



Statistical physics through the lens of real-space mutual information

Maciej Koch-Janusz



University of
Zurich^{UZH}

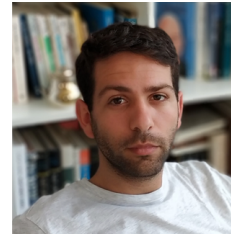


THE UNIVERSITY OF
CHICAGO

Zohar Ringel



Amit Gordon



Aditya Banerjee



- MKJ and Zohar Ringel, *Nature Physics* **14**, 578-582 (2018)
- A. Gordon, A. Banerjee, MKJ and Z. Ringel, “Relevance in RG and in Information Theory” *arXiv:2012.01447*

Doruk Efe Gokmen



Patrick Lenggenhager



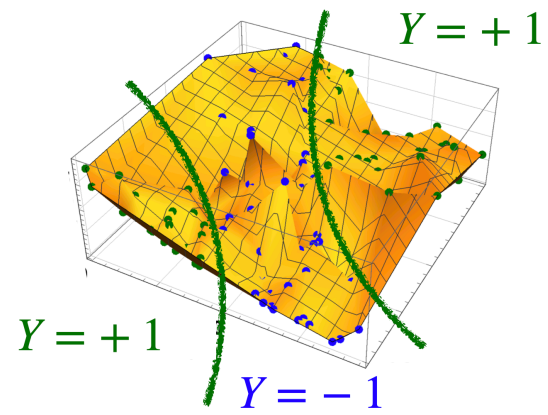
Sebastian D. Huber



- P. Lenggenhager, D.E. Gokmen, Z. Ringel, S.D. Huber and MKJ, *Phys. Rev. X* **10**, 011037 (2020)
- D.E. Gokmen, Z. Ringel, S.D. Huber and MKJ, “Statistical physics through the lens of real-space mutual information” *arXiv:2101.11633*

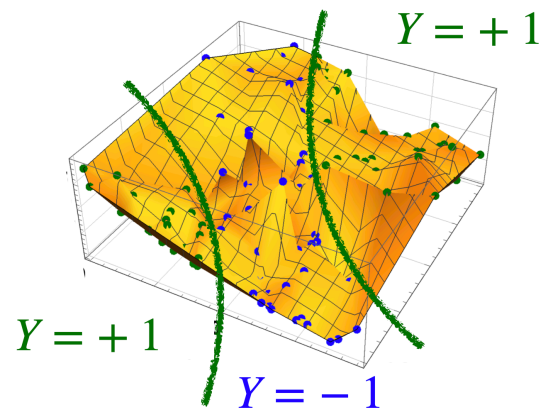
ML and physics

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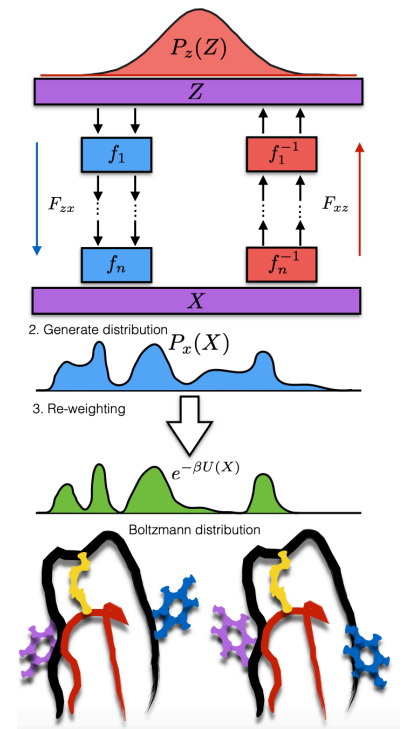


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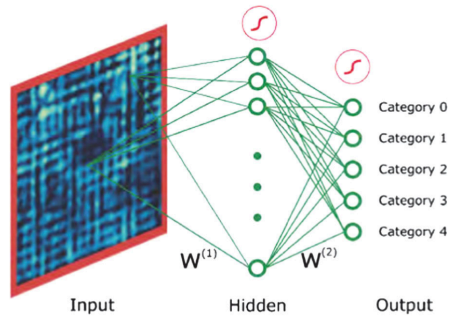
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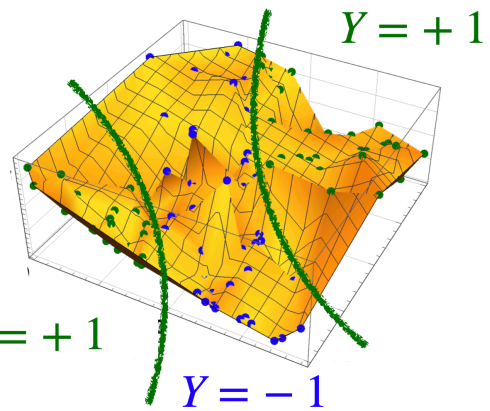
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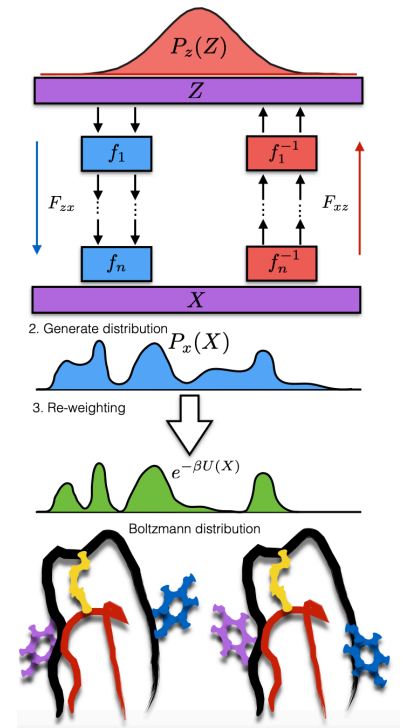


$Y = +1$

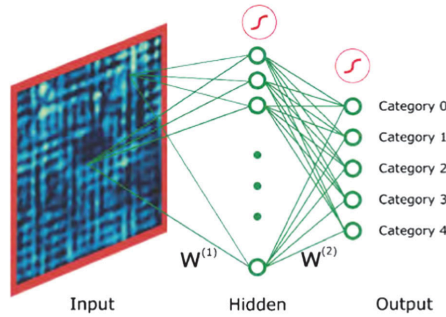


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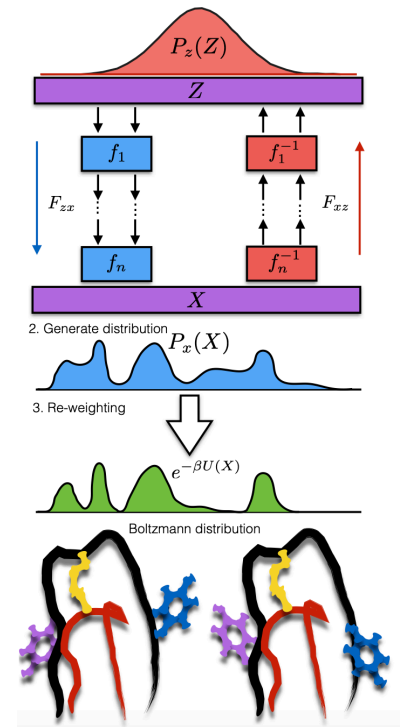
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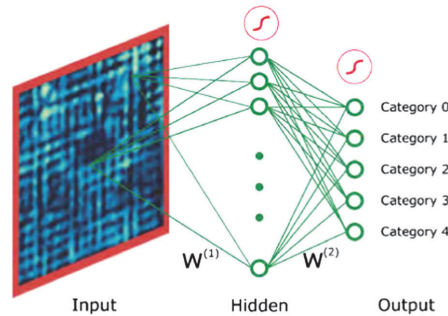
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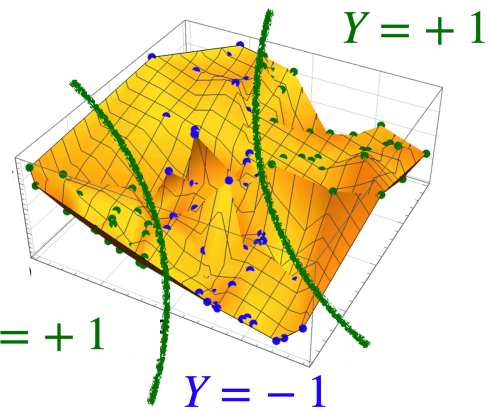


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- Juan Carrasquilla “Machine Learning for Quantum matter” *Advances in Physics: X*, 5:1 (2020)

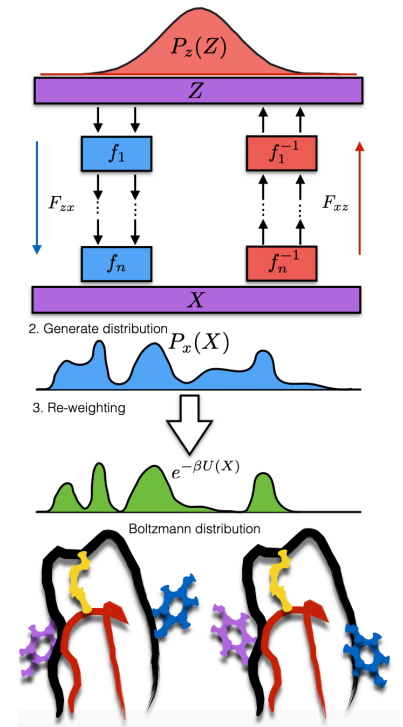
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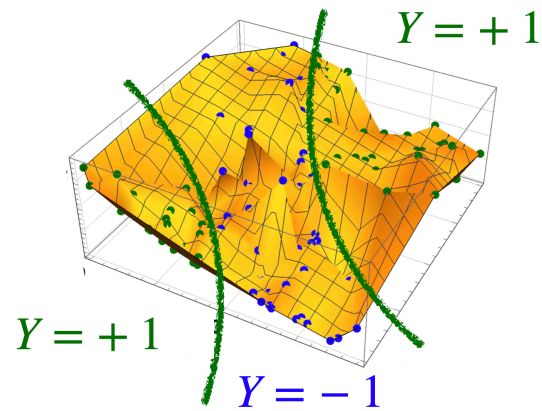
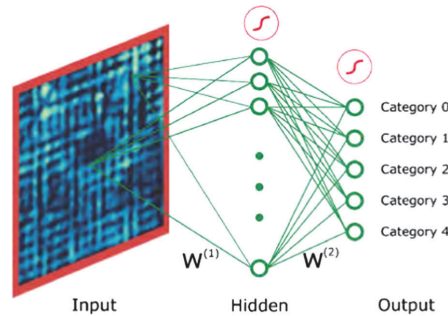
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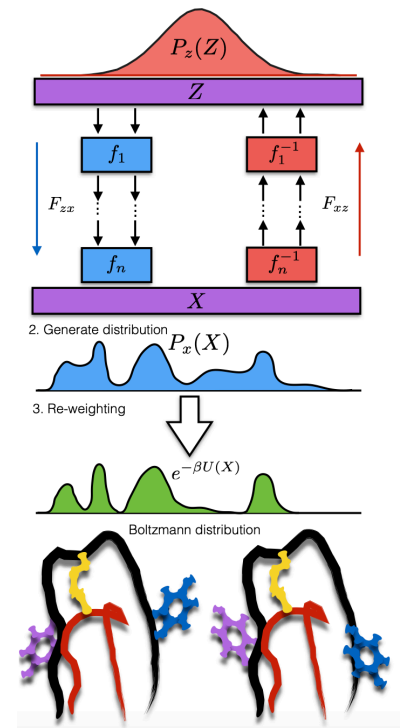
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- Challenges: reproducibility, interpretability, re-usability

ML and physics



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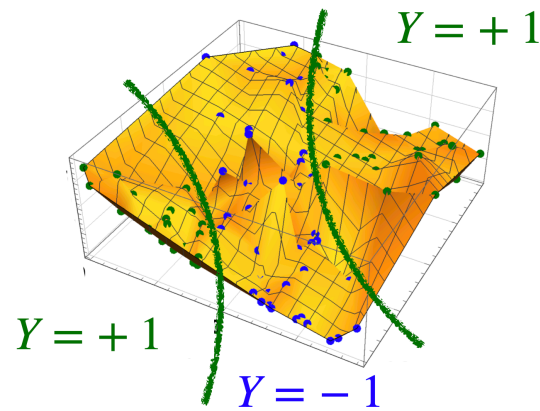
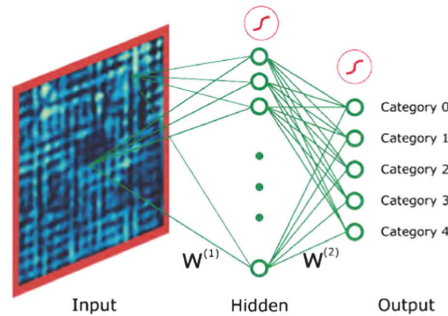


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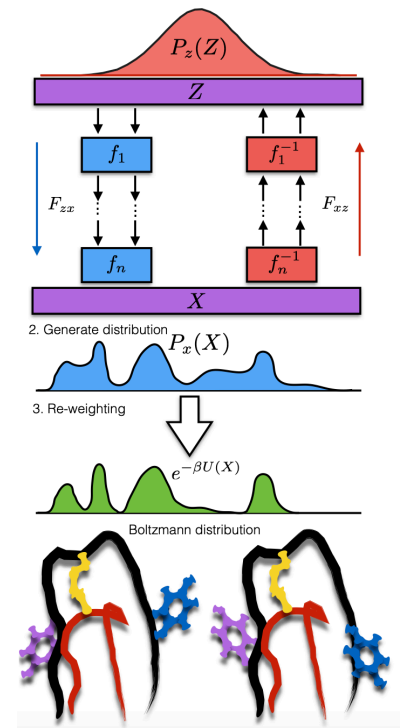


Automating theory-building

ML and physics



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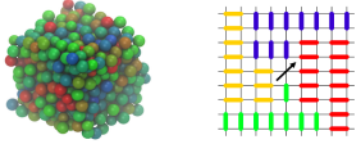
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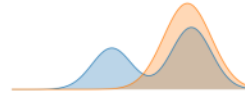
Automating theory-building

- **Formal** interpretability without prior knowledge

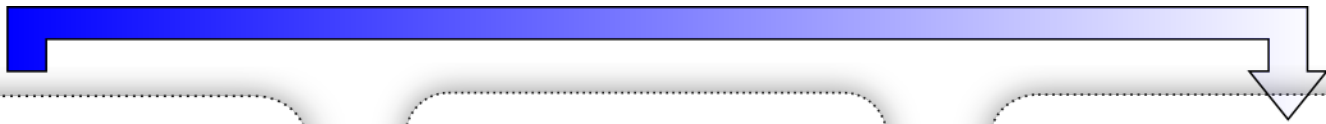
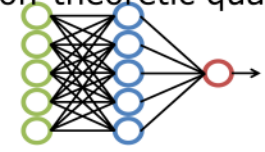
Using computational methods of
stat.mech. to improve ML



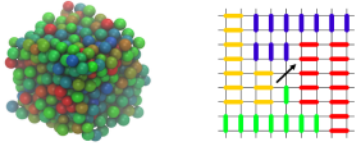
Applying information theory
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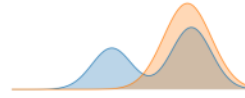
Using ML to approximate
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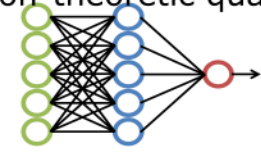
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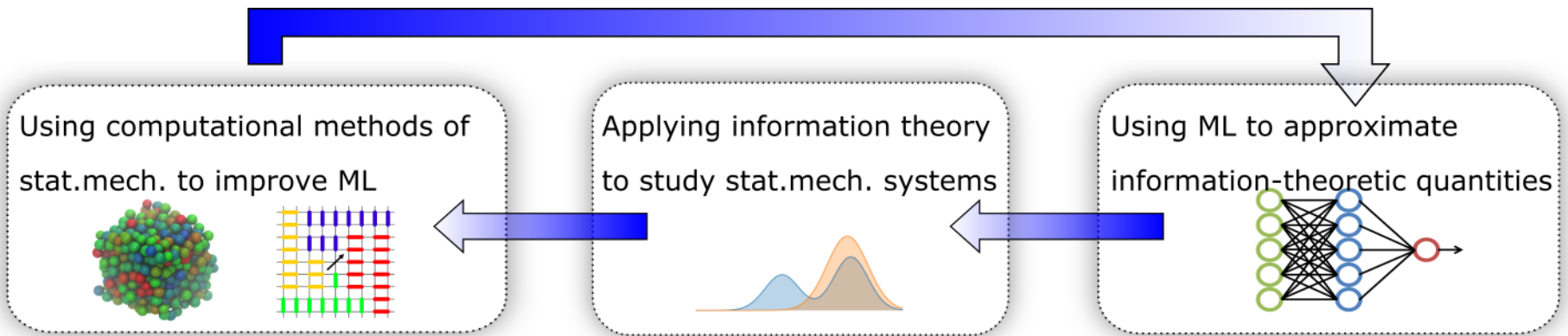
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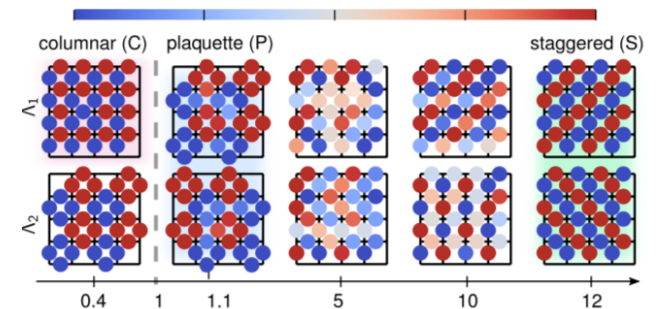


- Optimal RG transformation as a variational problem in information theory
- <https://github.com/RSMI-NE/RSMI-NE>
- Comprehensive view of long-distance physics
- Constructing the relevant operators
- Formal connection between compression theory and field theory formalism
- Possible extensions to non-equilibrium



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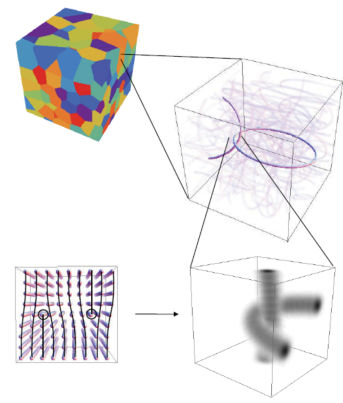
Renormalization Group

Renormalization Group

- Coarse-graining is important in theory/applications

Renormalization Group

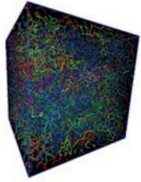
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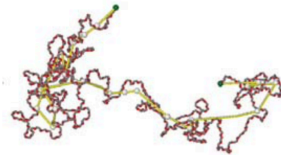
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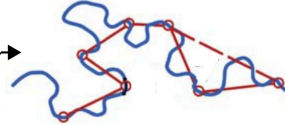
Atomistic simulations
of entangled polymer chains



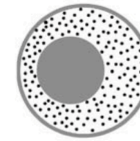
Primitive path analysis
to find model parameters



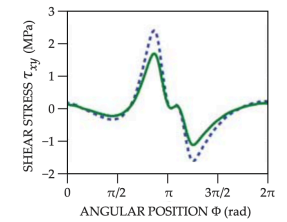
Discrete slip-link model
with parameters from
atomistic simulations



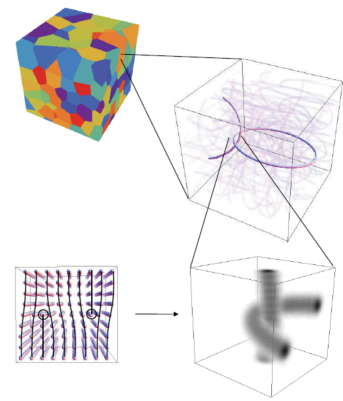
Macroscopic flow
simulation



Stress prediction in complex flow



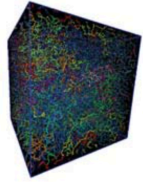
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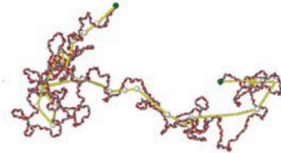
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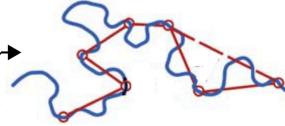
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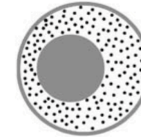
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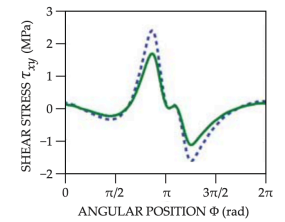
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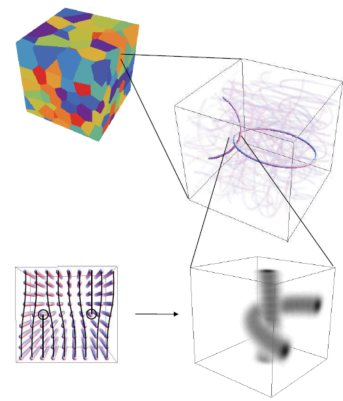
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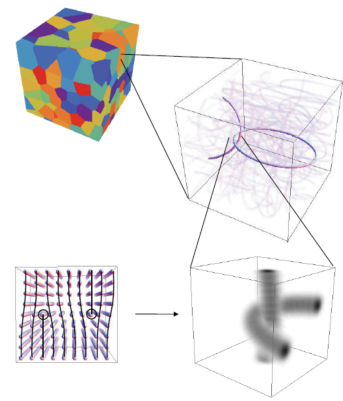


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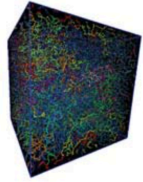


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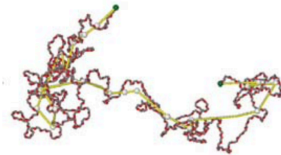
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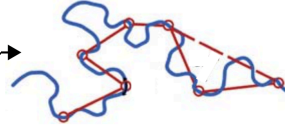
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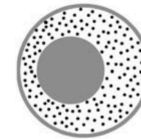
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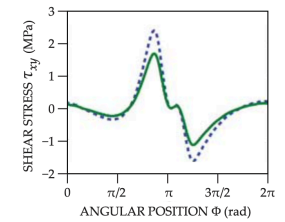
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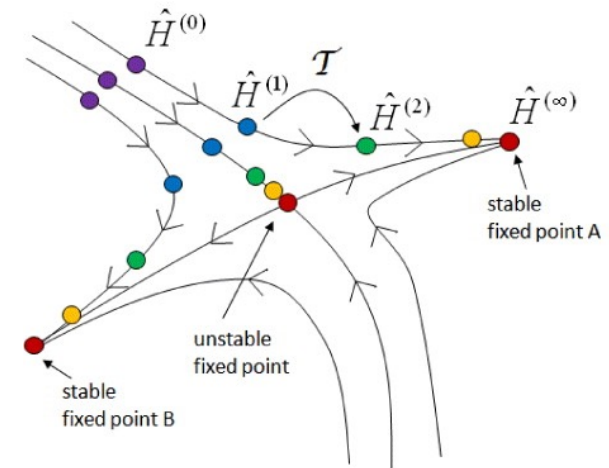
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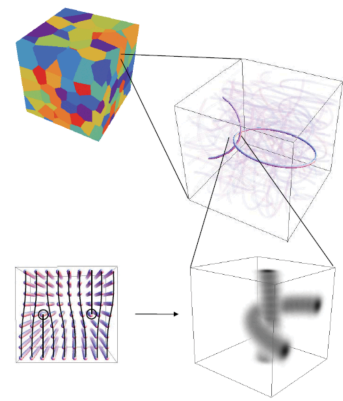


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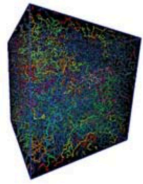


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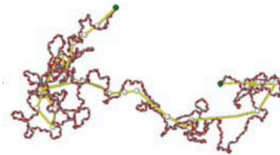
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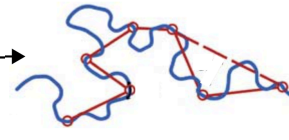
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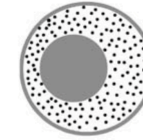
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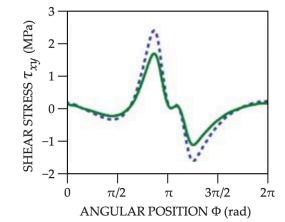
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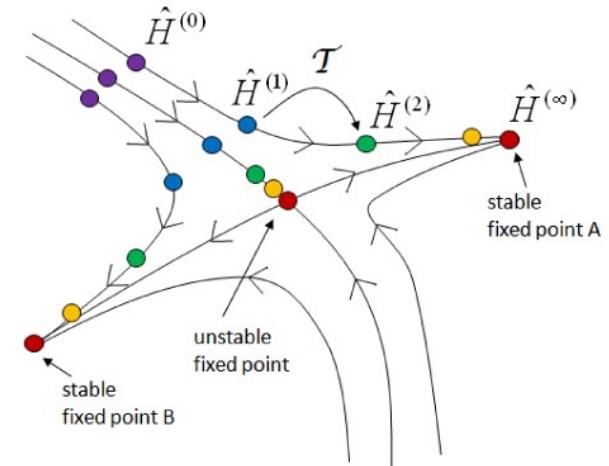


Stress prediction in complex flow



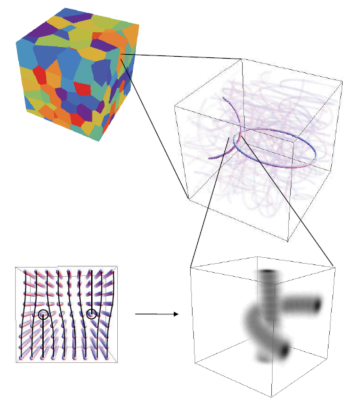
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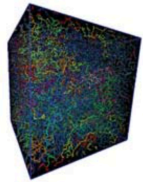


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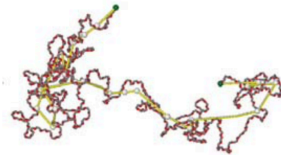
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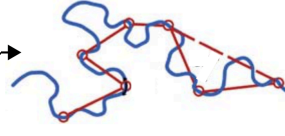
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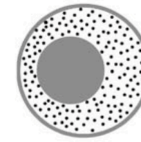
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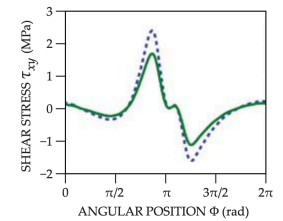
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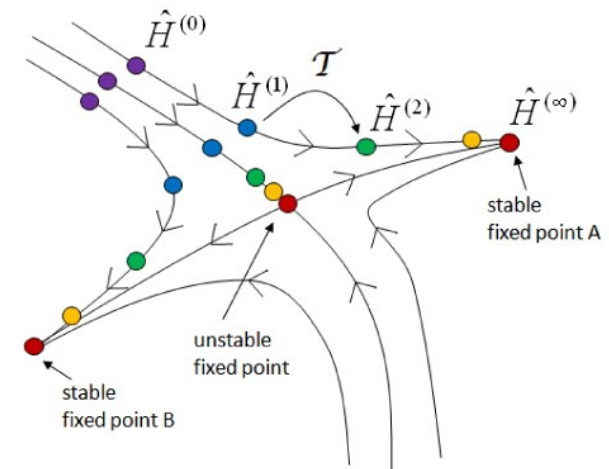


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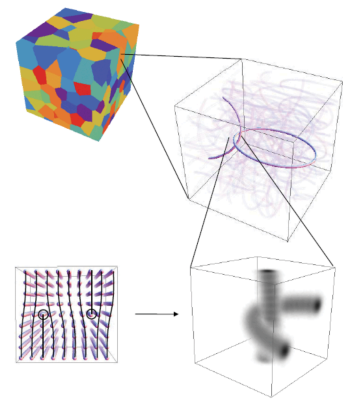
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- Many flavors: Wilsonian, DMRG, real-space,...

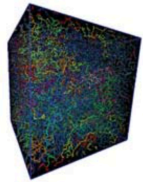


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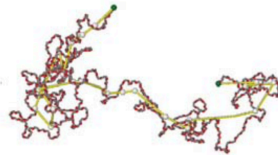
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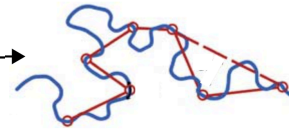
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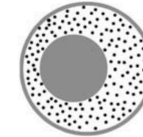
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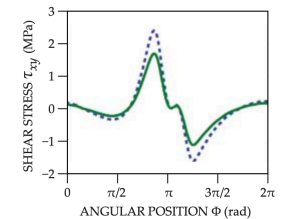
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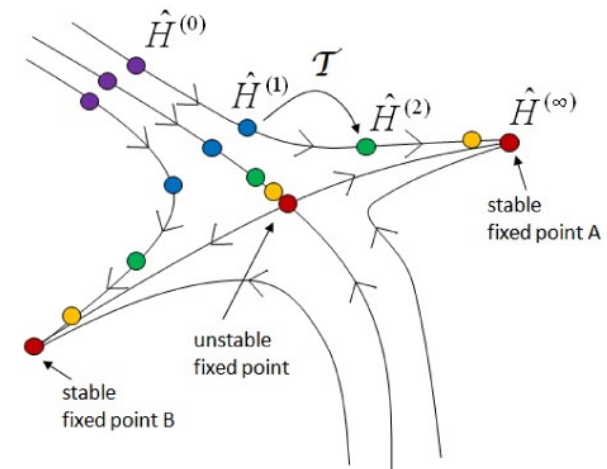


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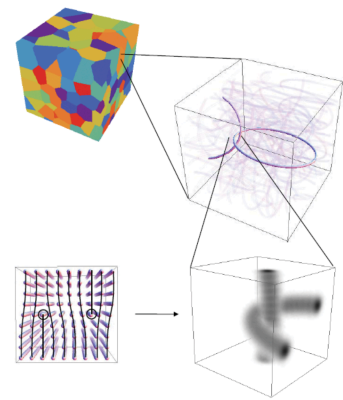
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- Many flavors: Wilsonian, DMRG, real-space,...
- Leitmotiv: integrate out DOFs to obtain effective theory of the remaining ones

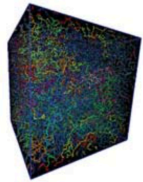


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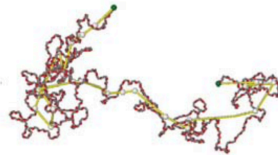
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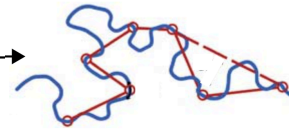
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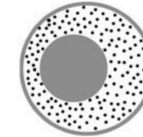
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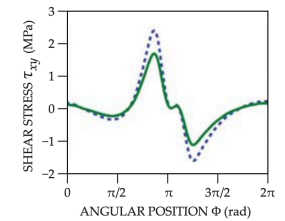
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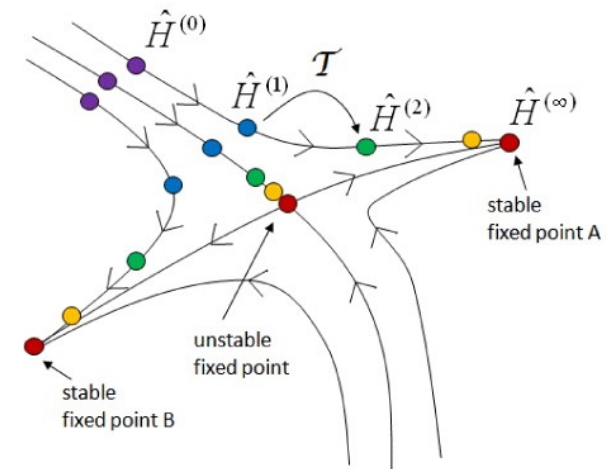
Stress prediction in complex flow



Schieber, Huetter, Physics Today (2020)

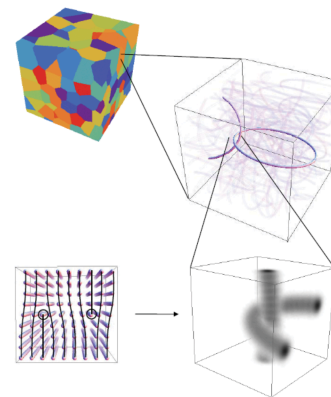
- Formalizes the notion of universality
- Many flavors: Wilsonian, DMRG, real-space,...
- Leitmotiv: integrate out DOFs to obtain effective theory of the remaining ones

The relation of RG to information theory is obvious but:

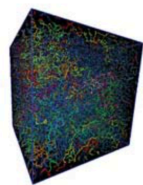


Renormalization Group

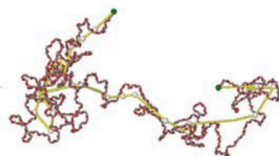
- Coarse-graining is important in theory/applications
- Deriving effective theories



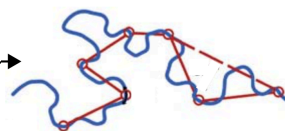
Atomistic simulations of entangled polymer chains



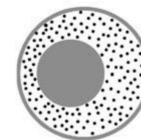
Primitive path analysis to find model parameters



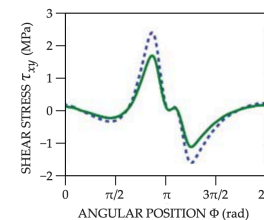
Discrete slip-link model with parameters from atomistic simulations



Macroscopic flow simulation



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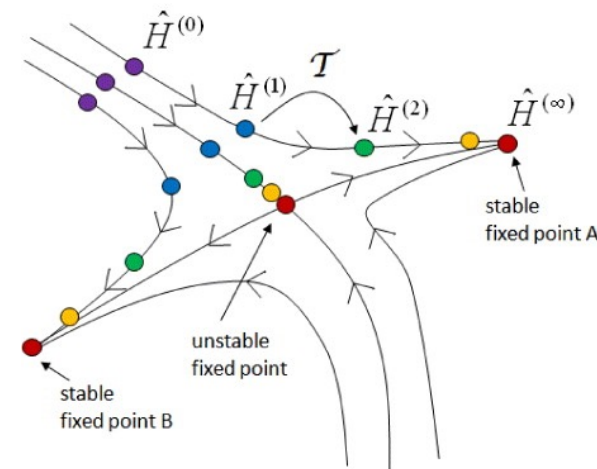


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The relation of RG to information theory is obvious but:

- Can this intuition be formalized?
- Is it useful in practice?

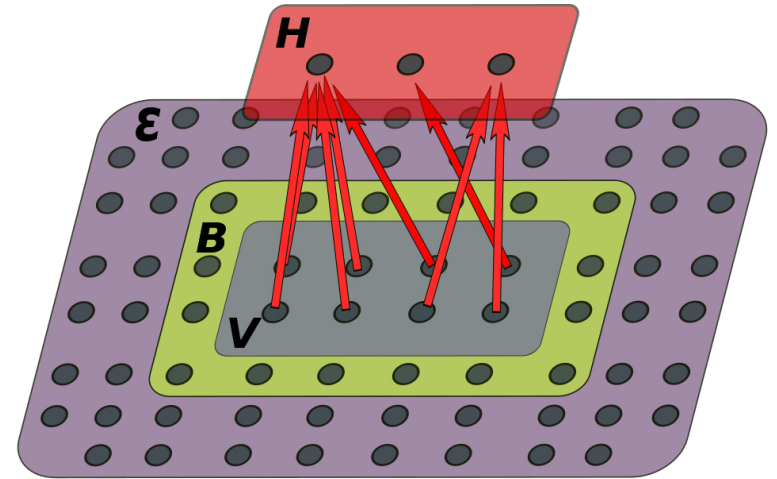


Outline

- The RSMI setup
- Efficient implementation with MINE-based methods
- Examples

- Relevance in RG and in information theory
- Optimality of RSMI
- Symmetries in IB and RG
- Future directions: Non-Eq?

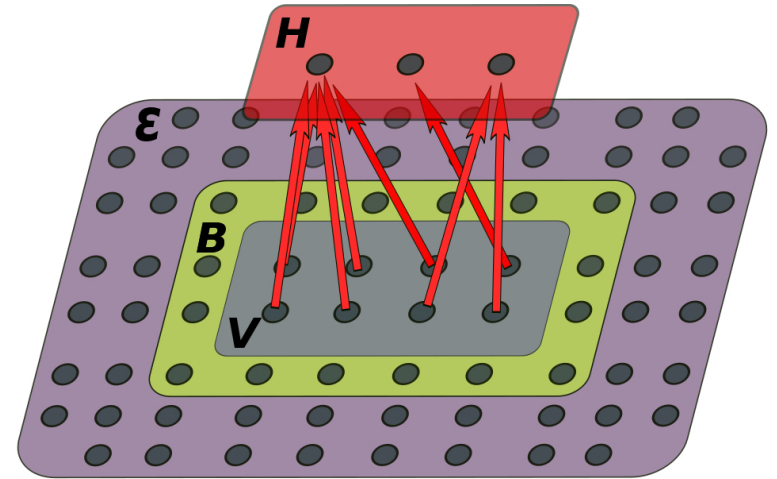
Real-space RG from Information Theory perspective



$$P(\mathcal{X}) = \frac{1}{Z} e^{\kappa(\mathcal{X})}$$

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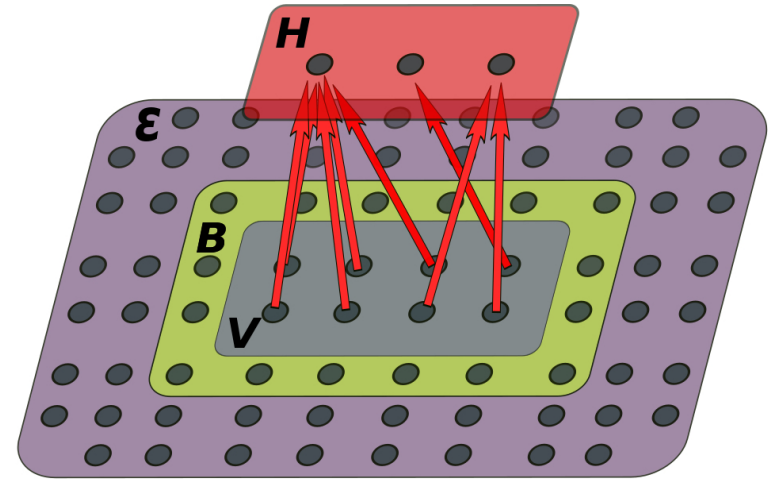
$$e^{\kappa'(\mathcal{X}')} = \sum_{\mathcal{X}} e^{\kappa(\mathcal{X})} P_{\Lambda}(\mathcal{X}'|\mathcal{X})$$



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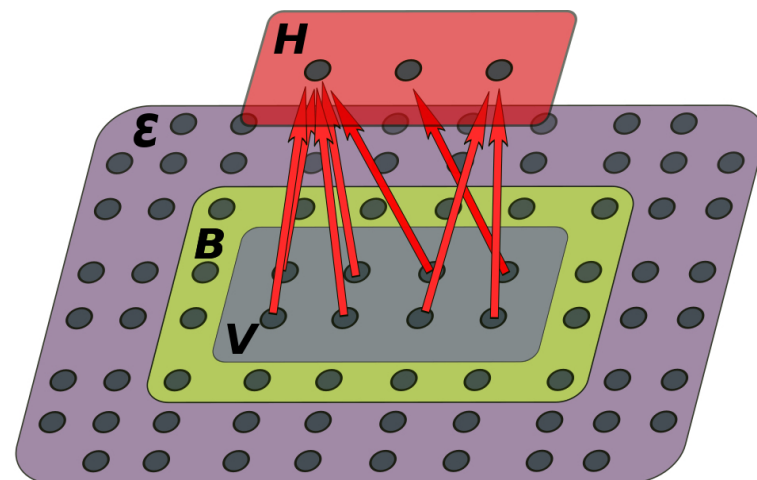


Task: Learn $P_{\Lambda}(\mathcal{H}|\mathcal{V})$ such that \mathcal{H} tracks the most relevant degrees of freedom within region \mathcal{V}

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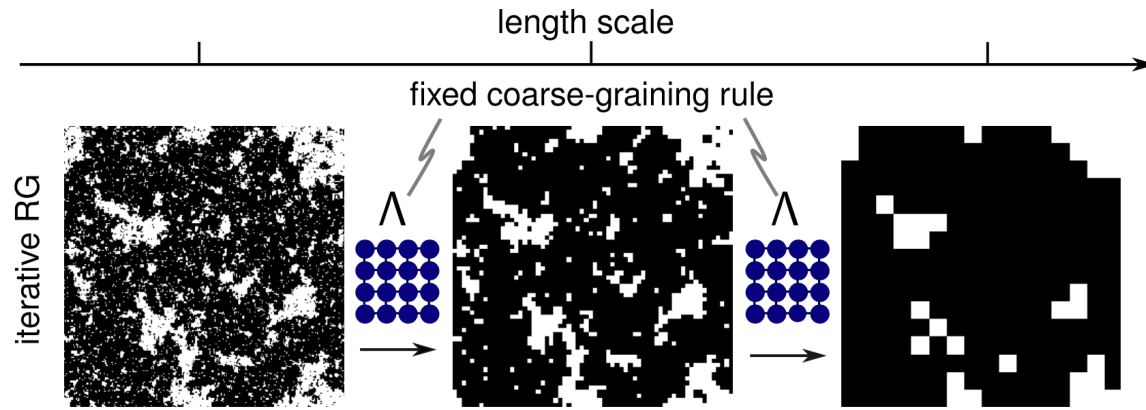
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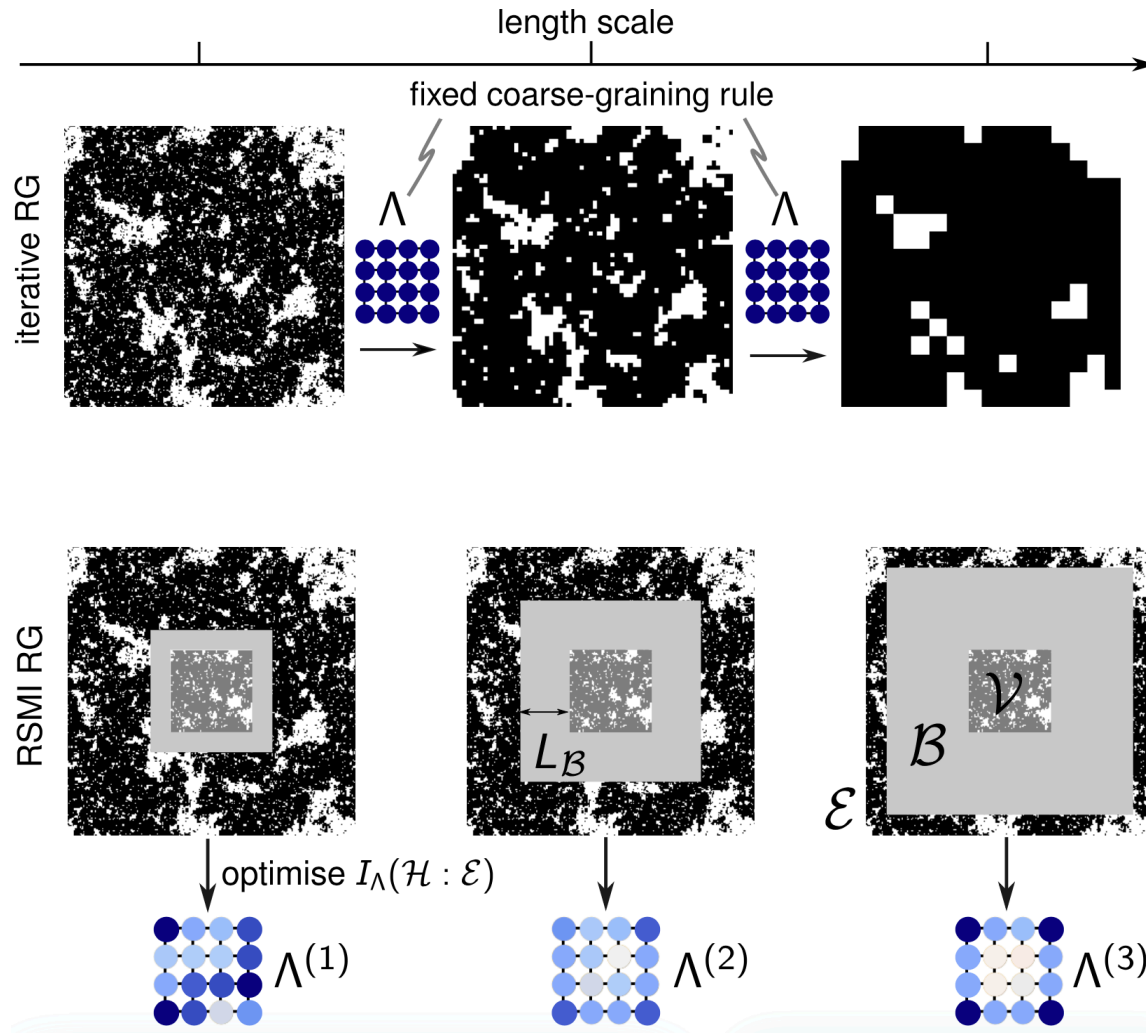
Method: find $\max[I_{\Lambda}(\mathcal{H}:\mathcal{E})]$ over parameters Λ

Iterative Fixed rs-RG vs RSMI

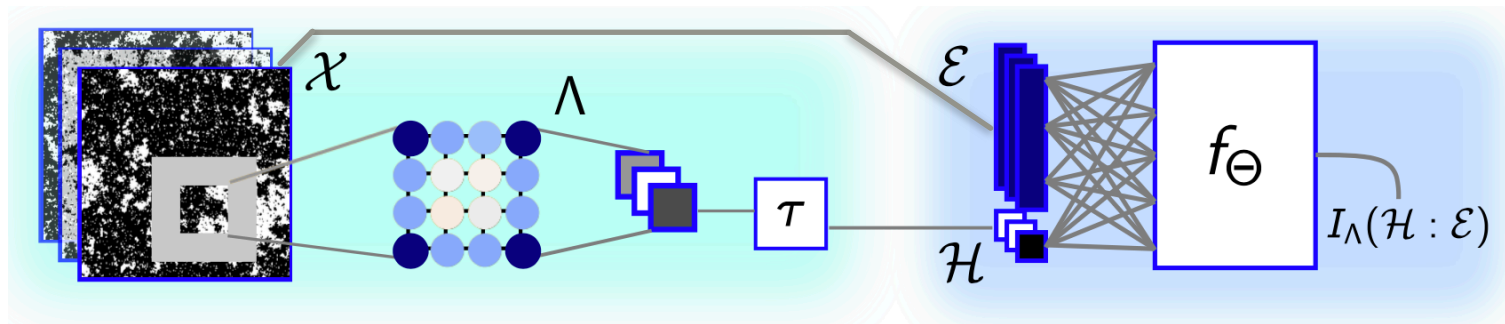
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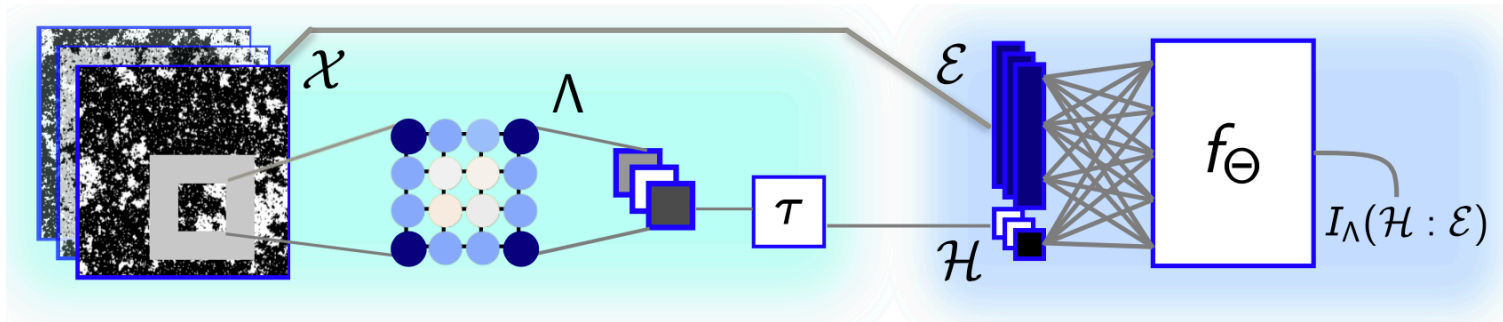


The essential ingredients



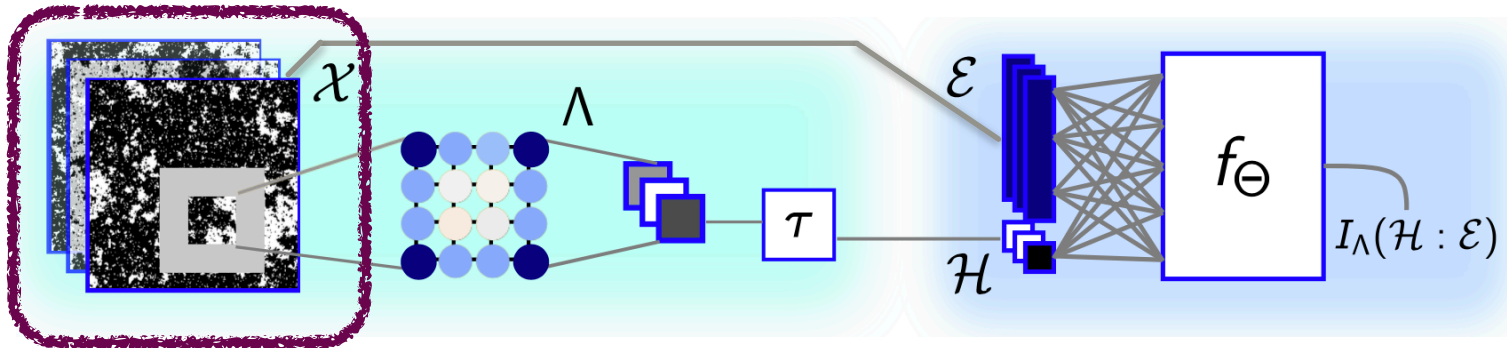
The essential ingredients

- The physical principle: “the cost function”



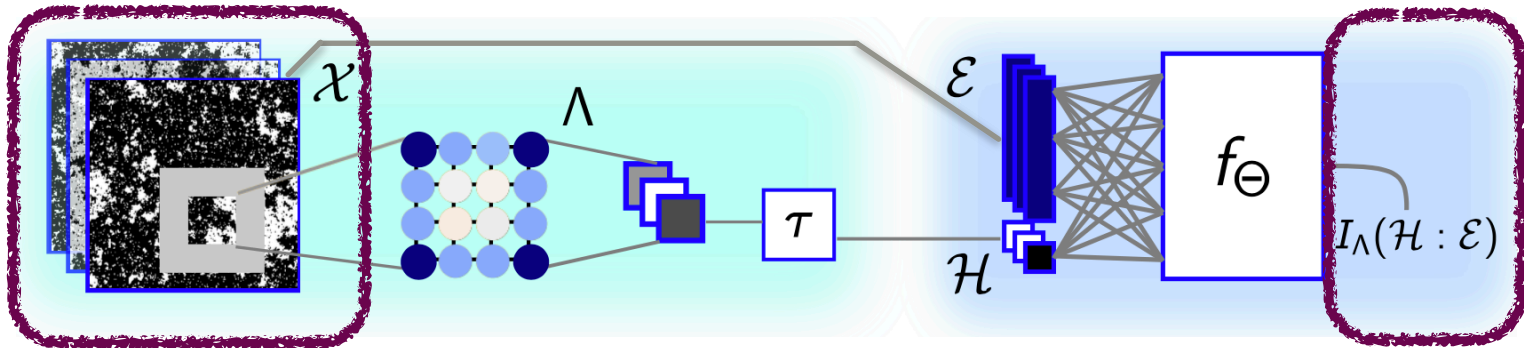
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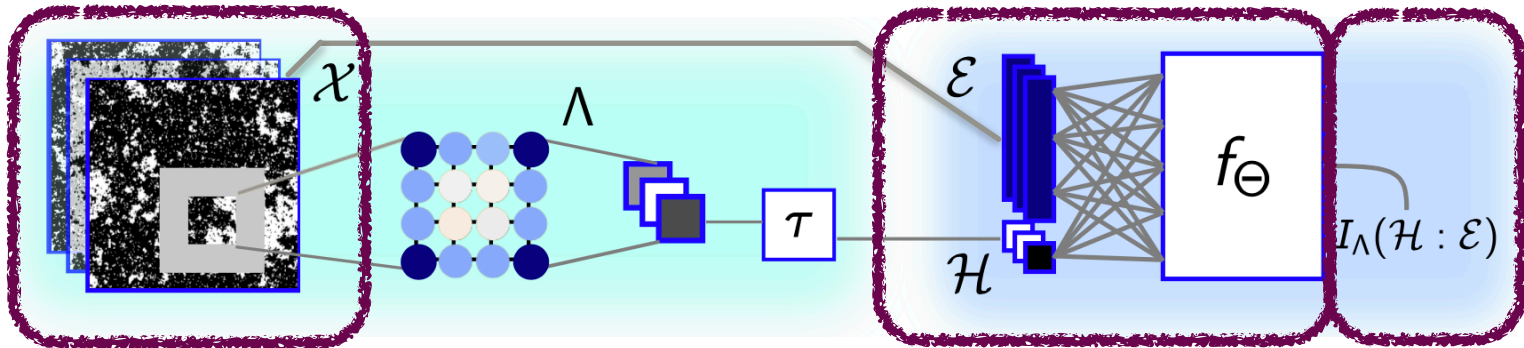
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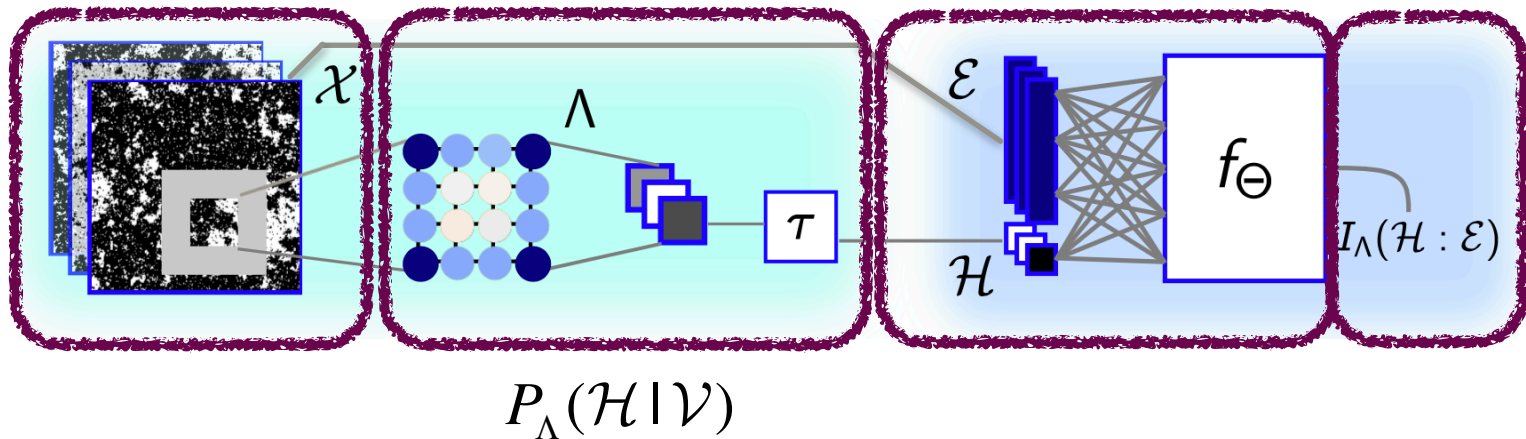
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The essential ingredients

- The physical principle: “the cost function”
- The MI estimator
- The RG ansatz



Estimating MI with neural networks

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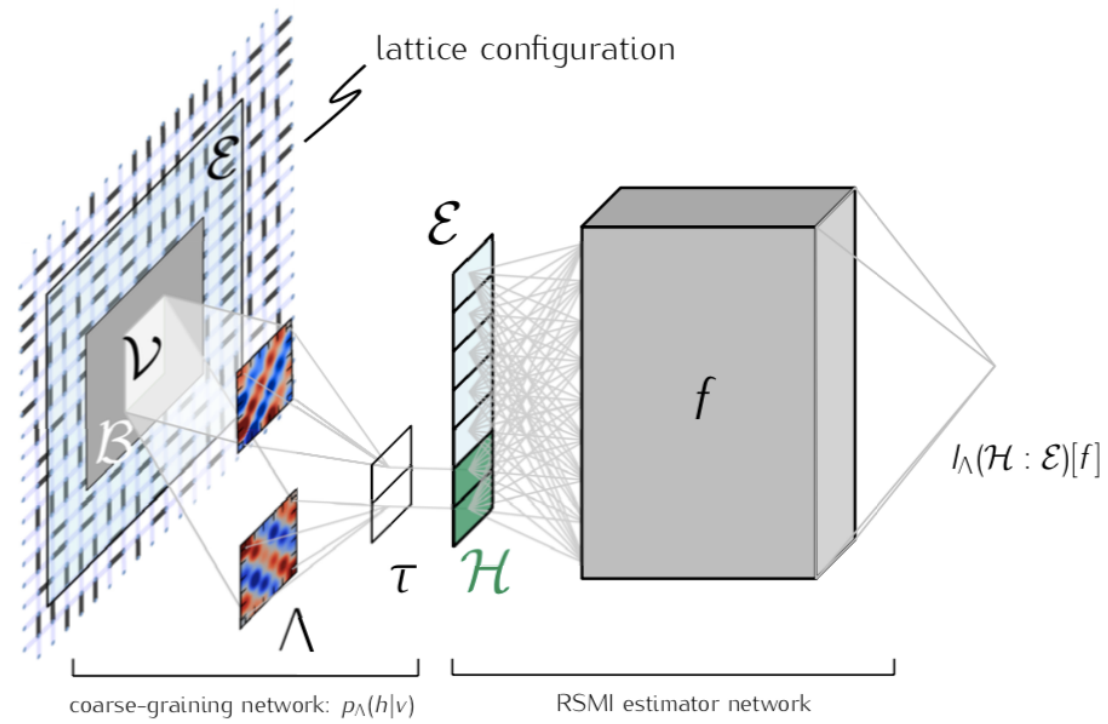
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InfoNCE, van den Oord et al. (2018)

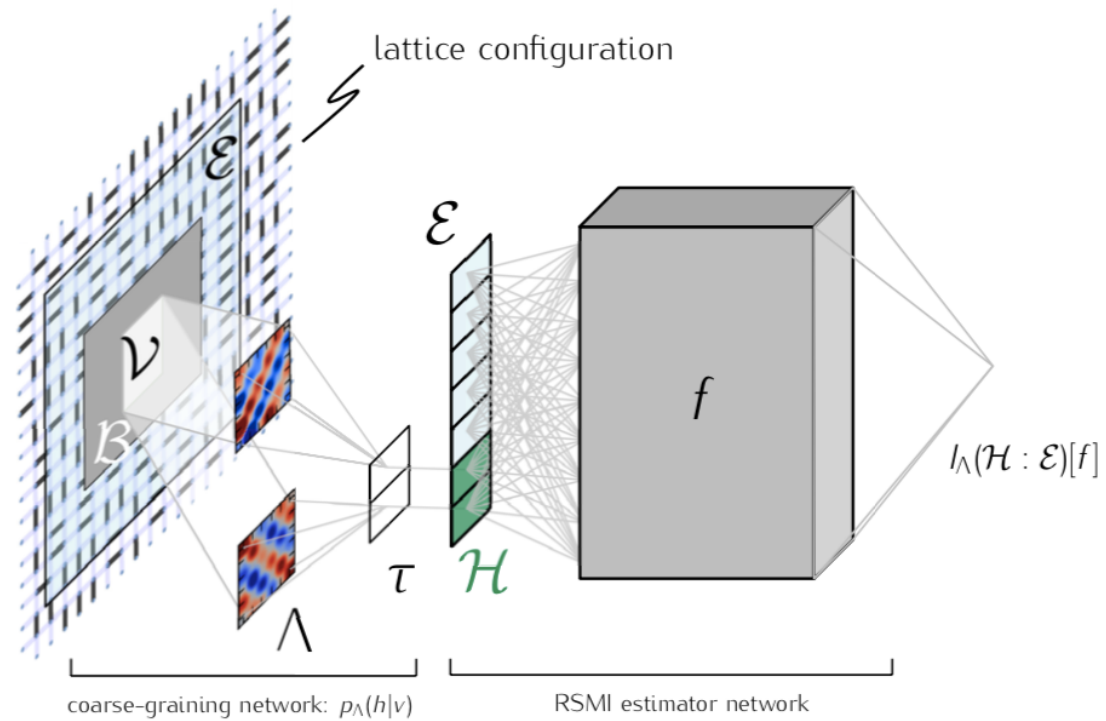
Poole et al. ICMLR (2019) "On variational bounds of mutual information"

The RSMI-NE network



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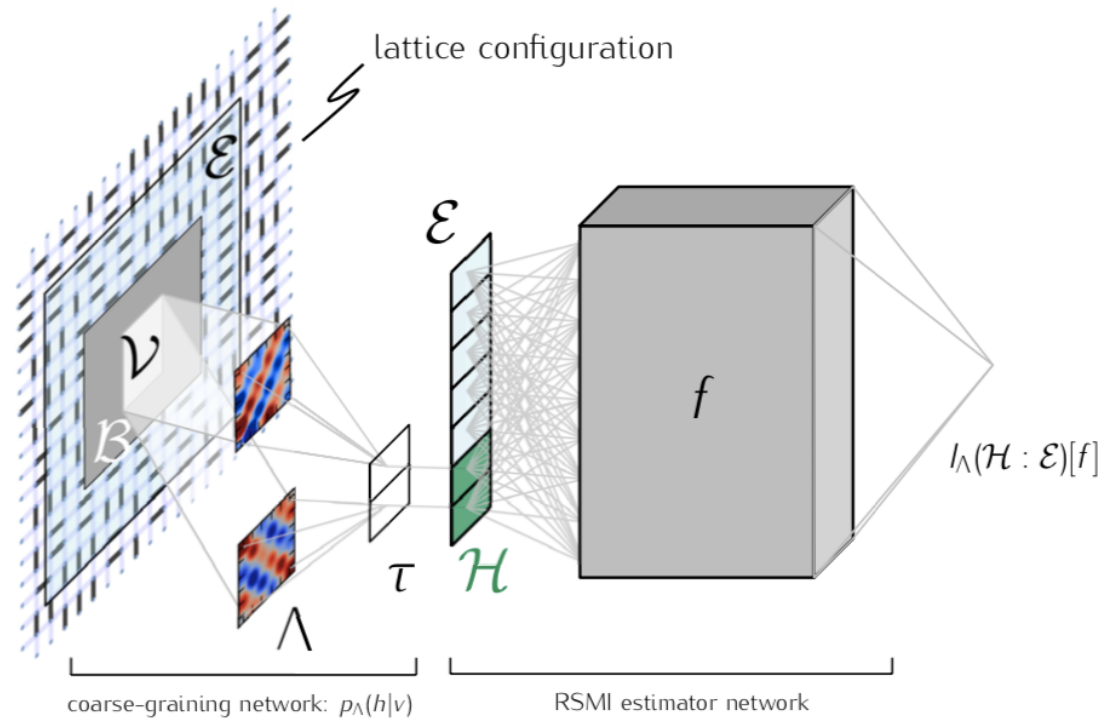
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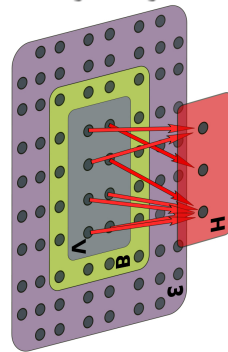
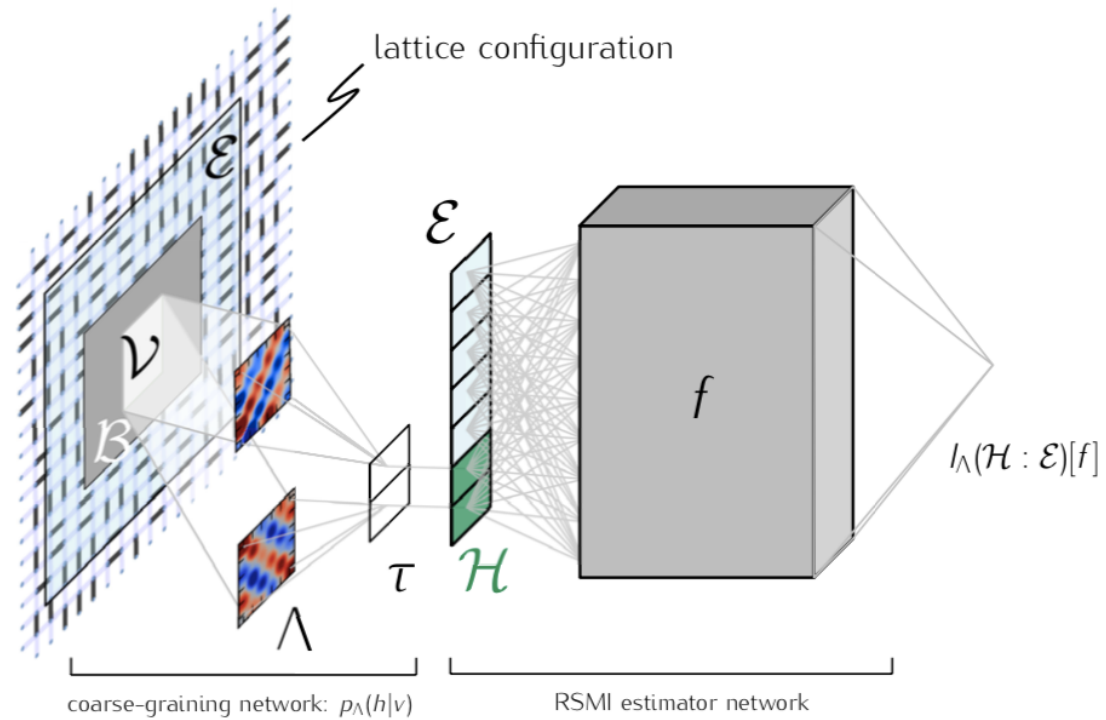
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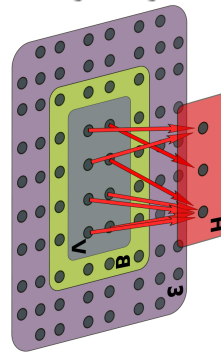
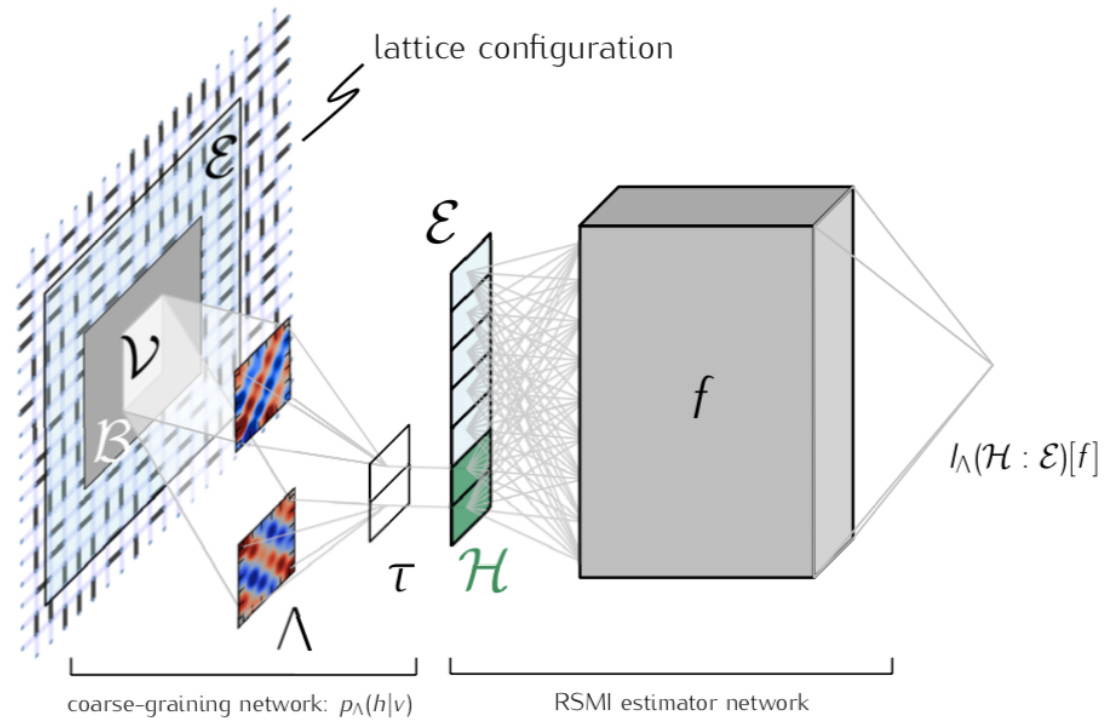
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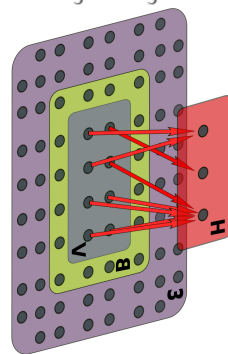
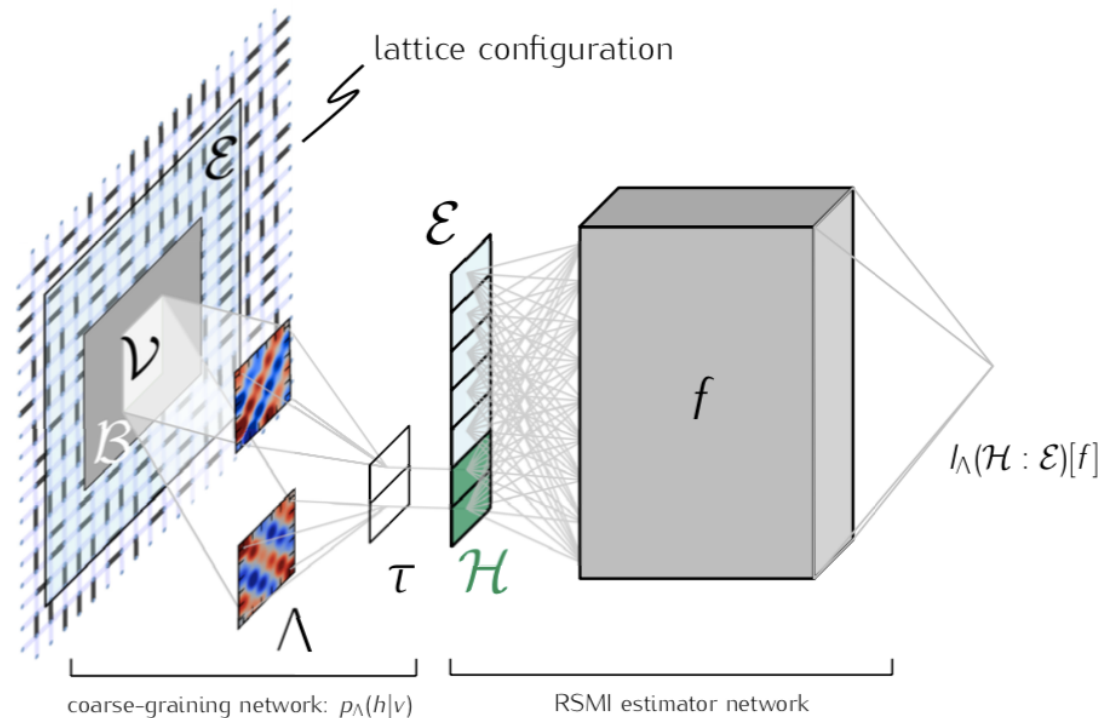
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Jang, Gu, Poole ICLR (2017)
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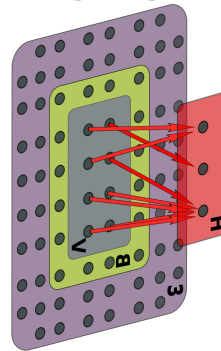
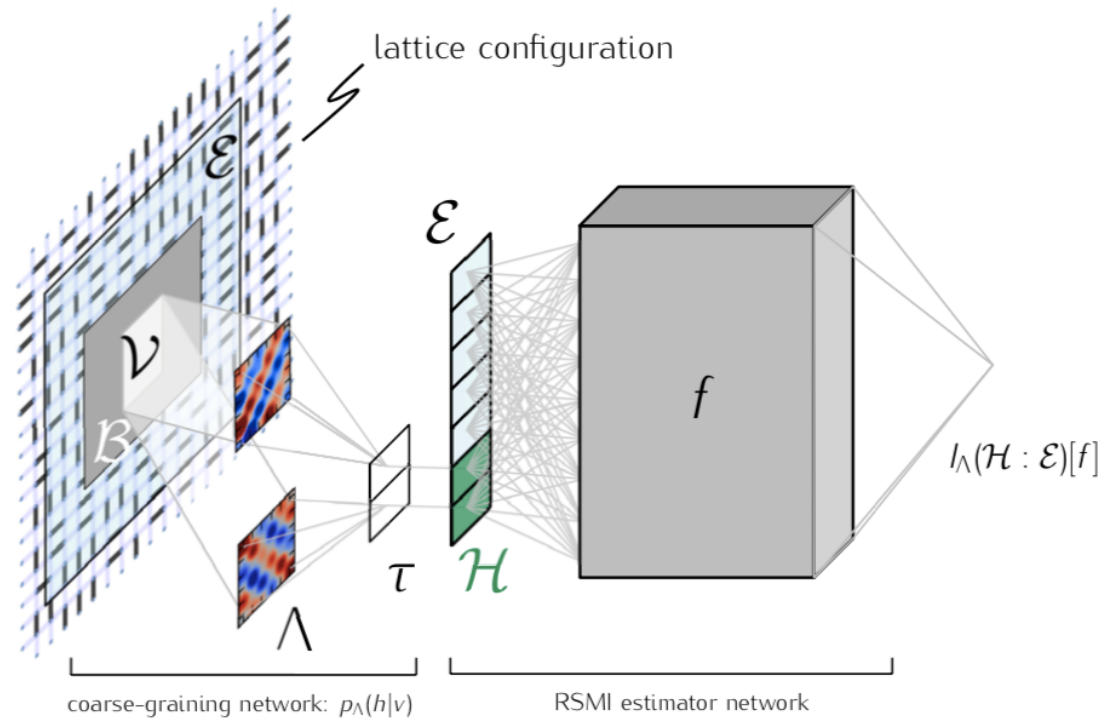
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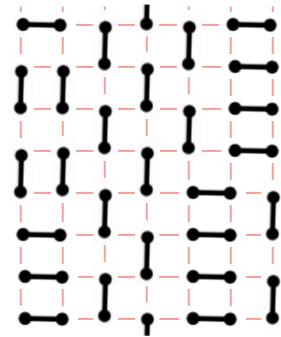
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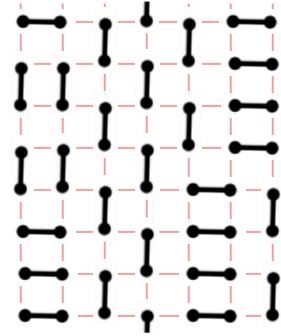
- The RSMI estimator and the coarse-graining Ansatz are chained together
- They are co-trained with SGD as a single network (**because: differentiable, upper bounded!**)

Example: interacting dimer model

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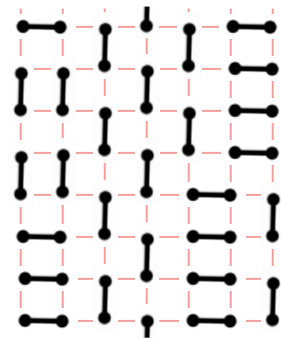
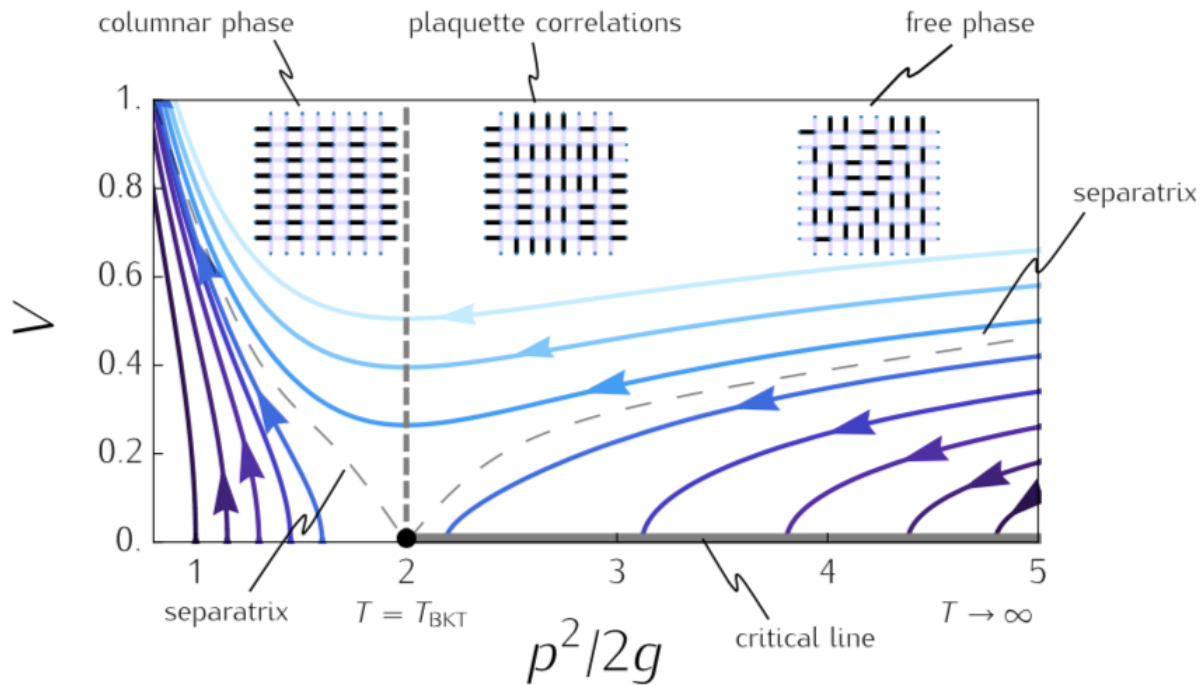
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$$Z = \sum_c \exp(-E_c/T),$$

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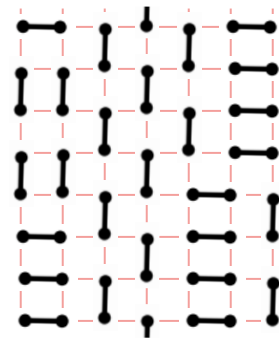
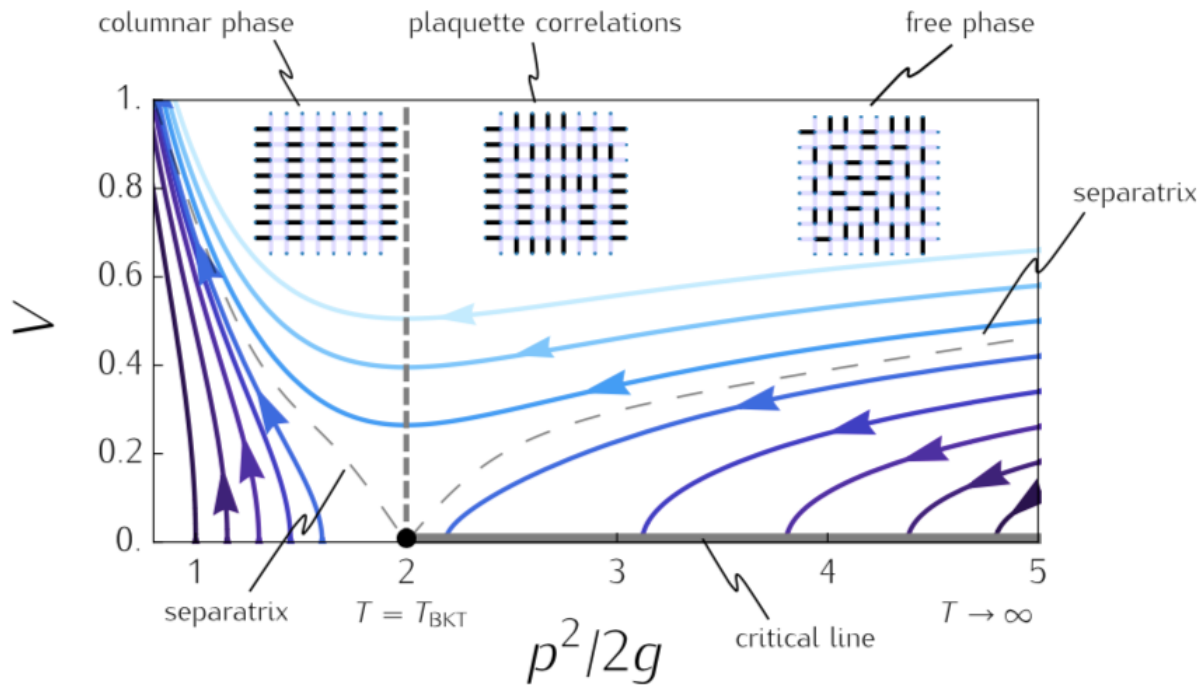
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Alet et al. PRE 74, 041124 (2006)

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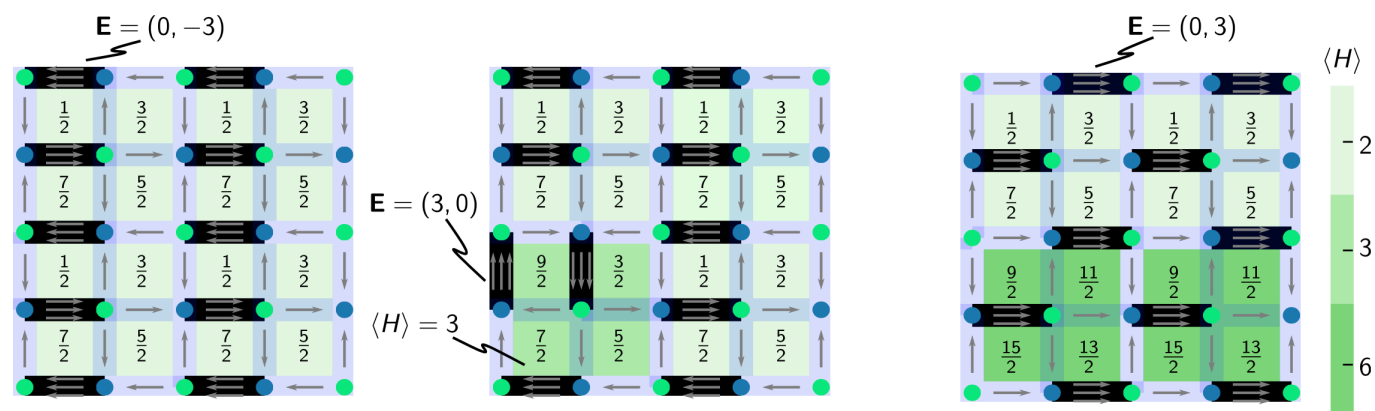
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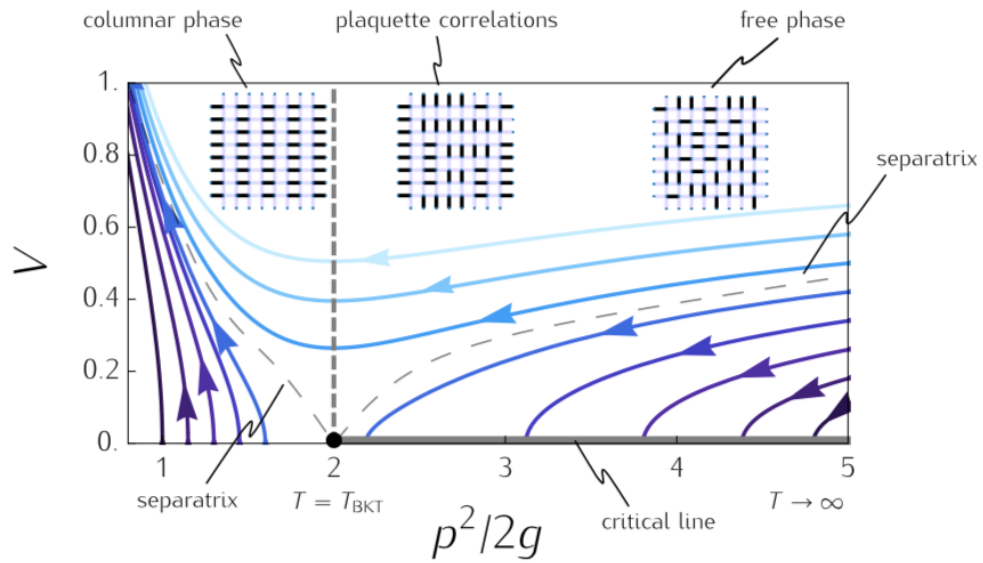
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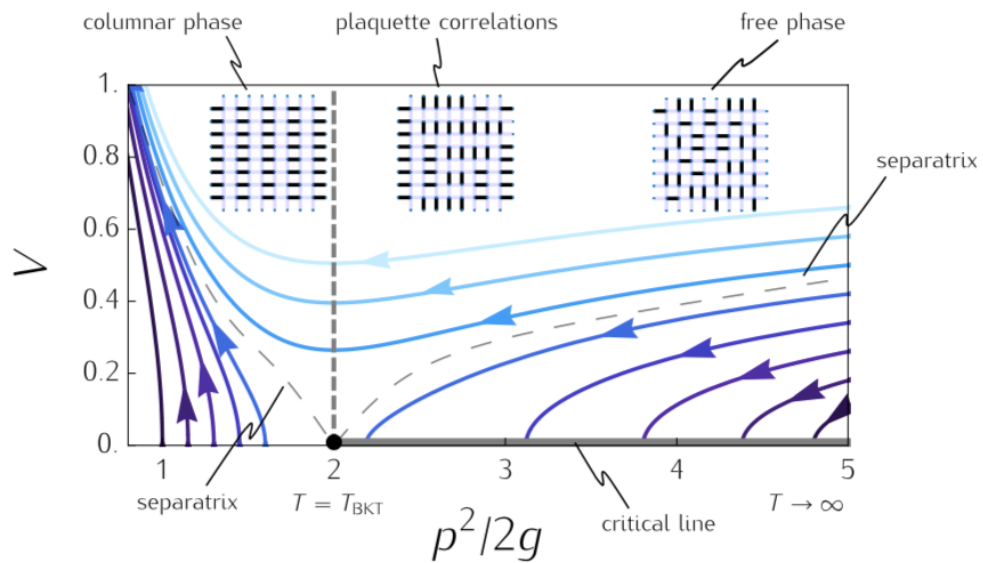
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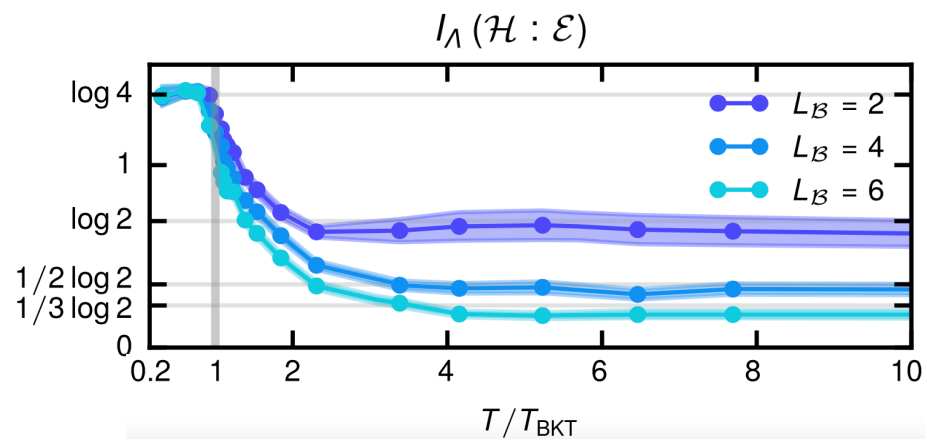
RG of dimer model:
mapping to height field

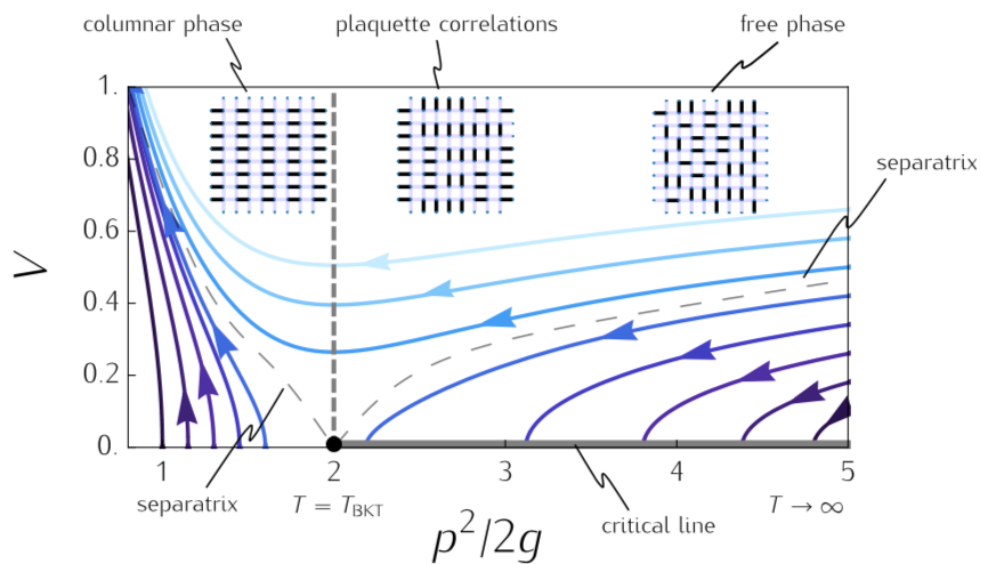




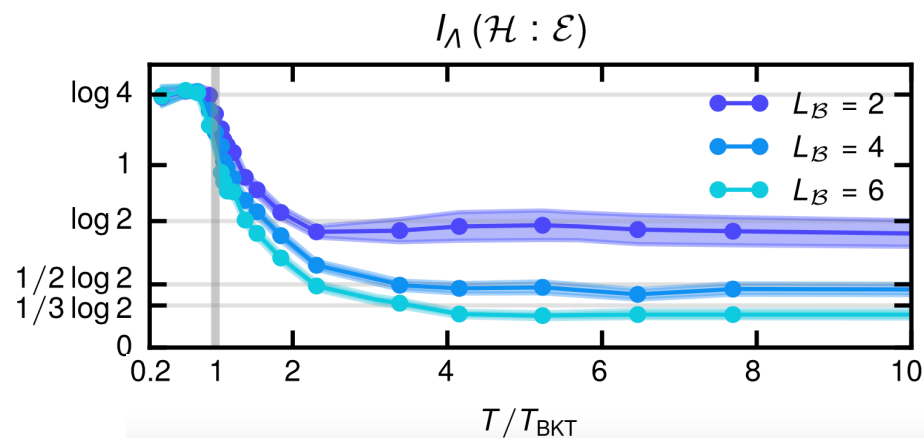


■ Total RSMI with the *optimal* filter

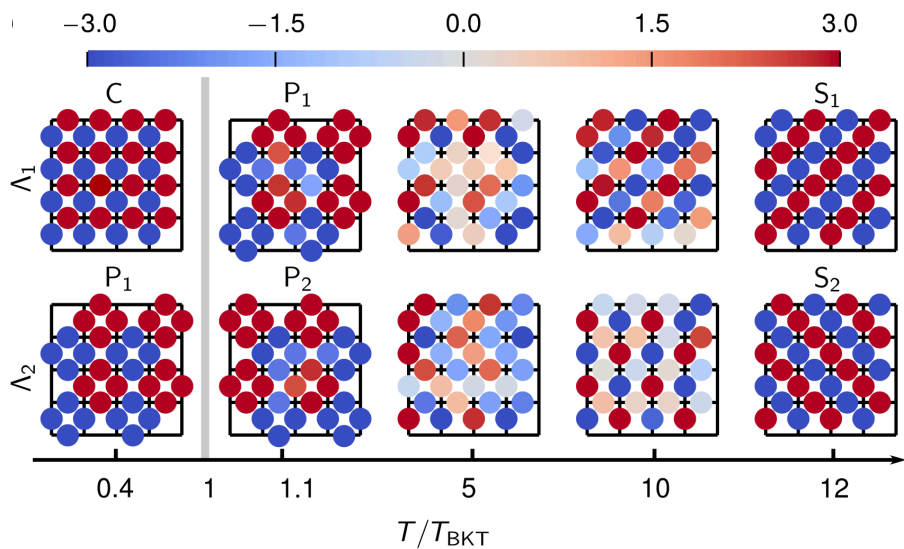


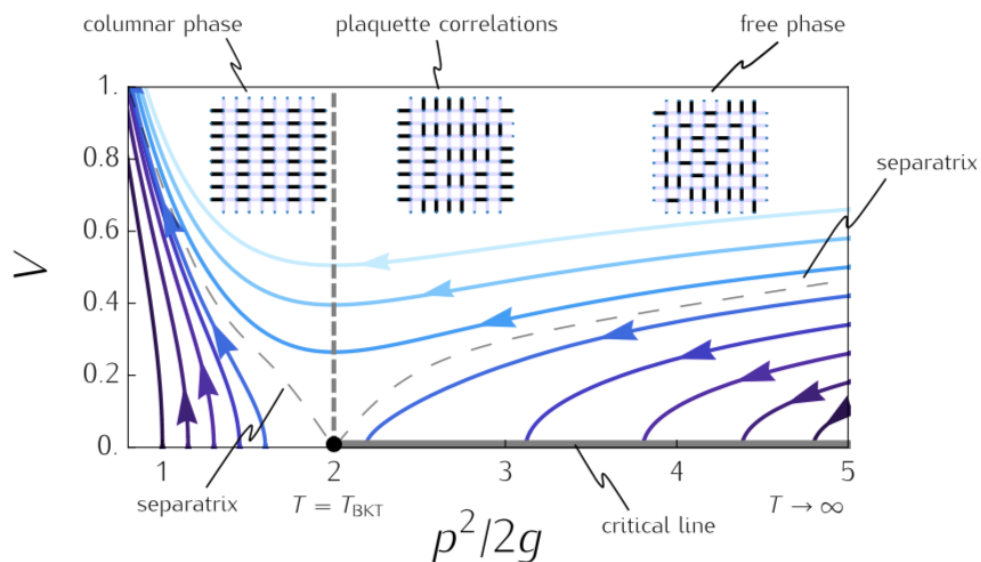


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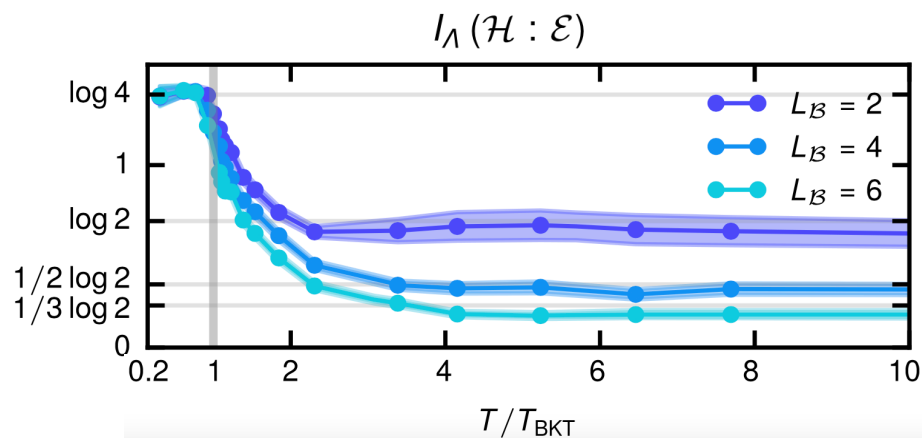


■ The optimal filters *depend* on T

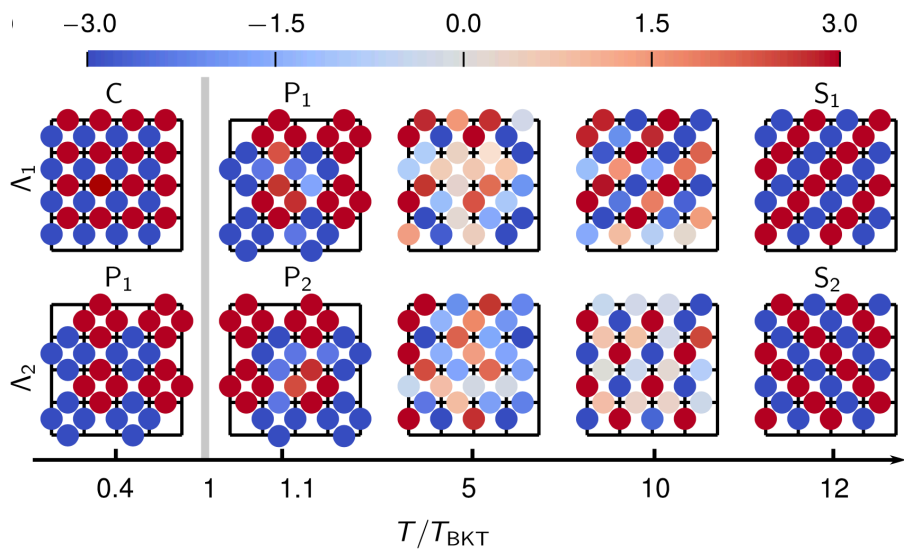




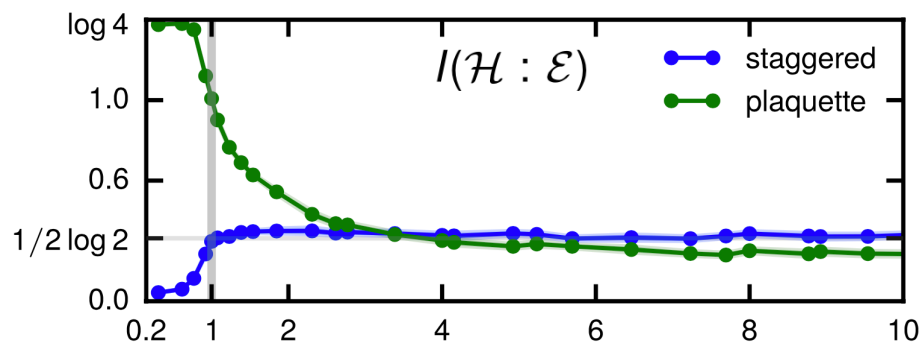
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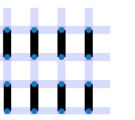
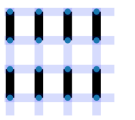
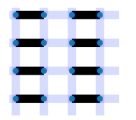
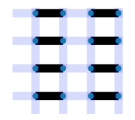
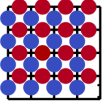
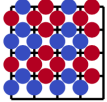
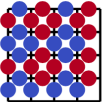
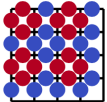
■ The optimal filters *depend* on T



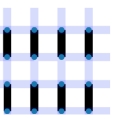
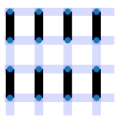
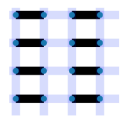
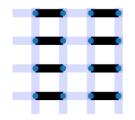
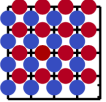
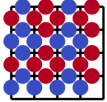
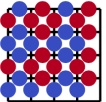
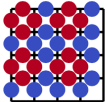
■ RSMI retrieved by pristine filters reflect **competing correlations**



- Pairs of C/P filters **label broken symmetry** states

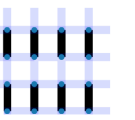
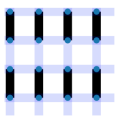
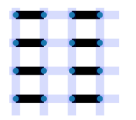
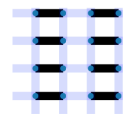
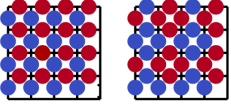
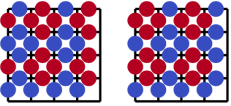
$C(r)$				
Λ_C Λ_{P1}  	$(-1, -1)$	$(-1, +1)$	$(+1, -1)$	$(+1, +1)$
Λ_{P1} Λ_{P2}  	$(-1, -1)$	$(+1, +1)$	$(-1, +1)$	$(+1, -1)$

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Λ_C Λ_{P1}  	$(-1, -1)$	$(-1, +1)$	$(+1, -1)$	$(+1, +1)$
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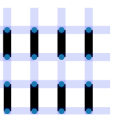
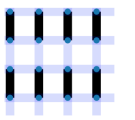
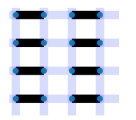
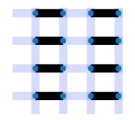
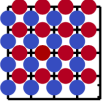
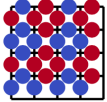
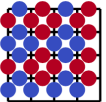
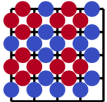
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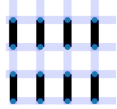
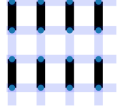
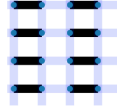
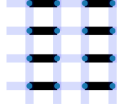
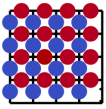
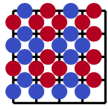
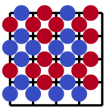
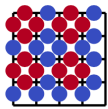
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Alet et al. PRE 74, 041124 (2006)

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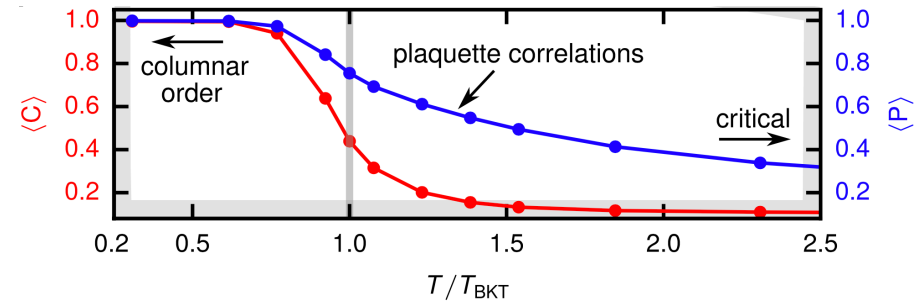
$C(r)$				
Λ_C Λ_{P1}				
	(-1, -1)	(-1, +1)	(+1, -1)	(+1, +1)
Λ_{P1} Λ_{P2}				
	(-1, -1)	(+1, +1)	(-1, +1)	(+1, -1)

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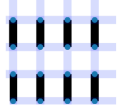
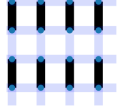
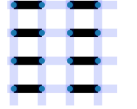
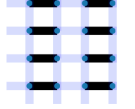
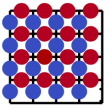
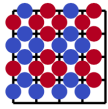
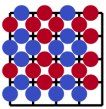
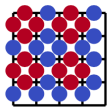
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Alet et al. PRE 74, 041124 (2006)



- Pairs of C/P filters **label broken symmetry** states

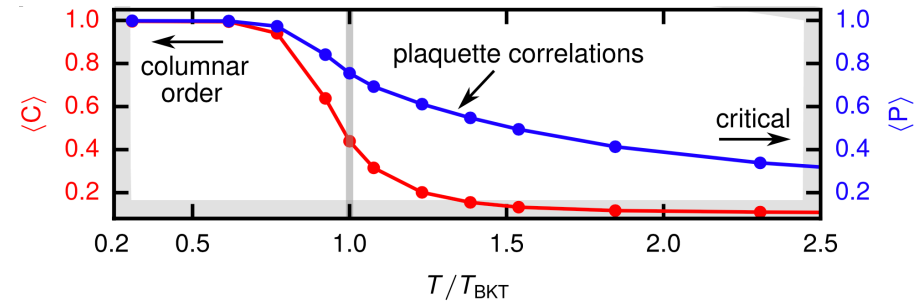
$C(r)$				
Λ_C Λ_{P1}				
	$(-1, -1)$	$(-1, +1)$	$(+1, -1)$	$(+1, +1)$
Λ_{P1} Λ_{P2}				
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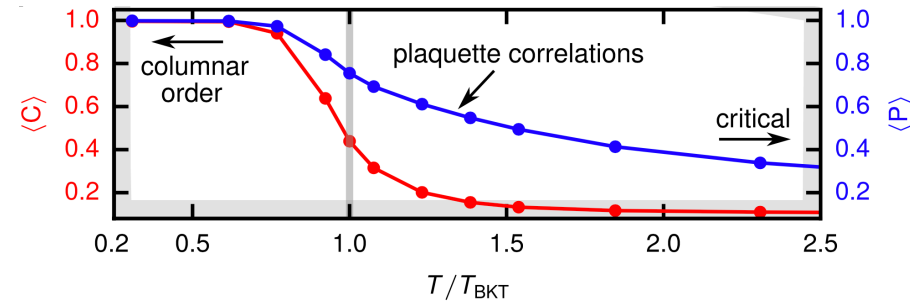
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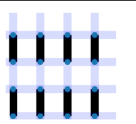
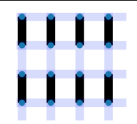
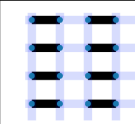
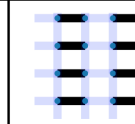
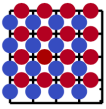
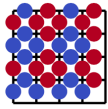
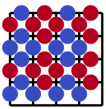
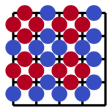


- Filters **are** relevant operators:

$$\mathcal{O}_n(\varphi) = (\cos(n\varphi), \sin(n\varphi))$$

Papanikolaou et al. PRB 76, 134514 (2007)

Pairs of C/P filters **label broken symmetry** states

$C(\mathbf{r})$				
Λ_C  Λ_{P1} 	$(-1, -1)$	$(-1, +1)$	$(+1, -1)$	$(+1, +1)$
Λ_{P1}  Λ_{P2} 	$(-1, -1)$	$(+1, +1)$	$(-1, +1)$	$(+1, -1)$
$\varphi(\mathbf{r})$	$\frac{\pi}{2}$	$\frac{3\pi}{2}$	π	0
$\mathcal{O}_1(\varphi) = (\cos \varphi, \sin \varphi)$	$(0, 1)$	$(0, -1)$	$(-1, 0)$	$(+1, 0)$
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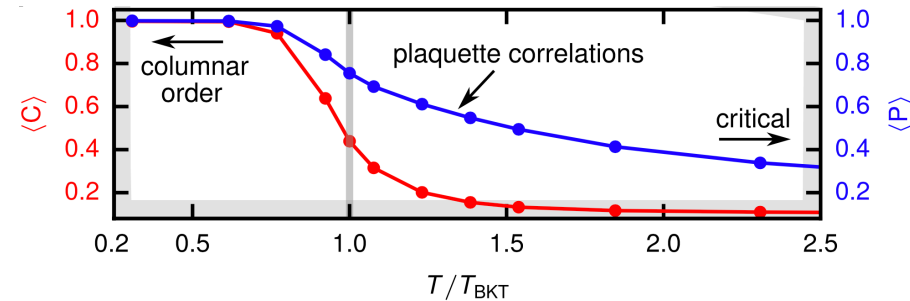
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Filters **define** order parameters:

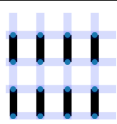
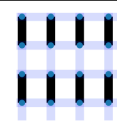
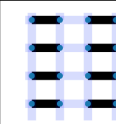
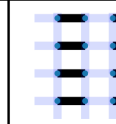
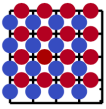
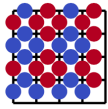
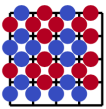
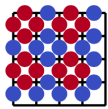
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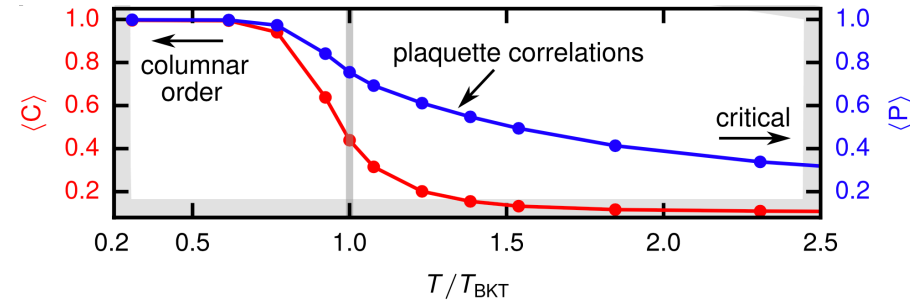
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Papanikolaou et al. PRB 76, 134514 (2007)

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Pairs of C/P filters **label broken symmetry** states

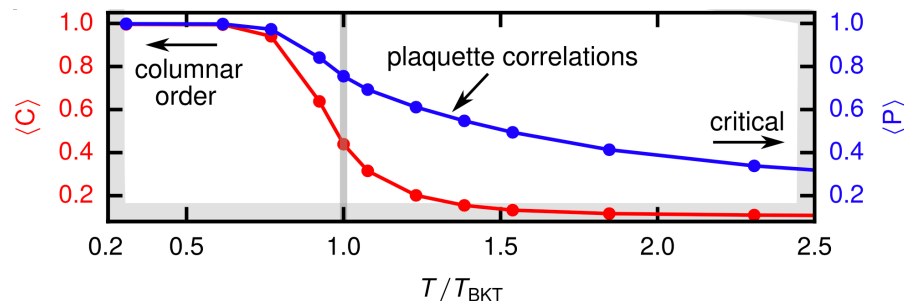
$C(r)$				
Λ_C Λ_{P1}	$(-1, -1)$	$(-1, +1)$	$(+1, -1)$	$(+1, +1)$
Λ_{P1} Λ_{P2}	$(-1, -1)$	$(+1, +1)$	$(-1, +1)$	$(+1, -1)$
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$\mathcal{O}_1(\varphi) = (\cos \varphi, \sin \varphi)$	$(0, 1)$	$(0, -1)$	$(-1, 0)$	$(+1, 0)$
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Filters **define** order parameters:

$$D_i := \mathbb{E} \left[\frac{1}{N_{\mathcal{V}}} \sum_k \tau \circ (\Lambda_i \cdot \mathcal{V}_k) \right]$$

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Alet et al. PRE 74, 041124 (2006)



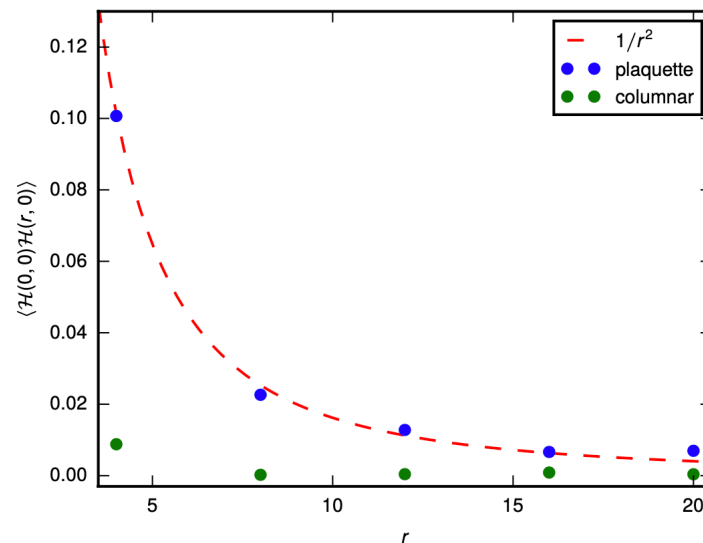
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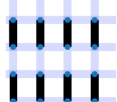
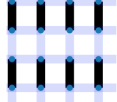
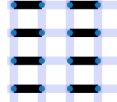

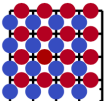
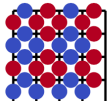
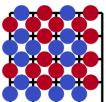
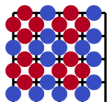
Papanikolaou et al. PRB 76, 134514 (2007)

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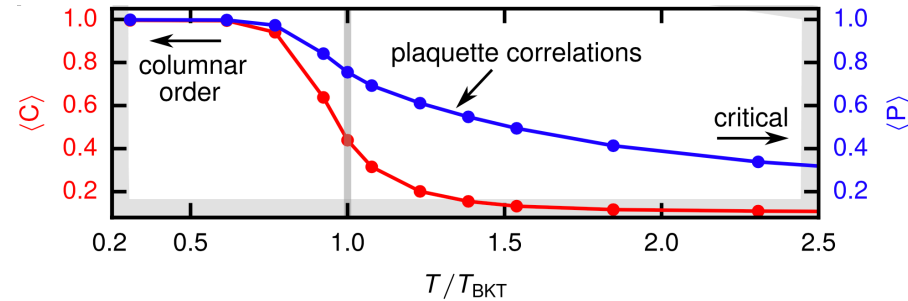
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Alet et al. PRE 74, 041124 (2006)



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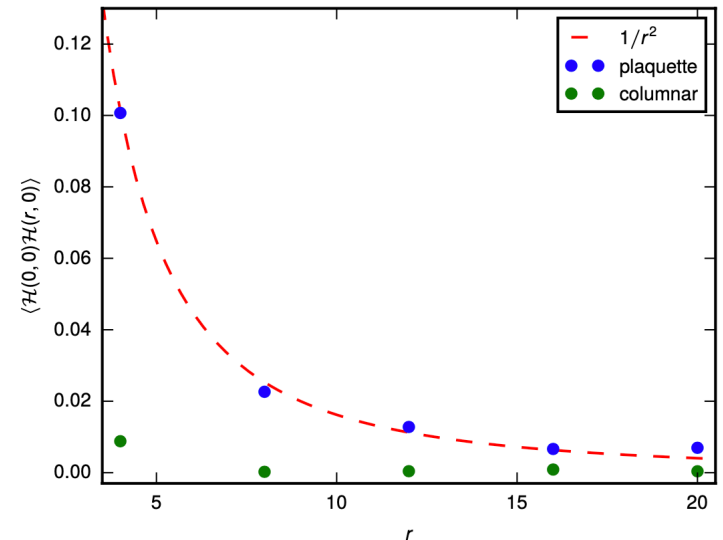
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They can be assigned scaling dimensions



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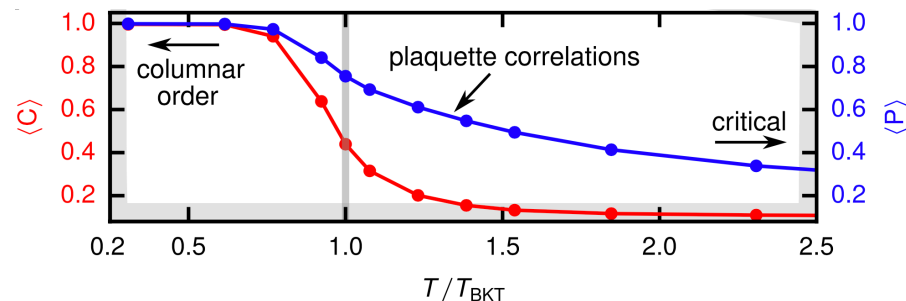
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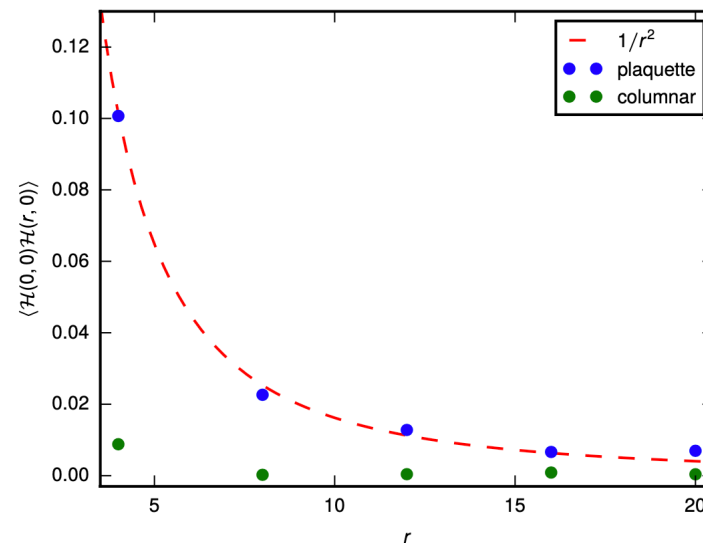
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(Also: staggered filters are gradients of the height field)

They can be assigned scaling dimensions



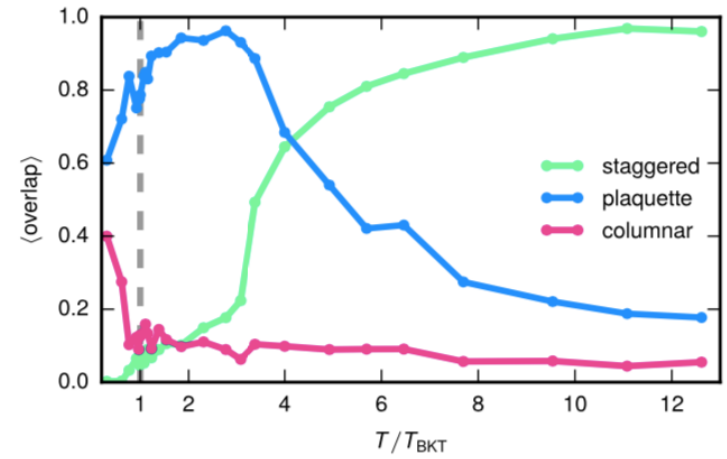
Data analysis of RMSI filter ensemble

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- In intermediate regimes and finite systems competing correlations yield mixtures of filters

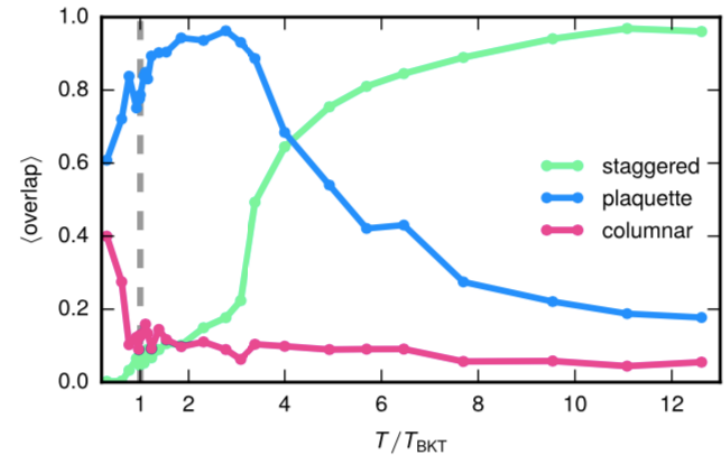
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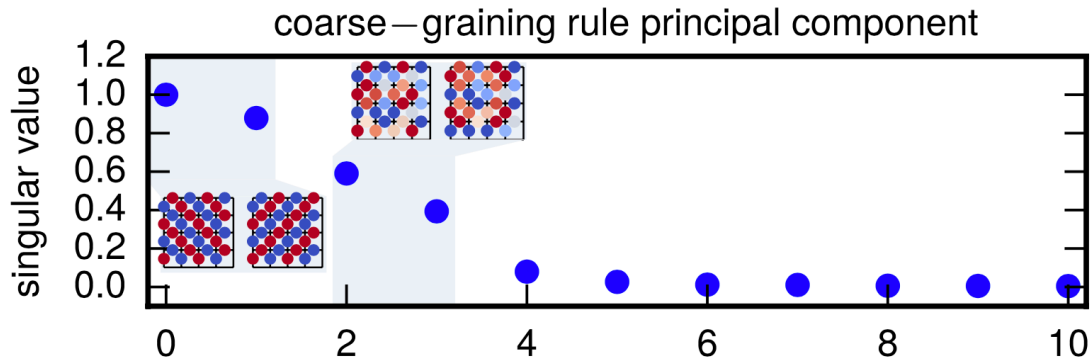
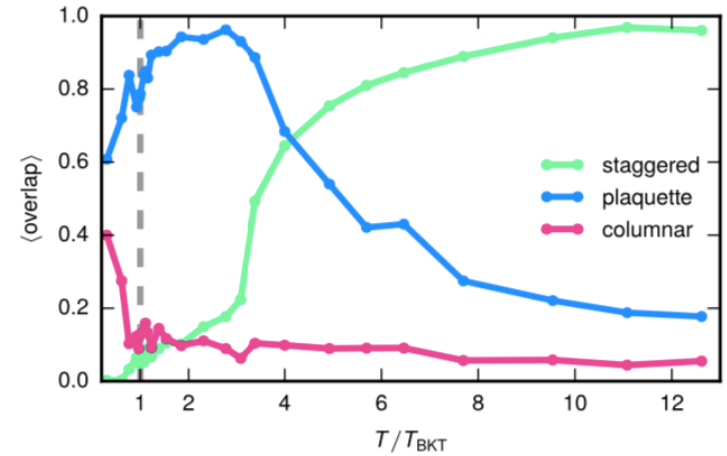
Data analysis of RMSI filter ensemble

- In intermediate regimes and finite systems competing correlations yield mixtures of filters
- They can be decoupled and recovered



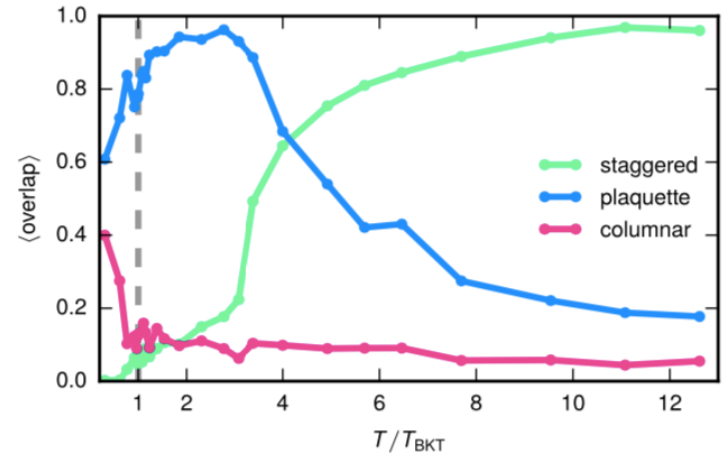
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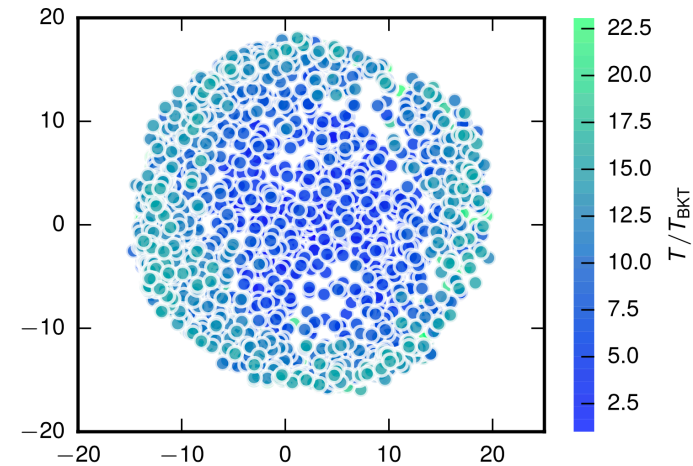
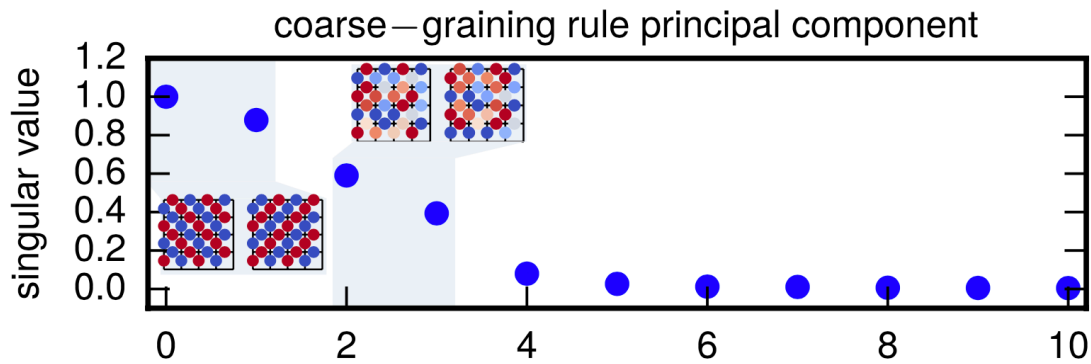


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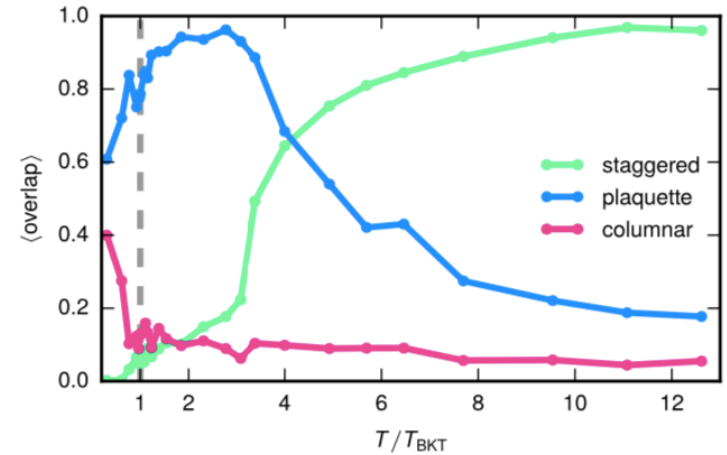


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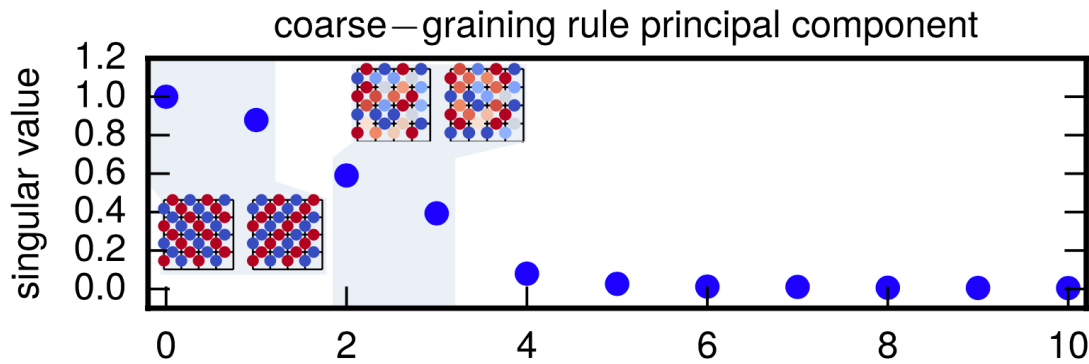


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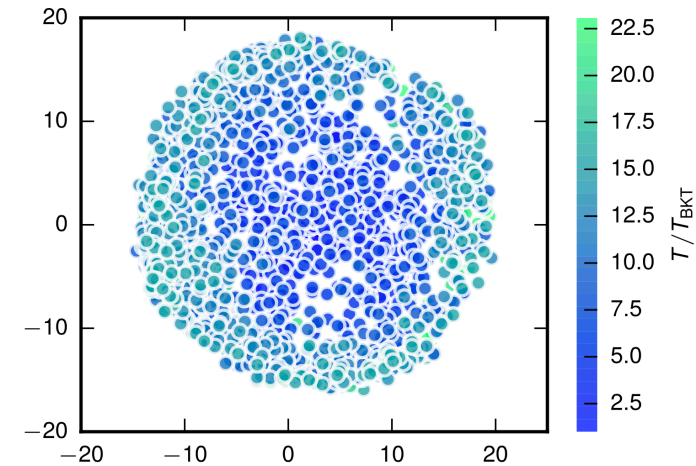
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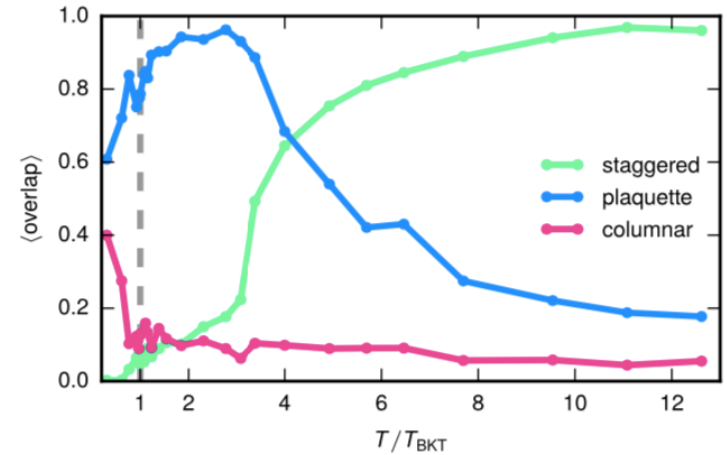


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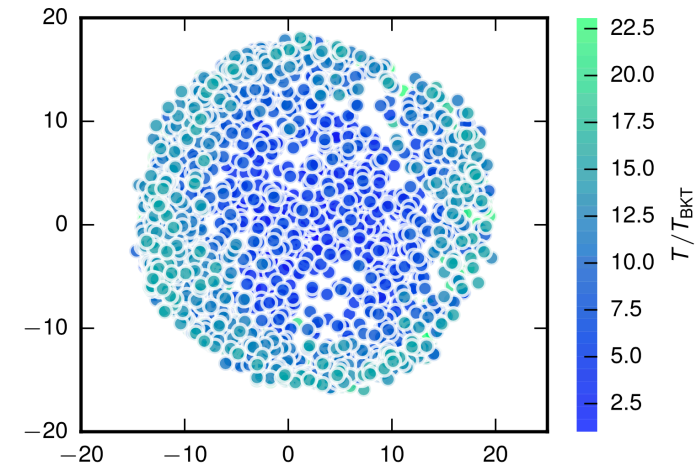
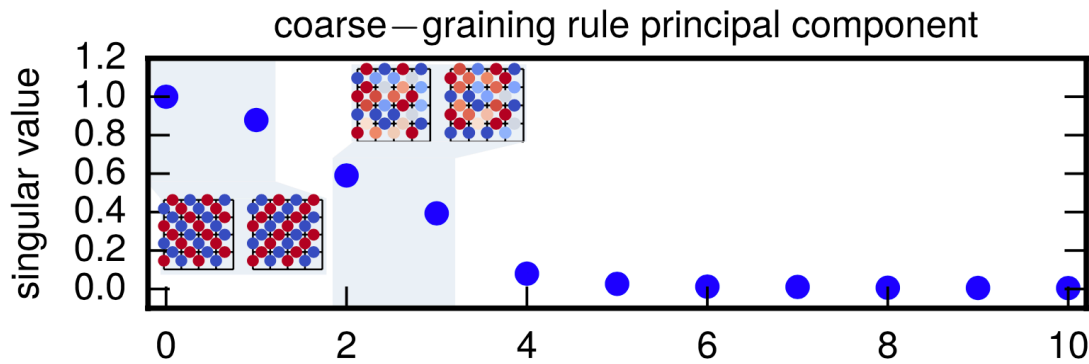


Data analysis of RMSI filter ensemble

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- They can be decoupled and recovered



- Works also from partial data
- As a function of disorder distribution?

The information bottleneck (IB) compression

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- “Relevance” defined implicitly, by correlations with a signal variable

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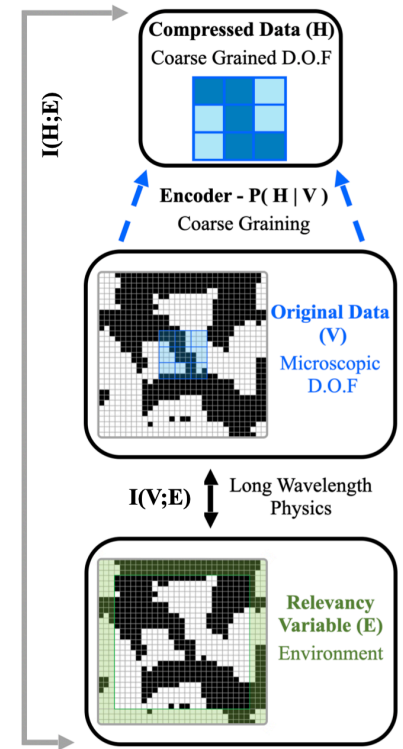
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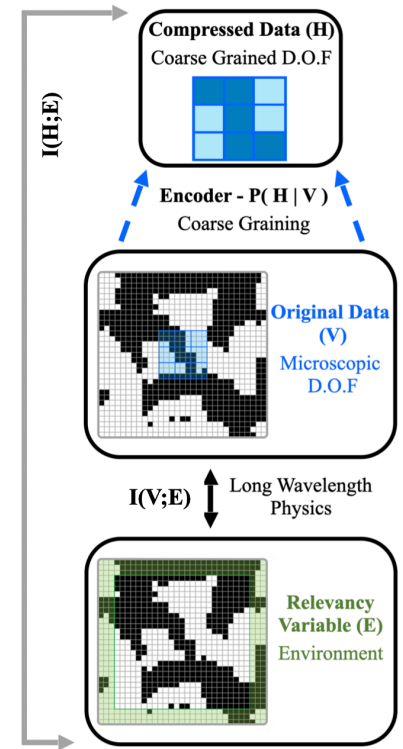


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- Optimal compression of relevant information is a variational problem

$$\min_{P(H|V)} \mathcal{L}_{IB}[P(H|V)] \equiv \min_{P(H|V)} I(V; H) - \beta I(H; E)$$

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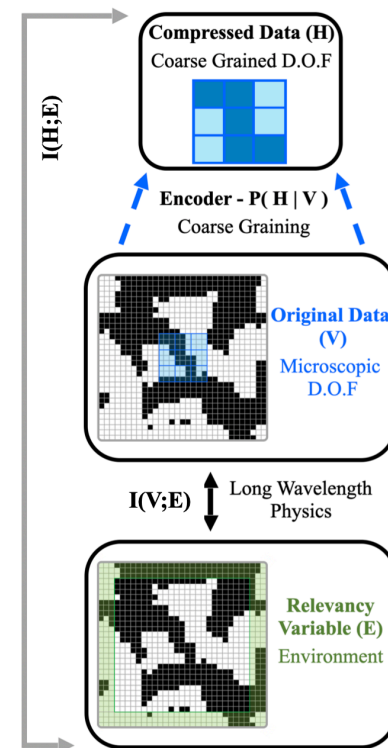
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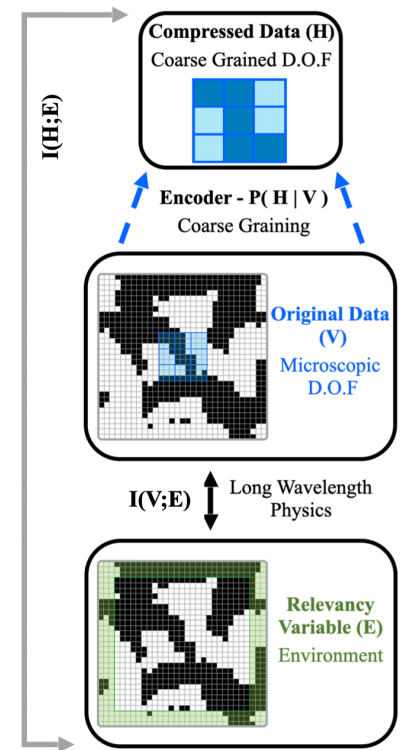
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Gedeon et al. *Entropy* (2012), 14(3) 456-479



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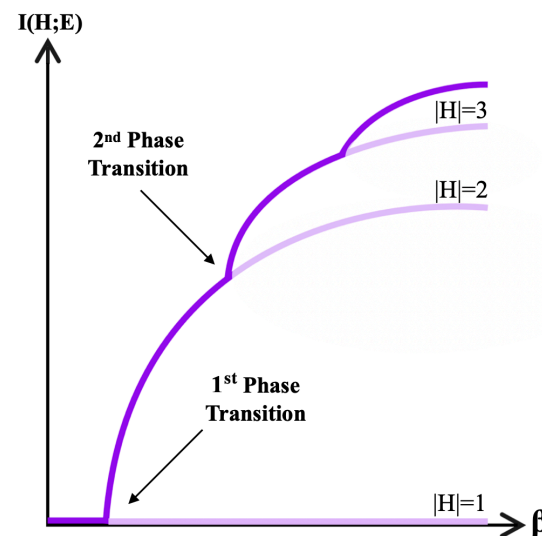
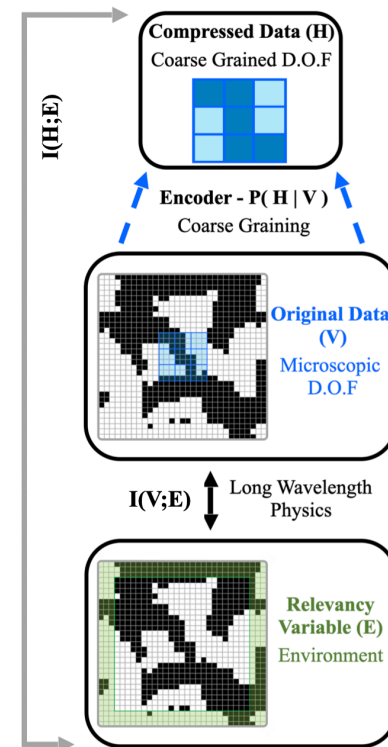
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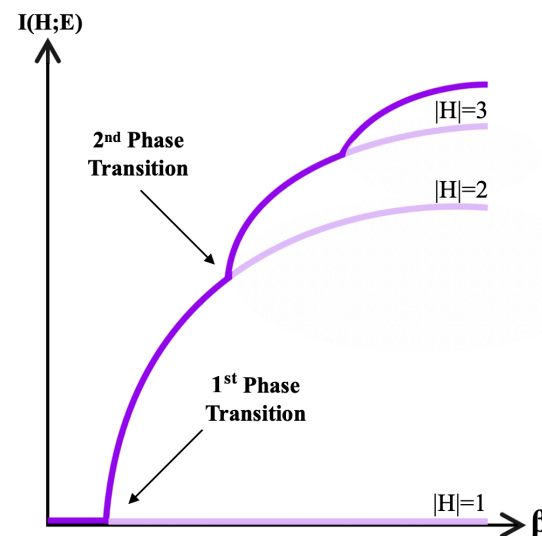
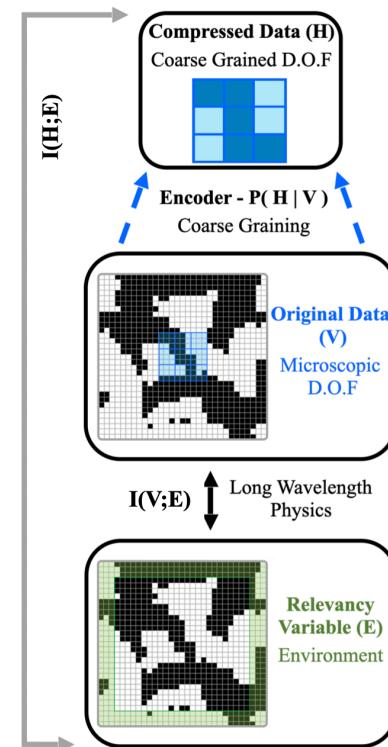
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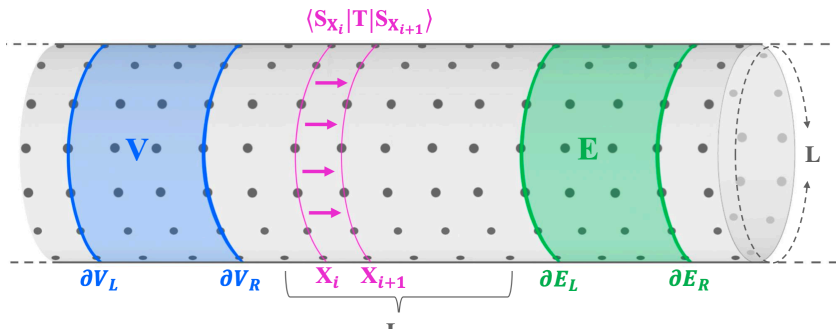
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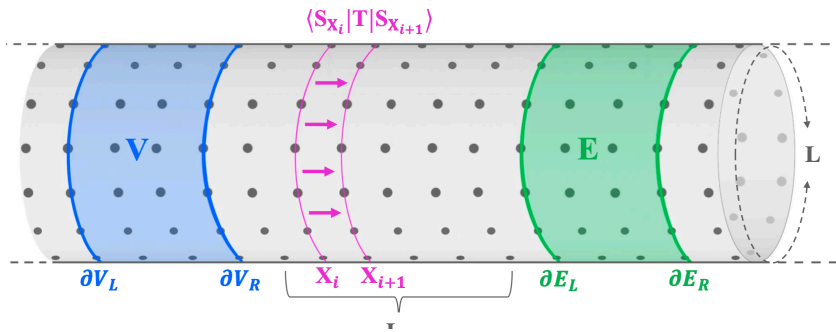
- RSMI arises in the infinite β limit, and finite alphabet



IB and the transfer matrix



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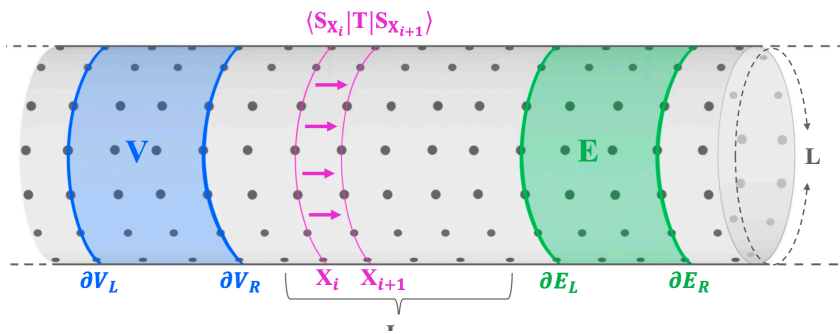


- We want to solve the IB eqs. for encoder

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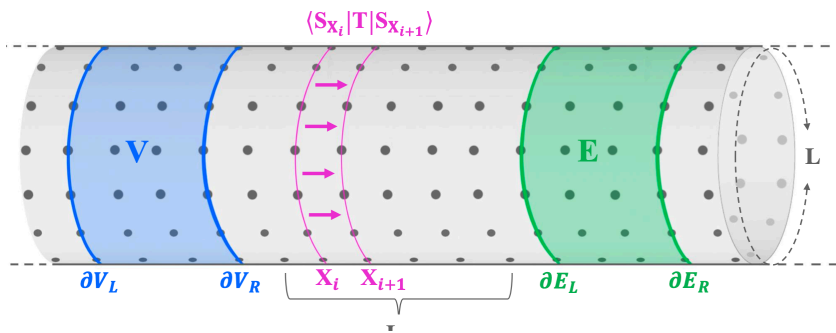
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Cardy J. Phys. A: Math. Gen. 17, L385 (1984)

Bloete et al. Phys. Rev.Lett. 56, 742 (1986)

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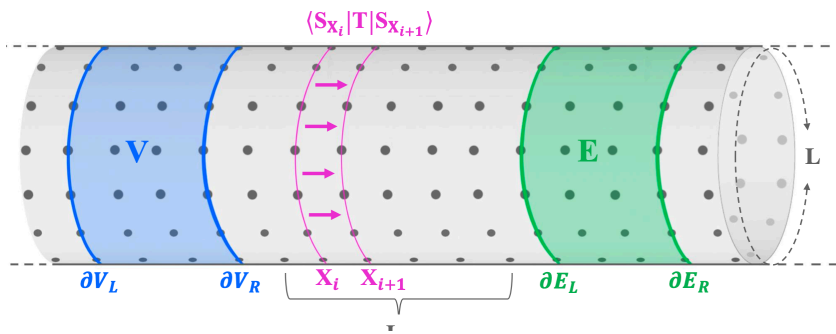
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$$= N^{-1} P(v) [1 + \epsilon r_e r_v]$$

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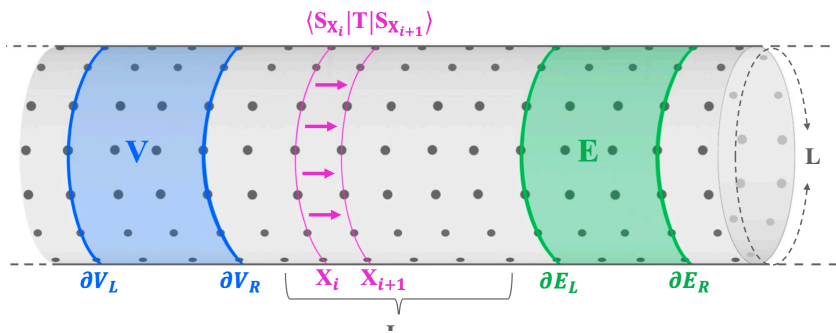
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- The encoder (needs to be solved self-consistently):

$$P(h|v) = P(h|r_v) \propto P(h) e^{\beta \epsilon^2 r_v \langle r_v \rangle_h}$$

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Differentiation from
trivial encoder



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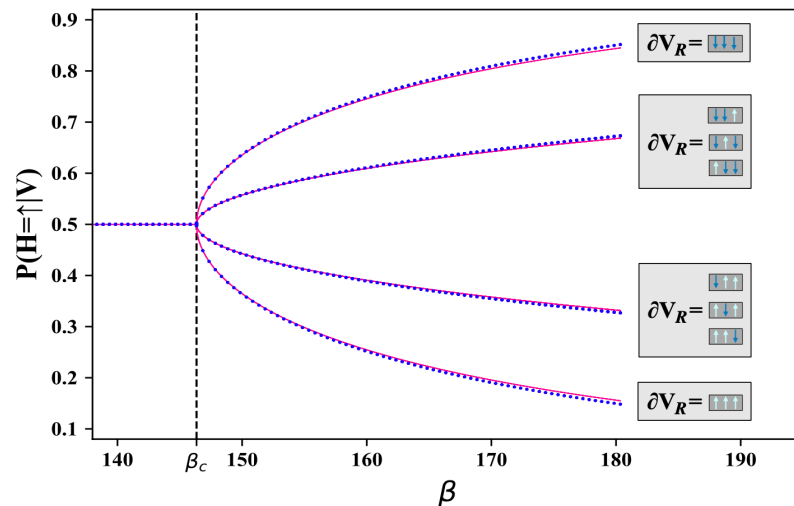
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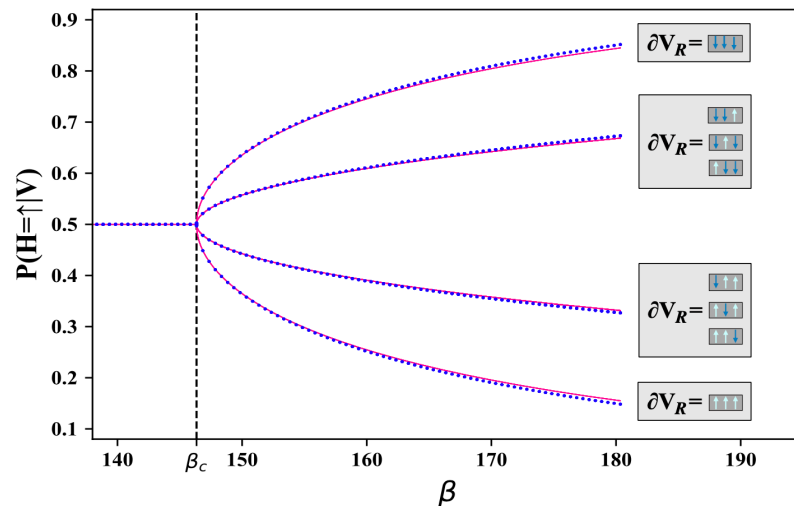


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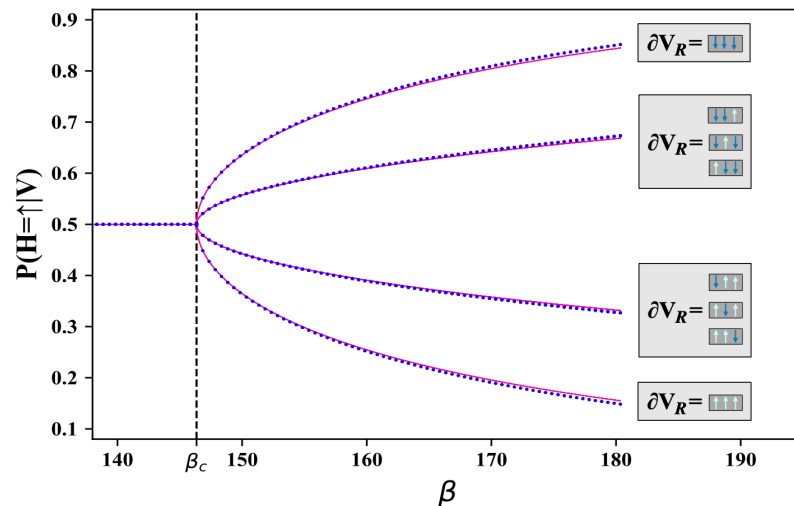
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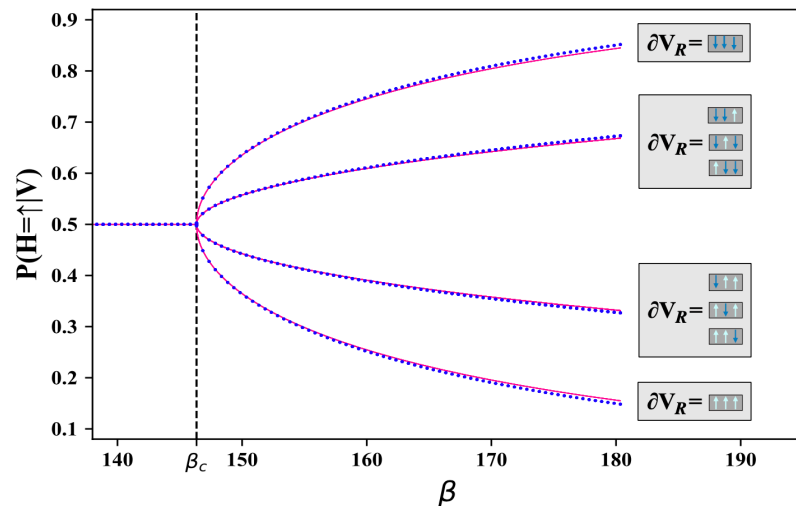
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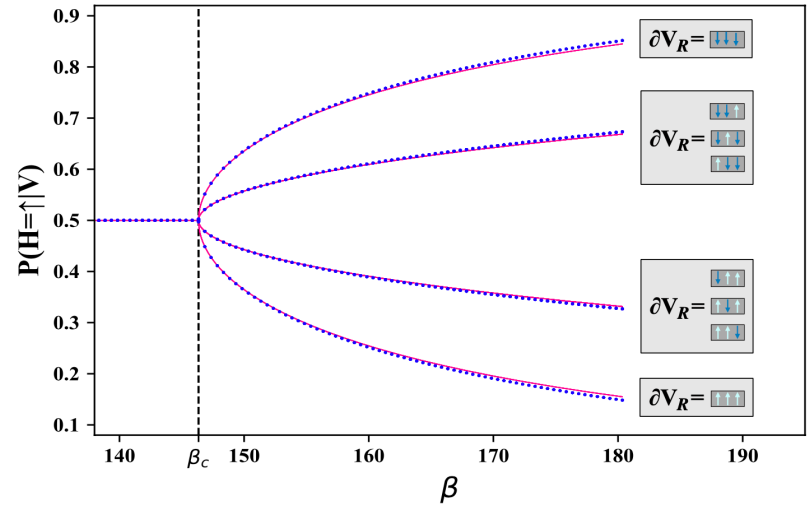
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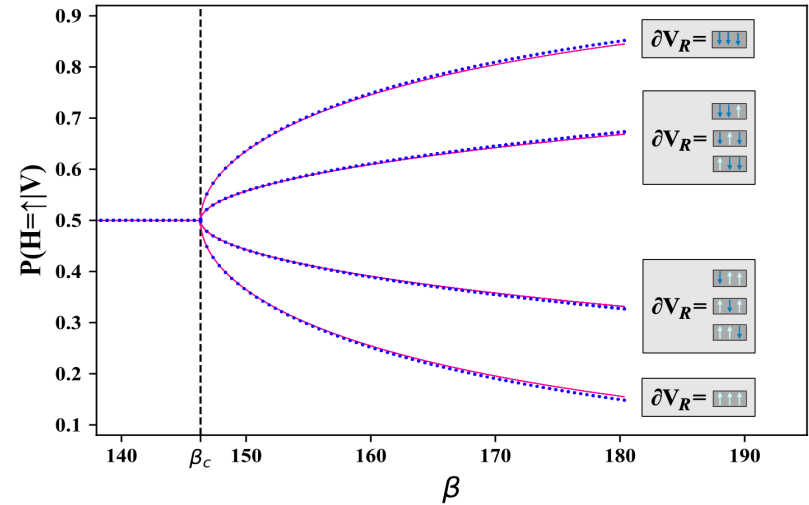
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- Can potentially be used to identify symmetries.

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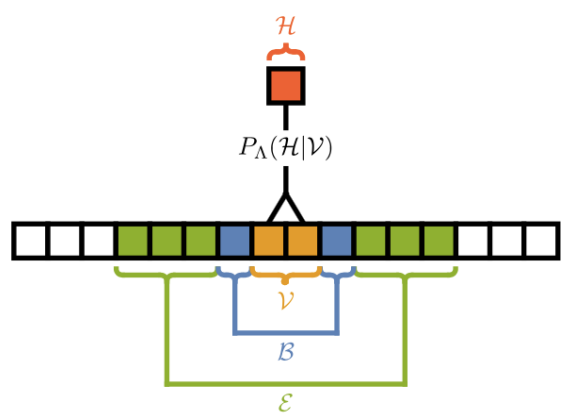
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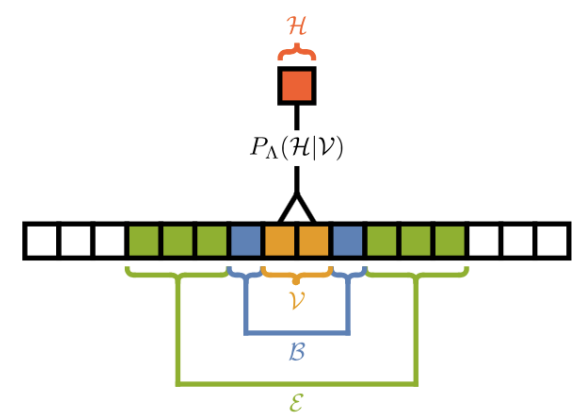
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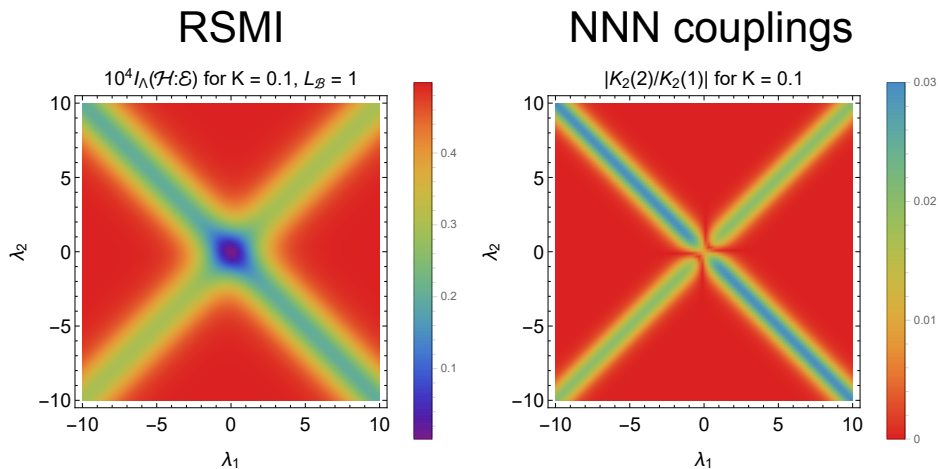
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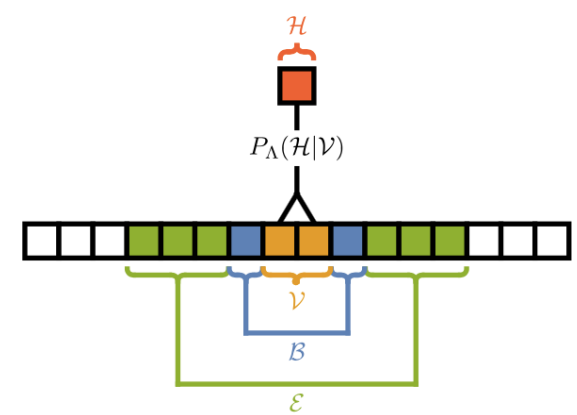
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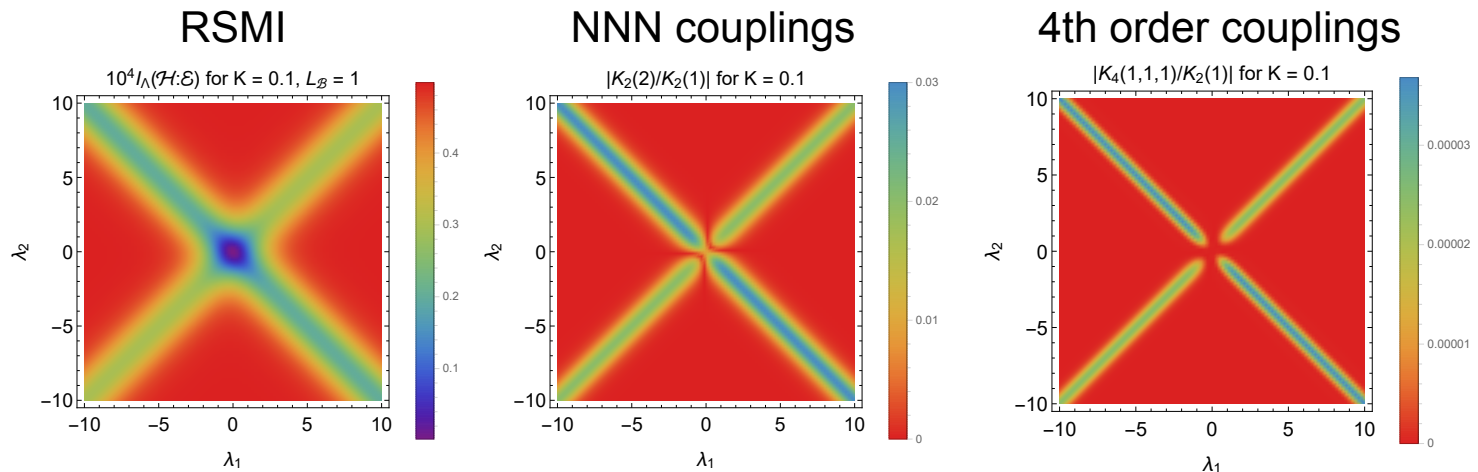


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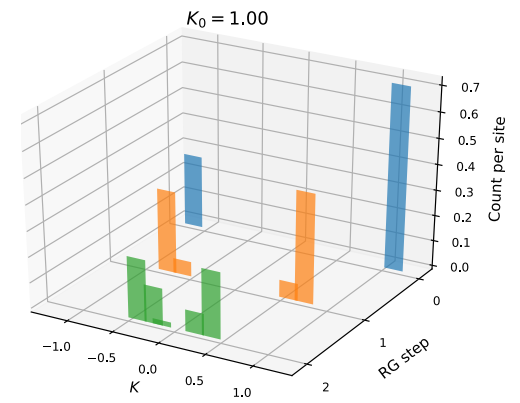
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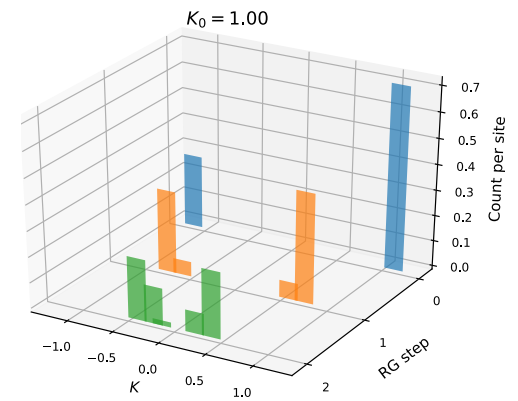
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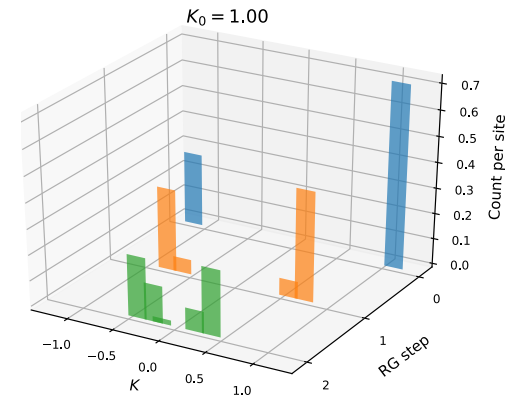
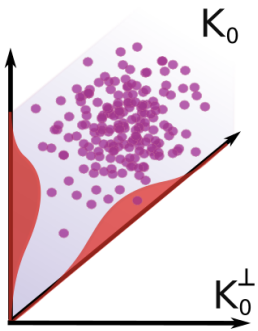
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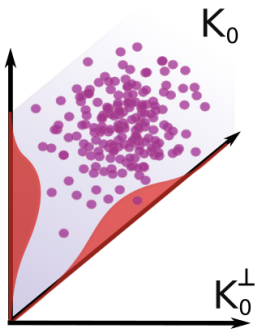
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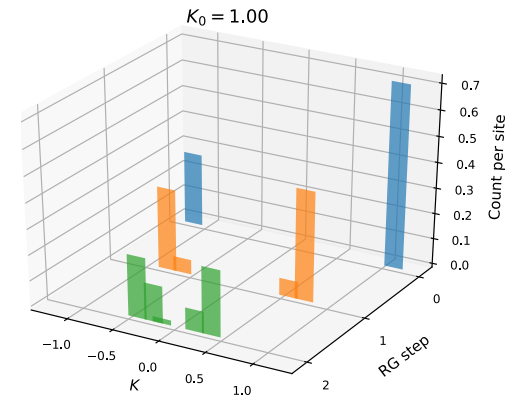


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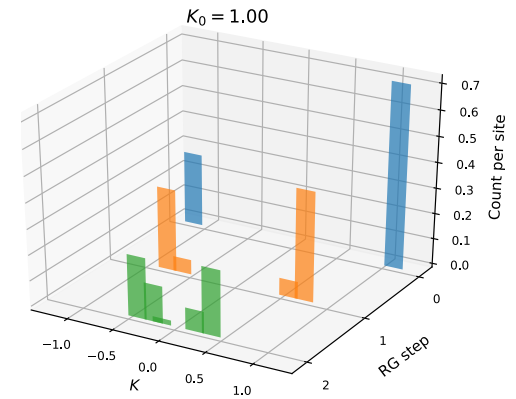
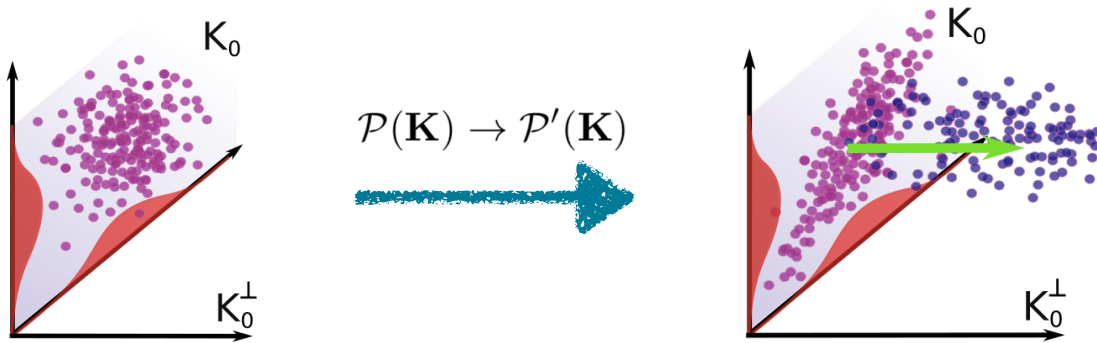


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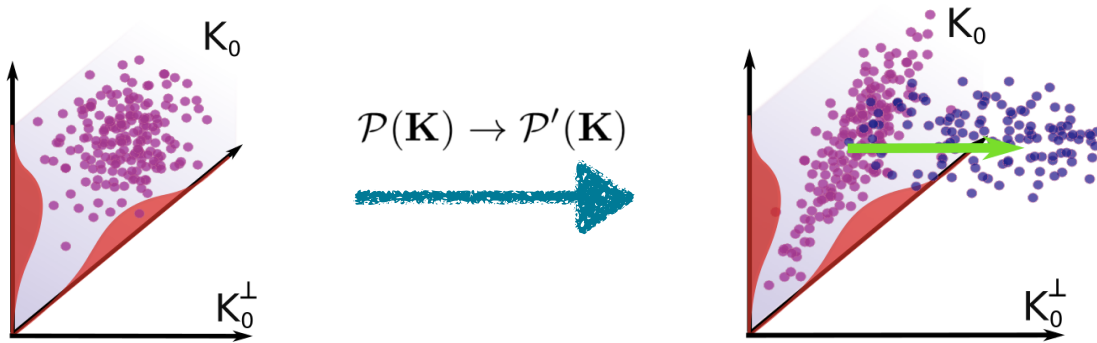
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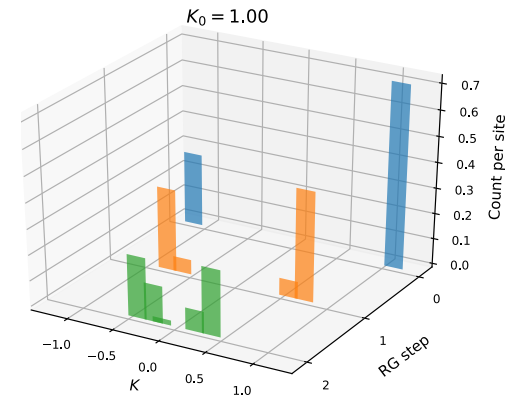


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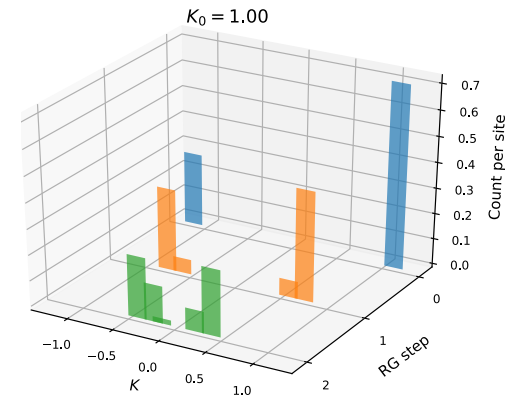
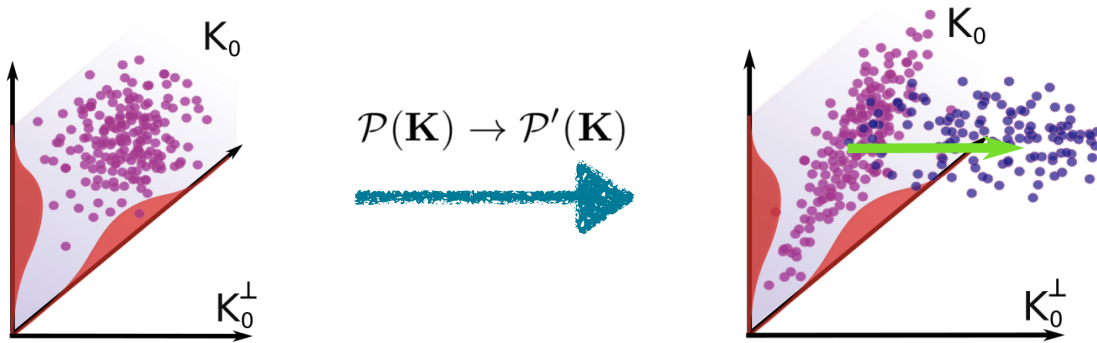


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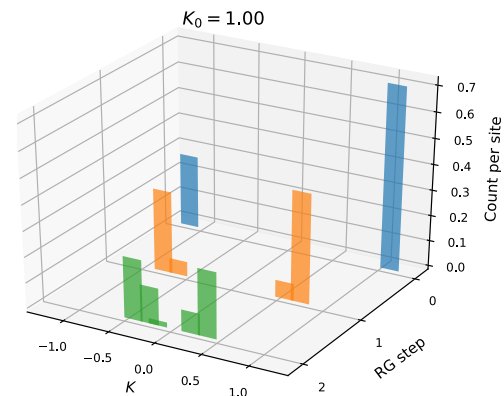
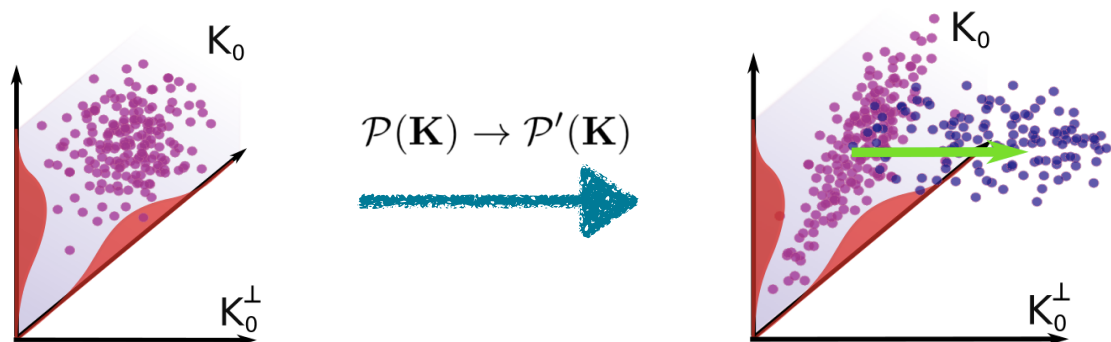


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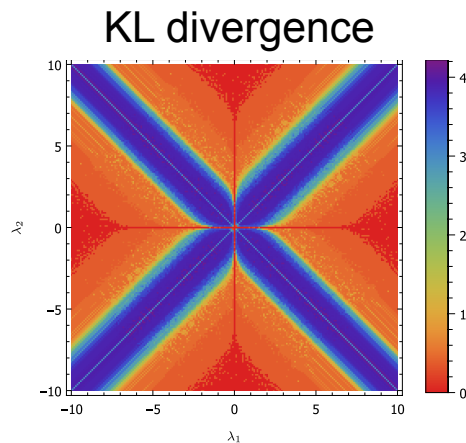
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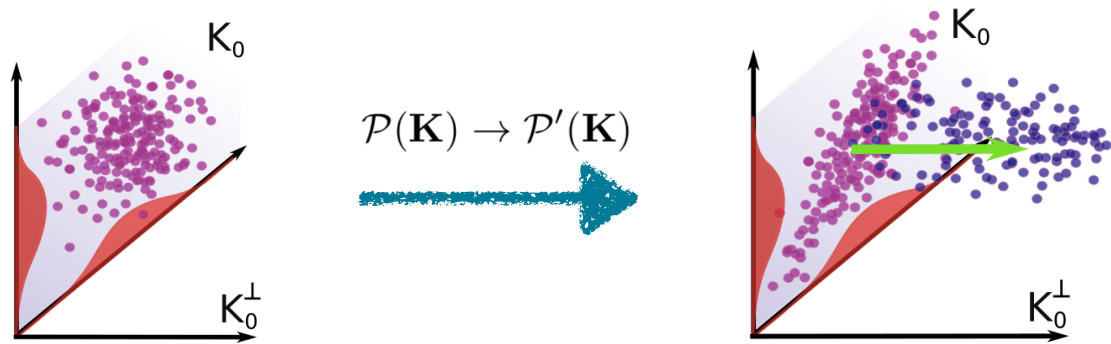
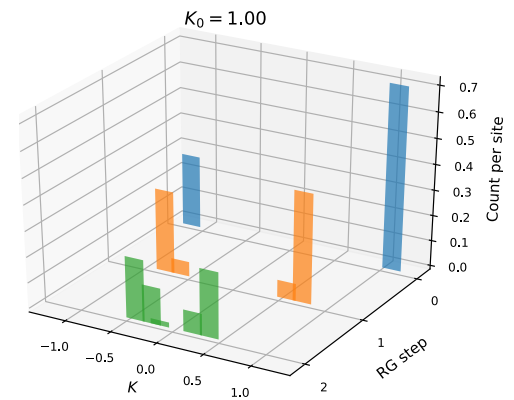
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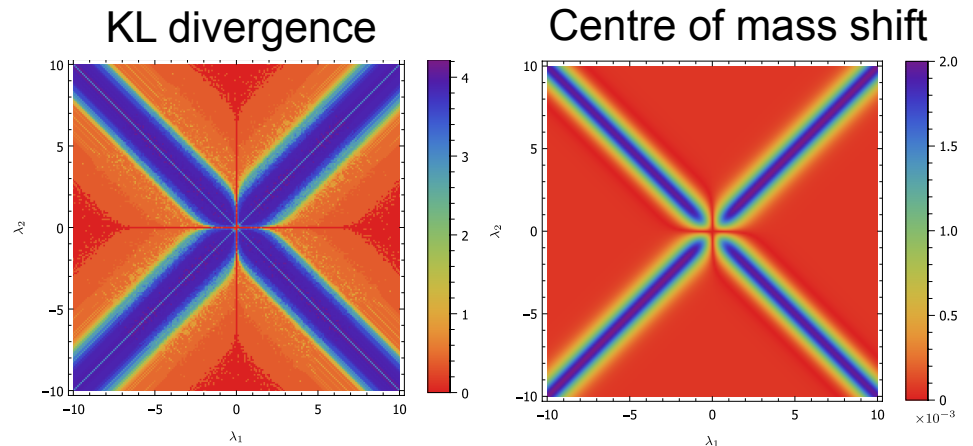
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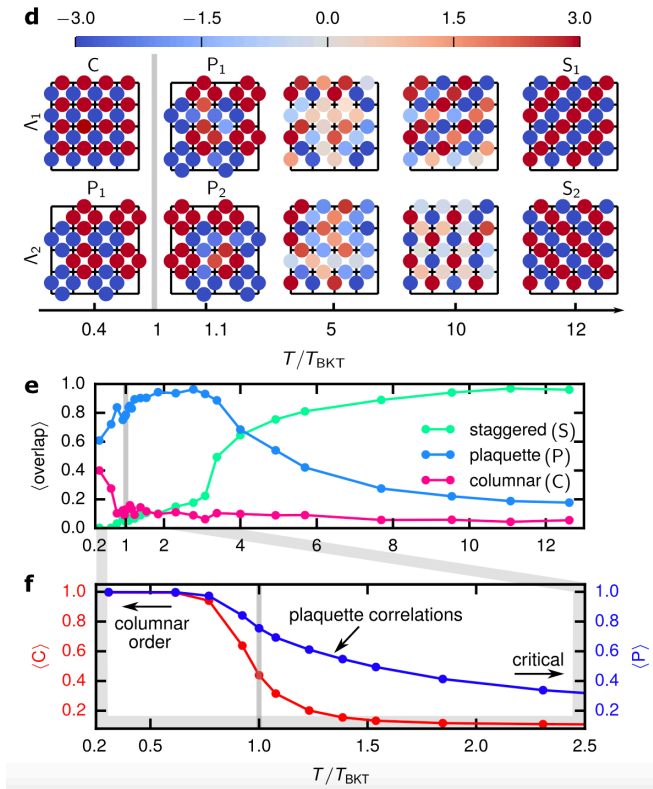
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Conclusions

- Constructing an optimal RG transformation as a variation problem in information theory
- <https://github.com/RSMI-NE/RSMI-NE>
- Comprehensive view of long-distance physics
- Constructing the relevant operators
- Formal connection between compression theory and field theory formalism



Outlook

- Extension to non-equilibrium
- Statistical models in 3D
- Correlations in experimental data: surface measurements, meteo, ...

Thank you!



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$$N_+(\mathbf{r}) = \frac{1}{4} + \frac{(-1)^{x+y+1}}{2\pi} \partial_x \varphi(\mathbf{r}) + (-1)^y \sin \varphi(\mathbf{r})$$

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Papanikolaou et al. **PRB 76**, 134514 (2007)

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- Expanding sin/cos and averaging we obtain:

$$\mathcal{H} \propto \tau \circ \nabla \langle \varphi(\mathbf{r}) \rangle_{\mathbf{r} \in \mathcal{V}}$$

Algorithm 3.1 One epoch for the unsupervised learning procedure for the RSMI-net using InfoNCE lower-bound

```

1:  $\eta =$  learning rate
2:  $\epsilon =$  relaxation parameter for Gumbel-softmax distribution
3:  $\mathbf{w}^0 \leftarrow$  random hyperparameter tensor  $\triangleright$  initialise InfoNCE ansatz  $f(h, e)$ 
4:  $\Lambda^0 \leftarrow$  random hyperparameter tensor  $\triangleright$  initialise coarse-graining filter
5: for  $s$  in  $1 : n$  do  $\triangleright$  loop over all  $n$   $K$ -replica samples for  $(\mathcal{V}, \mathcal{E})$ 
6:    $\epsilon^s \leftarrow$  reduce Gumbel-softmax relaxation parameter
7:    $\tau^s \leftarrow \tau(\epsilon^s)$   $\triangleright$  Anneal Gumbel-softmax layer
8:   for  $i$  in  $1 : K$  do
9:     for  $j$  in  $1 : K$  do
10:       $h_i^s[\Lambda^s] \leftarrow \tau^s(\Lambda^s \cdot v_i^s)$   $\triangleright$  Coarse-grain visible degrees of freedom
11:       $F_{ij}(\mathbf{w}^s, \Lambda^s) \leftarrow f(h_i^s[\Lambda^s], e_j^s; \mathbf{w}^s)$   $\triangleright$   $ij$ 'th element of scores matrix
12:    end for
13:  end for
14:   $Q(x_{1:K}, y_{1:K}; \mathbf{w}^s, \Lambda^s) \leftarrow \sum_{j=1}^K \frac{F_{ij}(\mathbf{w}^s, \Lambda^s)}{\sum_{i=1}^K \exp F_{ij}(\mathbf{w}^s, \Lambda^s)}$   $\triangleright$  InfoNCE "prediction"
15:   $\triangleright$  Update parameters of the RSMI estimator network:
16:   $\Delta \mathbf{w}^s \leftarrow \eta \nabla_{\mathbf{w}} [\log Q(\mathbf{w}, \Lambda^s)] \Big|_{\mathbf{w}=\mathbf{w}^s}$   $\triangleright$  automatic differentiation
17:   $\mathbf{w}^s \leftarrow \mathbf{w}^s + \Delta \mathbf{w}^s$   $\triangleright$  stochastic gradient-ascent
18:   $\triangleright$  Update parameters of the coarse-grainer network:
19:   $\Delta \Lambda^s \leftarrow \eta \nabla_{\Lambda} [\log Q(\mathbf{w}^s, \Lambda)] \Big|_{\Lambda=\Lambda^s}$ 
20:   $\Lambda^s \leftarrow \Lambda^s + \Delta \Lambda^s$ 
21: end for
22:  $\tilde{\mathcal{I}}_{\Lambda}(\mathcal{H} : \mathcal{E}) = \frac{1}{n} \sum_{t=1}^n \log Q(x_{1:K}, y_{1:K}; \mathbf{w}^t, \Lambda^t) + \log K$   $\triangleright$  average over  $n$  samples
23: return  $\tilde{\mathcal{I}}_{\Lambda}(\mathcal{H} : \mathcal{E}), \Lambda^n$ 

```

RSMI training

