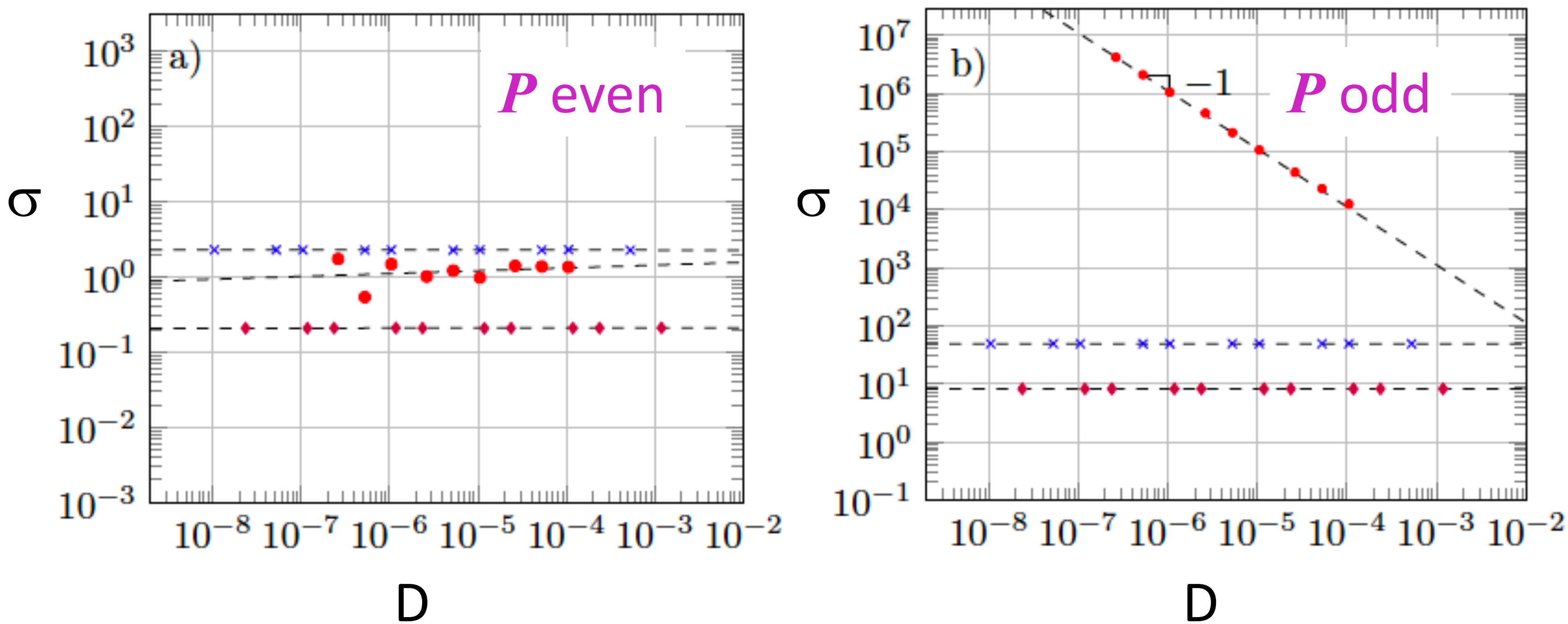


isotropic:	D^0	∅	PT
polar liquid:	D^0	T	PT
polar μp / cl:	D^{-1}	**PT**	
static crystal:	D^0	∅	PT

Borthne, Fodor + MEC NJP 2000

Active Vector Fields

Diffusive Flocking Model eliminating *J*



isotropic:	D^0	∅	PT	D^0	∅	PT
polar liquid:	D^0	T	PT	D^0	T	PT
polar μp / cl:	D^{-1}	**PT**		D^{-1}	**PT**	
static crystal:	D^0	∅	PT	D^{-1}	**PT**	

Borthne, Fodor + MEC NJP 2000

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Summary: EPR as $D \to 0$

- D^{-1} from broken PT in ground state (steady $\boldsymbol{J}$, asymmetric waves...)
- D^{0} from broken PT at leading order in fluctuations
- D^{1} when PT broken only at next order
- Results depend on whether $\boldsymbol{P}$ even/odd and whether $\boldsymbol{J}$ retained

Borthne, Fodor + MEC NJP 2000

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- Results depend on whether $\boldsymbol{P}$ even/odd and whether $\boldsymbol{J}$ retained

Compare scalar models

Active B/B+: uniform D^1 , interface D^0

Model A+B ($\mu_2 \neq \mu_1 + \alpha\phi$): uniform D^1

nonuniform D^0 (for ϕ only) , D^{-1} (for ϕ, $\boldsymbol{J}$)

Borthne, Fodor + MEC NJP 2000

Conclusions

EPR generically calculable for active Langevin fields

EPR has informative scalings in low-noise expansion

- D^{-1}: finite dissipation, e.g. macro currents, at mean-field level
- D^{0} : finite EPR even as fluctuations become small
- D^{1} : equilibrium-like approach to low noise limit

Cause: broken PT at the given order

EPR depends on degrees of freedom retained (e.g. A+B, RG flow)

EPR depends on time-signature of vector fields:

- forward equations alone do not determine (ir)reversibility

EPR nontrivial at critical point even in a 'passive' universality class

- $\xi^{-(d+z)}$ scaling ($d > d_c$) or new exponent ($d < d_c$) expected

Borthne, Fodor + MEC NJP 2000

EPR in Active Field Theories

- Entropy Production: General Formalism
- Field Theories of Active Matter
  - Active Model B/B+
  - Model A+B: microphase separation
  - Hydrodynamic Vicsek / Diffusive flocking model
  - Active B (and Active A) near critical point
- Conclusions

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