Unsupervised Learning of Phase Transitions

arxiv: 1812.00895

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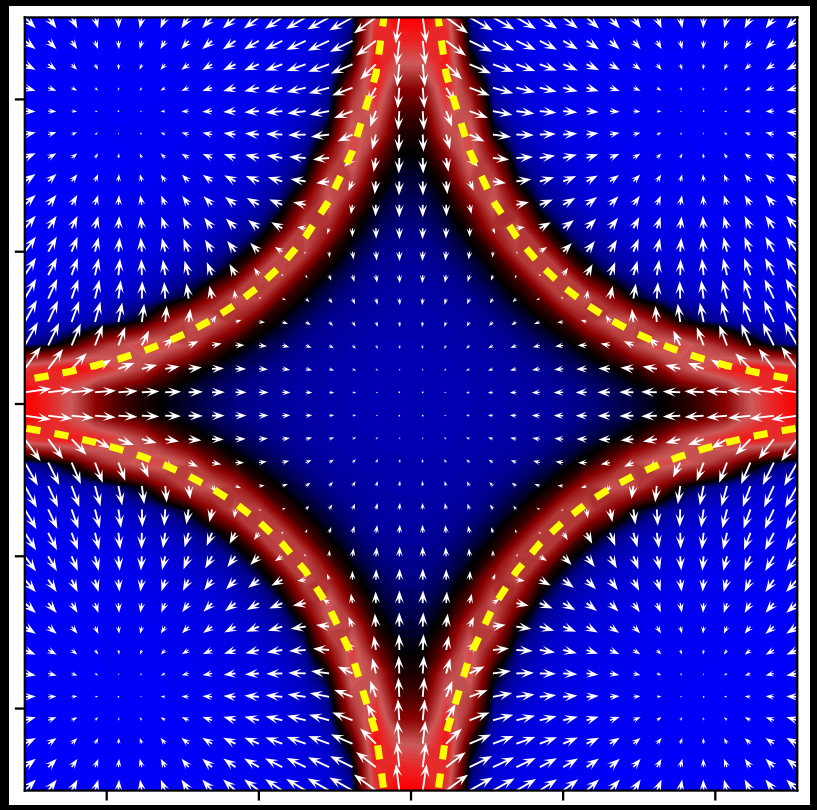
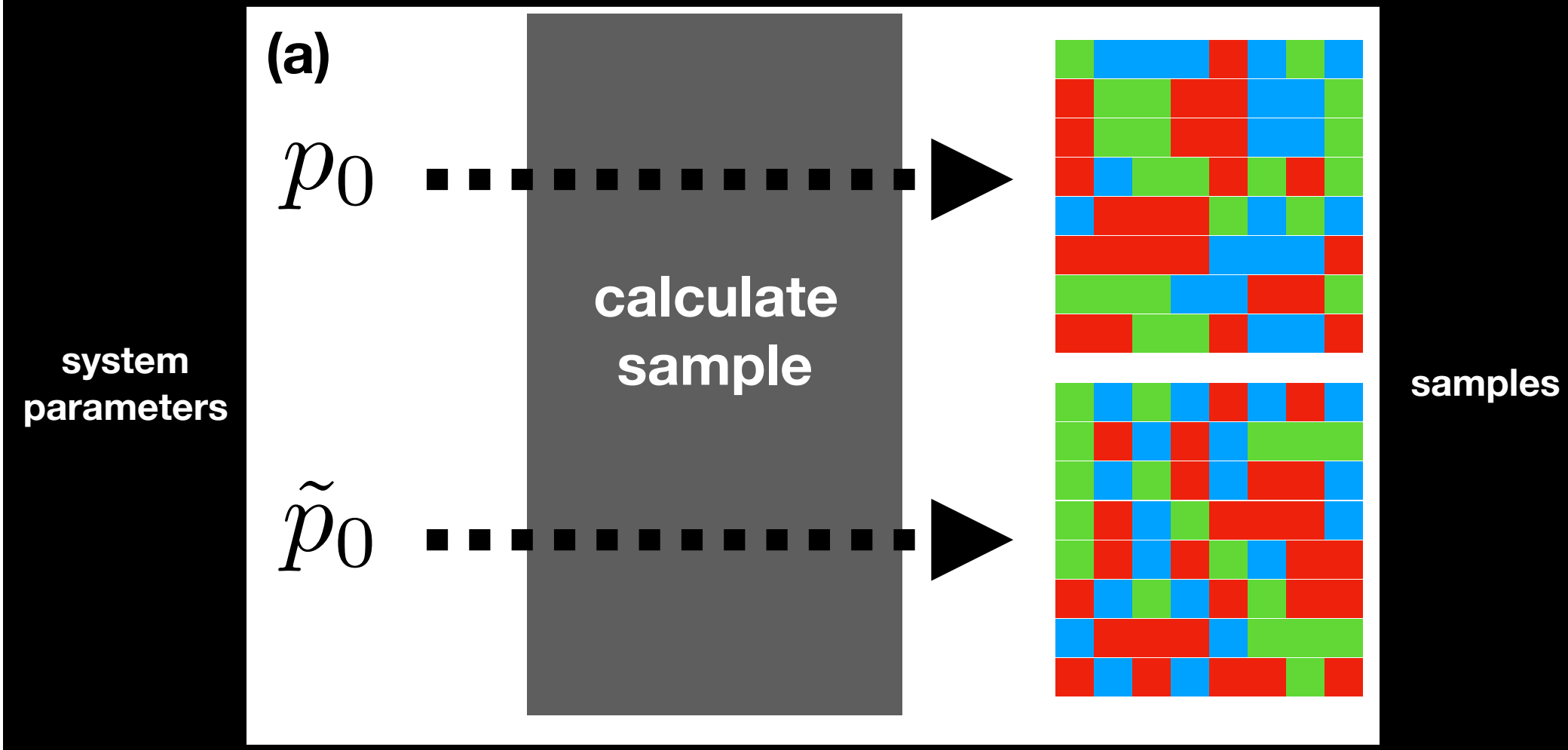


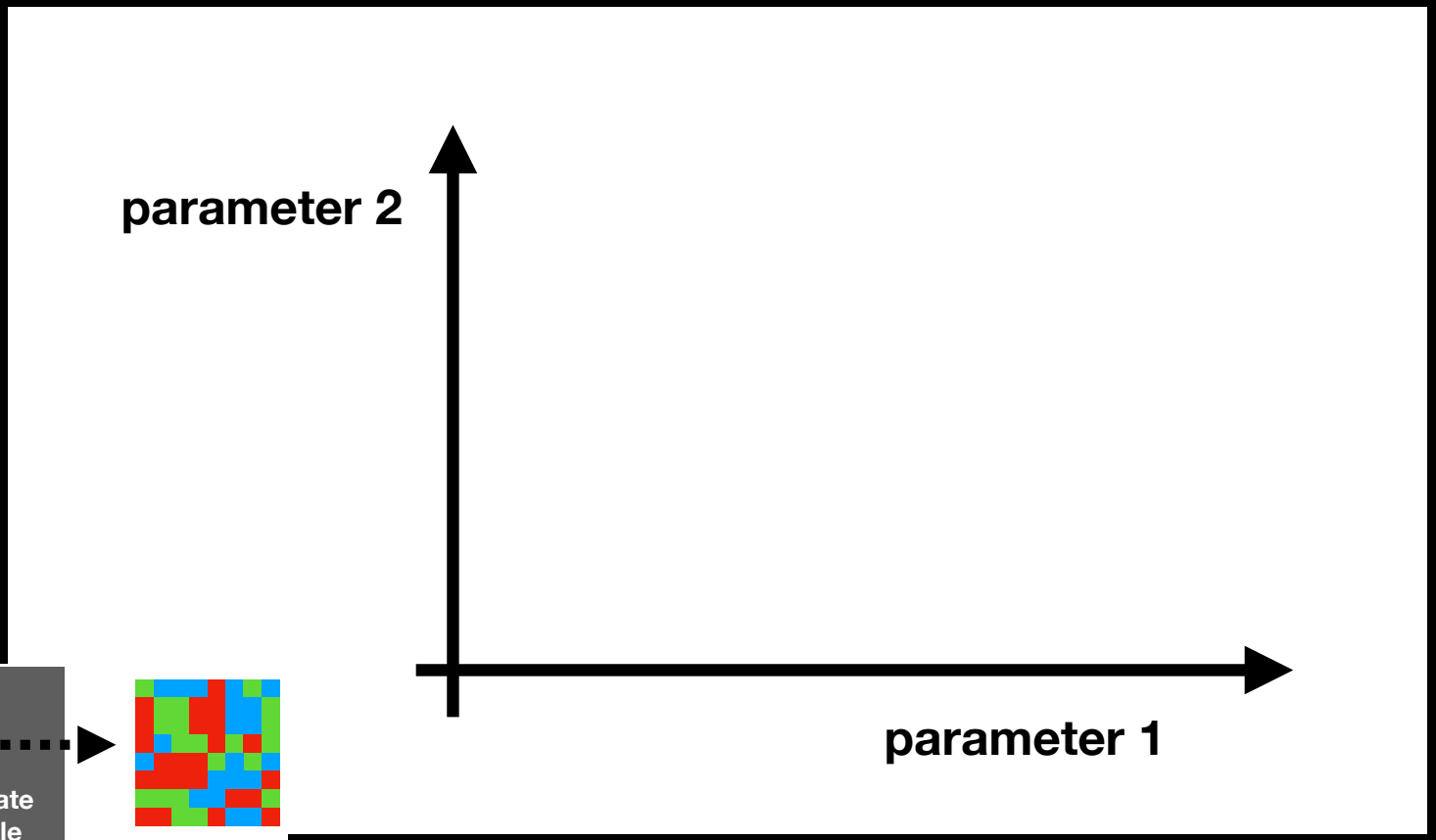
Introduction

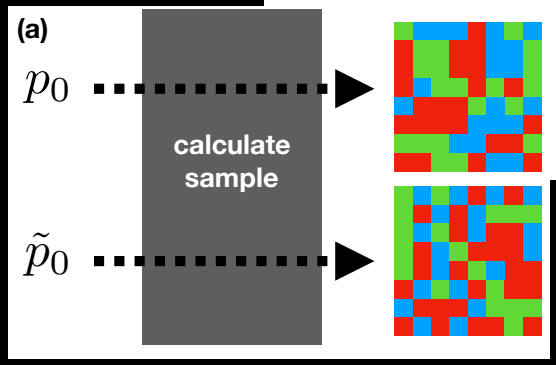
Scenario



"sample state of a system as a function of parameters"

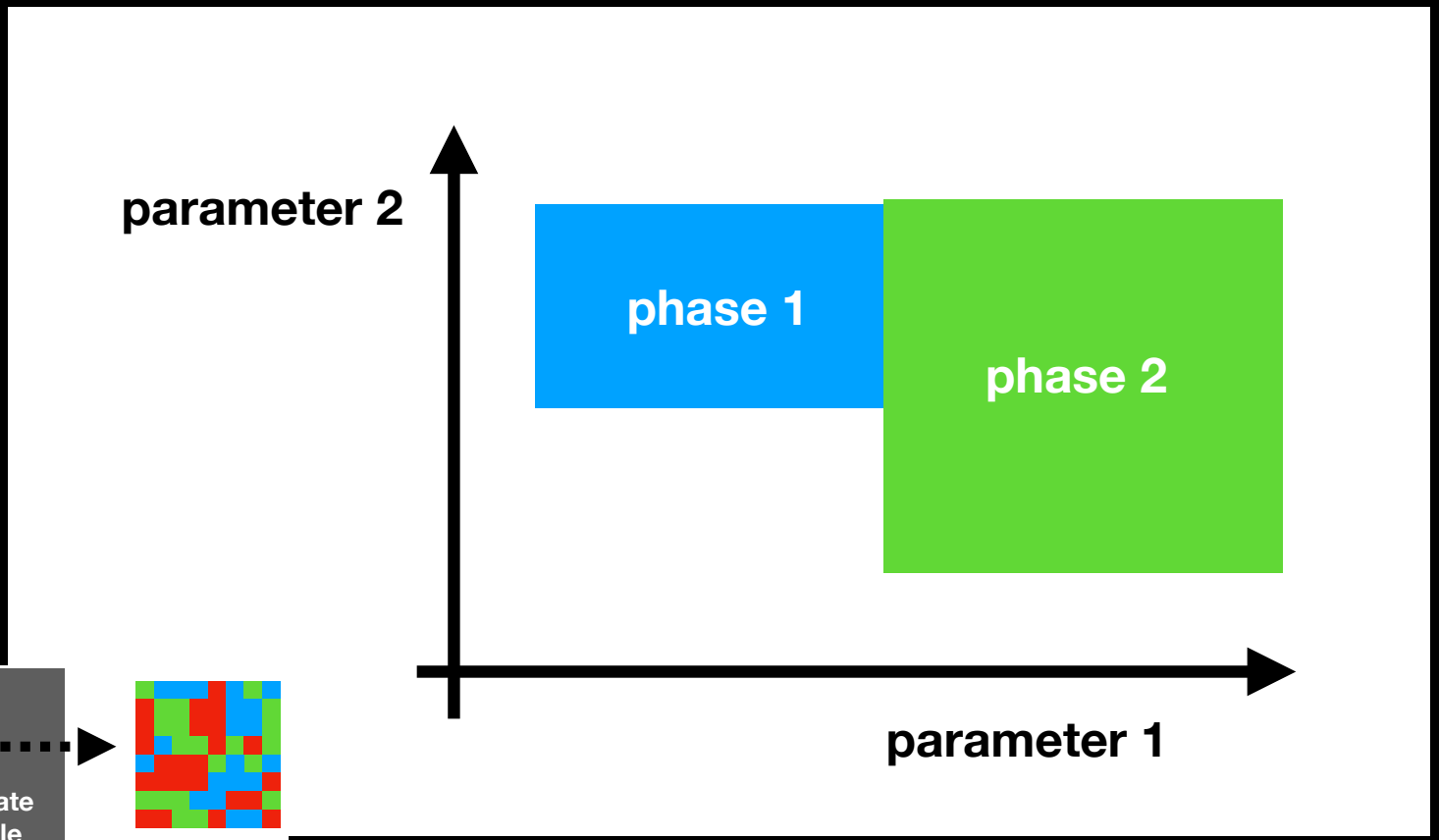
Motivation

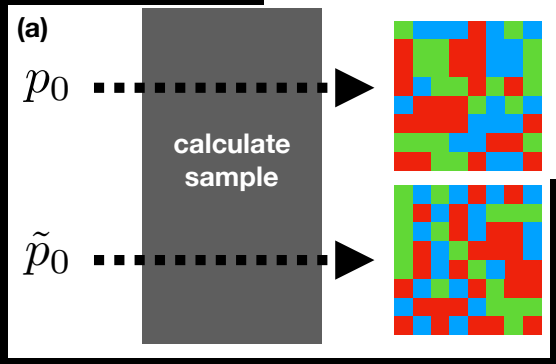




"we know nothing about phase diagram"

Motivation

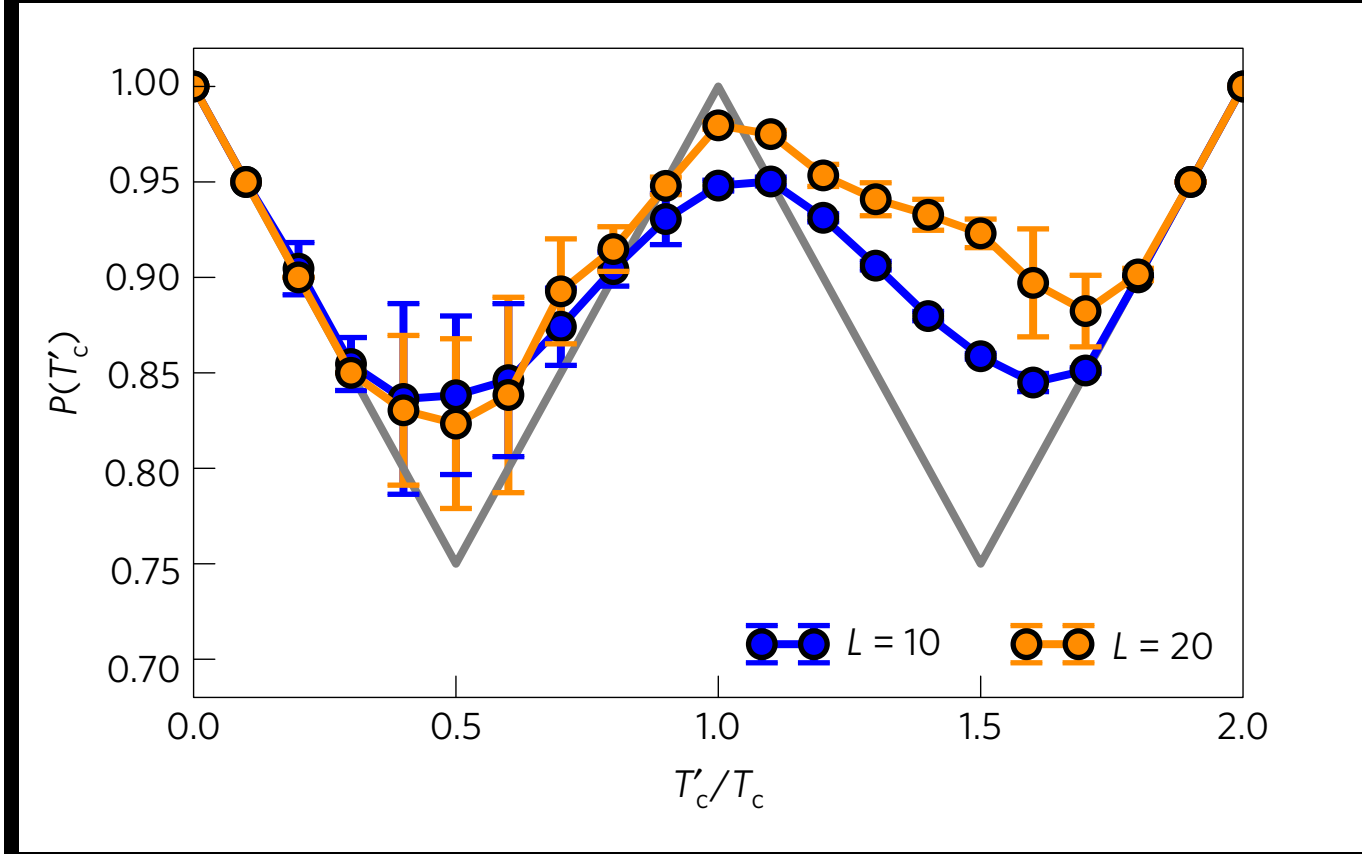




aim: infer phase diagram

Introduction

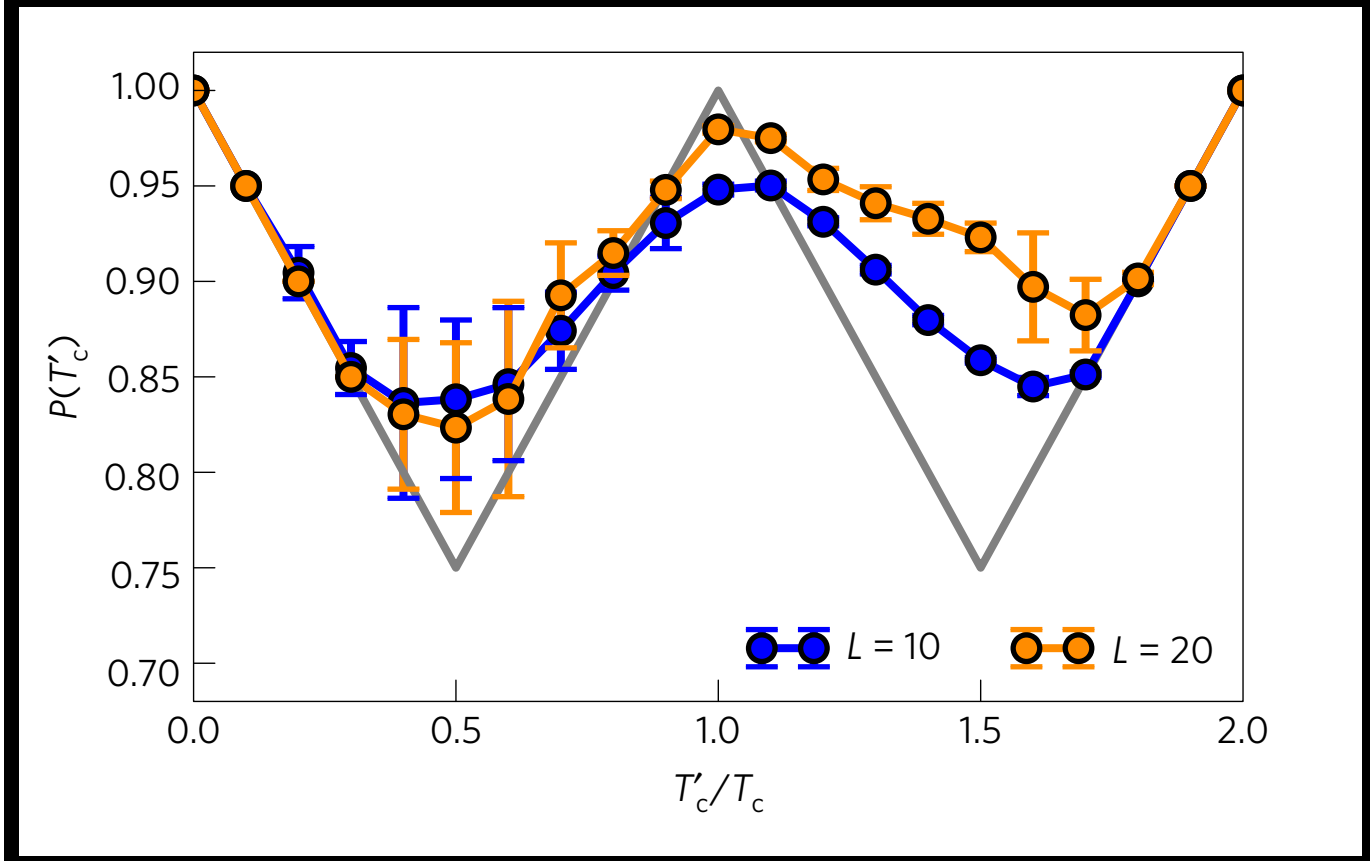
Idea: Use tentative labels, use labels with best predictive model performance

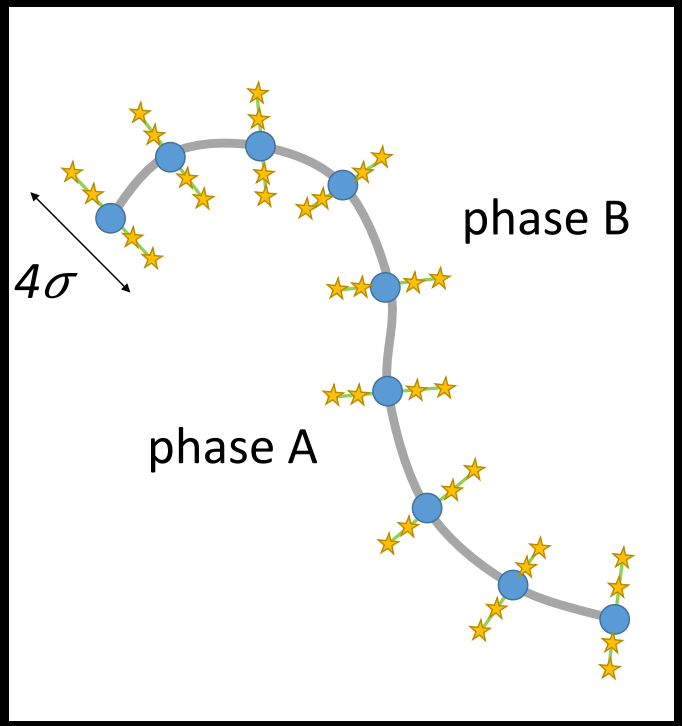


Evert van Nieuwenburg, Yehua Liu, Sebastian Huber, Nature Physics (2017), doi:10.1038/nphys4037

Introduction

Idea: Use tentative labels, use labels with best predictive model performance





Evert van Nieuwenburg, Yehua Liu, Sebastian Huber, Nature Physics (2017), doi:10.1038/nphys4037

Yehua Liu, Evert van Nieuwenburg, Phys. Rev. Lett. 120, 176401 (2018)

Now:
Can we do this in a single shot?

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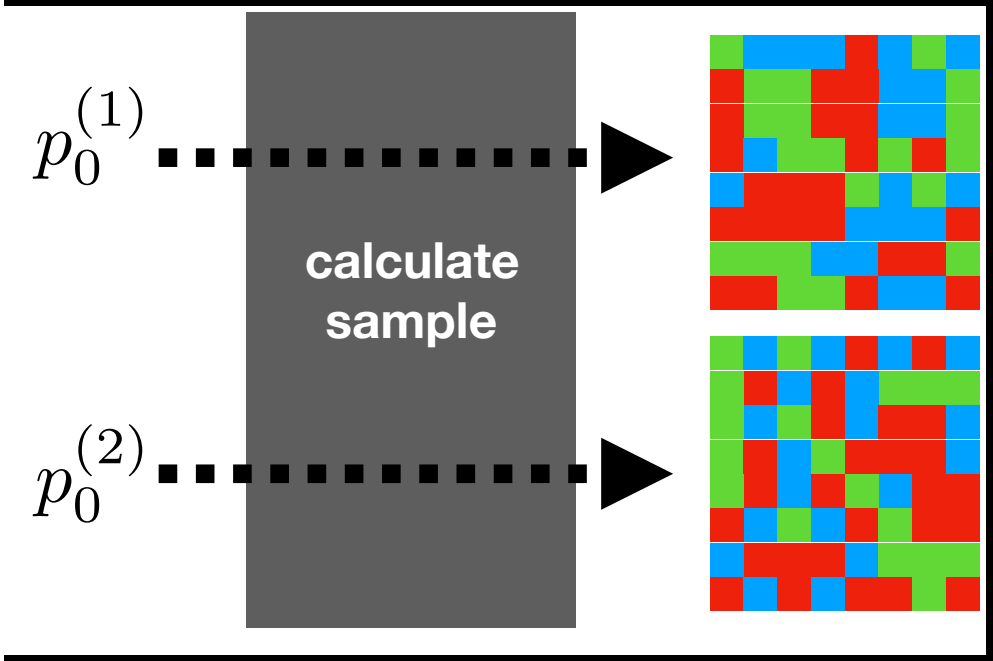
predictive model m learns parameters p of samples S



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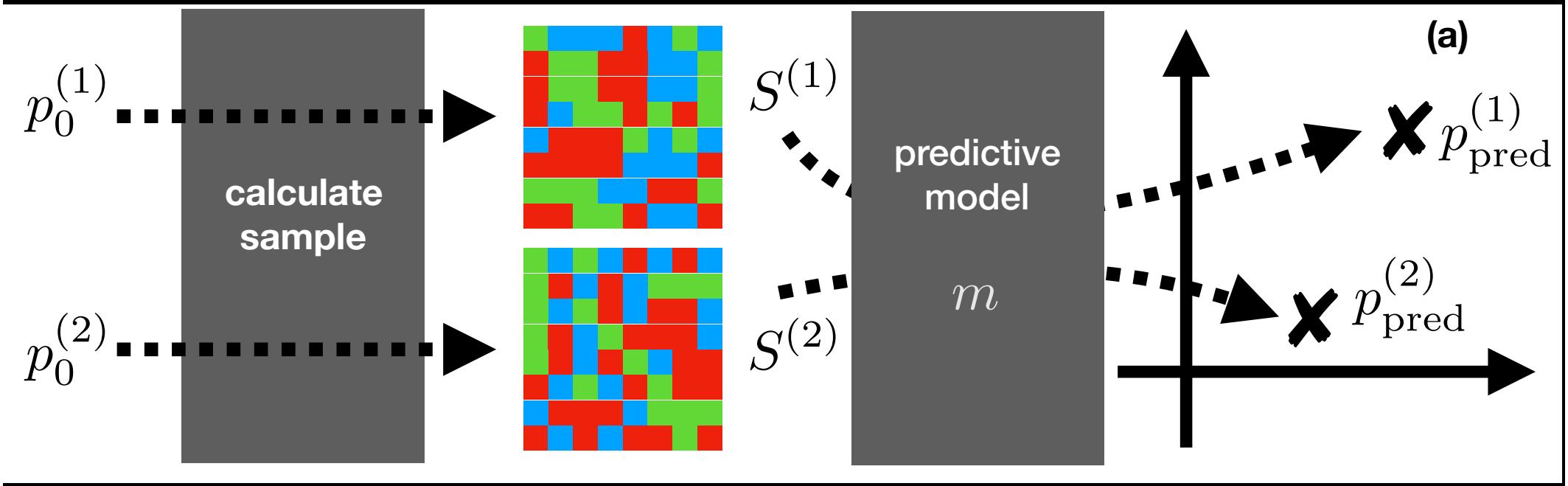
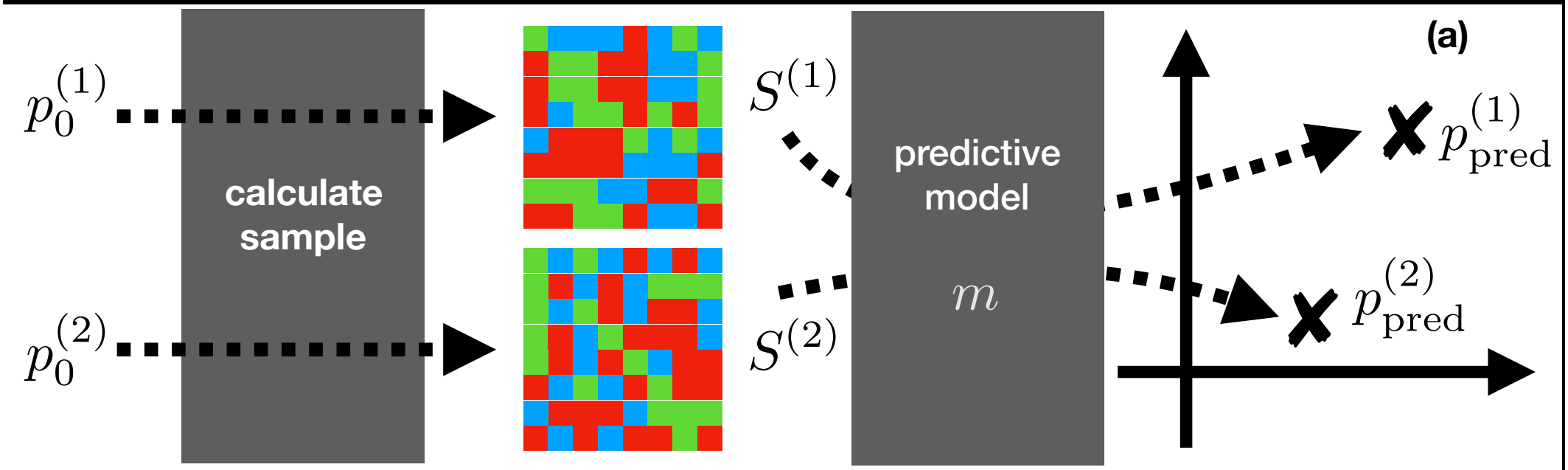
predictive model m learns parameters p of samples S



"first step towards unsupervised learning of phases: supervised learning of system parameters"

arxiv: 1812.00895

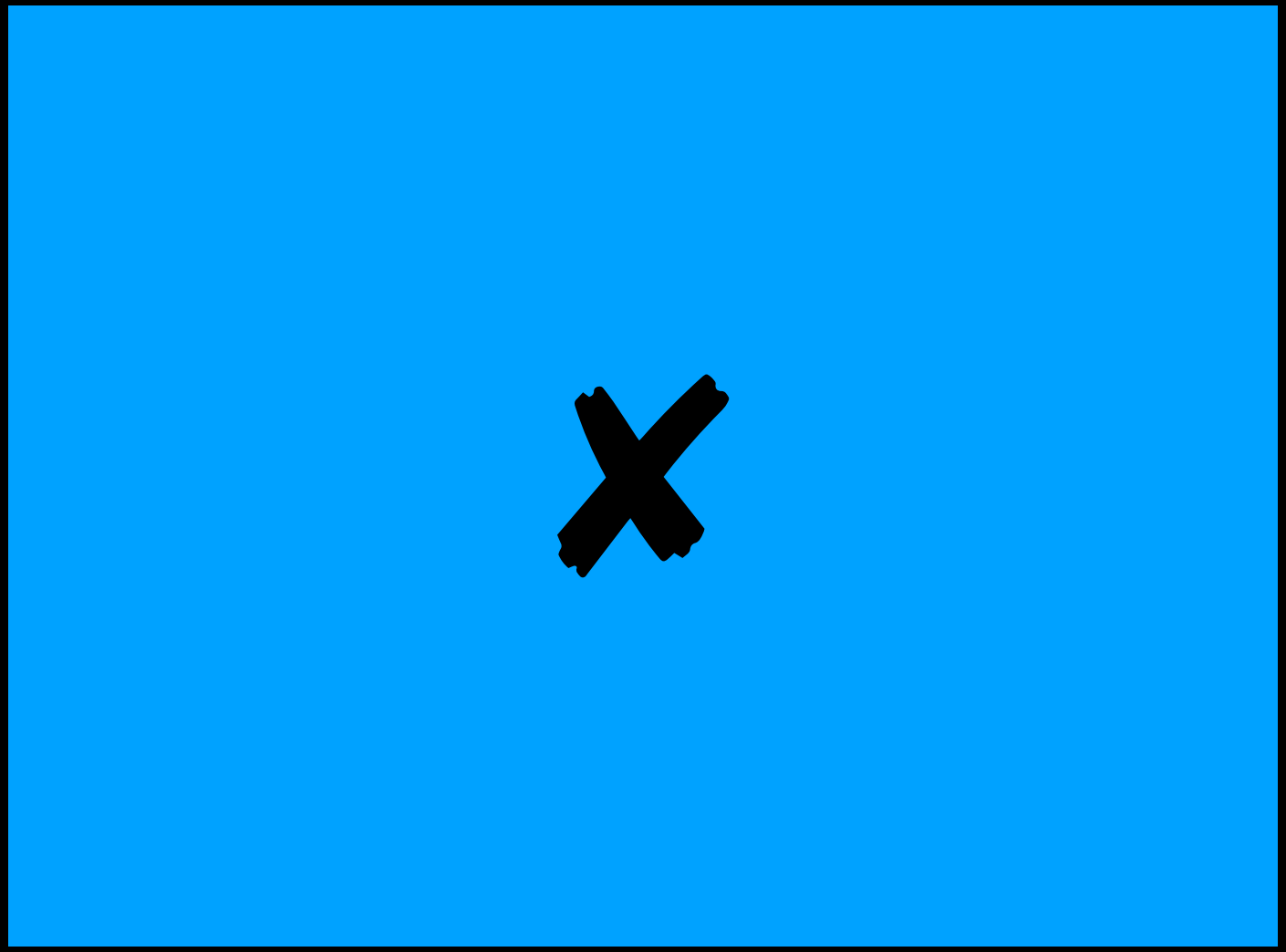
predictive model m learns parameters p of samples S



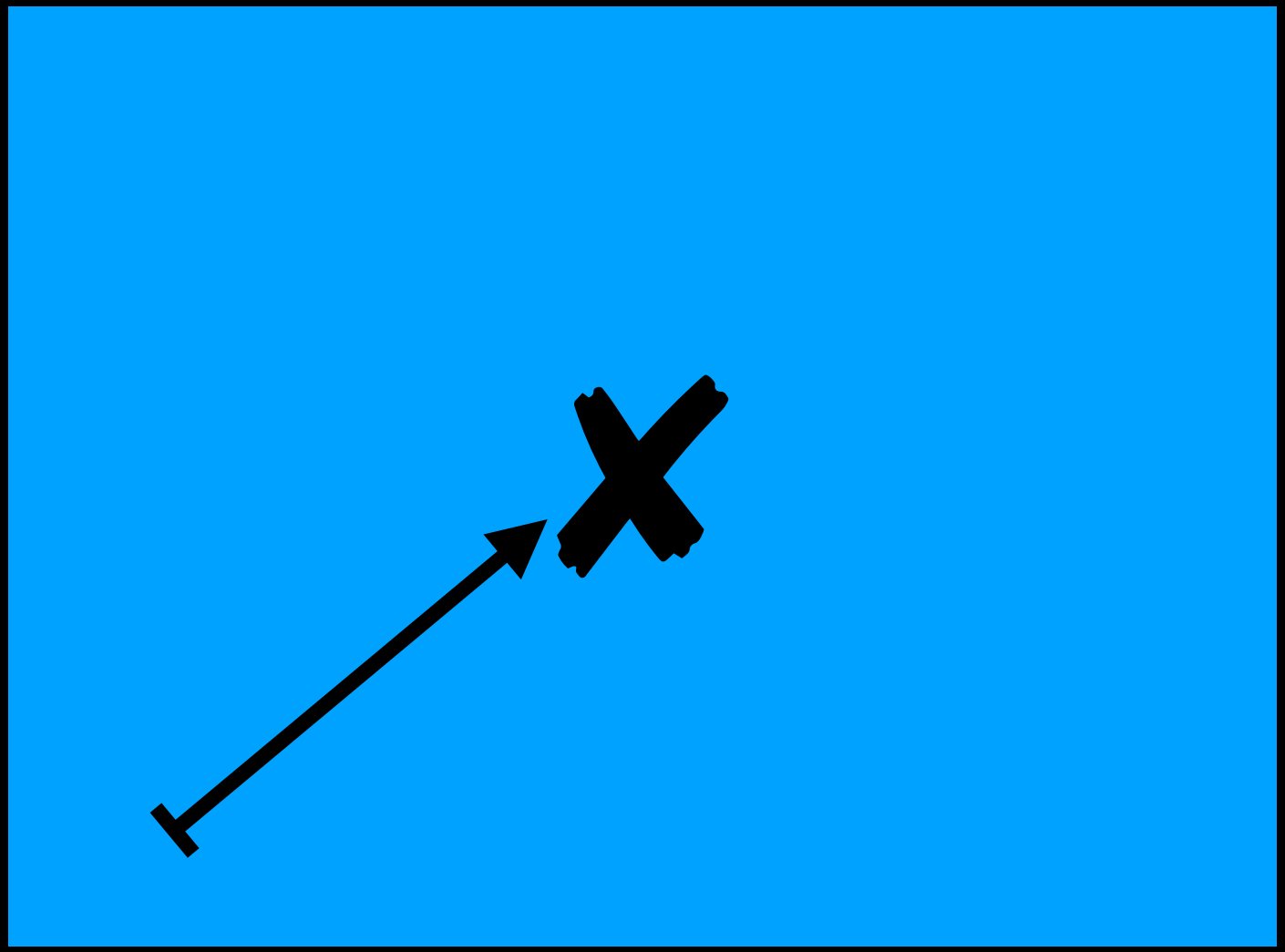
loss function: $\left|p_{\mathrm{pred}} - p_0\right|^2$

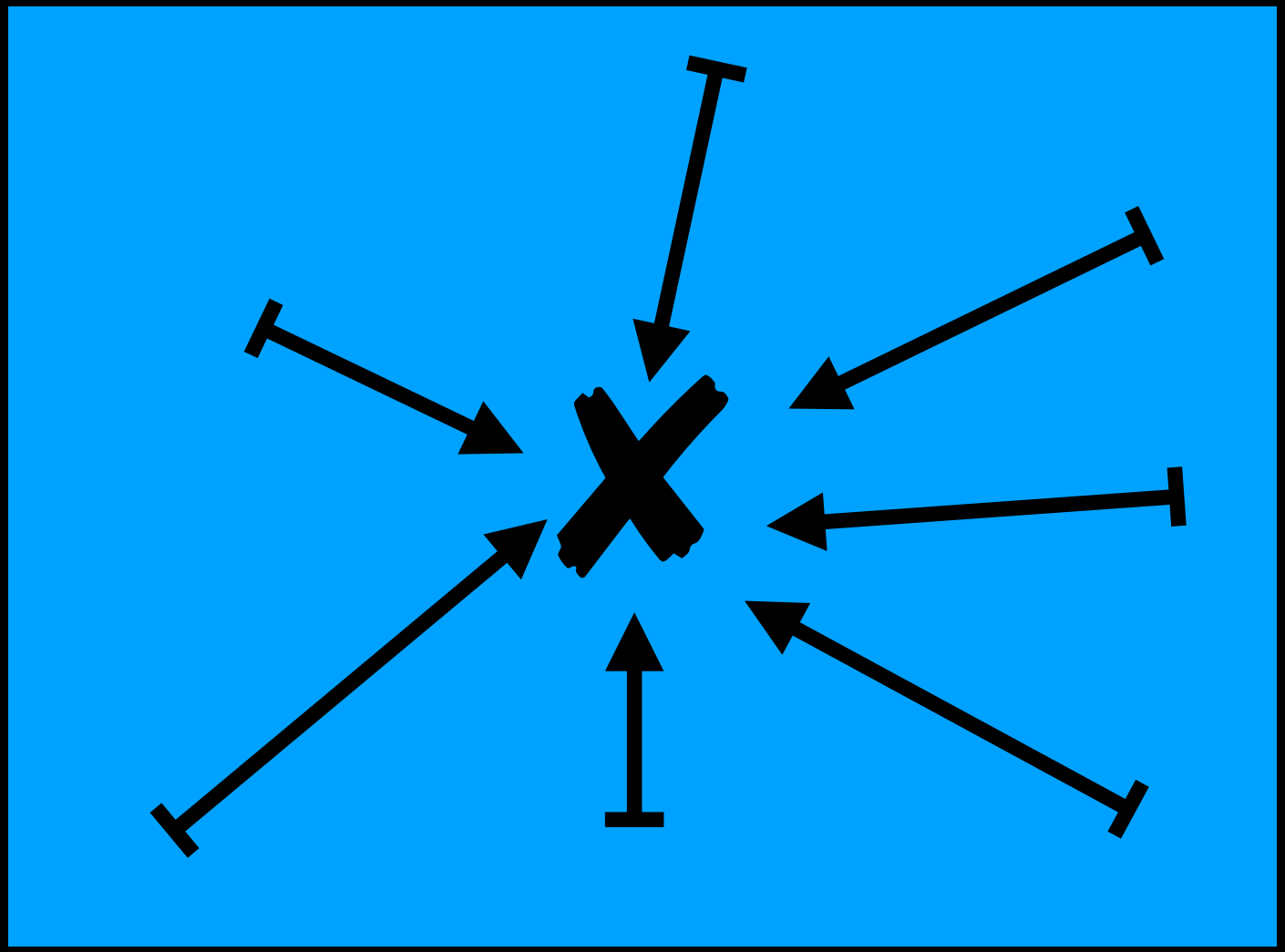
"needs to be distance for our method to work"

“what would a model with zero understanding of the system do?”

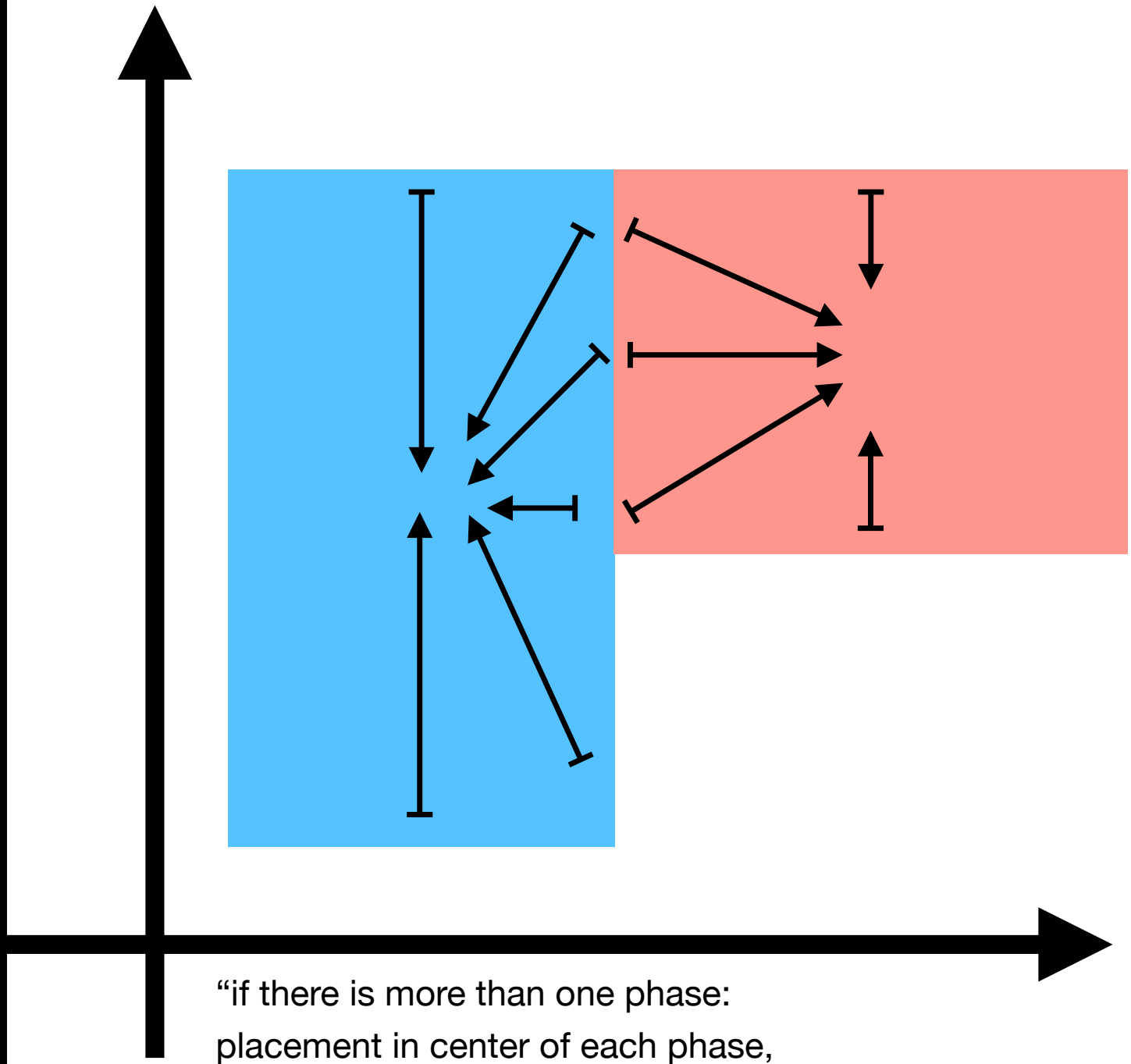


“what would a model with zero understanding of the system do?”
-> “place every guess in the center, to minimize average distance”

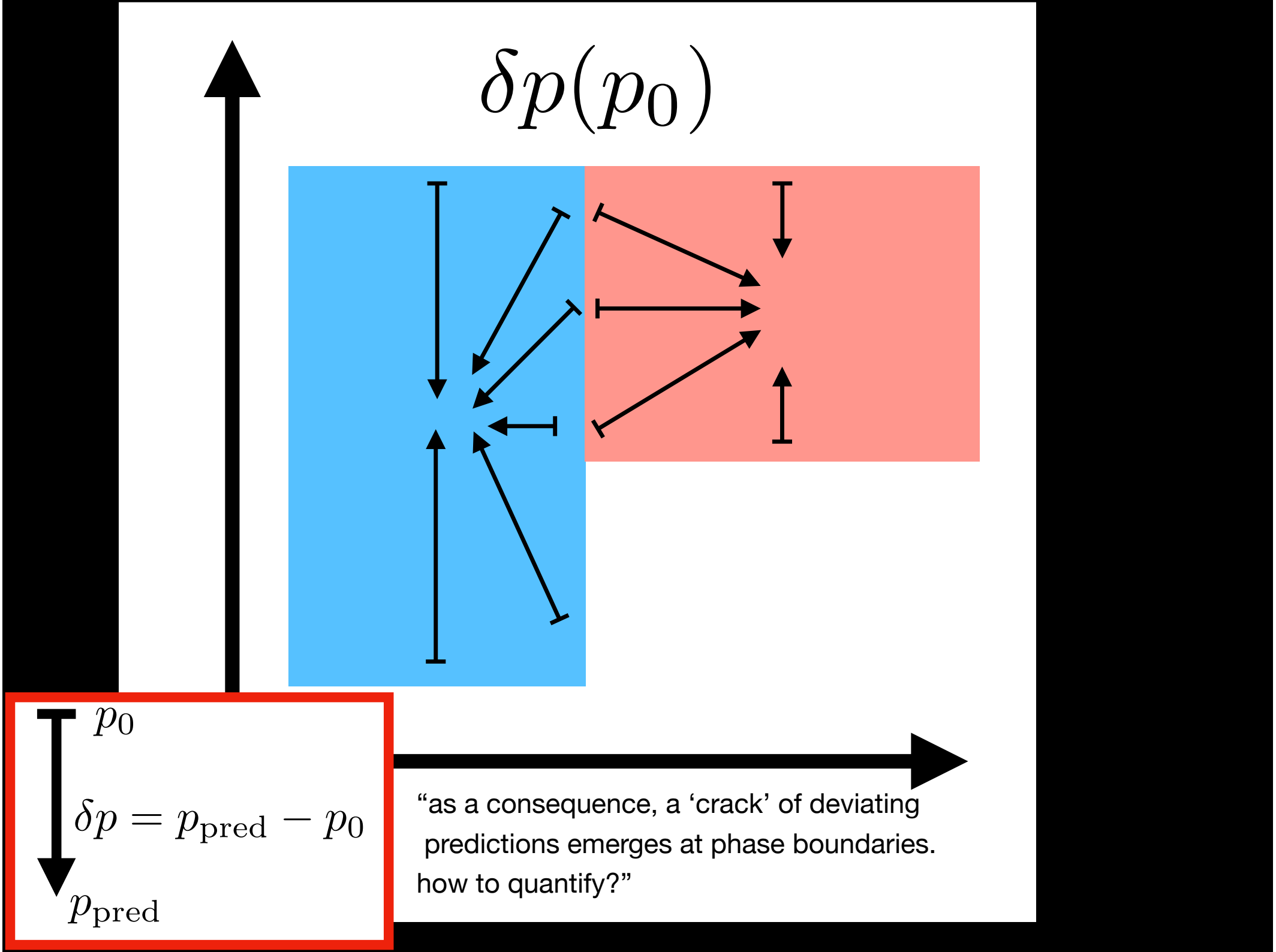




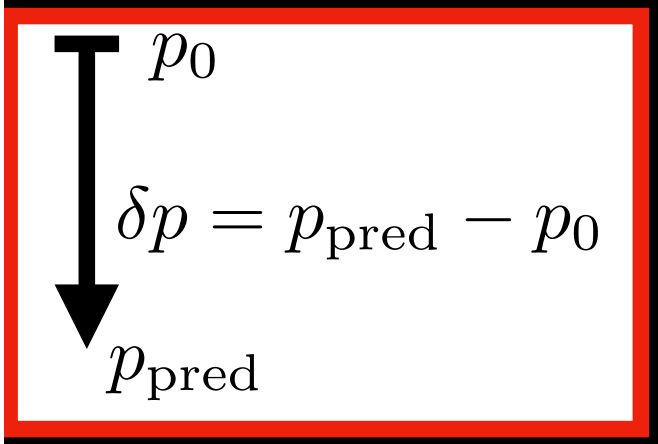
“such a vector field emerges for the model’s predictions”



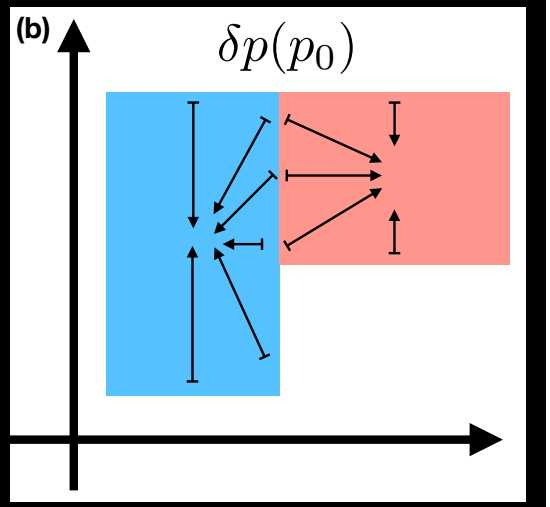
“if there is more than one phase:
placement in center of each phase,
if network cannot distinguish within phase”


$\delta p(p_0)$
p_0
$\delta p = p_{\mathrm{pred}} - p_0$
p_{pred}
“as a consequence, a ‘crack’ of deviating predictions emerges at phase boundaries. how to quantify?”

Quantify via <u>vector</u> divergence



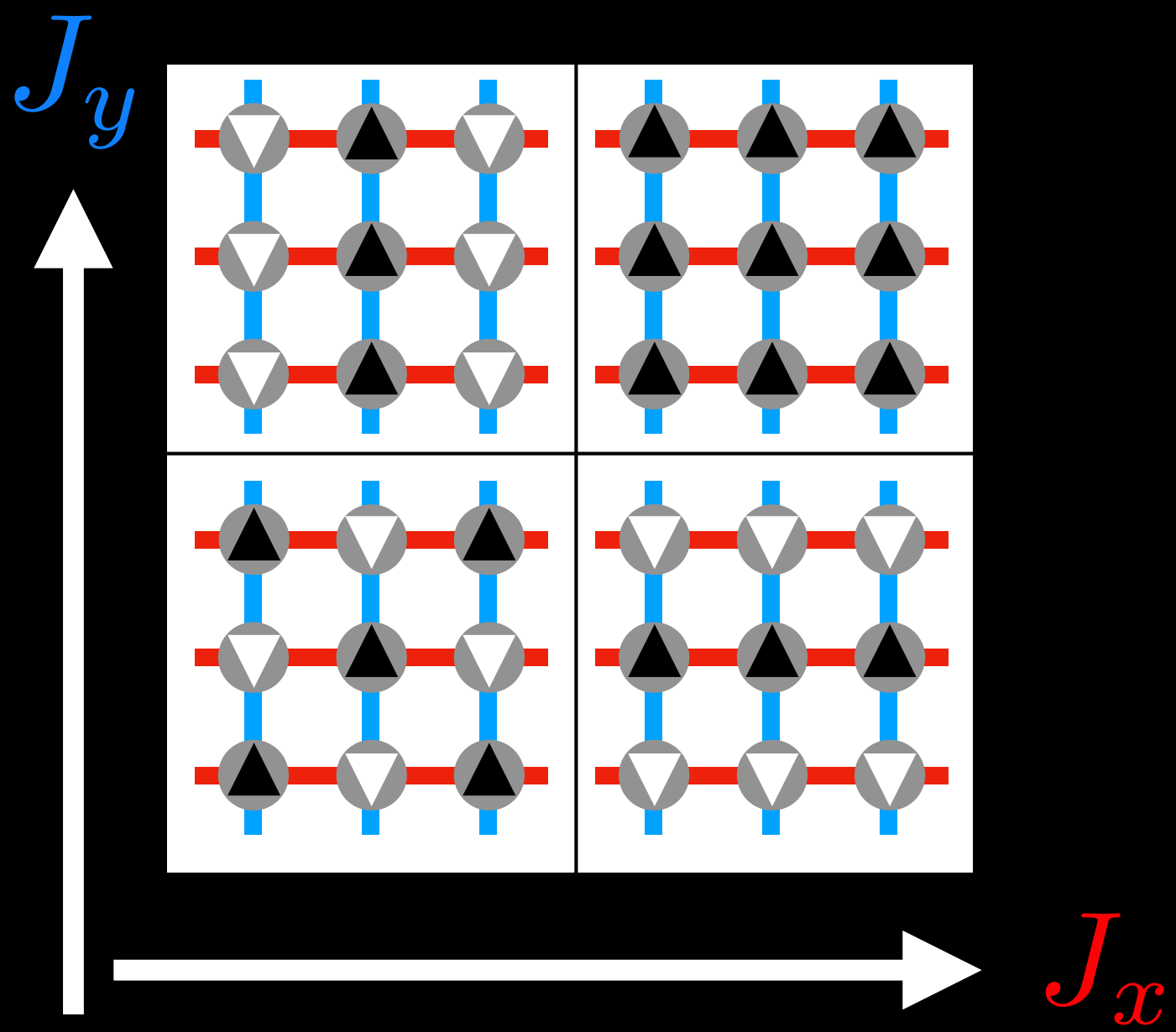
$$\vec{\nabla}_{\vec{p}_0} \cdot \delta\vec{p}$$

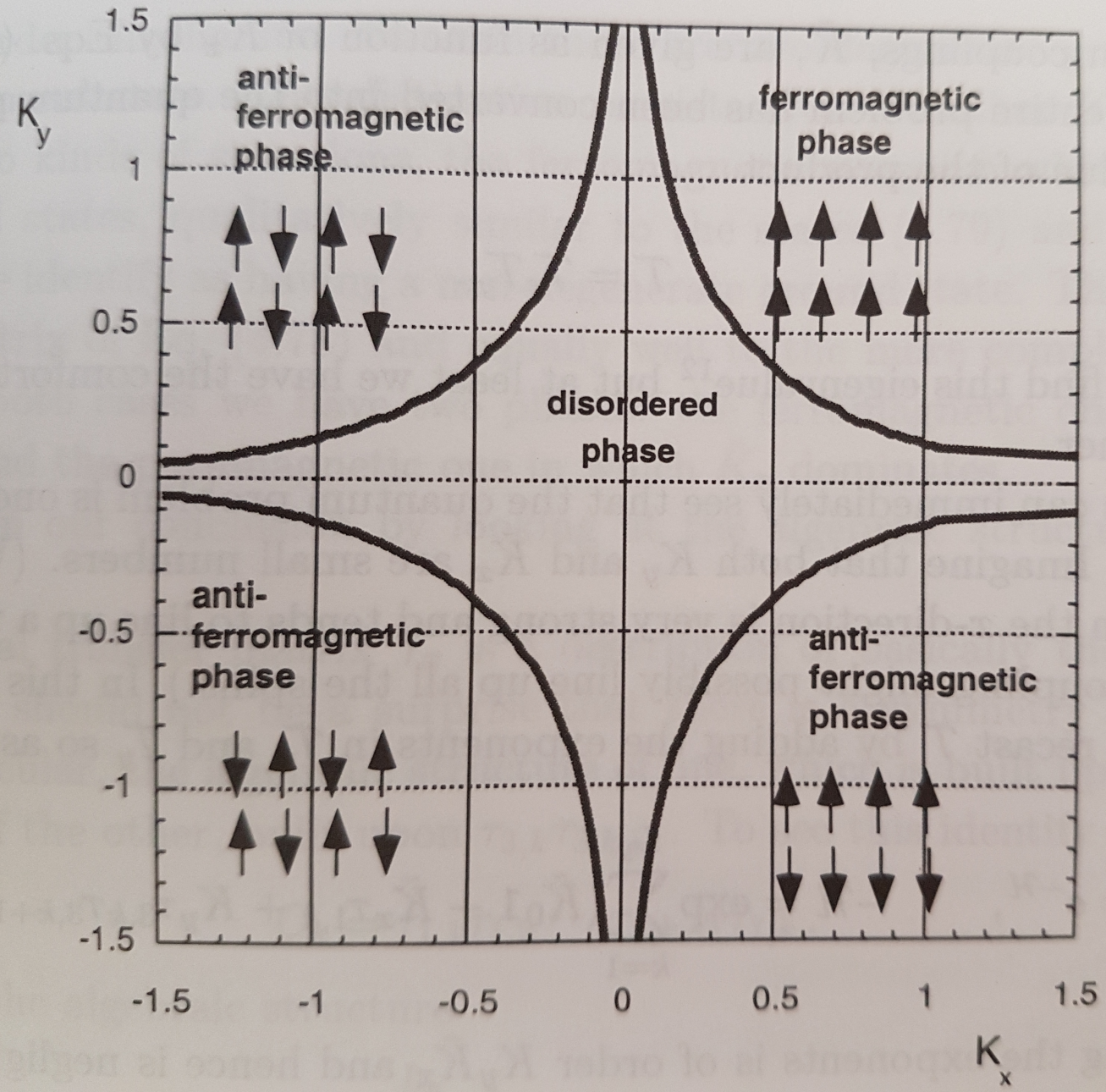


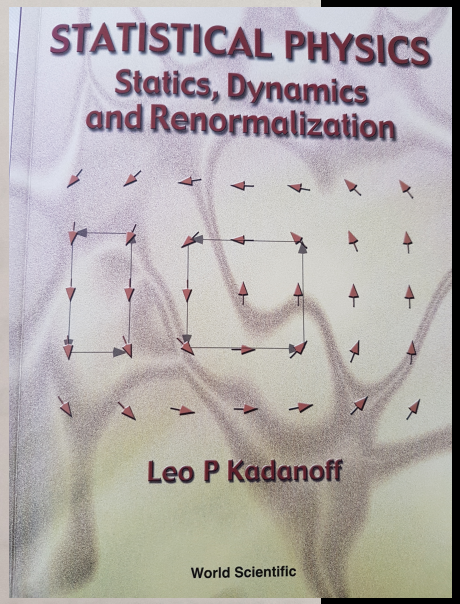
where $\delta\vec{p}$ are the deviations of the predictions

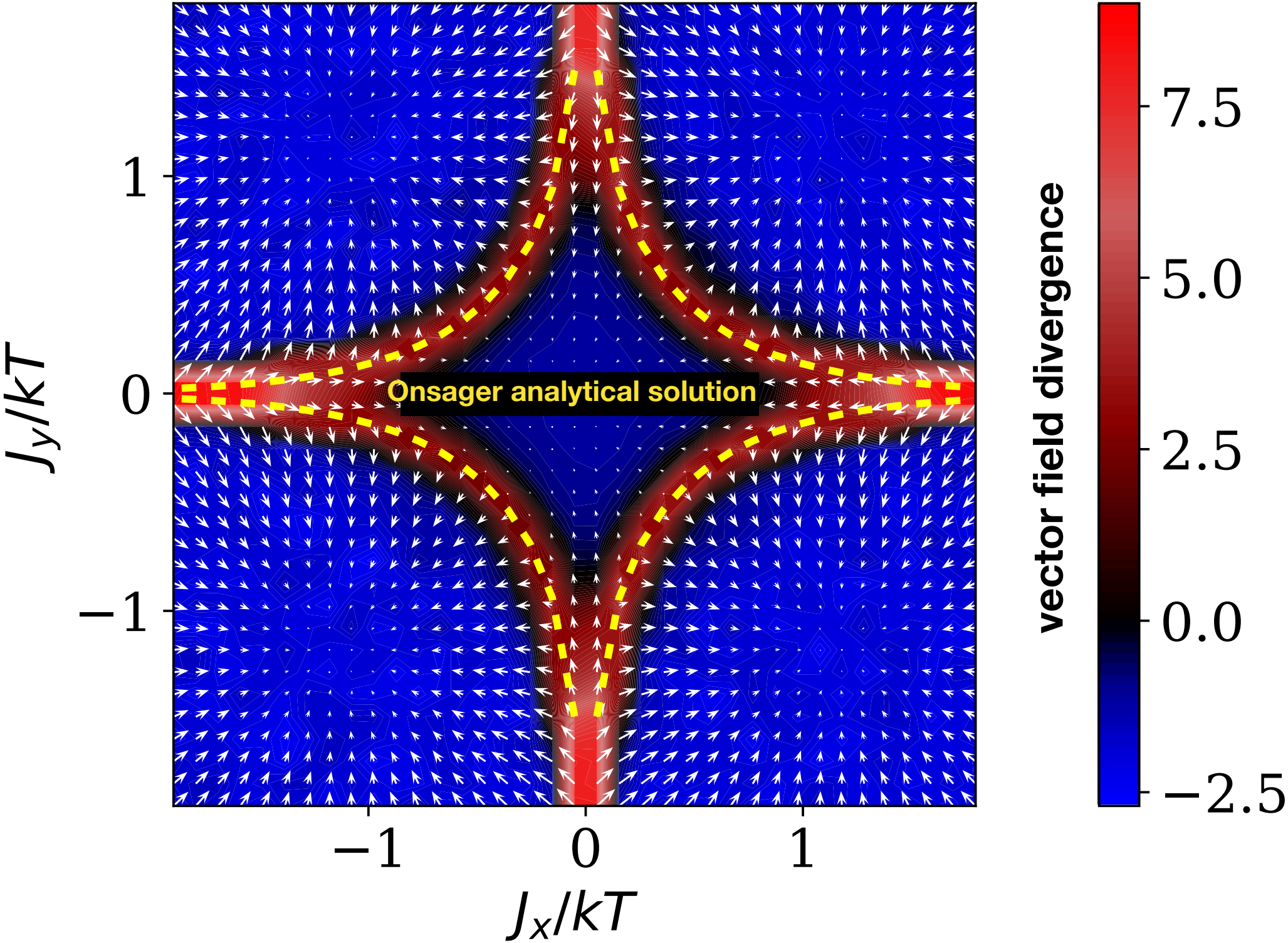
Numerical Experiment: Ising model

test on 2d Ising model

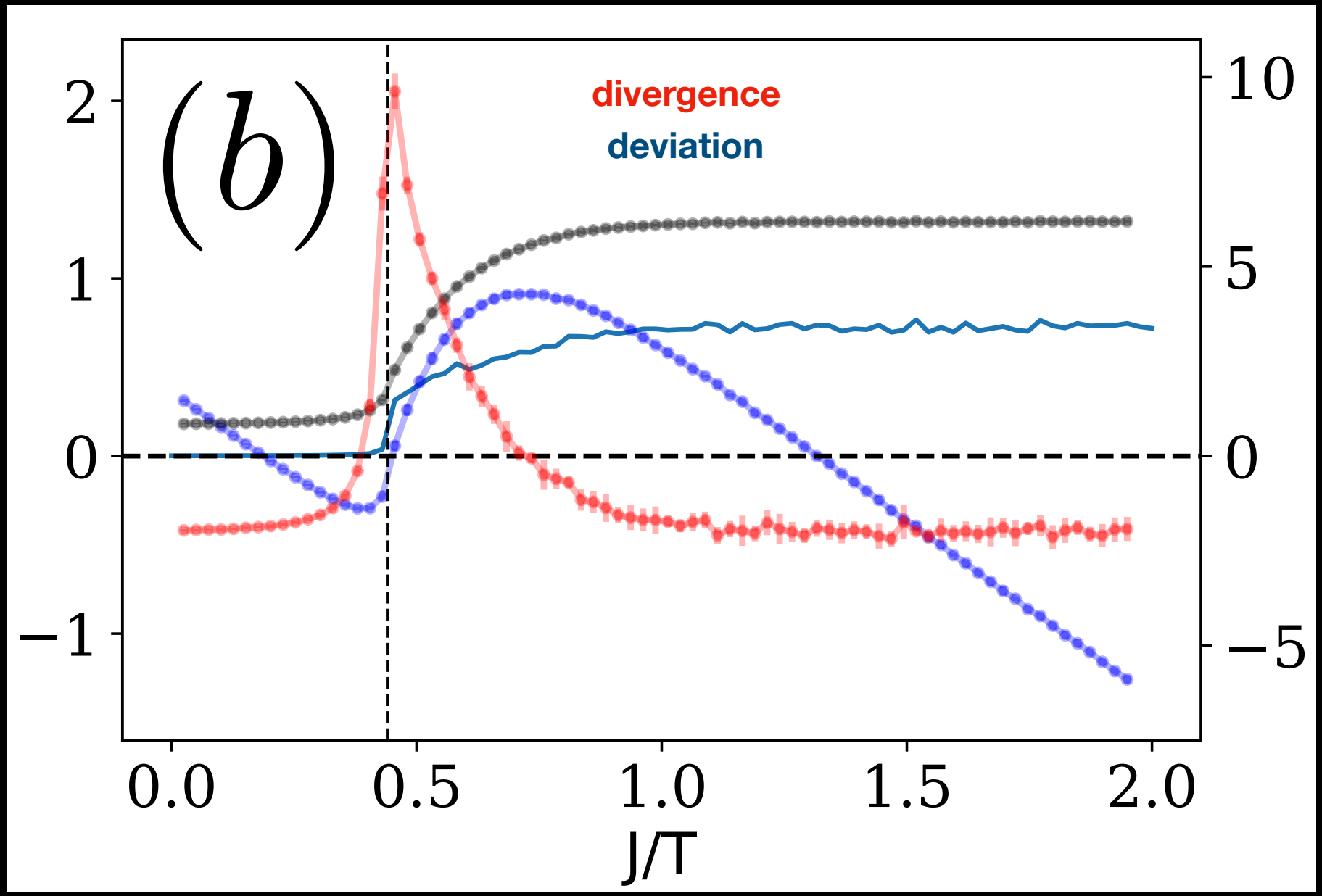



anti-
ferromagnetic
phase
ferromagnetic
phase
disordered
phase
anti-
ferromagnetic
phase
anti-
ferromagnetic
phase
K_y
K_x
1.5
1
0.5
0
-0.5
-1
-1.5
-1.5
-1
-0.5
0
0.5
1
1.5

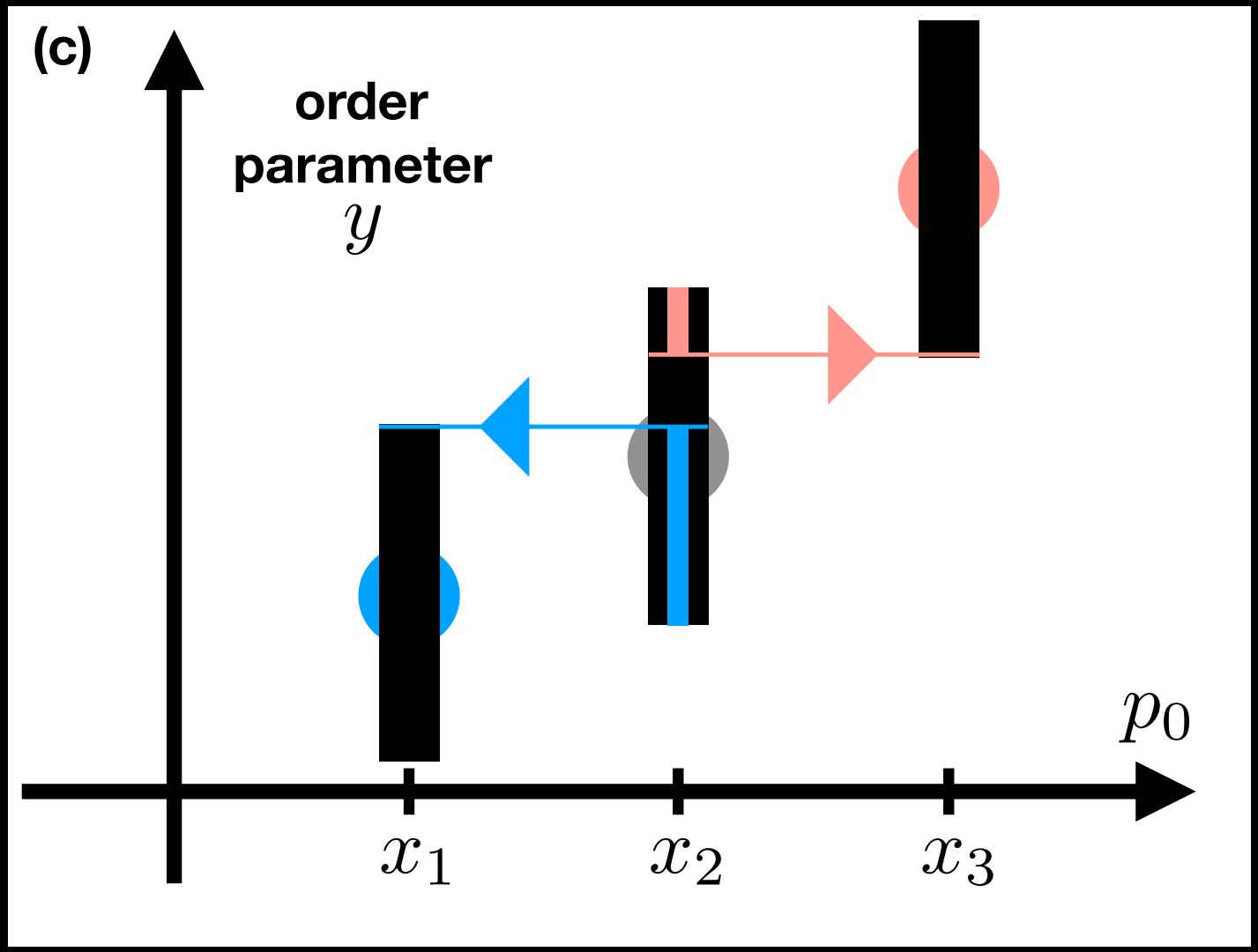

STATISTICAL PHYSICS
Statics, Dynamics
and Renormalization
Leo P Kadanoff
World Scientific


Onsager analytical solution
J_y/kT
J_x/kT
1
0
−1
−1
0
1
vector field divergence
7.5
5.0
2.5
0.0
−2.5

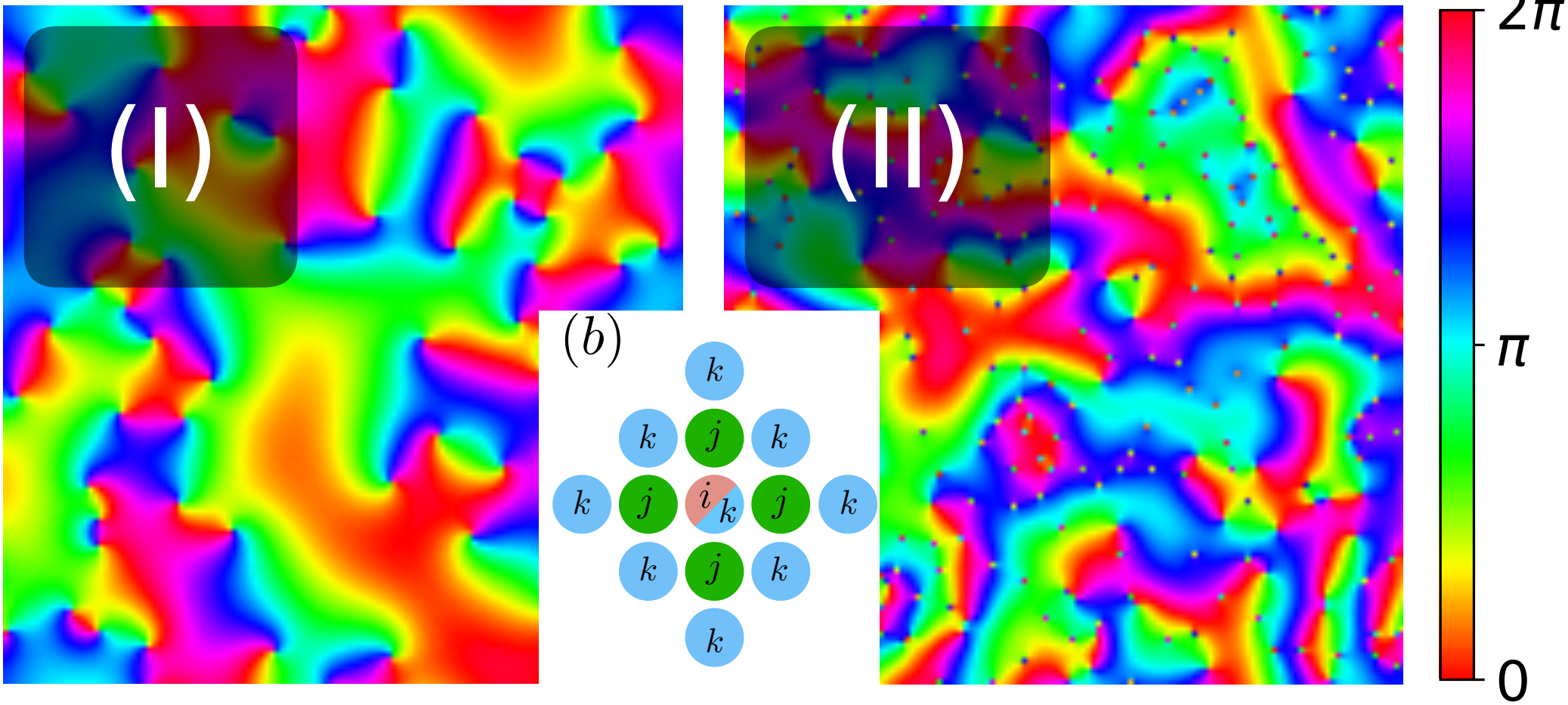
1d Ising model



high resolution limit



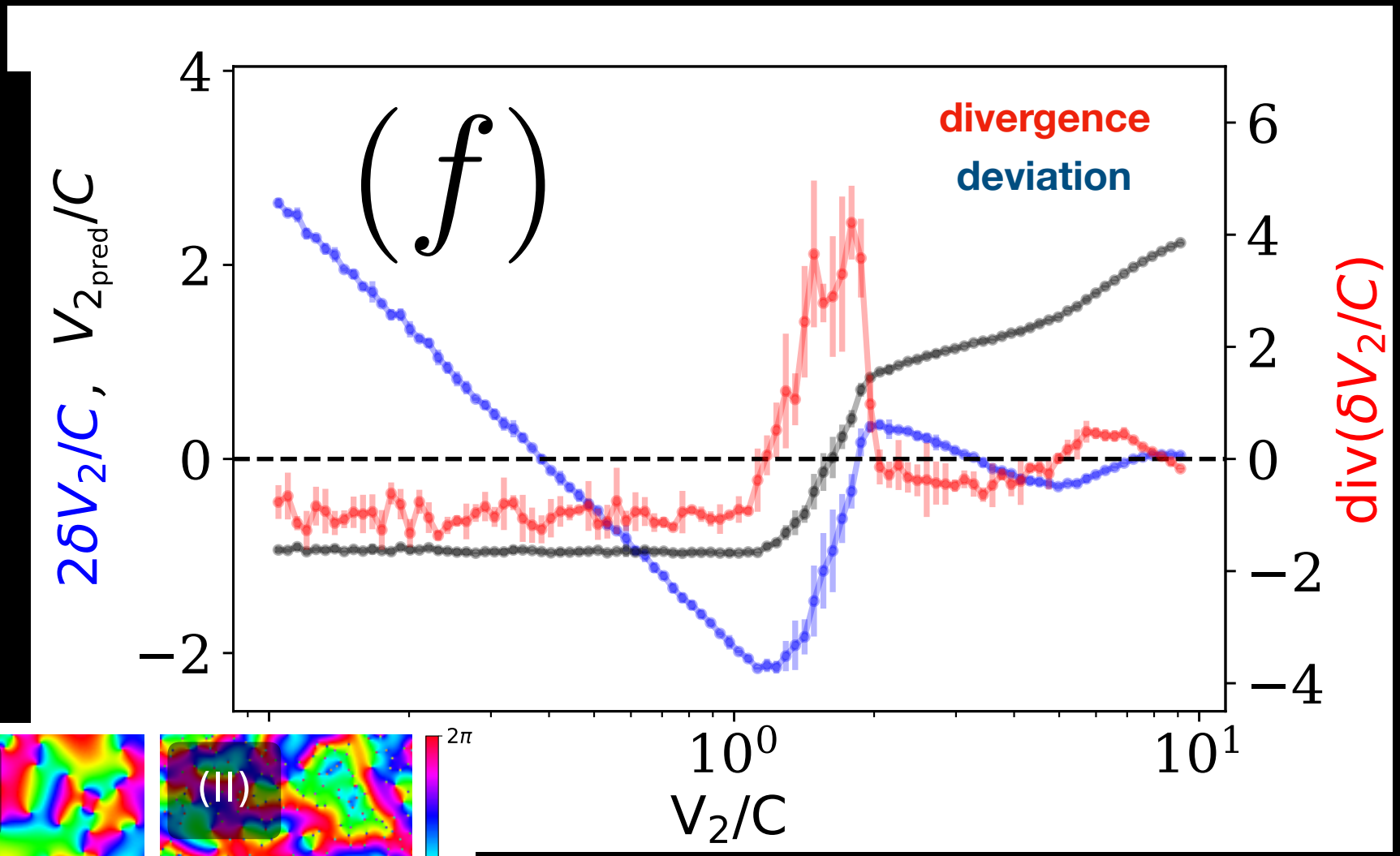
Kuramoto-Hopf model

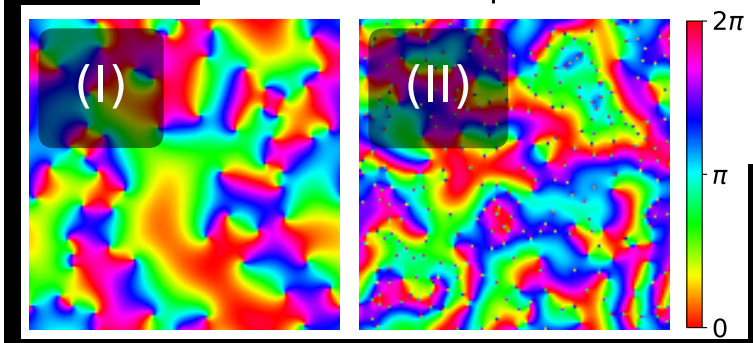


Roland Lauter, Christian Brendel, Steven Habraken, Florian Marquardt, PRE 92, 012902 (2015)

Matthew Matheny et al., *Science* 363 [6431], eaav7932 (2019)

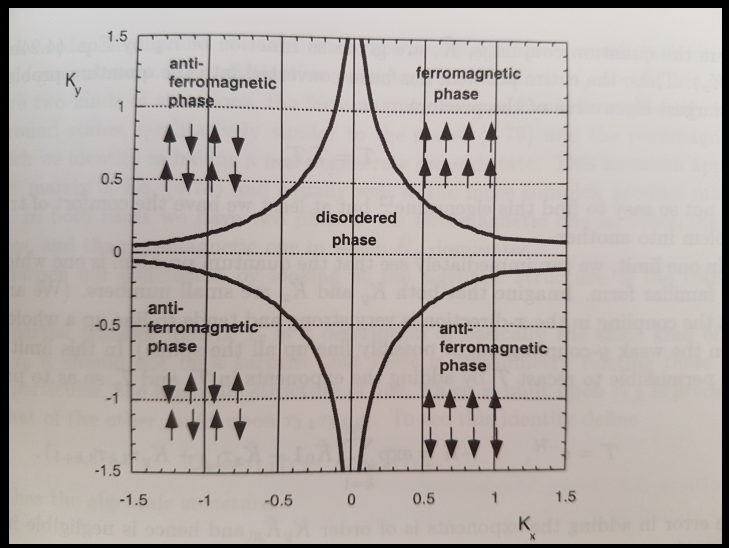
Kuramoto Hopf

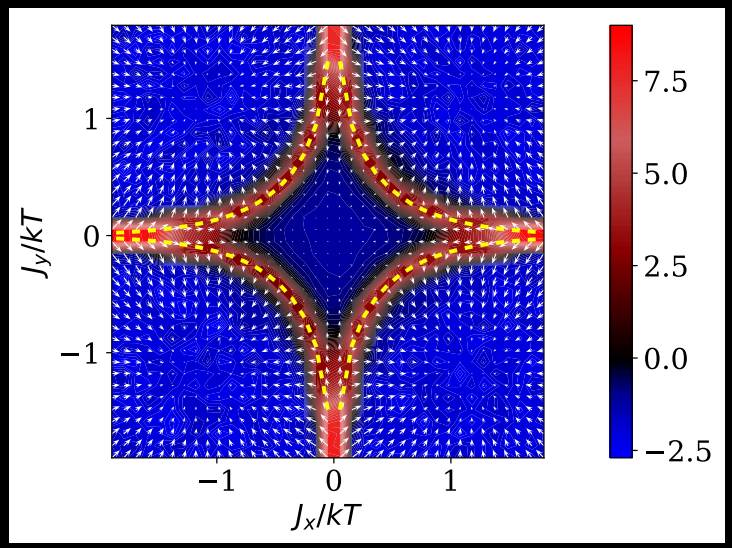




Conclusion and Outlook

- Addition to unsupervised learning toolbox
- Apply this method to less understood systems
- Regularization for regime of high resolution





Frank Schäfer, Niels Lörch, arxiv: 1812.00895