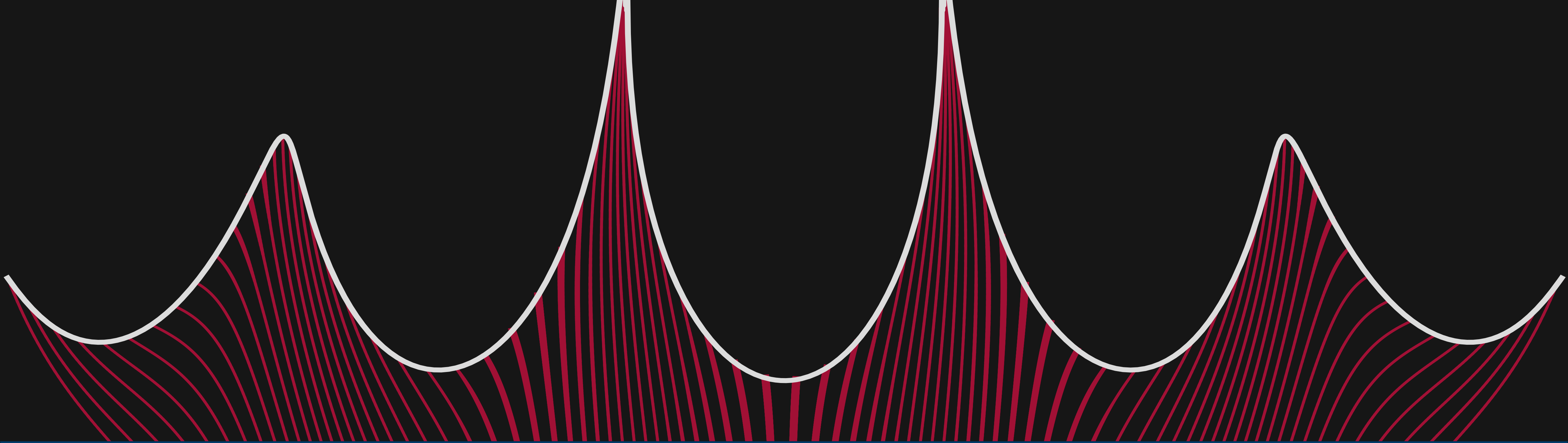
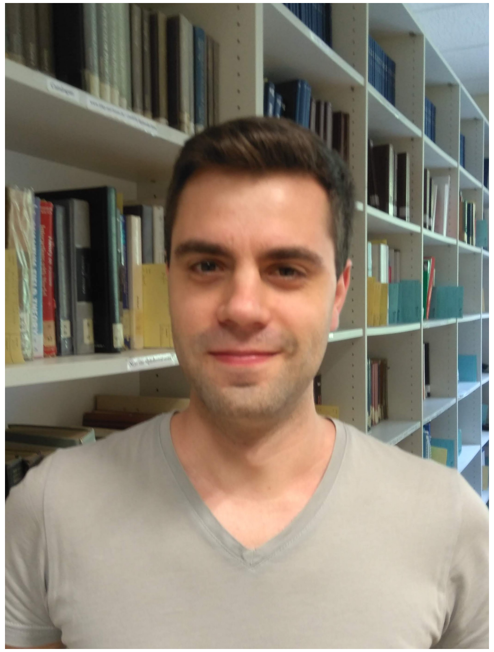


ALLEVIATING THE SIGN PROBLEM WITH HOLOMORPHIC FLOW: AN EXERCISE IN MACHINE LEARNING

TBILISI, GEORGIA, 09.2019

THOMAS LUU, IKP-3/IAS-4, FZJ/ HISKP, UNIVERSITÄT BONN

MY PARTNERS IN CRIME . . .



Jan-Lukas Wynen

Evan Berkowitz

Christopher Körber

Shout outs also go to:

Stefan Krieg, Timo Lähde, Johann Ostmeyer, Marcel Rodekamp, Carsten Urbach, Xiaonu Xiong

IF ONLY THERE WASN'T ANY SIGN PROBLEM. . .

- Path-integral formalism

$$\langle \hat{O} \rangle = \frac{1}{Z} \int_{\phi\in\mathbb{R}^N} \mathcal{D}[\phi]\ e^{-S[\phi]} O[\phi]$$

$$= \int_{\phi\in\mathbb{R}^N} \mathcal{D}[\phi]\ \mathbb{P}[\phi] O[\phi]$$

"Probability density"

Note: If $S[\phi] = S_R[\phi] + i\, S_I[\phi]$ then $\mathbb{P}[\phi]\mathcal{D}[\phi] \notin [0, \infty)$

Question: How do we interpret such "Probabilities"?

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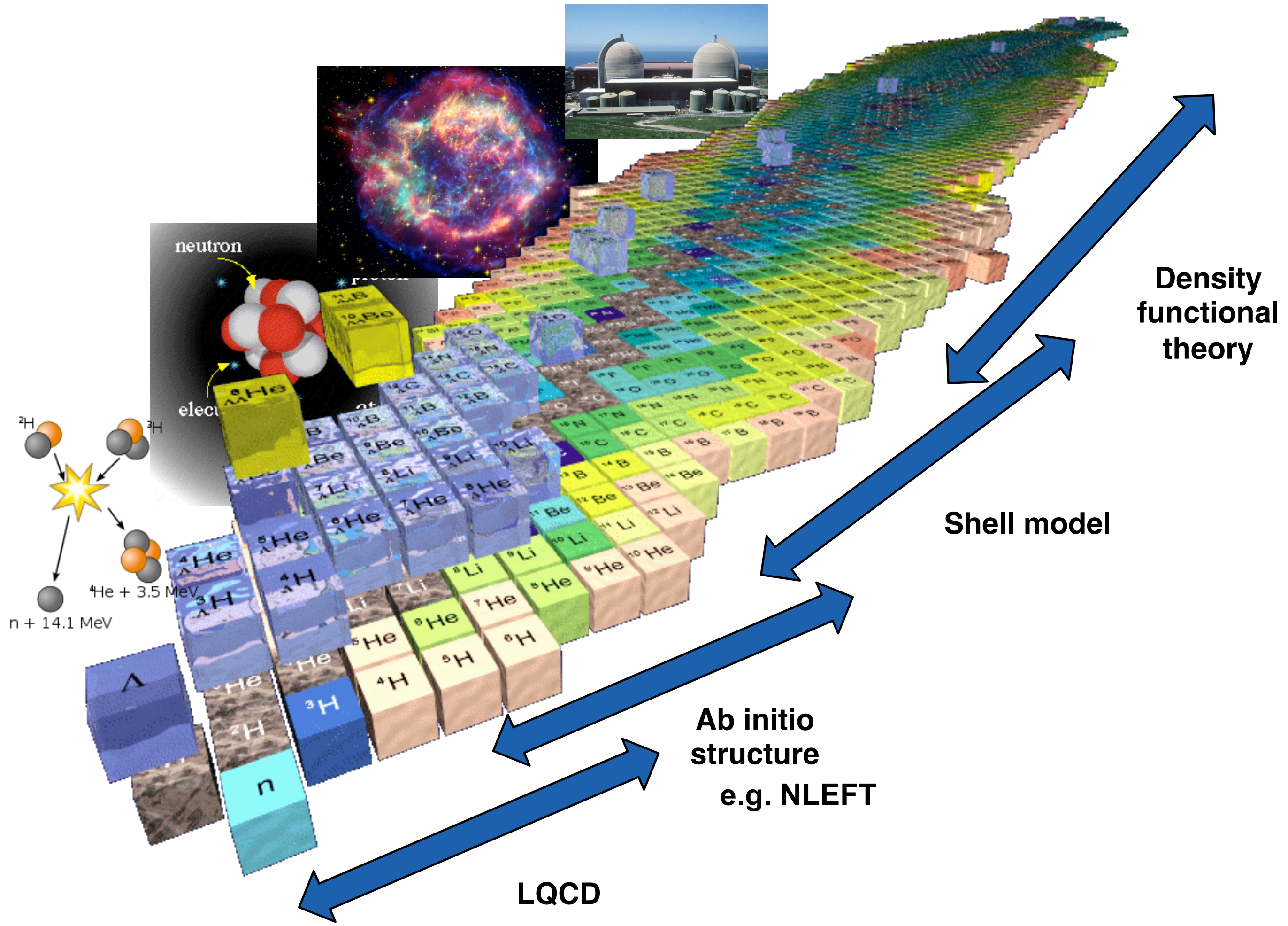
"Complex Phase sign problem"

WHEN DOES THE SIGN PROBLEM SHOW UP?

- Life in Minkowski space
- Finite density field theory
  - What are the phases of quark matter at high density?
  - Baryon chemical potential
- Complex term in Lagrangian (even after Wick rotation)
  - QCD theta term
- Stochastic calculations of neutron rich nuclei



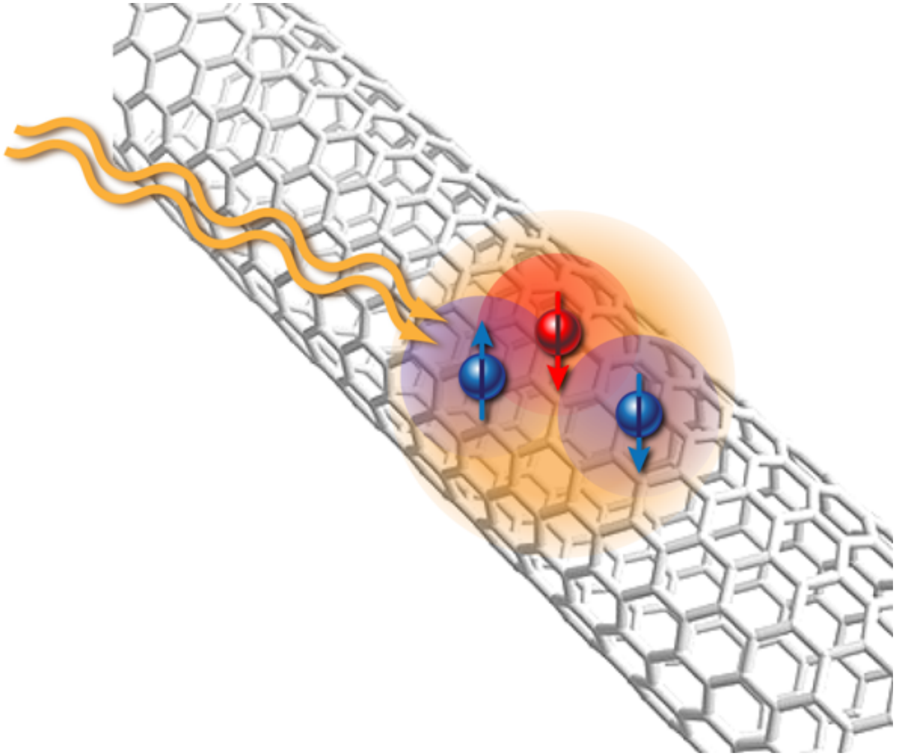
Sign problem shows up in the *most interesting problems in nuclear physics!!*

JÜLICH Forschungszentrum

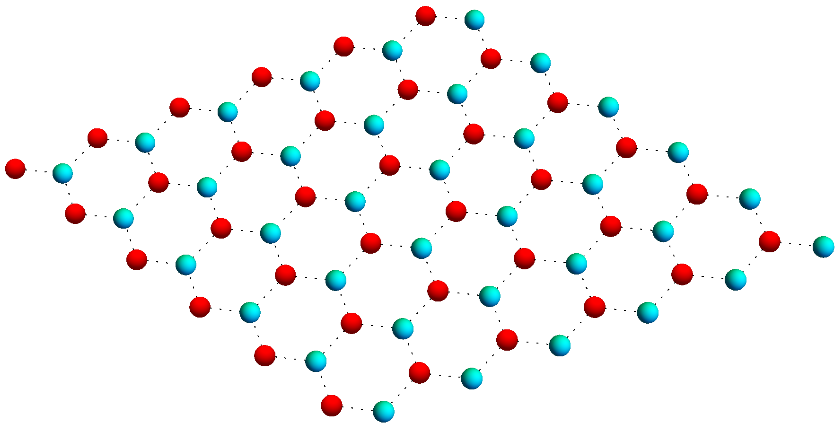
BUT THE SIGN PROBLEM IS NOT UNIQUE TO NUCLEAR PHYSICS. . .

Condensed matter/solid state communities also share our pain. . .

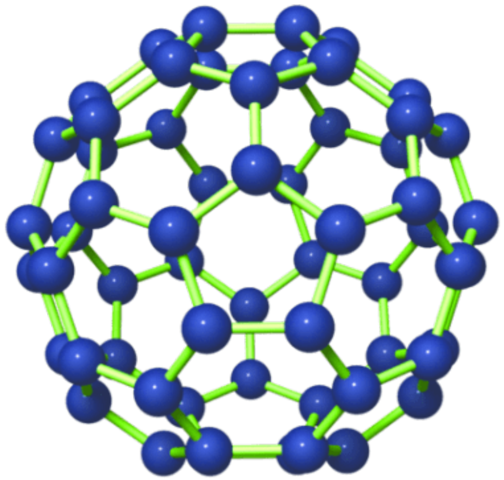
- High density strongly correlated electrons
- Doped systems
  - Electron chemical potential



THE TYPE OF THE LATTICE ALSO CAN INFLUENCE THE SIGN PROBLEM



bipartite lattice



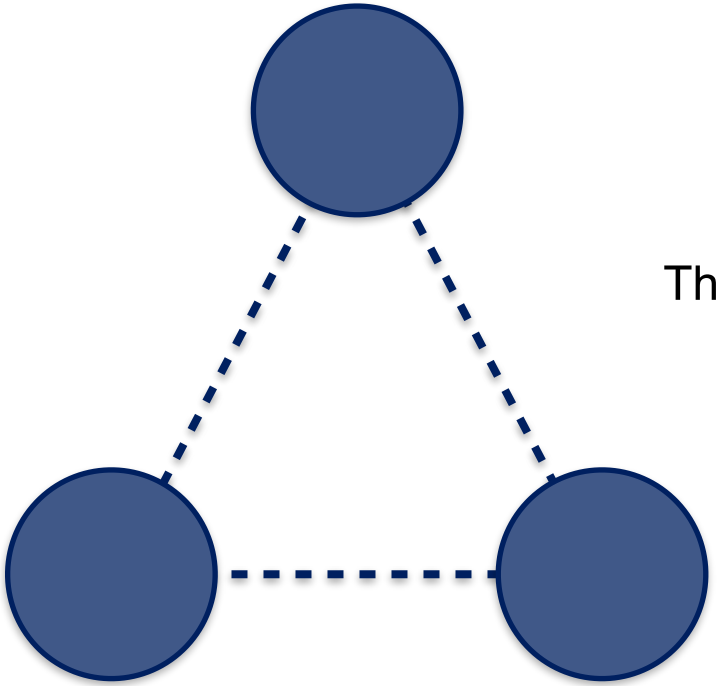
non-bipartite lattice

$$\mathbb{P}[\phi] \propto \det\left(M[\phi]M^\dagger[\phi]\right) \geq 0$$

$$\mathbb{P}[\phi] \propto \det\left(M[\phi,\kappa]M[-\phi,-\kappa]\right) \in (-\infty,\infty)$$

THE (NEXT TO) SIMPLEST NON-BIPARTITE LATTICE: THE TRIANGLE

- Can be solved exactly via direct diagonalization
  - Can immediately test new methods
- Severity of sign problem controlled by strength of interaction and temperature of system
- No need to introduce chemical potential



Three-site problem

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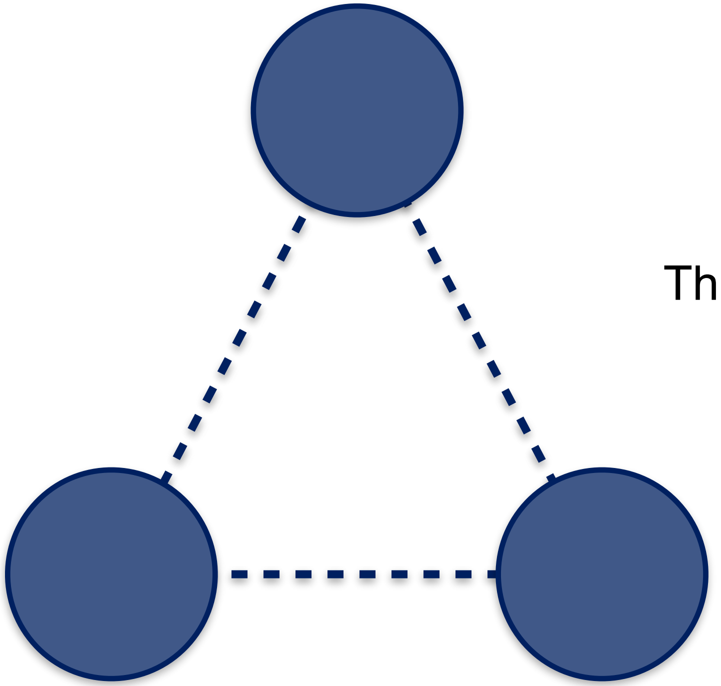

Three-site problem

Numerical examples shown in this talk will be done on this system

THE SIGN PROBLEM IS NOT NEW, AND HAS BEEN TACKLED BEFORE. . .

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  - Discuss in the next slide

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  - Assume the quantity causing the sign problem is "small" and expand in this quantity
    - Expand in μ (baryon chemical potential)
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Holomorphic flow (Lefschetz Thimbles)
The subject of this talk. . .

HUBBARD MODEL ON A NON-BIPARTITE LATTICE

Introducing the Hamiltonian

$$H = -\sum_{x,y}\left(a_x^\dagger \kappa_{xy} a_y + b_x^\dagger \kappa_{xy} b_y\right) + \frac{U}{2}\sum_x \left(n_x - \tilde{n}_x\right)^2$$

$$Z = \mathrm{Tr}\; e^{-\beta H}$$

Goal: Apply PI formalism

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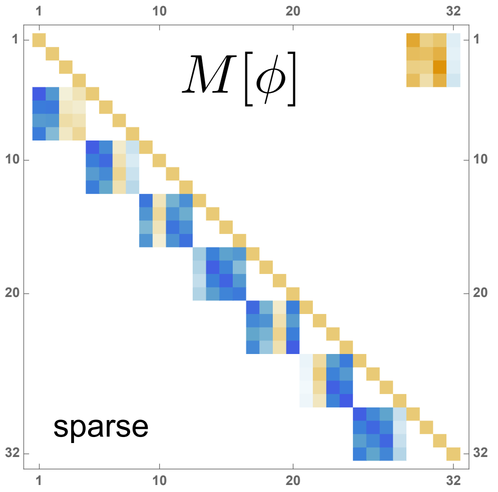

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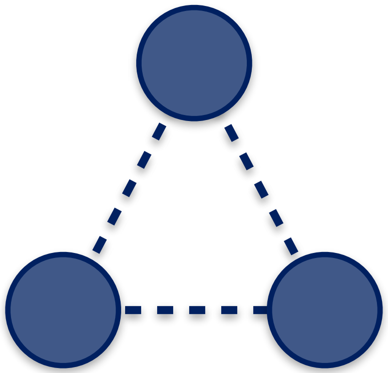

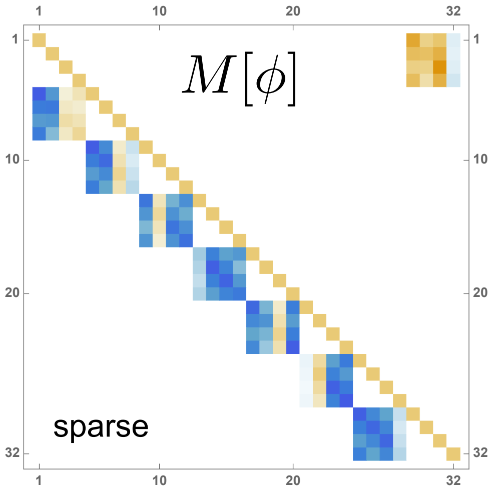

RE-WEIGHTING IS THE STANDARD “GO-TO” METHOD

$$\mathbb{P}[\phi] = \det\left(M[\phi,\kappa]M[-\phi,-\kappa]\right) e^{\left(-\frac{1}{2\tilde{U}}\sum_{x,t}\phi_{xt}^2\right)} = e^{-S_R[\phi]}e^{-iS_I[\phi]}$$

No longer positive definite! = “sign problem”

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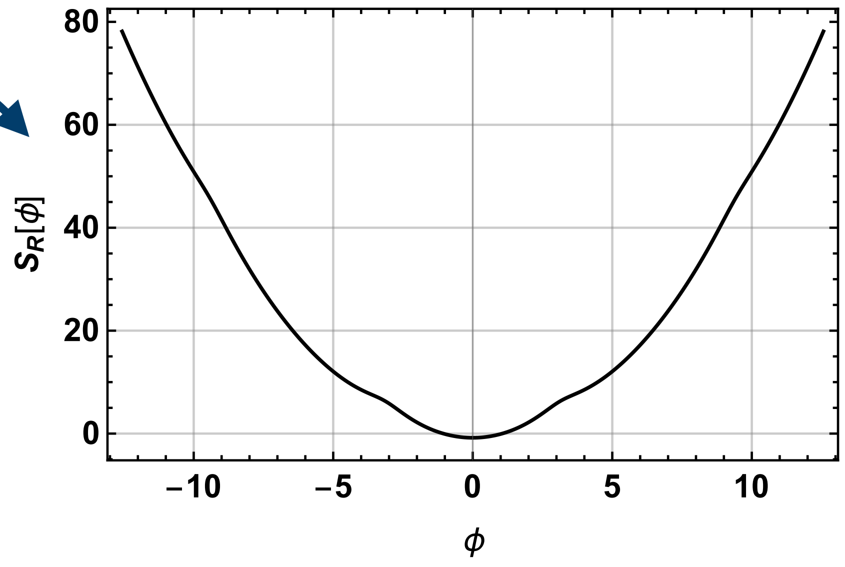

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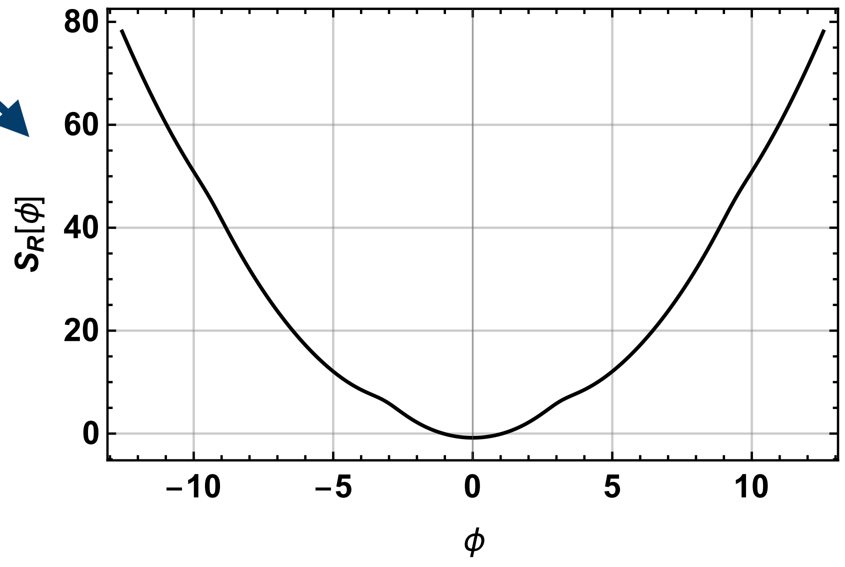

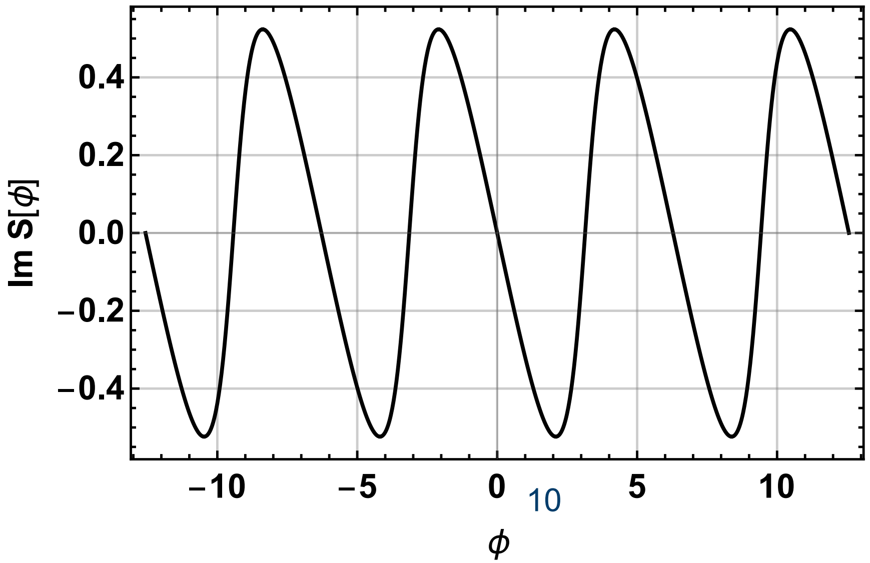

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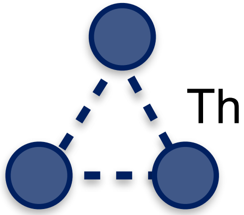
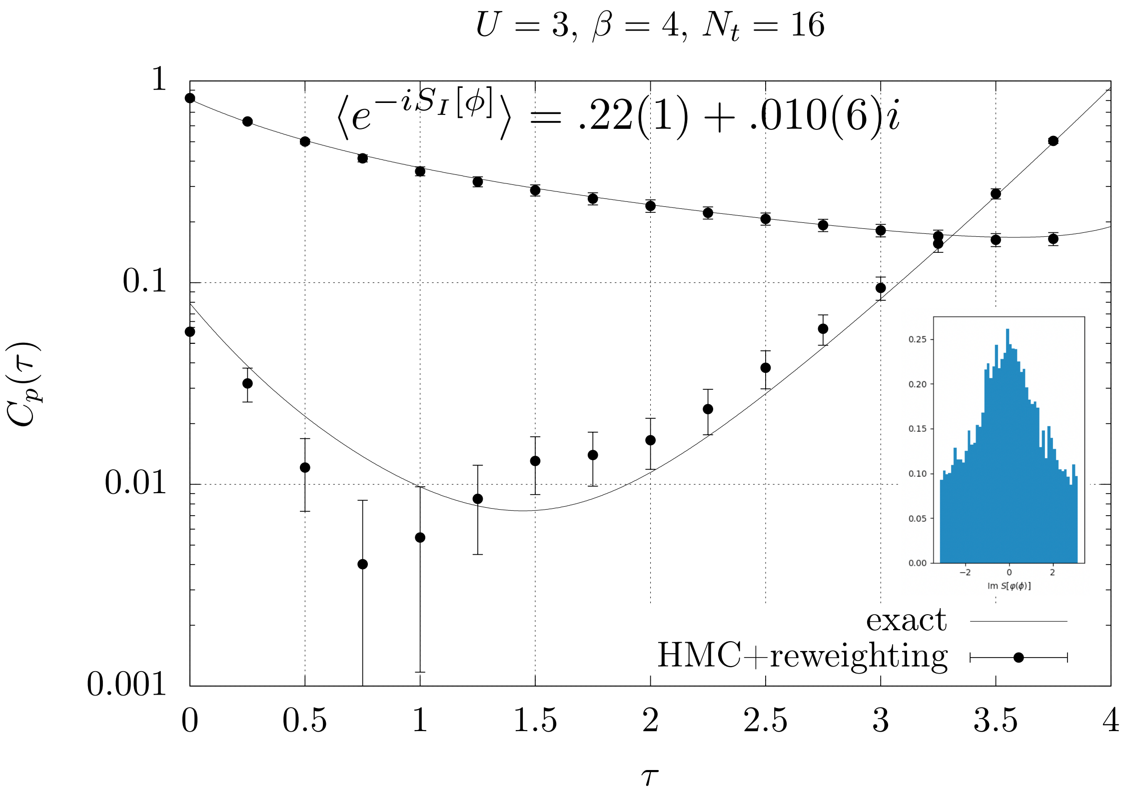
RE-WEIGHTING WORKS GREAT WHEN IT WORKS, BUT. . .



Three-site problem



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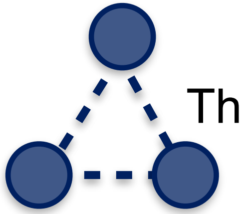

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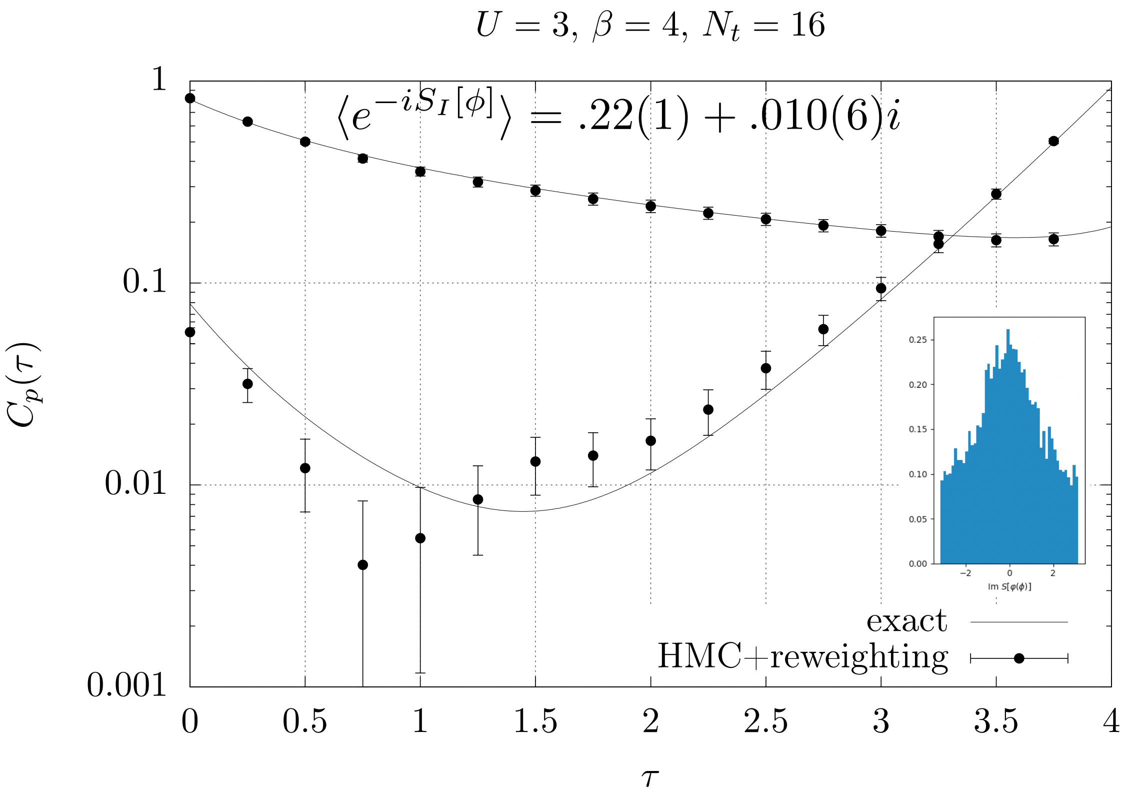
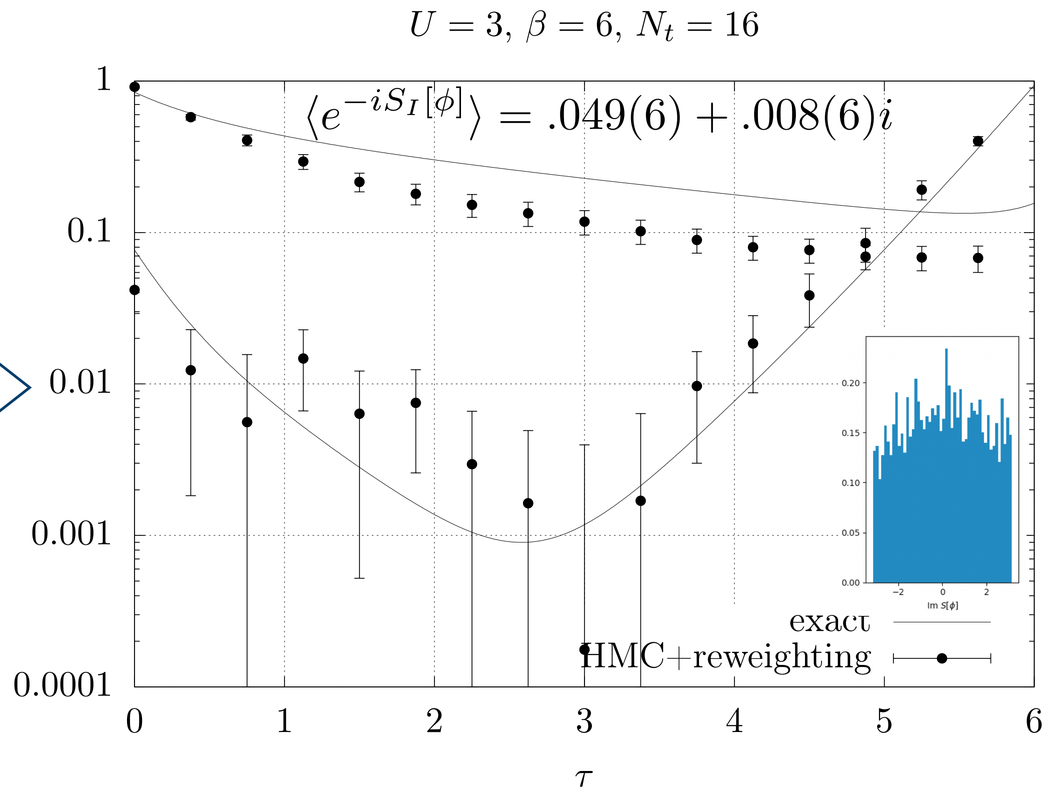


Increase system size



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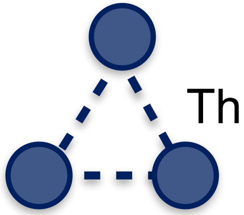
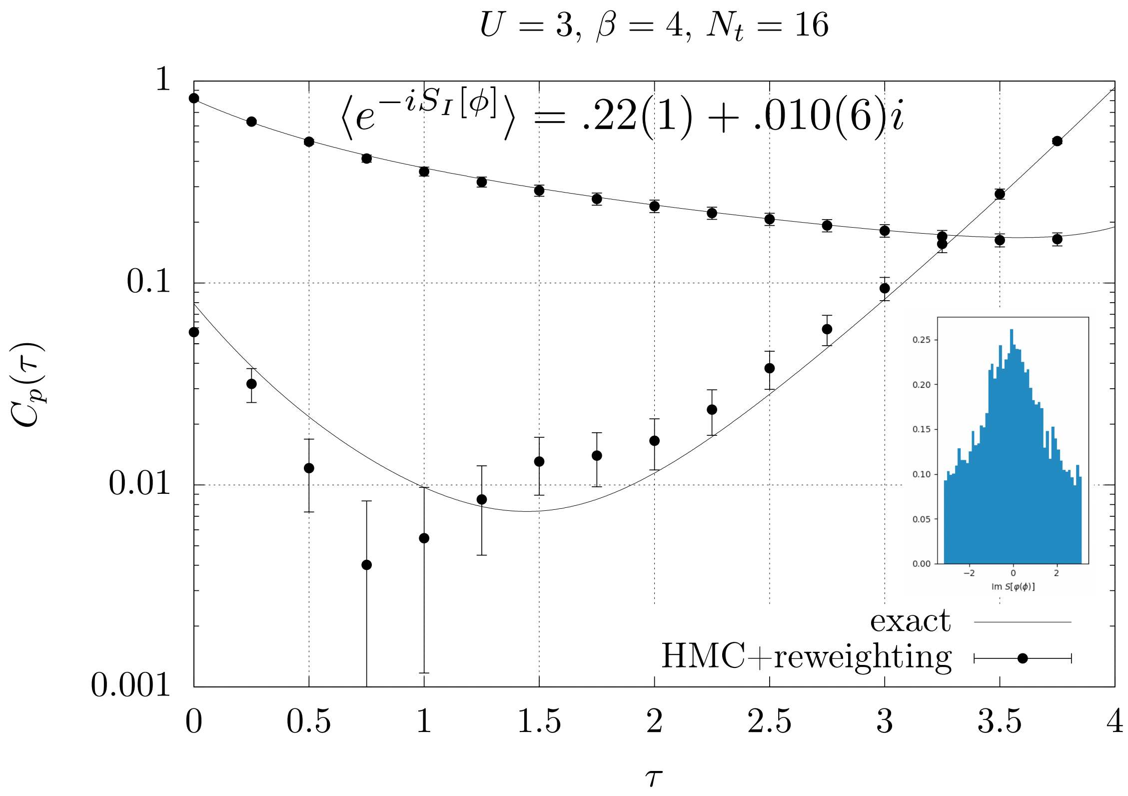
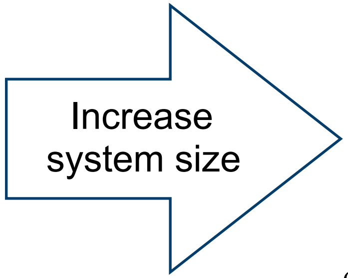
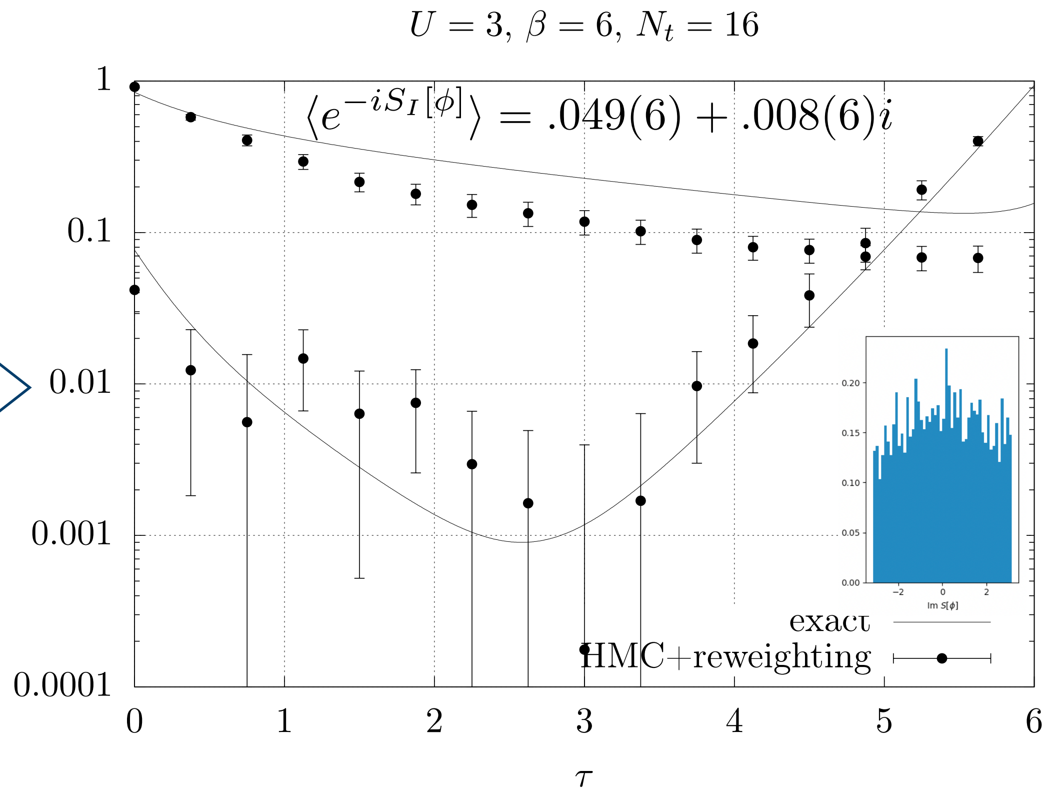






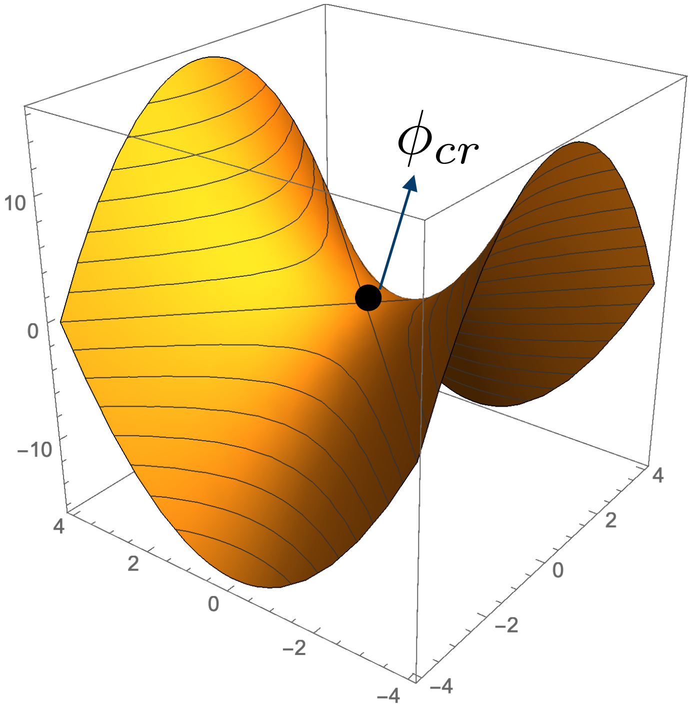


Phase fluctuations scale with the system size (extensive quantity). The larger the system, the worse the fluctuations $\Longrightarrow$ re-weighting will inevitably fail for large enough system sizes

ALLEVIATING THE SIGN-PROBLEM VIA HOLOMORPHIC FLOW

- Recall the stationary phase approximation:

$$\int \mathcal{D}[\phi] e^{-S[\phi]} = e^{-S[\phi_{cr}]} \int \mathcal{D}[\phi] e^{-\delta S[\phi]}$$



Critical point:

$$\left.\frac{\partial S(\phi)}{\partial \phi}\right|_{\phi=\phi_{cr}} = 0$$

Kanazawa & Tanizaki [arXiv:1412.2802]

Alexandru et al., [arXiv:1510.03258] [arXiv:1512.08764]

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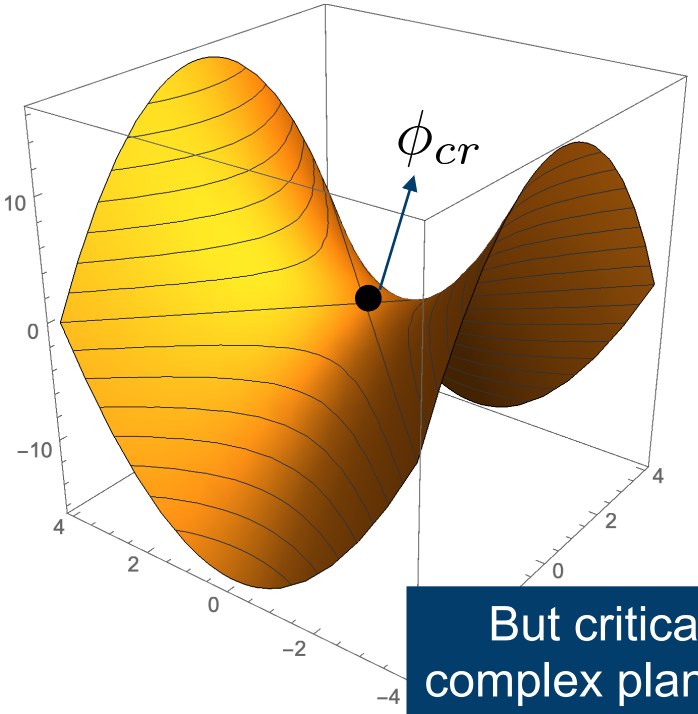

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But critical points are in the complex plane (and there can be more than one!)

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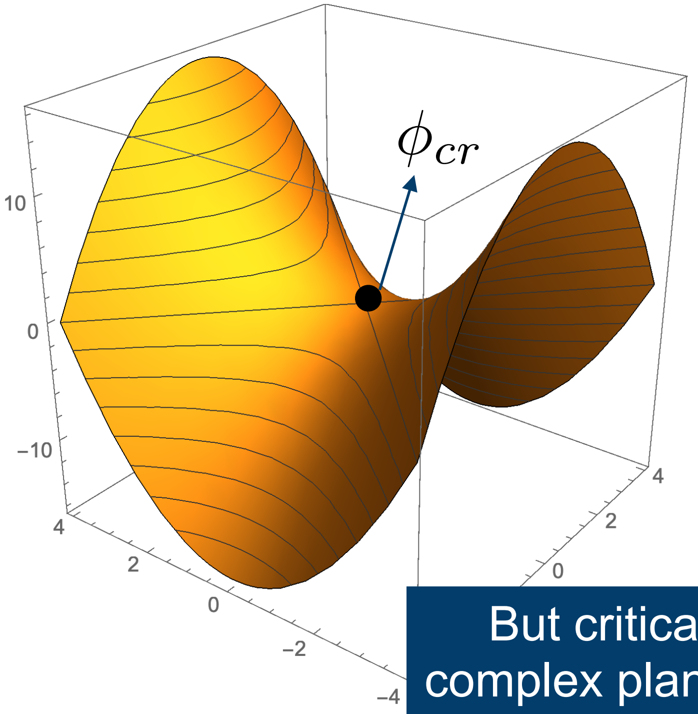
  - Cauchy's theorem tells us our integral will remain the same as long as we don't cross any singularities
  - Preserve homology class of kernel

How does this help the sign problem?

- ∃ particular manifolds in the complex plane that ***intersect*** ϕ_{cr} and have $S_I[\phi]$ is constant!
  - Lefschetz thimbles



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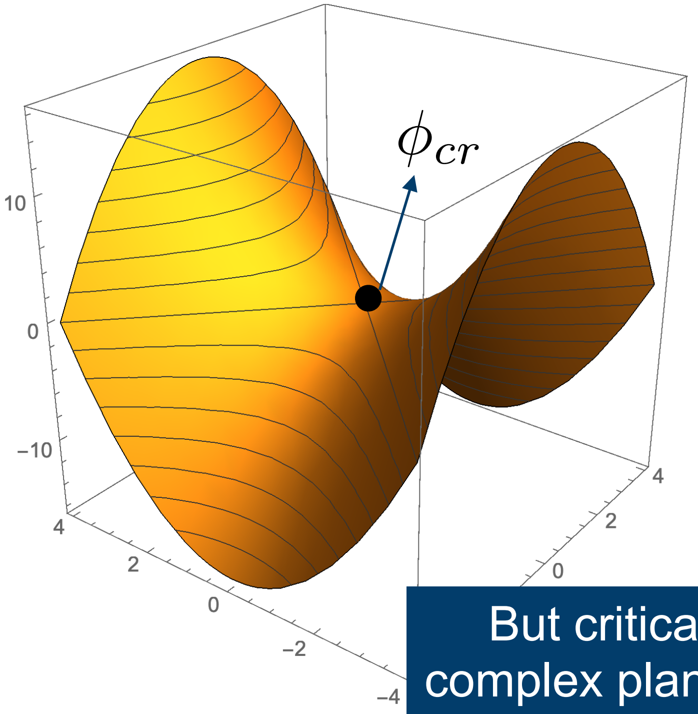

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$$\int_{\phi\in\mathbb{R}^N} \mathcal{D}[\phi] e^{-S[\phi]} \rightarrow e^{-iS_I^{\mathcal{T}}} \int_{\varphi\in\mathcal{T}\subset\mathbb{C}^N} D[\varphi] e^{-S_R[\varphi]}$$

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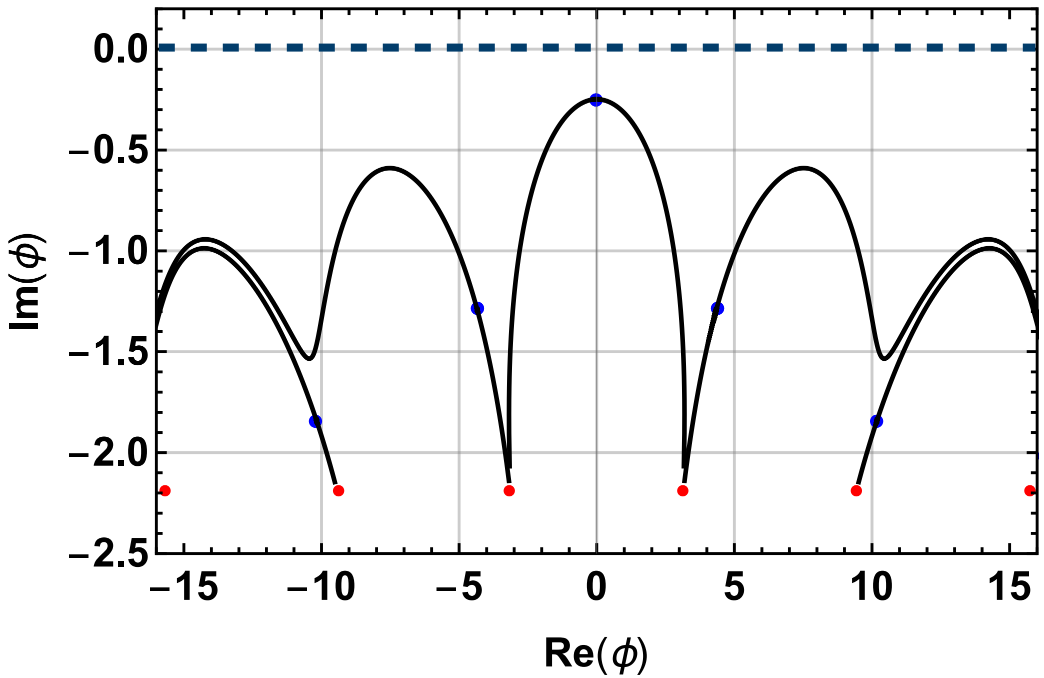
MORE ON LEFSCHETZ THIMBLES

1d example: $S(\phi) = \frac{1}{20}\left(\phi + \frac{3i}{2}\right)^2 - \log\left(1 + \frac{1}{2}e^{i\left(\phi+\frac{3i}{2}\right)}\right)$



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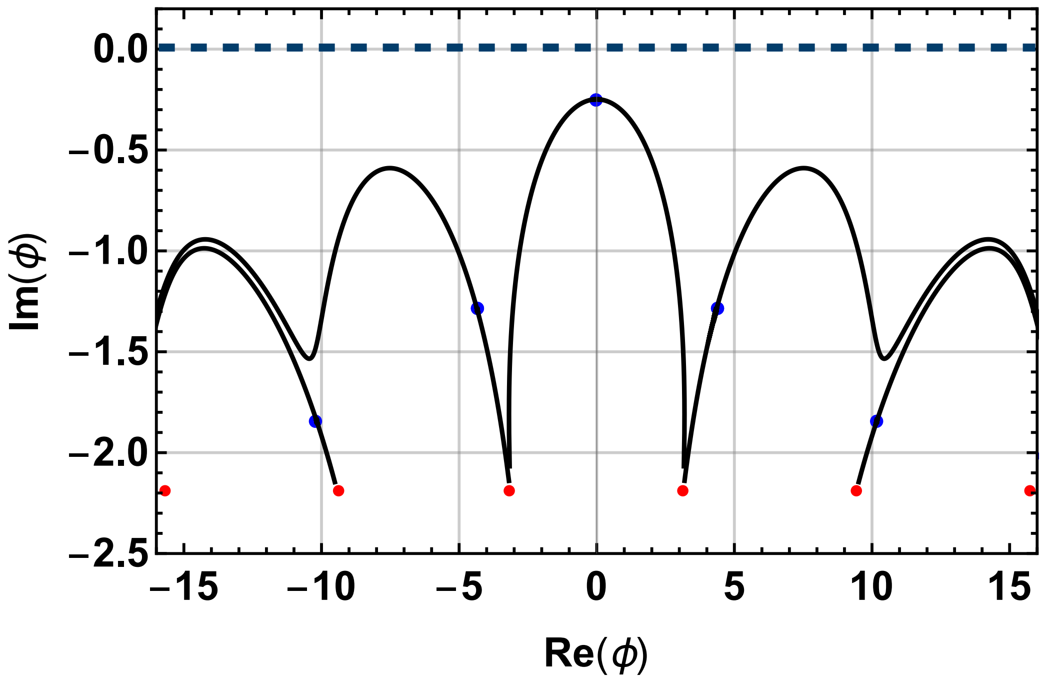
MORE ON LEFSCHETZ THIMBLES

Each critical point has an associated thimble

$$\mathcal{J}(\phi_{cr}) = \{\phi \mid \lim_{t\to\infty} \phi(t) = \phi_{cr}\}$$

1d example: $S(\phi) = \frac{1}{20}\left(\phi + \frac{3i}{2}\right)^2 - \log\left(1 + \frac{1}{2}e^{i\left(\phi+\frac{3i}{2}\right)}\right)$



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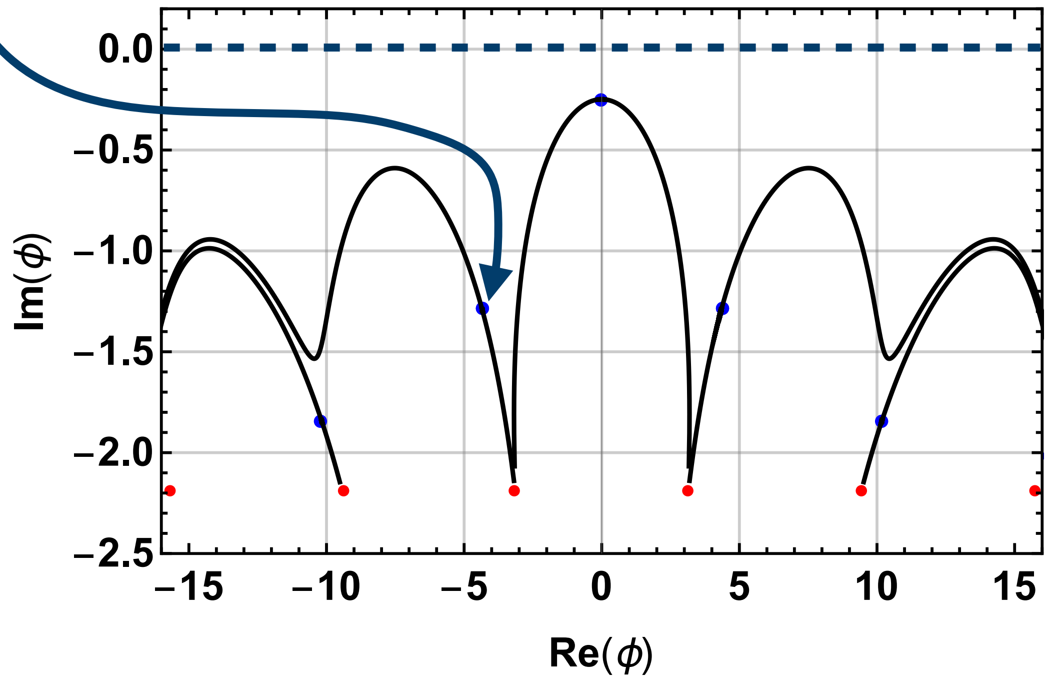

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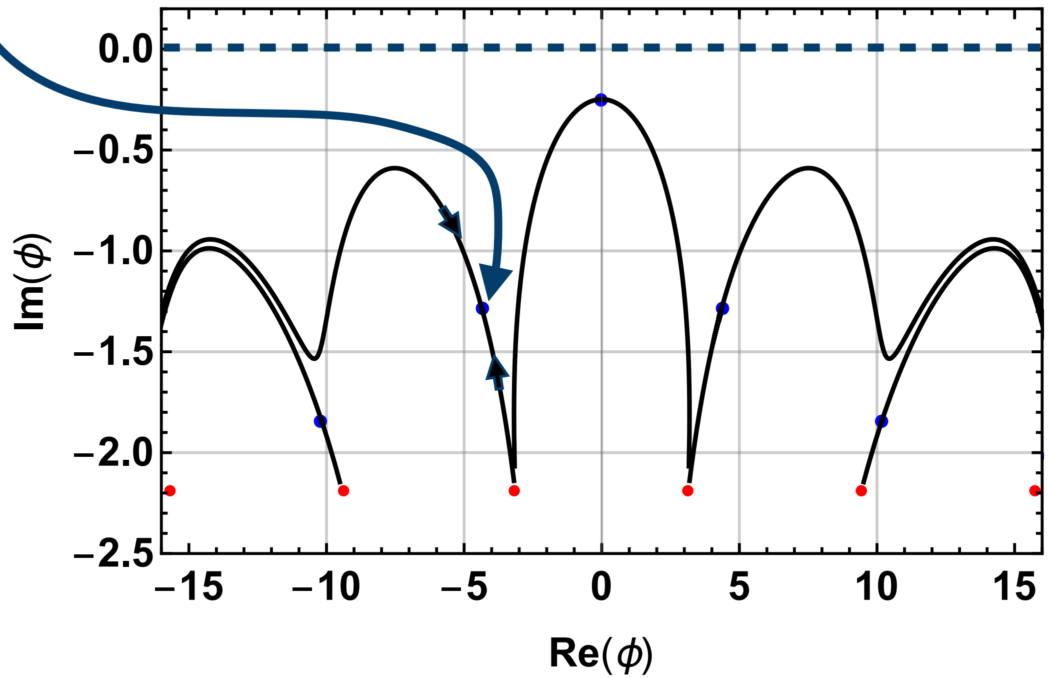

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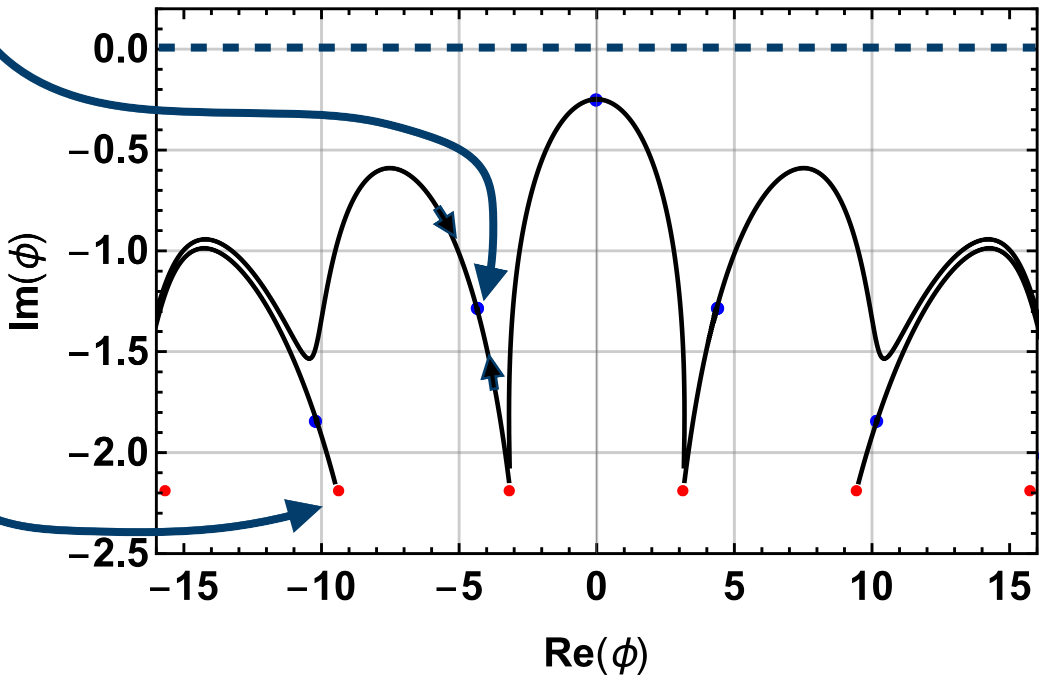

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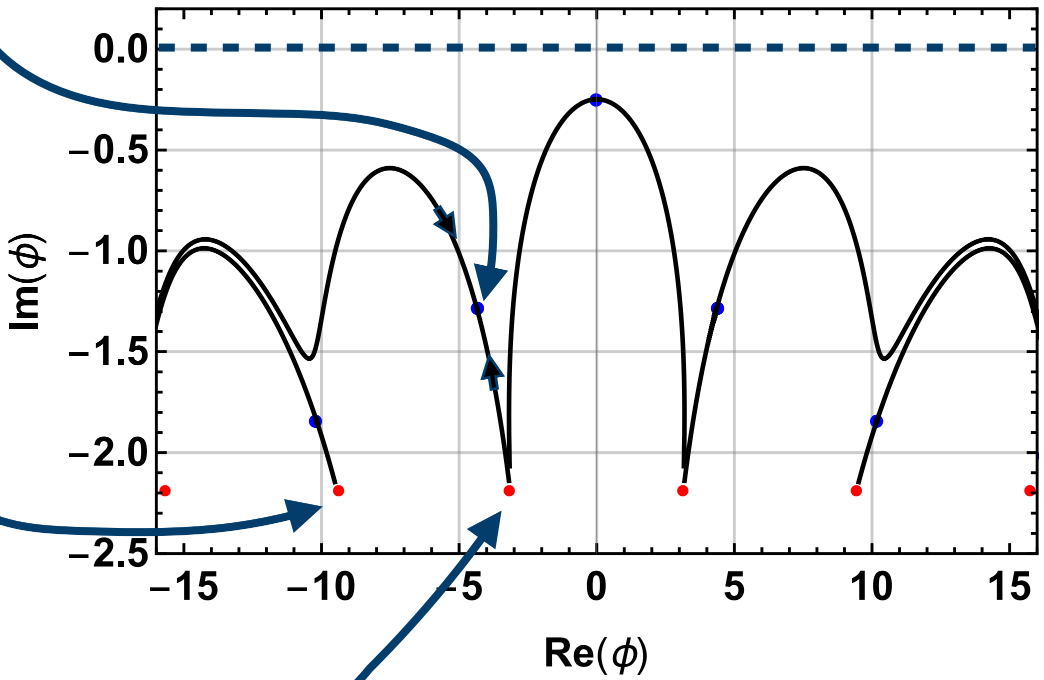

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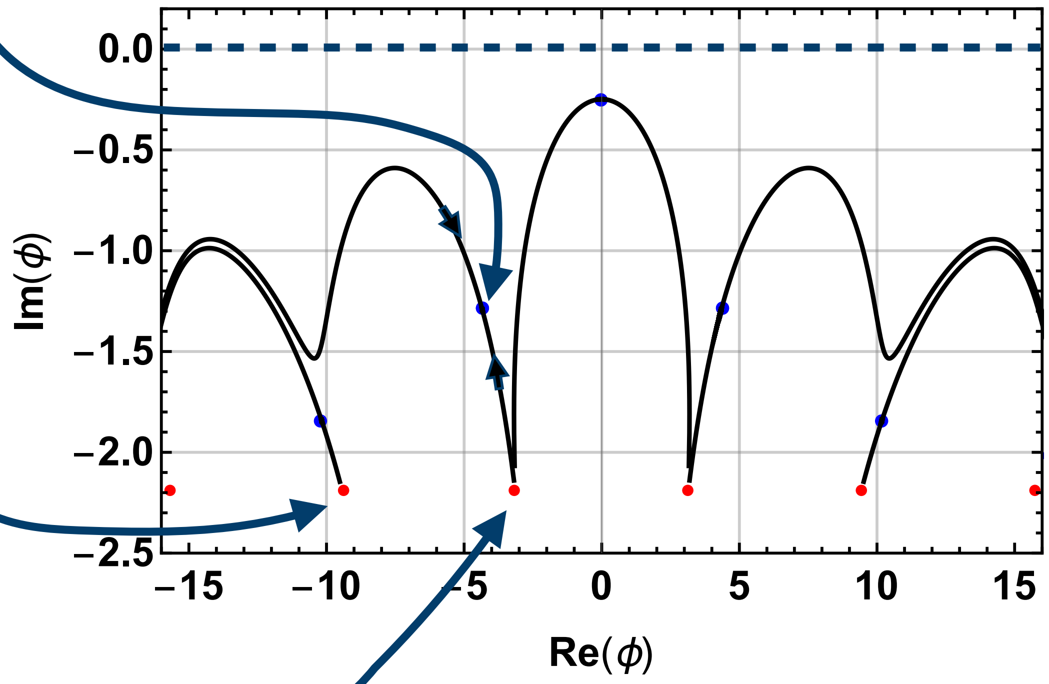

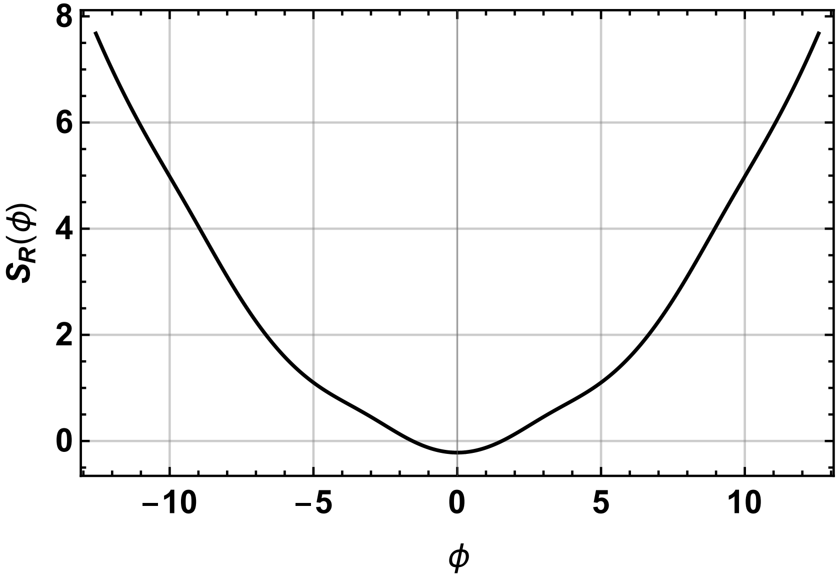

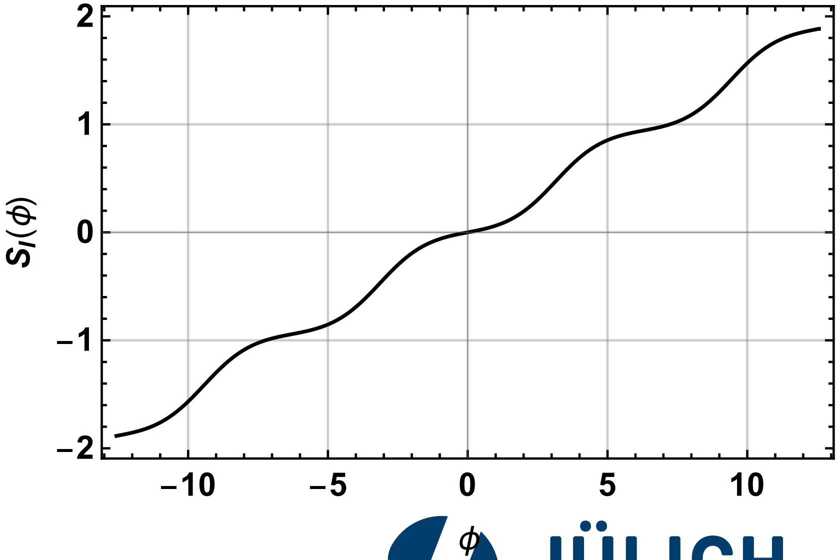

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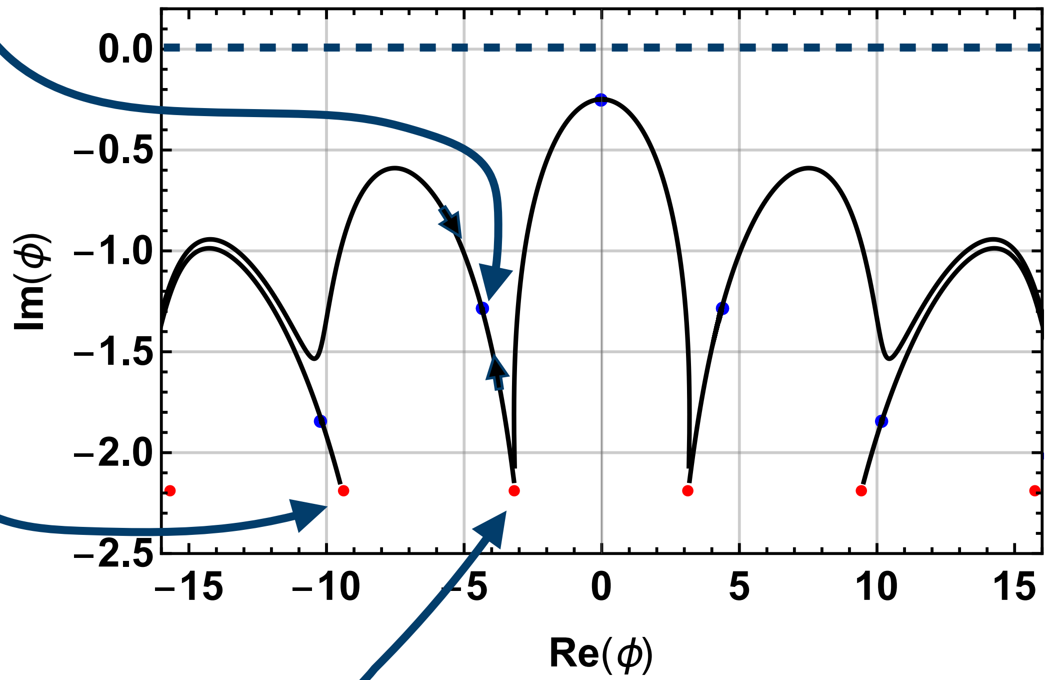

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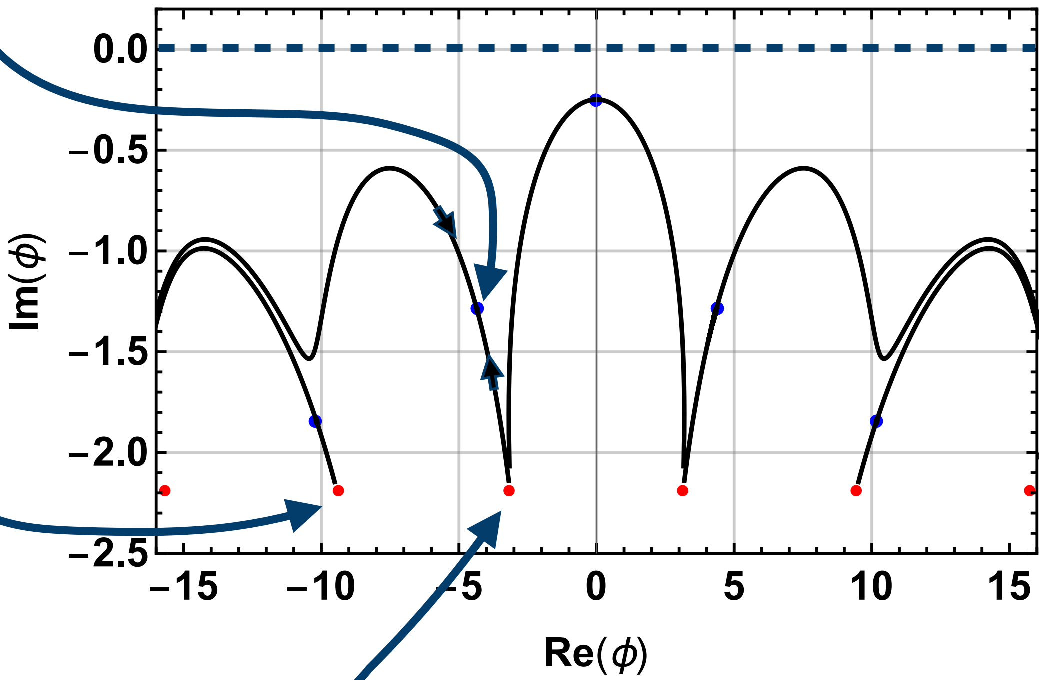

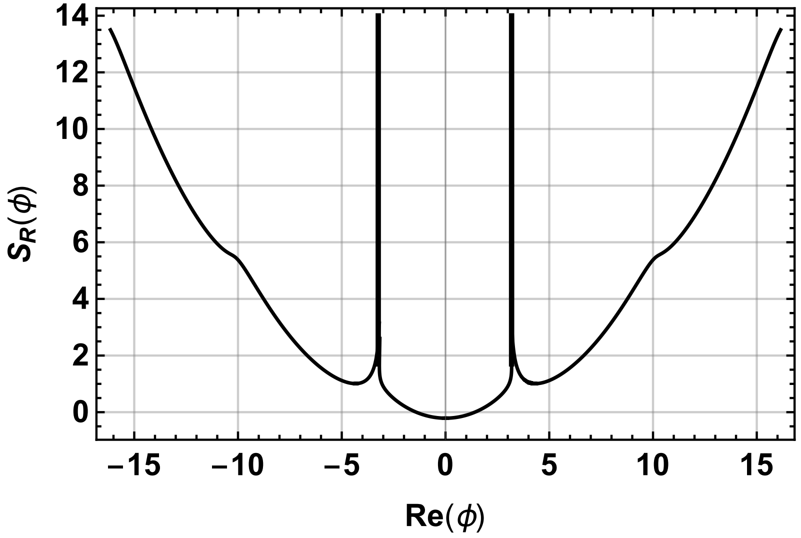

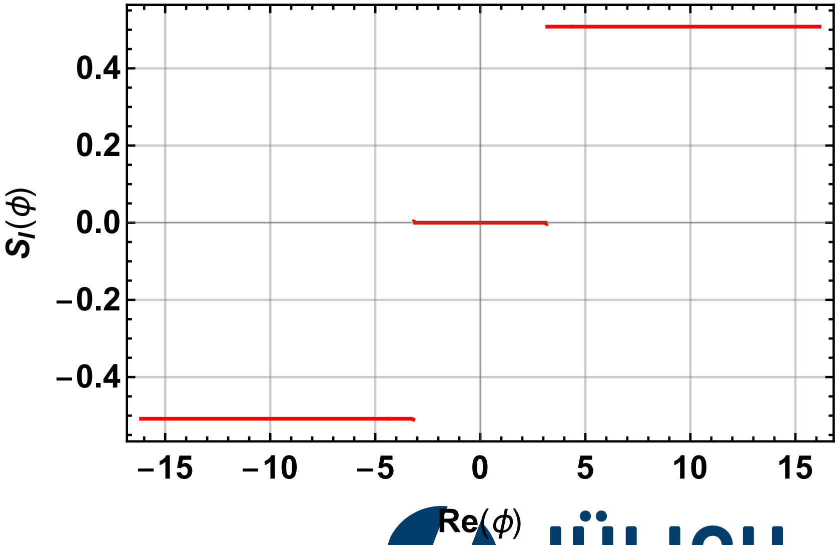

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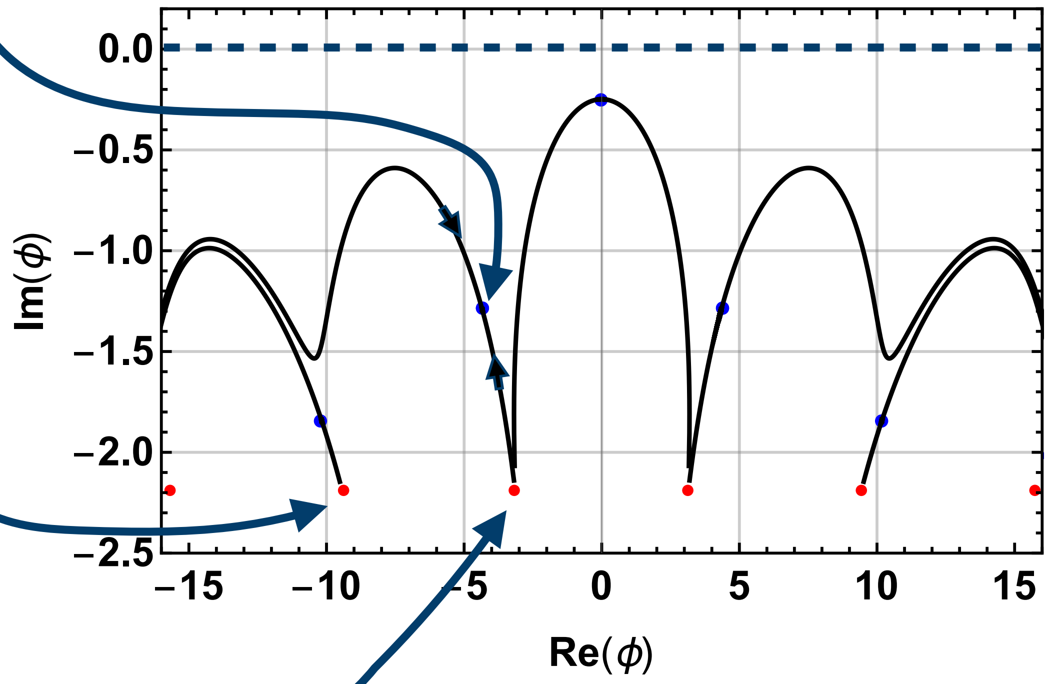

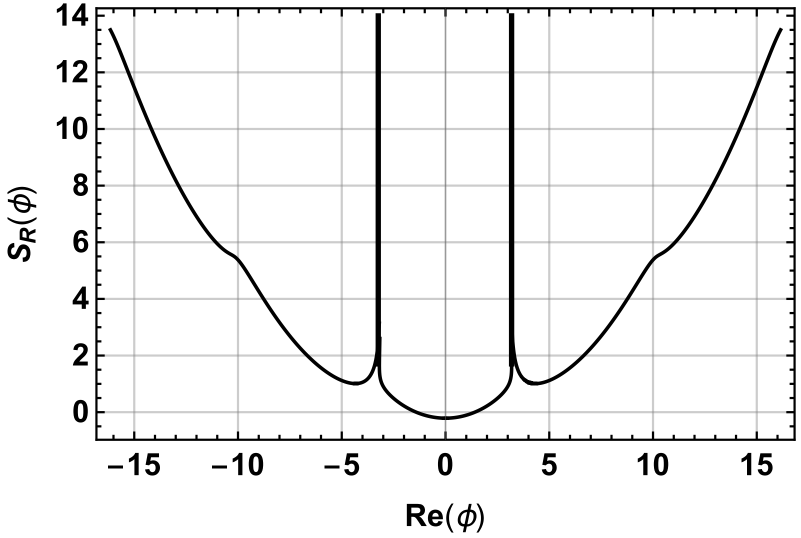

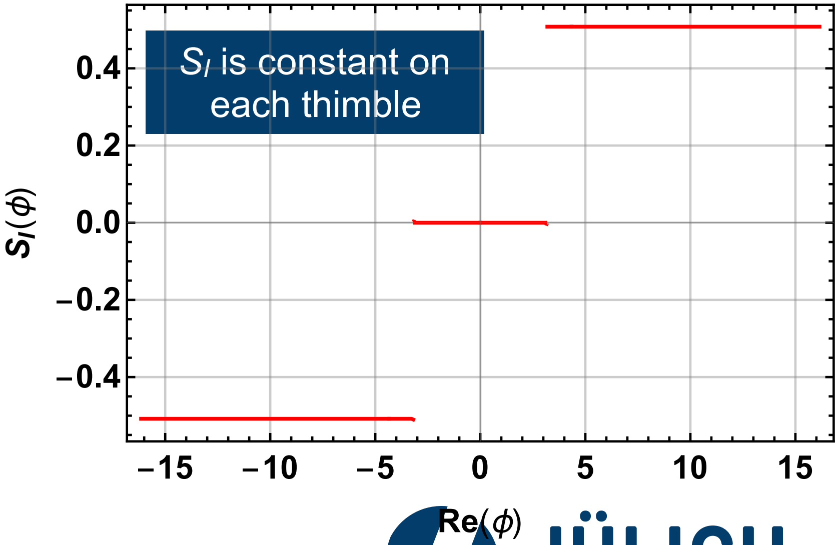

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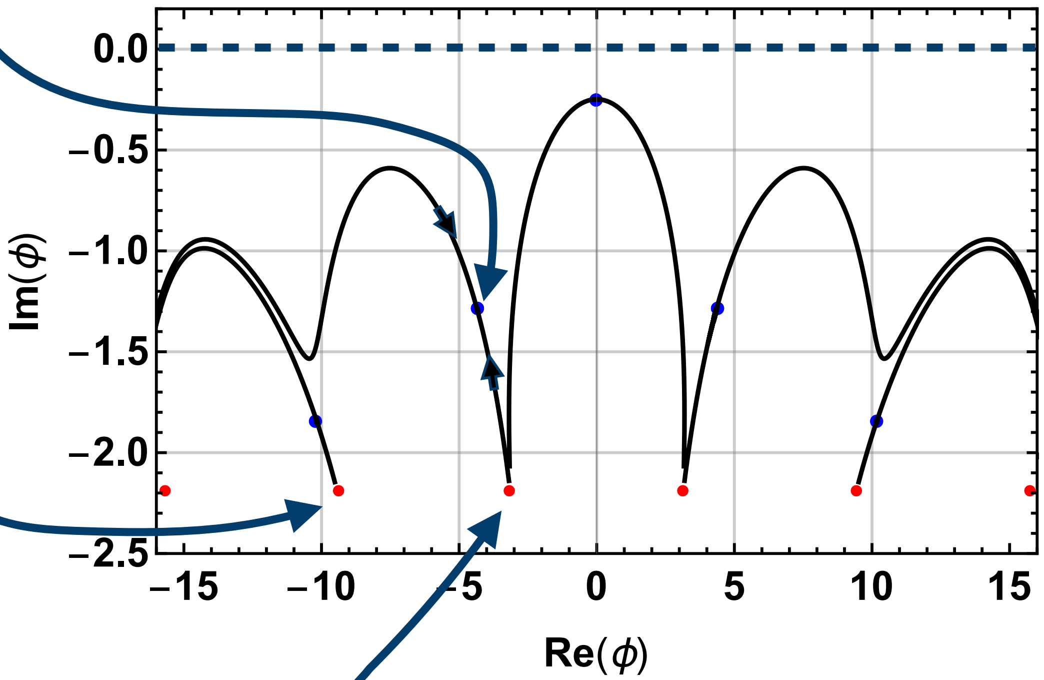
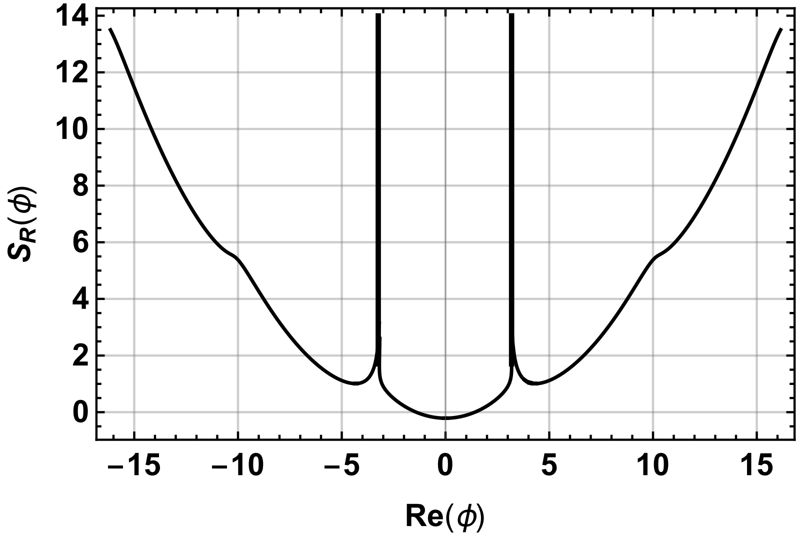
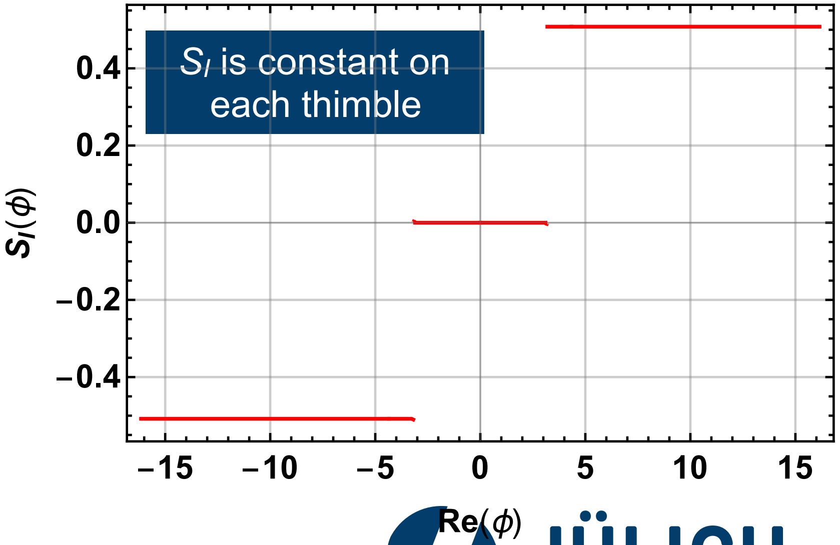






S_I is constant on each thimble

But we don't know *a priori* where these thimbles are!

BUT WE CAN APPROXIMATE THIMBLES BY FLOWING FROM REAL PLANE

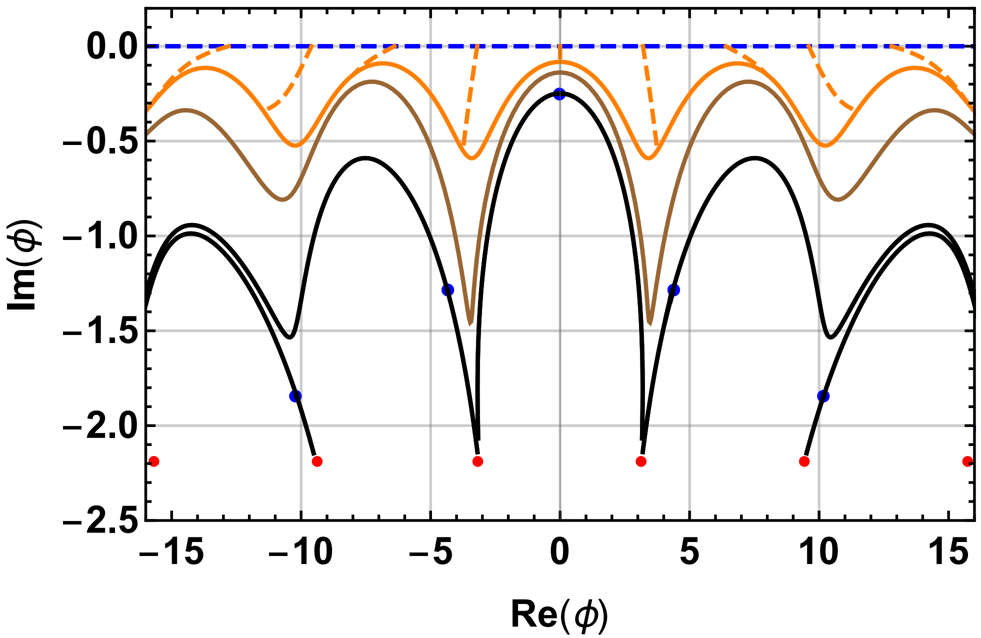
$$\dot{\phi} = \left(\nabla_\phi S[\phi]\right)^*$$

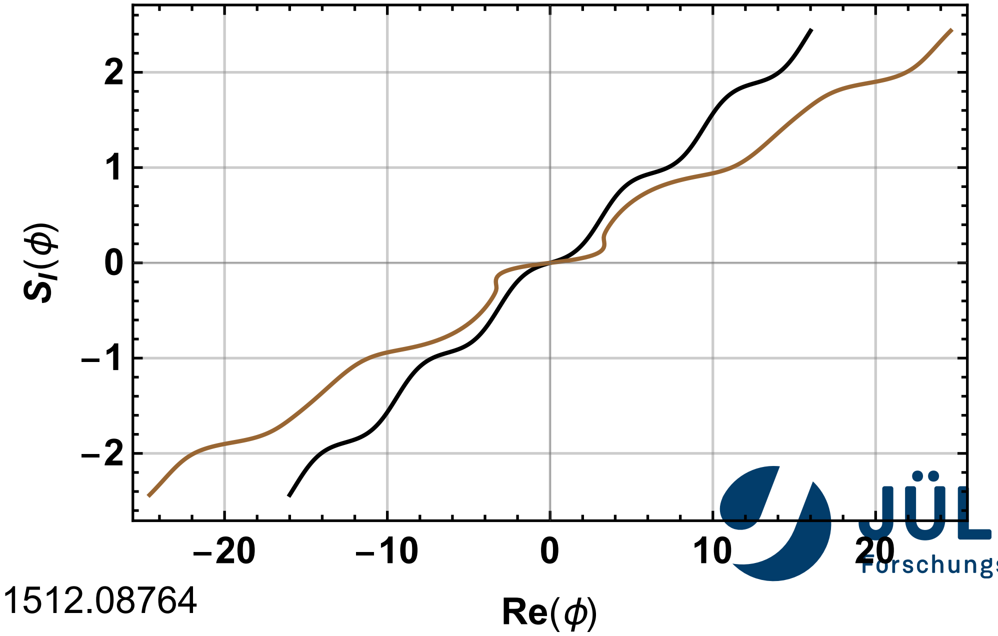
- Flow equations respect the homology class

- Starting from any point on the real plane, the flow will approach some point on the thimble manifolds
    - In the limit of infinite flow time, one recovers the exact thimbles (care must be taken in presence zeros)

- For finite flow time, one has an approximation to the thimbles
    - Sign problem has been alleviated
    - Re-weighting should work!

“Generalized Thimble” approach





Nishimura & Shimasaki, 1703.09409

Alexandru et al., 1512.08764

HOW DO WE SAMPLE FROM THE MANIFOLDS?

$$\underbrace{\frac{1}{\mathcal{Z}_{\mathcal{T}}}\int_{\mathcal{T}} D[\varphi]O[\varphi]\exp\{-S[\varphi]\}}_{\text{Integration on manifolds}} \;\longrightarrow\; \underbrace{\frac{1}{\mathcal{Z}_{\mathcal{T}}}\int_{\mathbb{R}} D[\phi]O[\varphi(\phi)]\exp\{-S[\varphi(\phi)]\}\det J[\varphi(\phi)]}_{\text{Integration on real plane}}$$

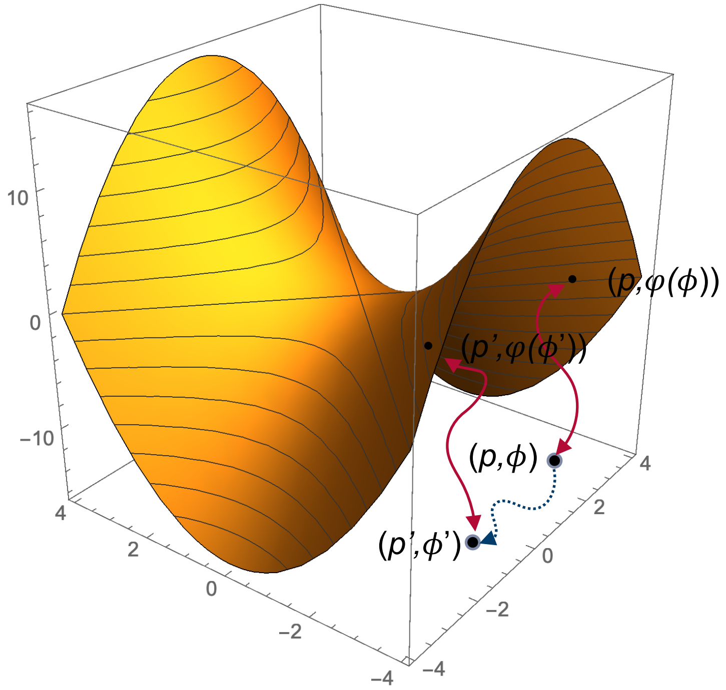
$$\frac{1}{\mathcal{Z}_{\mathcal{T}}}\int_{\mathcal{T}} D[\varphi]O[\varphi]\exp\{-S[\varphi]\} = \frac{1}{\mathcal{Z}_{\mathcal{T}}}\int_{\mathbb{R}} D[\phi]O[\varphi(\phi)]\exp\{-S[\varphi(\phi)]\}\det J[\varphi(\phi)]$$
$$= \frac{1}{\mathcal{Z}_{\mathcal{T}}}\int_{\mathbb{R}} D[\phi]O[\varphi(\phi)]\exp\{-S_{eff}[\varphi(\phi)]\}$$

$$S_{eff}[\varphi(\phi)] \equiv S[\varphi(\phi)] - \log\det J[\varphi(\phi)]$$

Jacobian is induced due to the change of variables from the manifold to the real plane

HMC WITH HOLOMORPHIC FLOW

- Perform HMC on the real plane to make proposal $(p,\phi) \rightarrow (p',\phi')$
- Then flow up (close) to manifold $\varphi(\phi')$
- Accept/reject with $\mathbb{P}_{a/r} = \min\left(1, \dfrac{e^{-p'^2/2 - \mathrm{Re}S_{eff}[\varphi(\phi')]}}{e^{-p^2/2 - \mathrm{Re}S_{eff}[\varphi(\phi)]}}\right)$
- Reversible, satisfies detailed balance



HMC directly on the thimble:
Ulybyshev et al. [arXiv:1906.02726]

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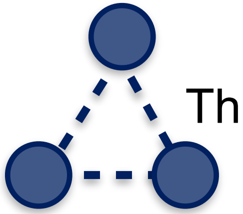
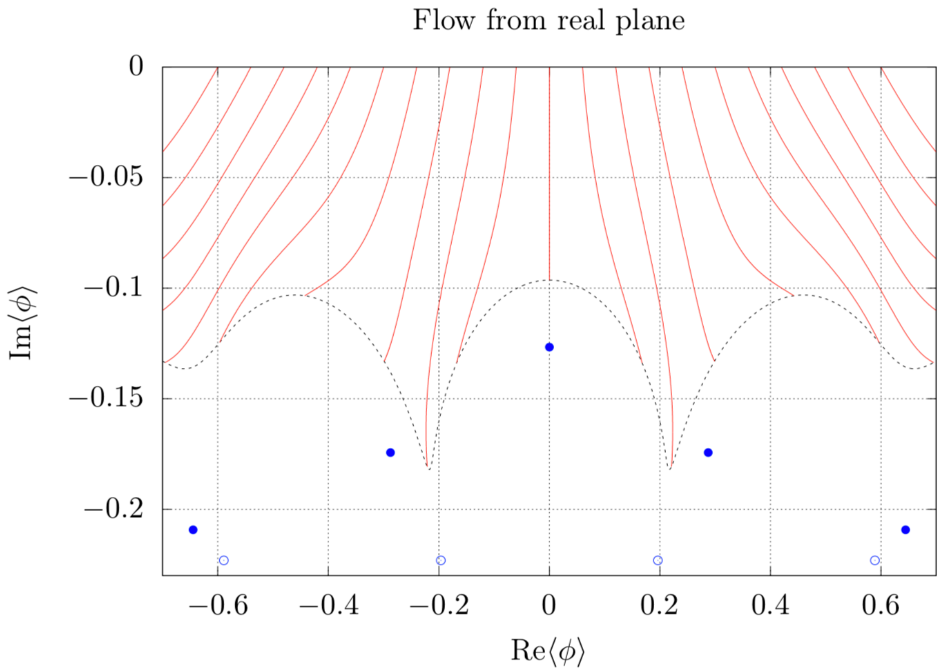
FLOWING THE ACTION

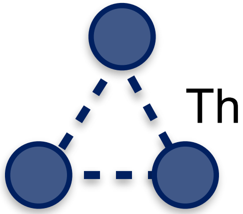


Flow from real plane $\dot{\phi} = (\nabla_\phi S[\phi])^*$



FLOWING THE ACTION

Three-site problem



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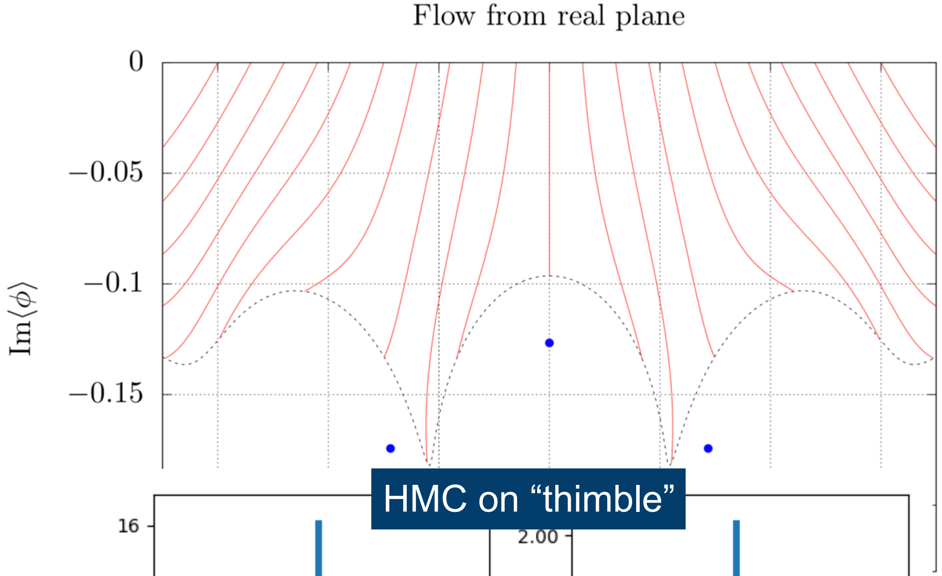
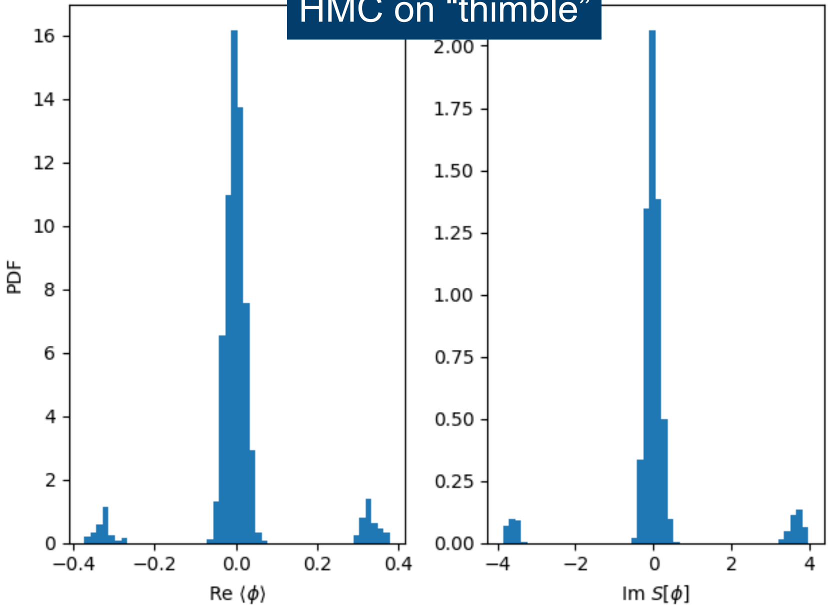


HMC on “thimble”



FLOWING THE ACTION

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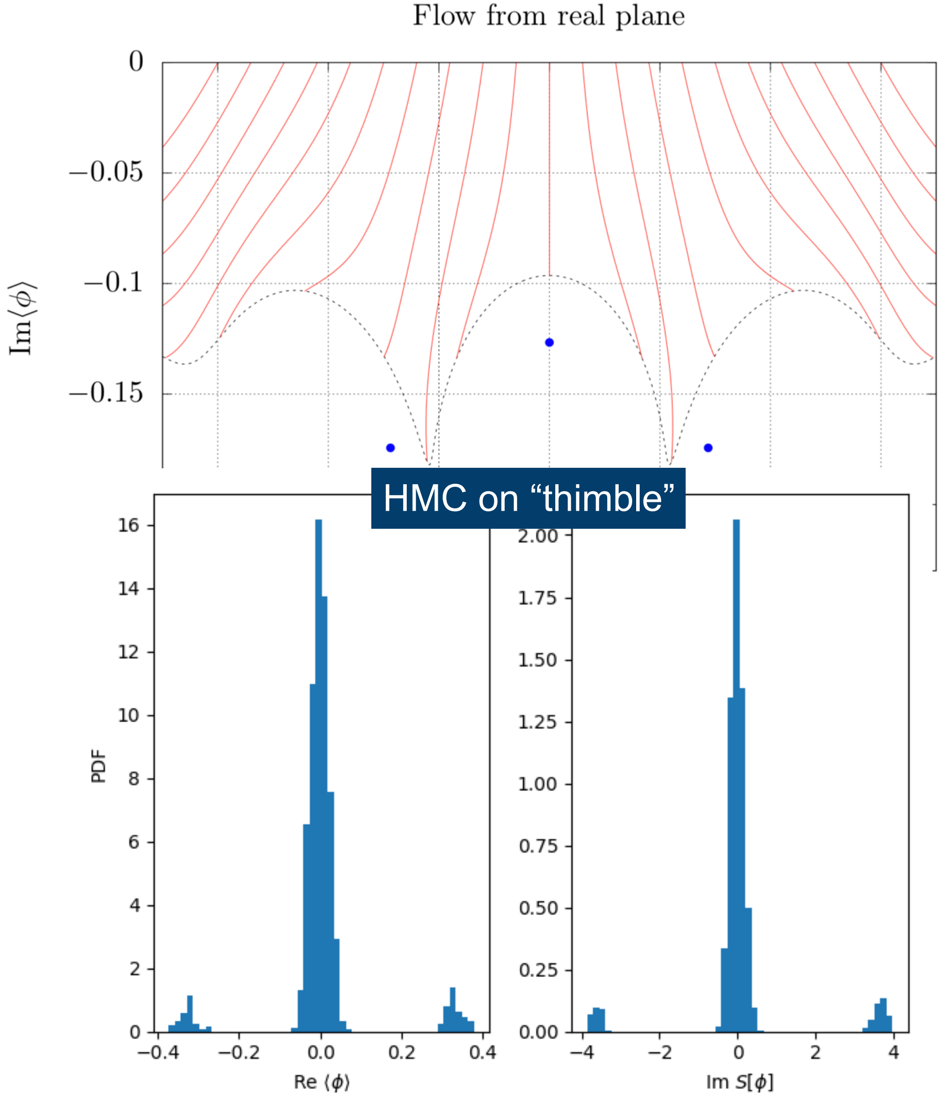
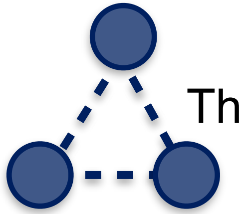
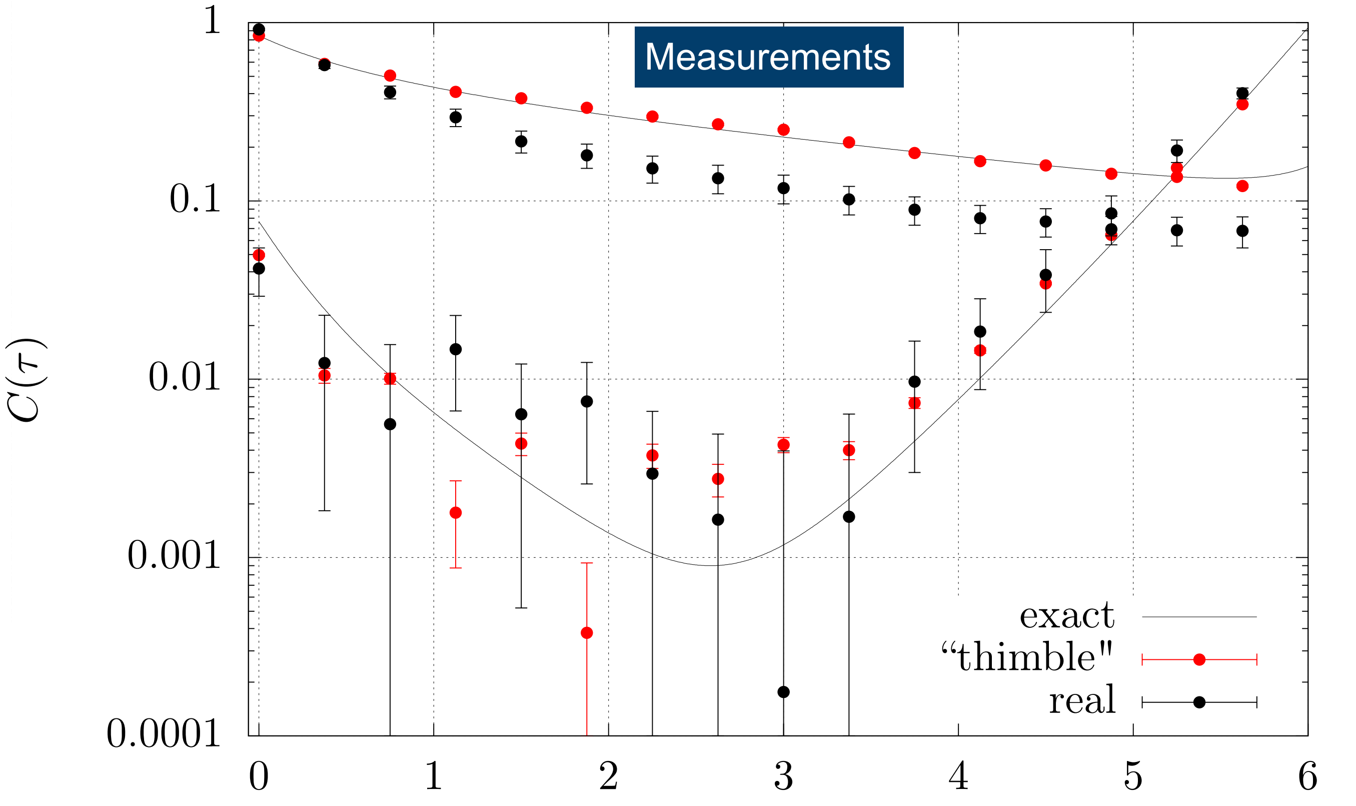




Three-site problem

$U = 3, \beta = 6, N_t = 16$



$\langle e^{-iS_I[\phi]} \rangle = .800(6) + .006(2)i$

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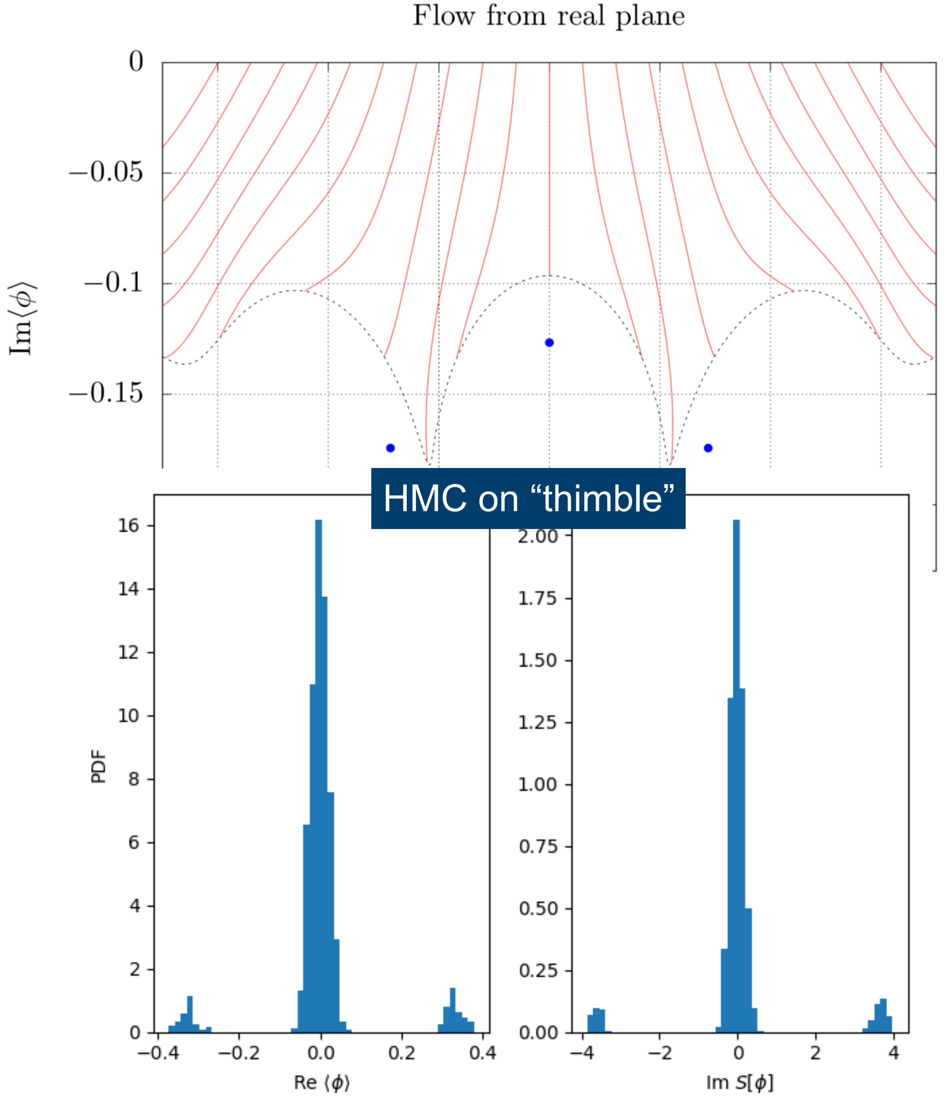
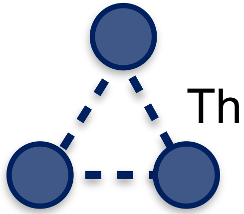


HMC on “thimble”



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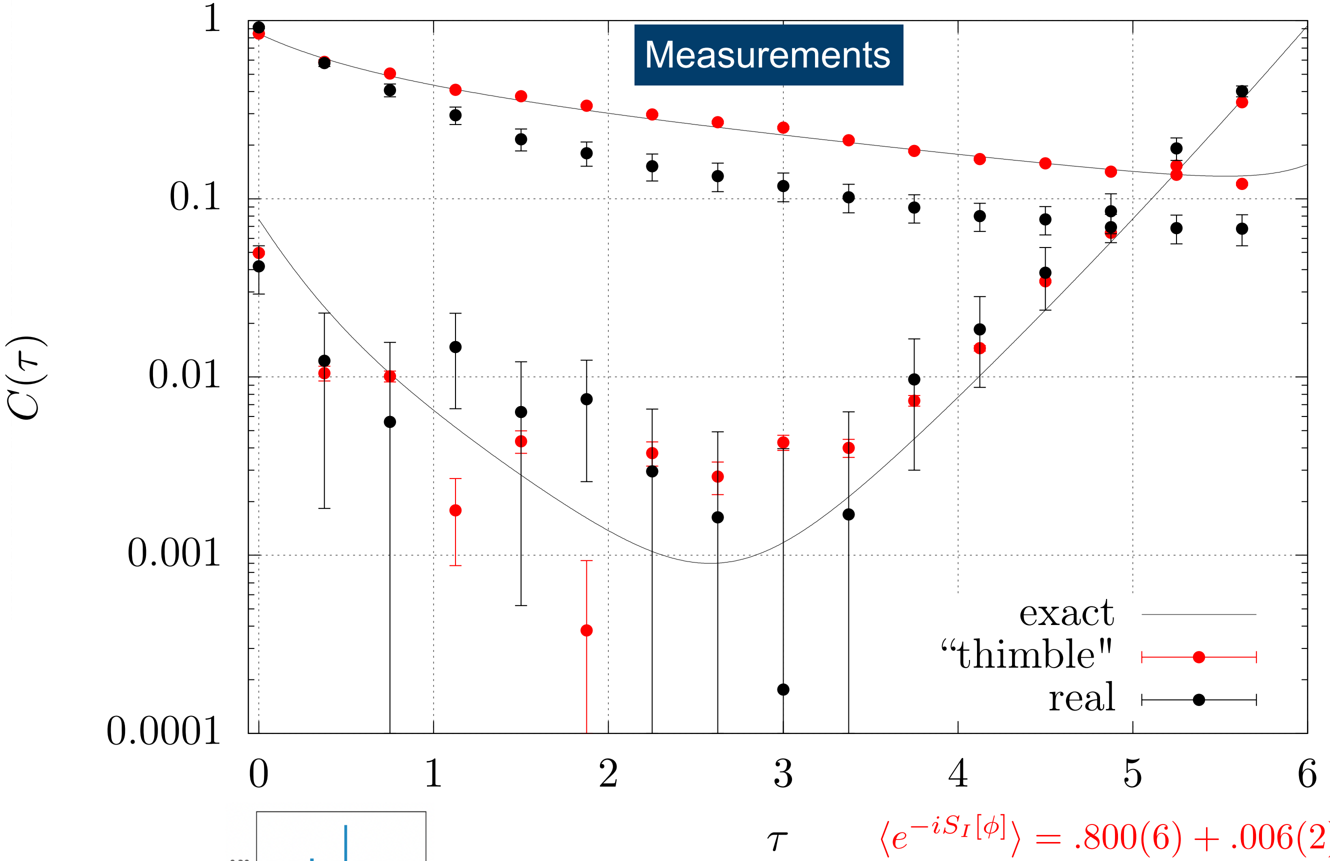
Measurements



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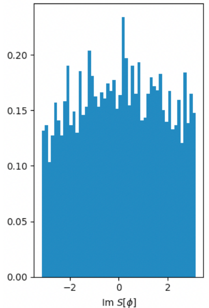


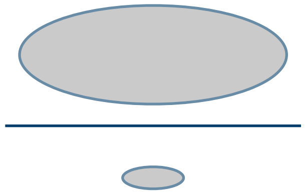
$\langle e^{-iS_I[\phi]} \rangle = .049(6) + .008(6)i$

UNFORTUNATELY, THIS “SOLUTION” IS NOT VIABLE NUMERICALLY

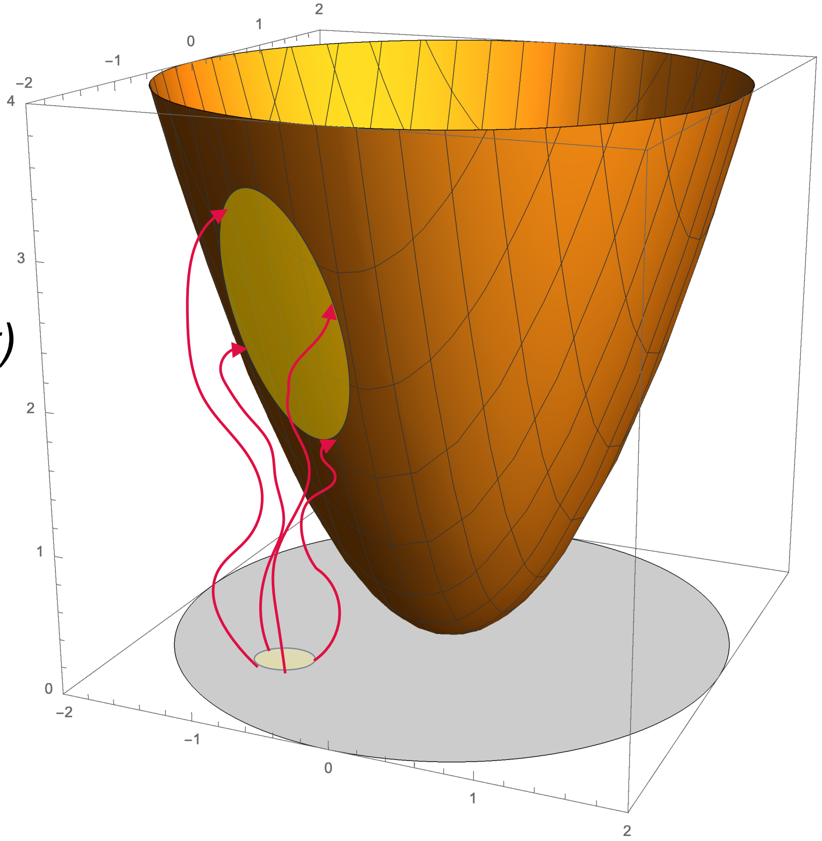
“No free lunch theorem”

$$\dot{\phi}(t) = [\nabla_\phi S[\phi(t)]]$$

$$\dot{J}(t) = [H[\phi(t)]J(t)]^*$$



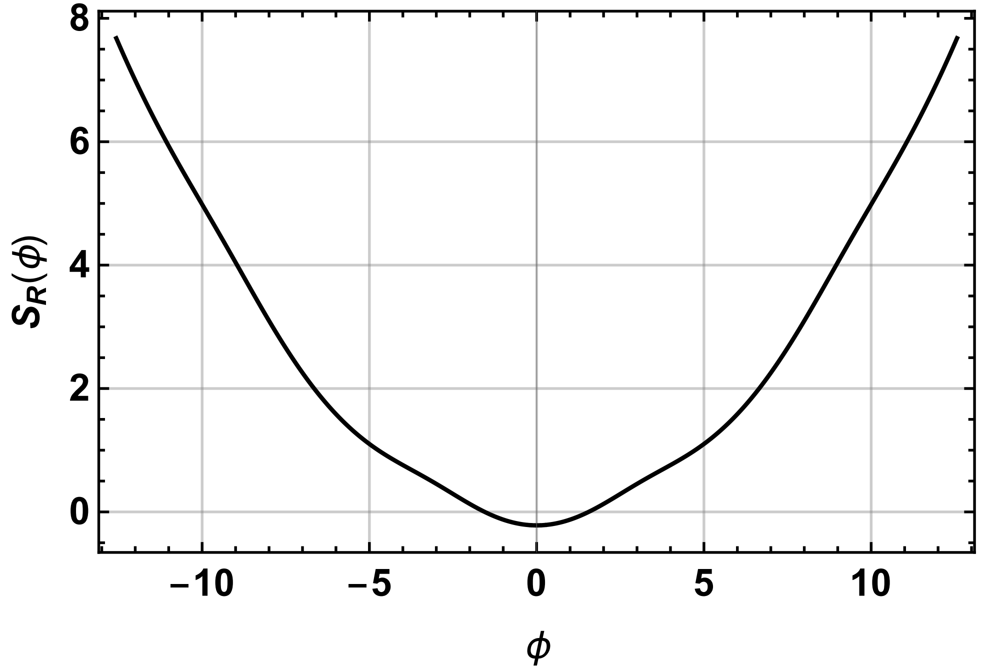
= det *J(t)*



- Calculation of Jacobian due to flow is extremely time consuming!
  - At every step of the flow integration, must compute a dense matrix!

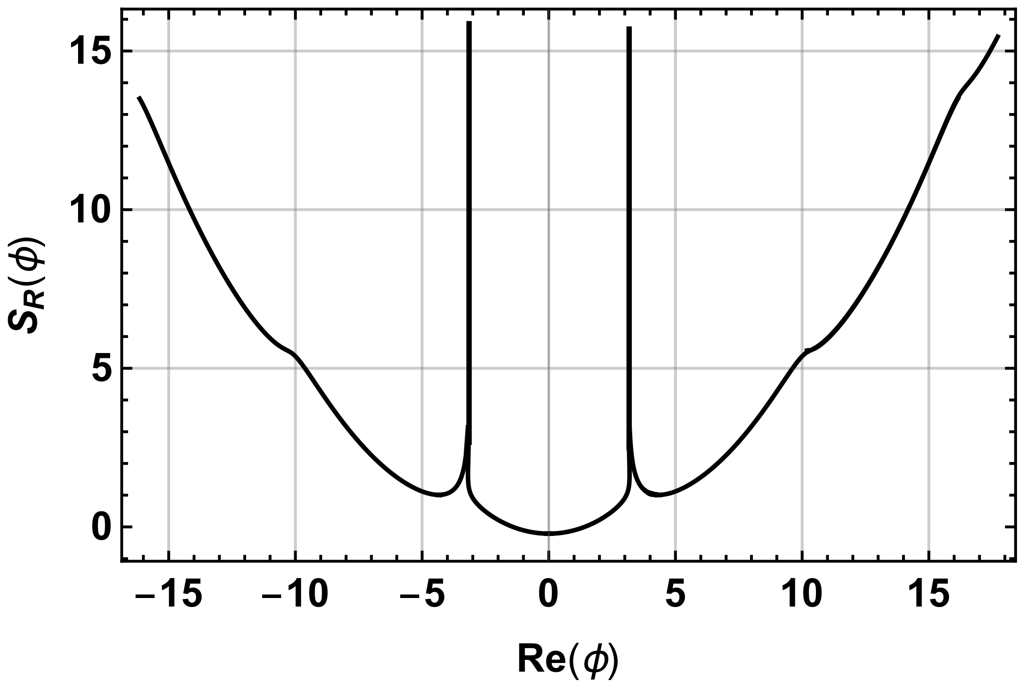
UNDER THE FLOW, MUST BE LEERY OF INFINITIES

no ergodicity issues, but sign problem



$$\dot{\phi} = (\nabla_\phi S[\phi])^*$$
$$\lim_{t_f \to \infty}$$

no sign problem, but ergodicity issues



Wynen, **TL**, et al. [arXiv:1812.09268] Phys.Rev. **B100** (2019) 075141

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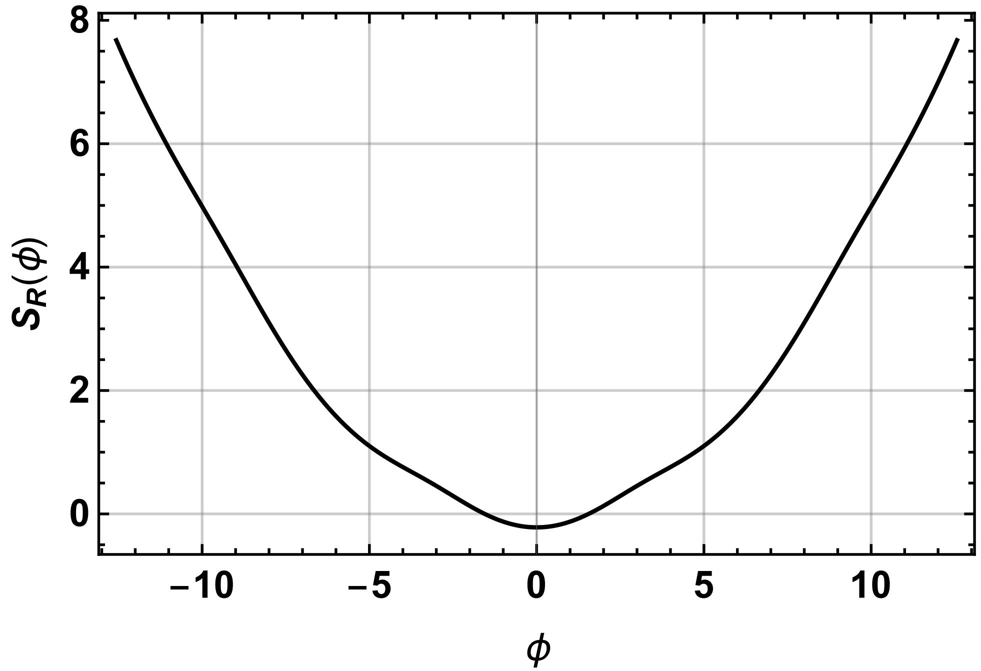

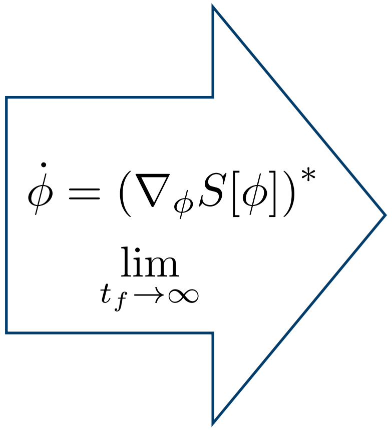

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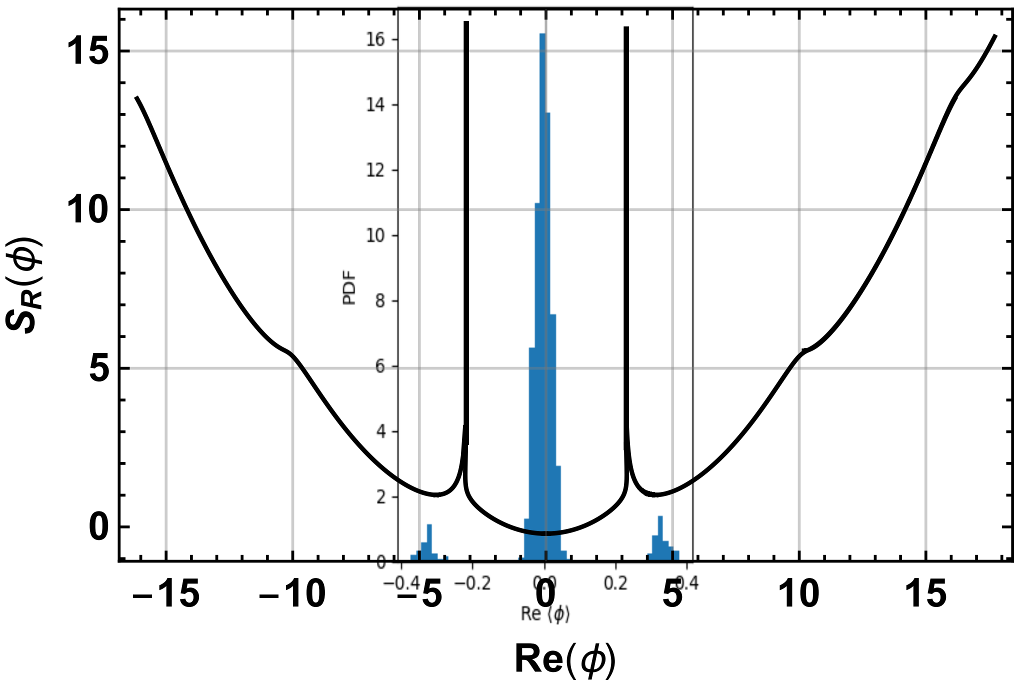

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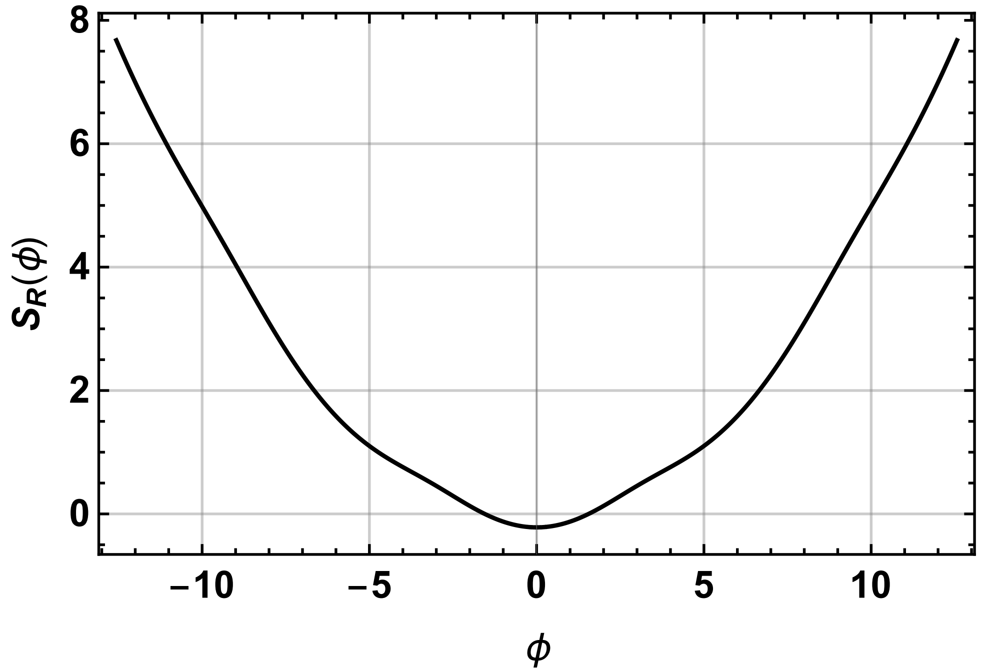

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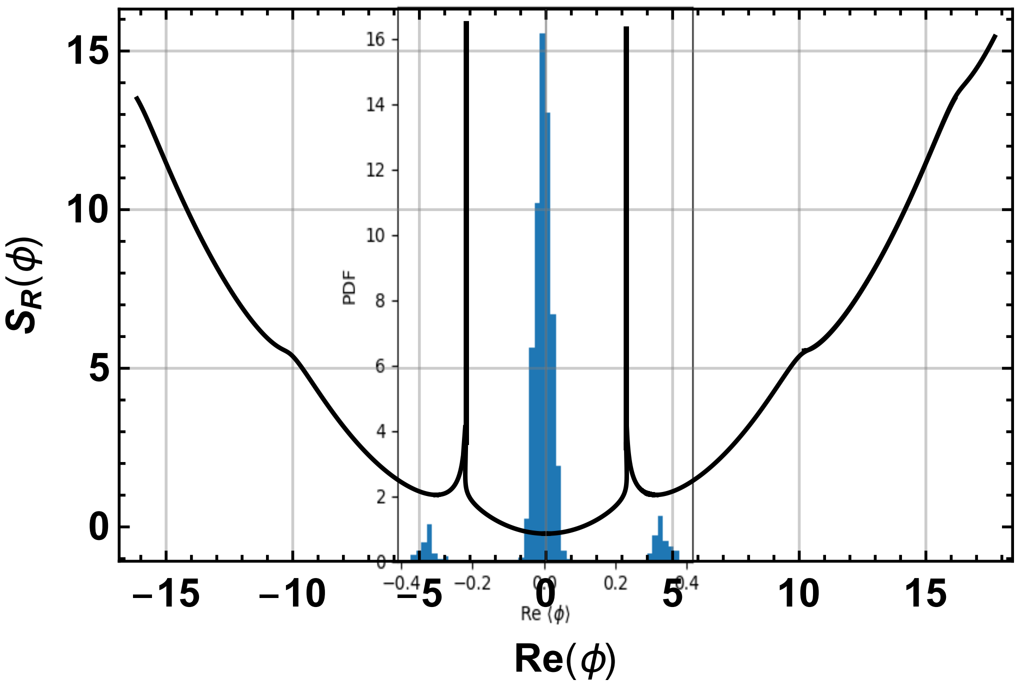
no sign problem, but ergodicity issues



Distributions become highly multi-modal (ergodicity issues)

Wynen, **TL**, et al. [arXiv:1812.09268] Phys.Rev. **B100** (2019) 075141

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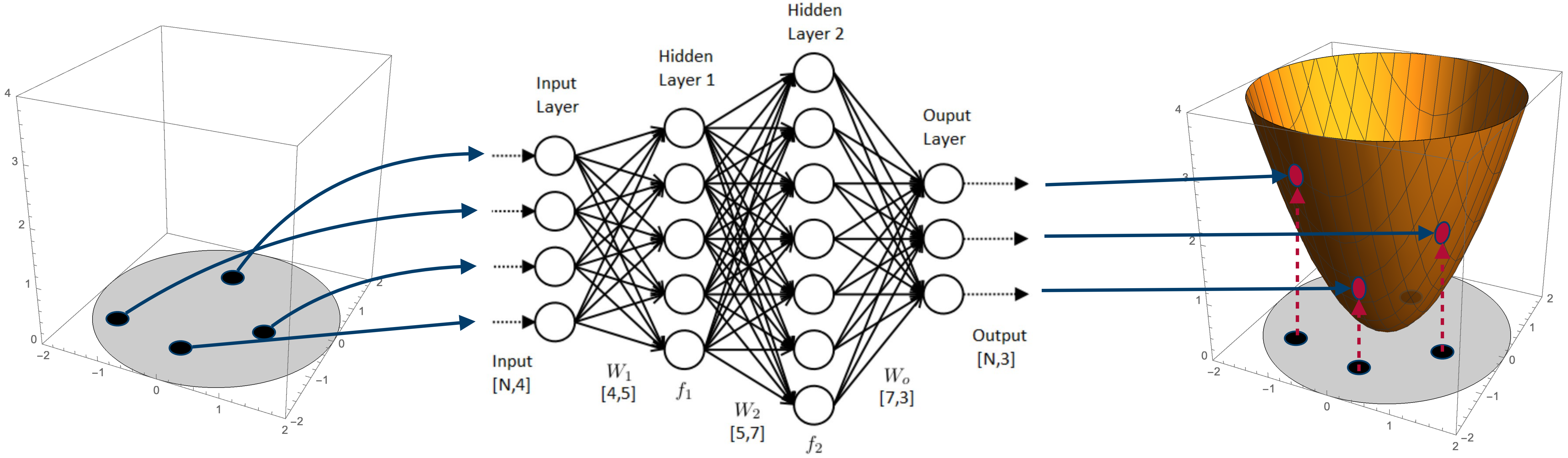
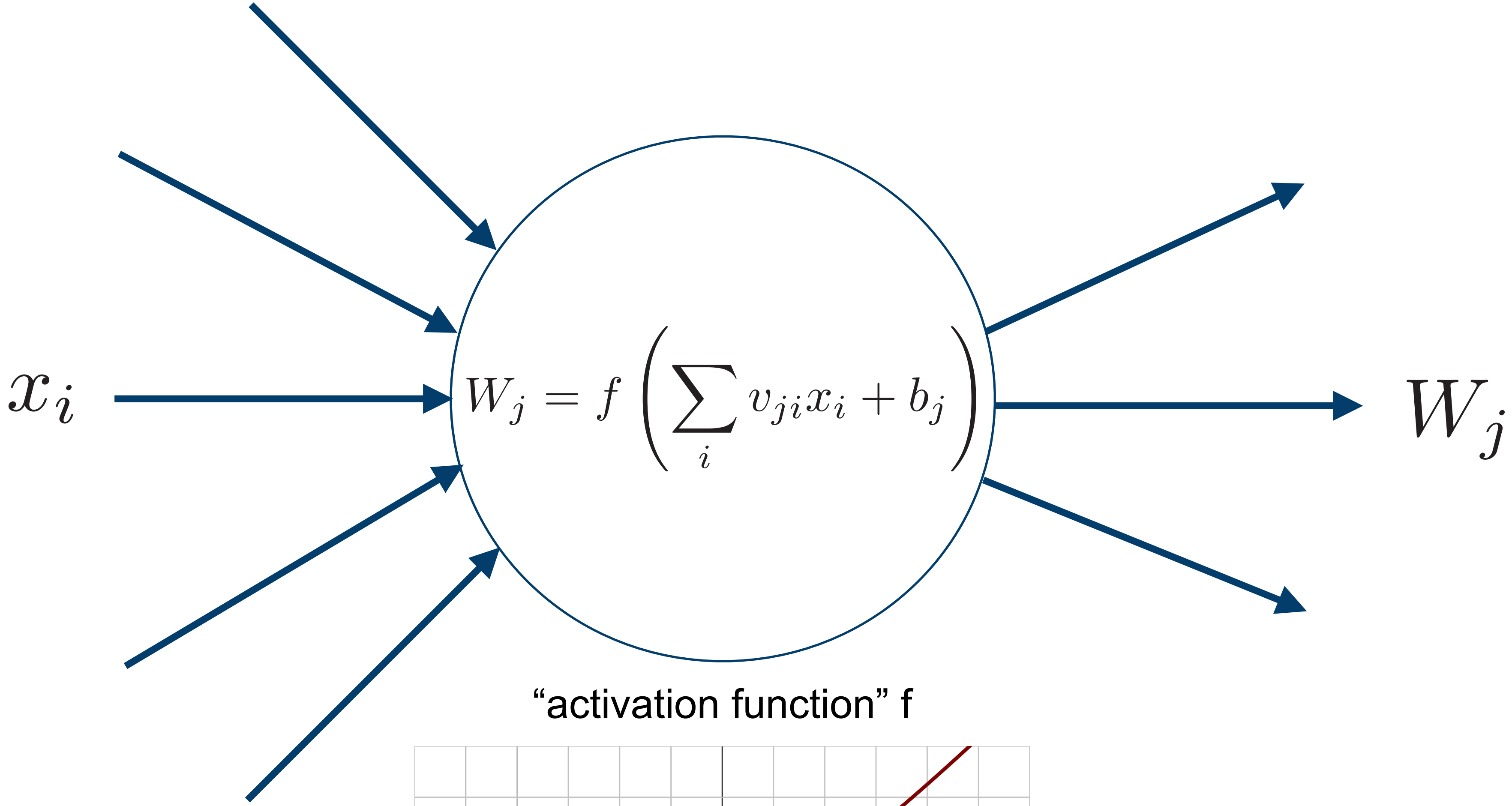
MACHINE LEARNING TO THE RESCUE!

Pushing all our ignorance into one black box called a neural network (NN)

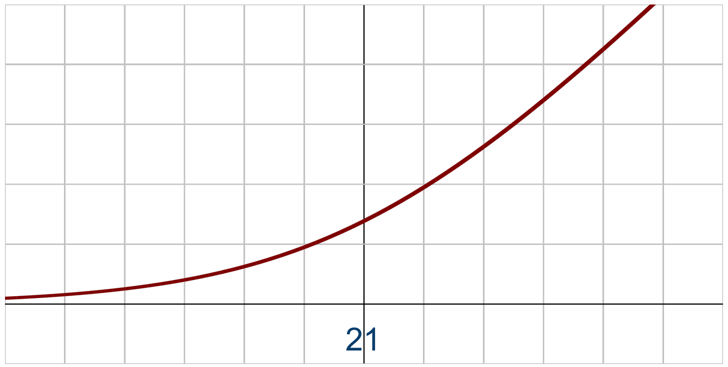


Alexandru et al., [arXiv:1709.01971] Phys.Rev. **D96** (2017) 094505

COMPOSITION OF A NEURONAL NODE



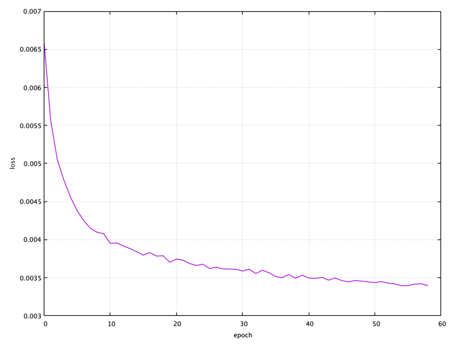
“activation function” f

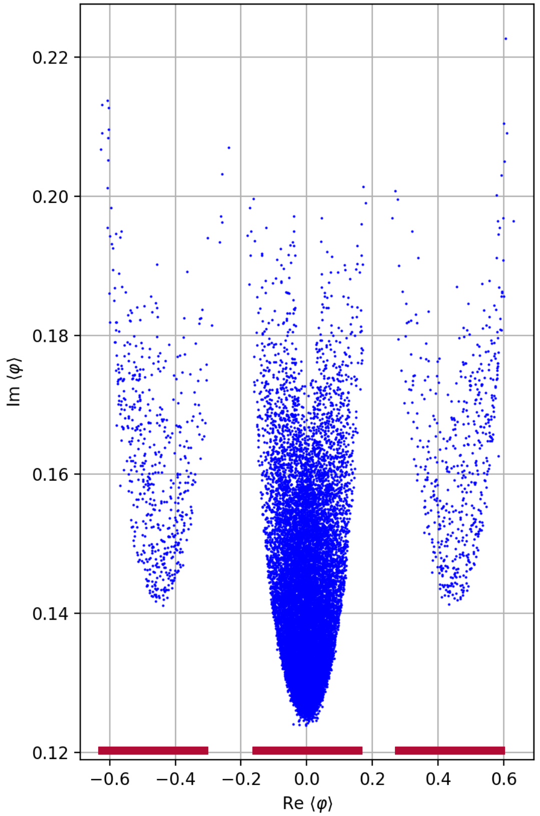


TRAINING THE NETWORK

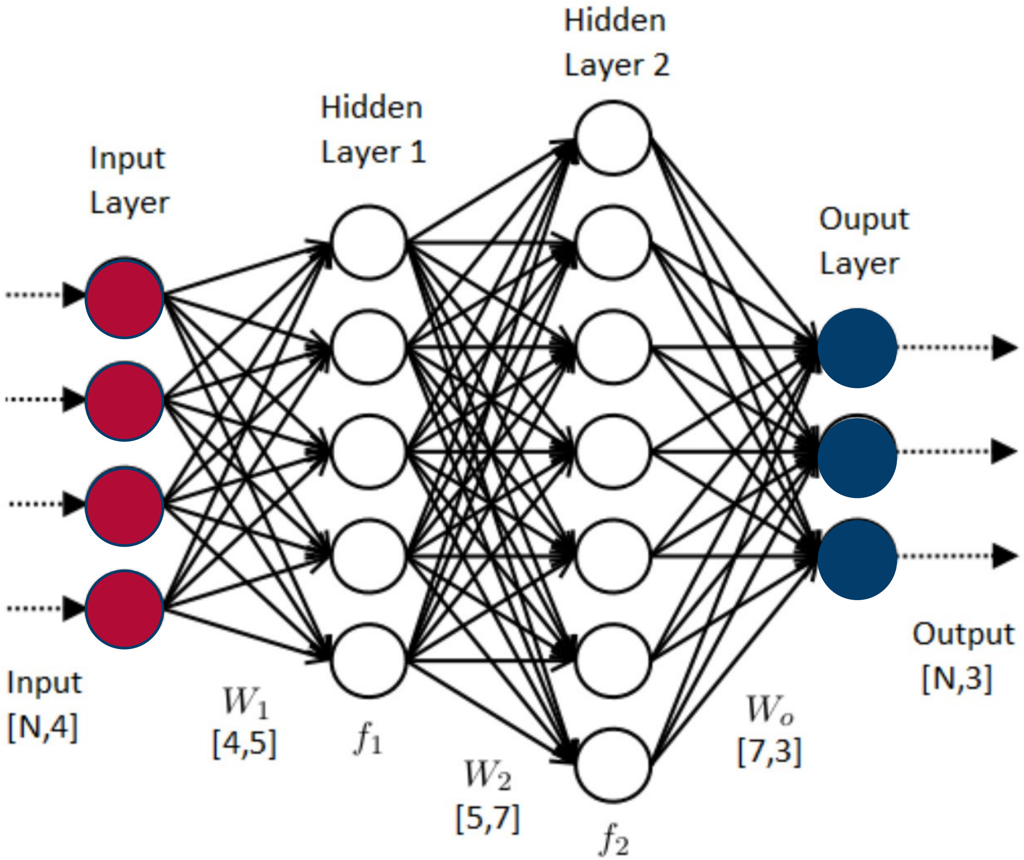
Trying to get a computer to do what you want. . .

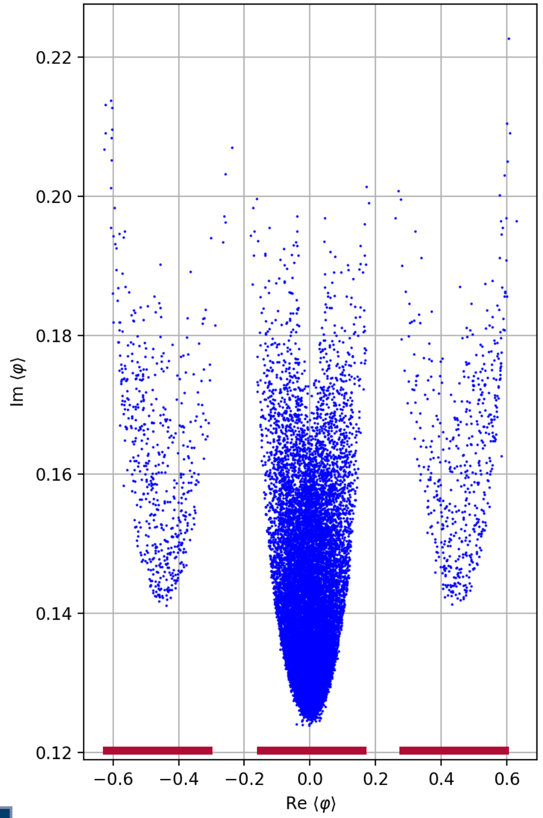
Single dense layer
“softmax” activation





training data



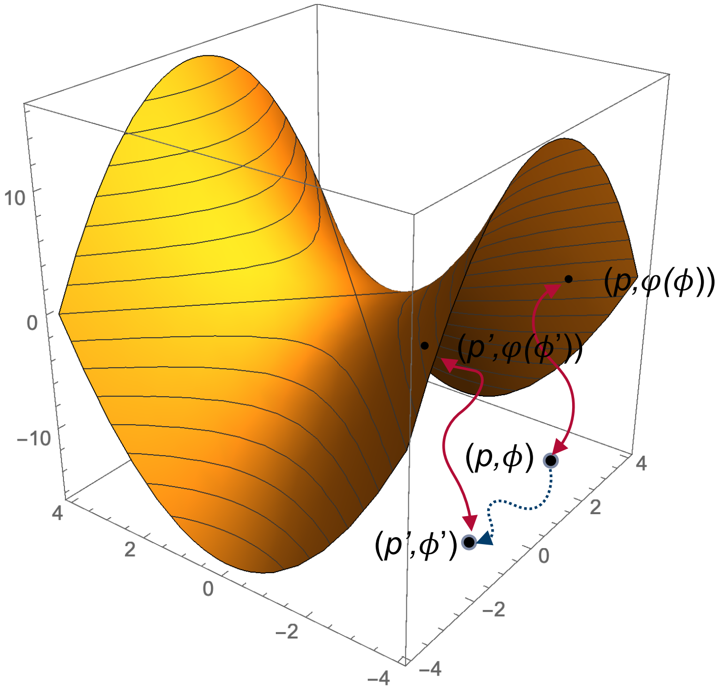


- Minimization of loss function
- Parameters tuned via stochastic gradient descent
- “Supervised training”

Alexandrou et al., [arXiv:1903.03506] unsupervised learning of phase transitions

HMC WITH NEURAL NETWORKS

- Perform HMC on the real plane to make proposal $(p,\phi) \rightarrow (p',\phi')$
- $\phi' \rightarrow$ NN $\rightarrow \varphi(\phi')$
- Accept/reject with $\mathbb{P}_{a/r} = \min\left(1, \frac{e^{-p'^2/2 - \mathrm{Re}S_{eff}[\varphi(\phi')]}}{e^{-p^2/2 - \mathrm{Re}S_{eff}[\varphi(\phi)]}}\right)$
- Reversible, satisfies detailed balance



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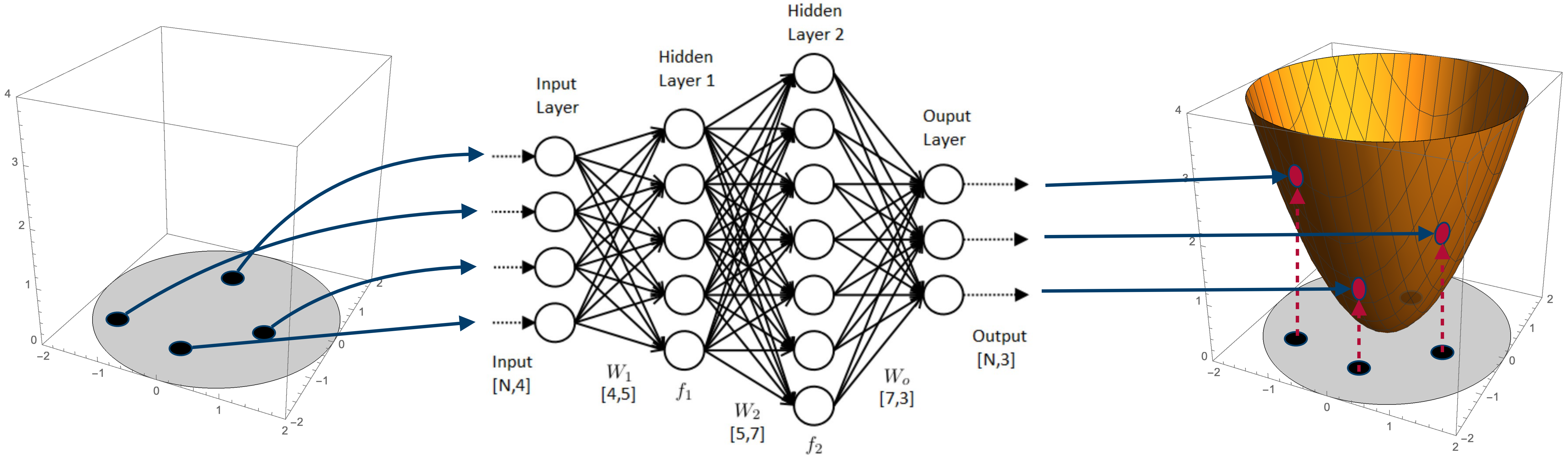
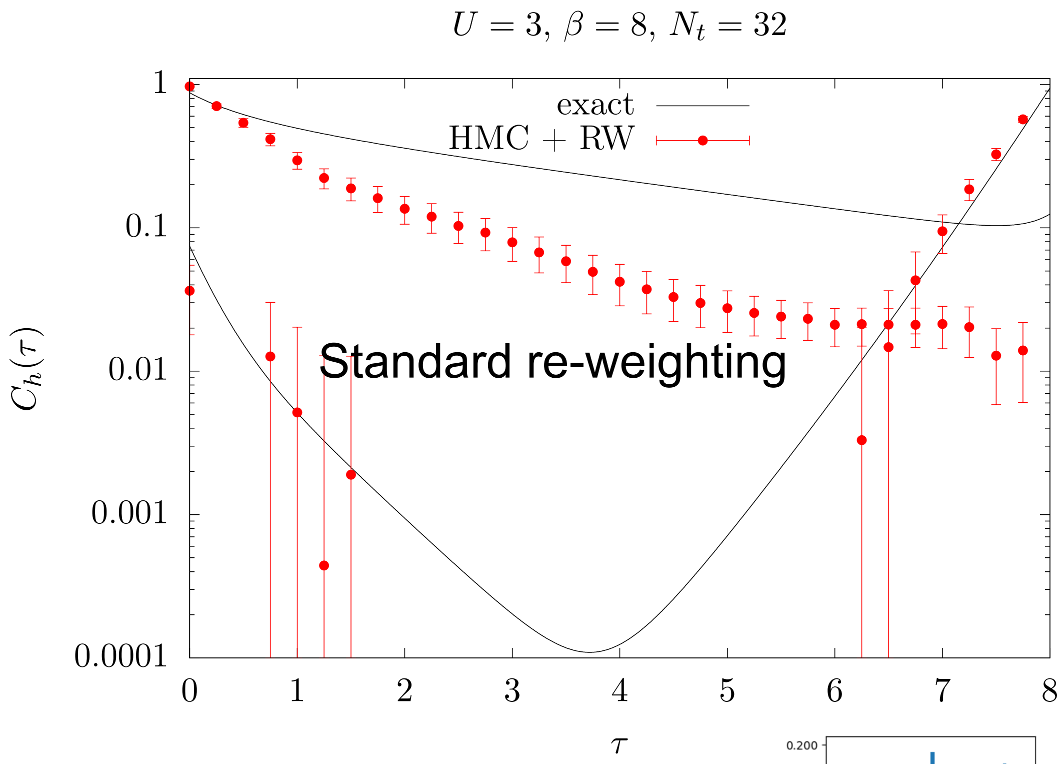
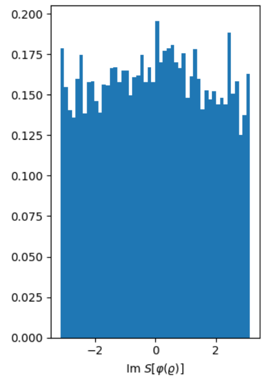
WHY IS THE NN USEFUL?

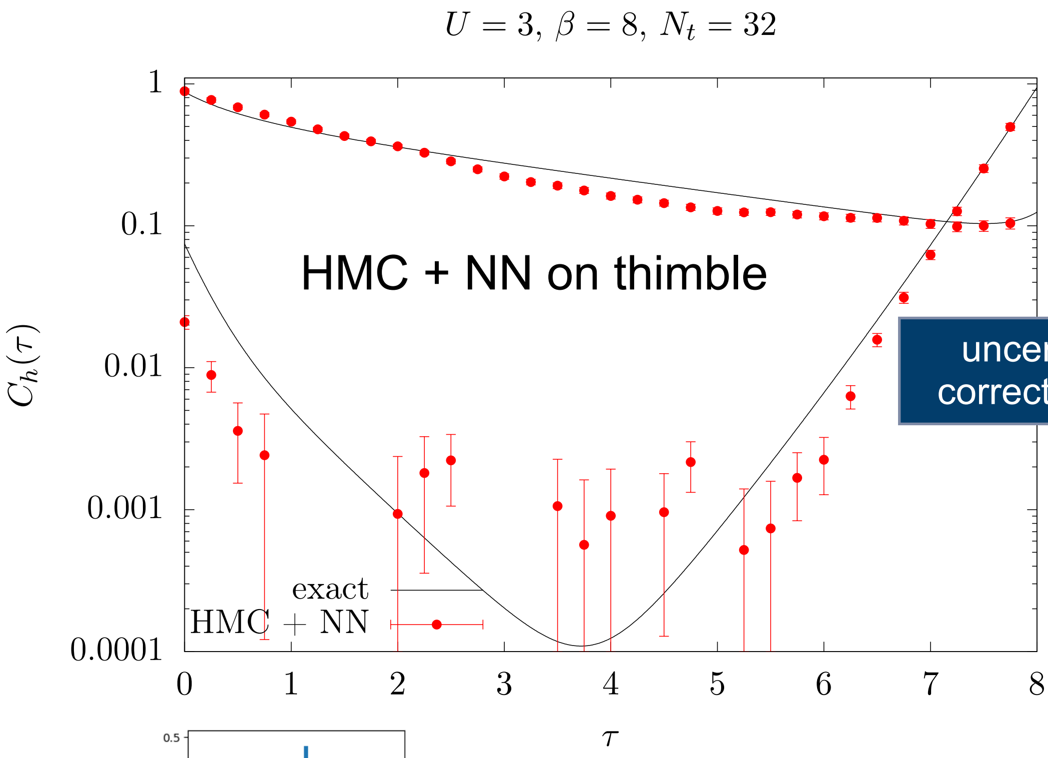


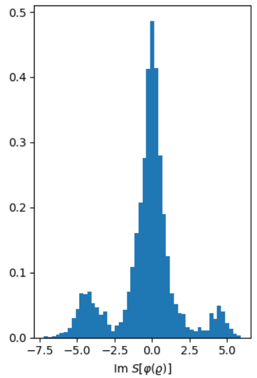
- Essentially a great big non-linear interpolation routine
  - Fast & efficient
- Calculation of Jacobian is *much* faster!
- Greatly alleviates ergodicity problem

SOME LIMITED SUCCESS SO FAR. . .





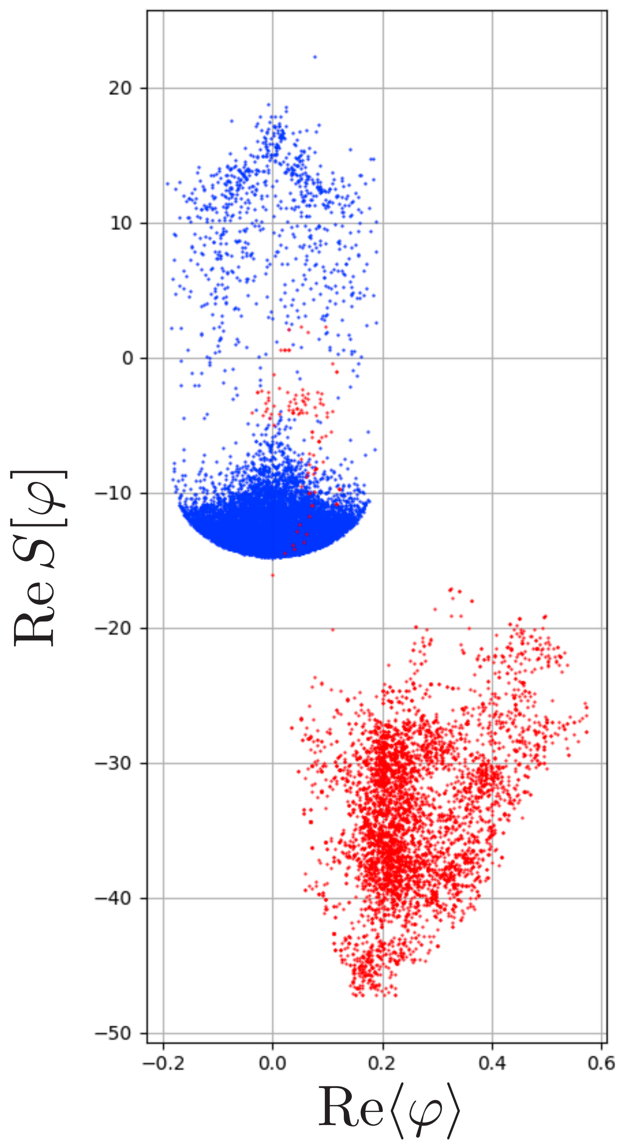




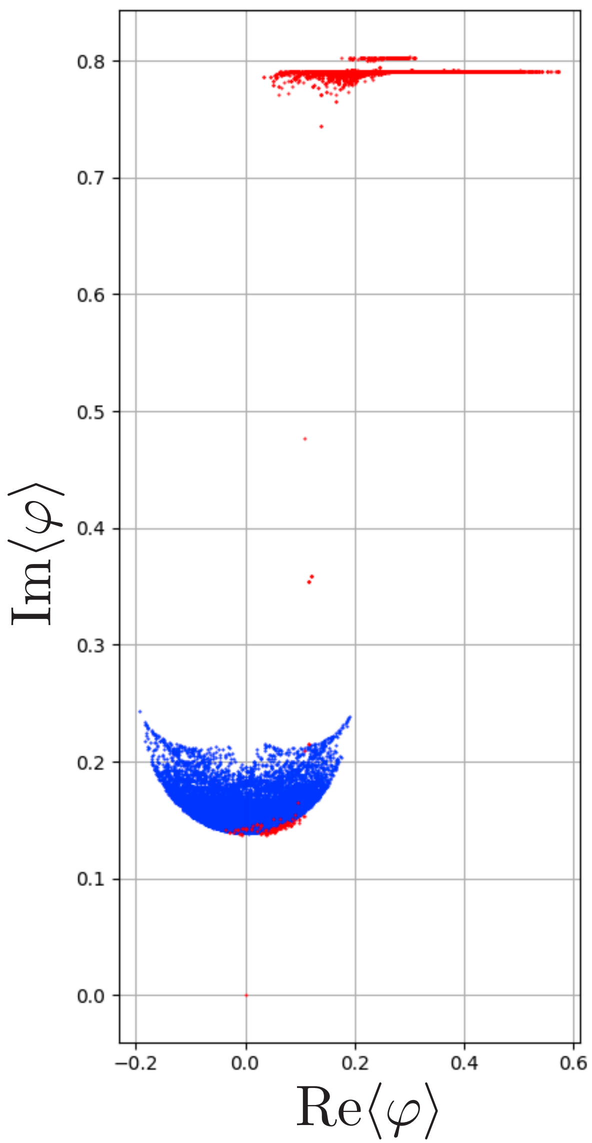
uncertainties not correctly assessed!

THE NN IS ONLY AS GOOD AS YOUR TRAINING DATA

Lessons learned so far. . .



Training data (blue)
HMC + NN run (red)



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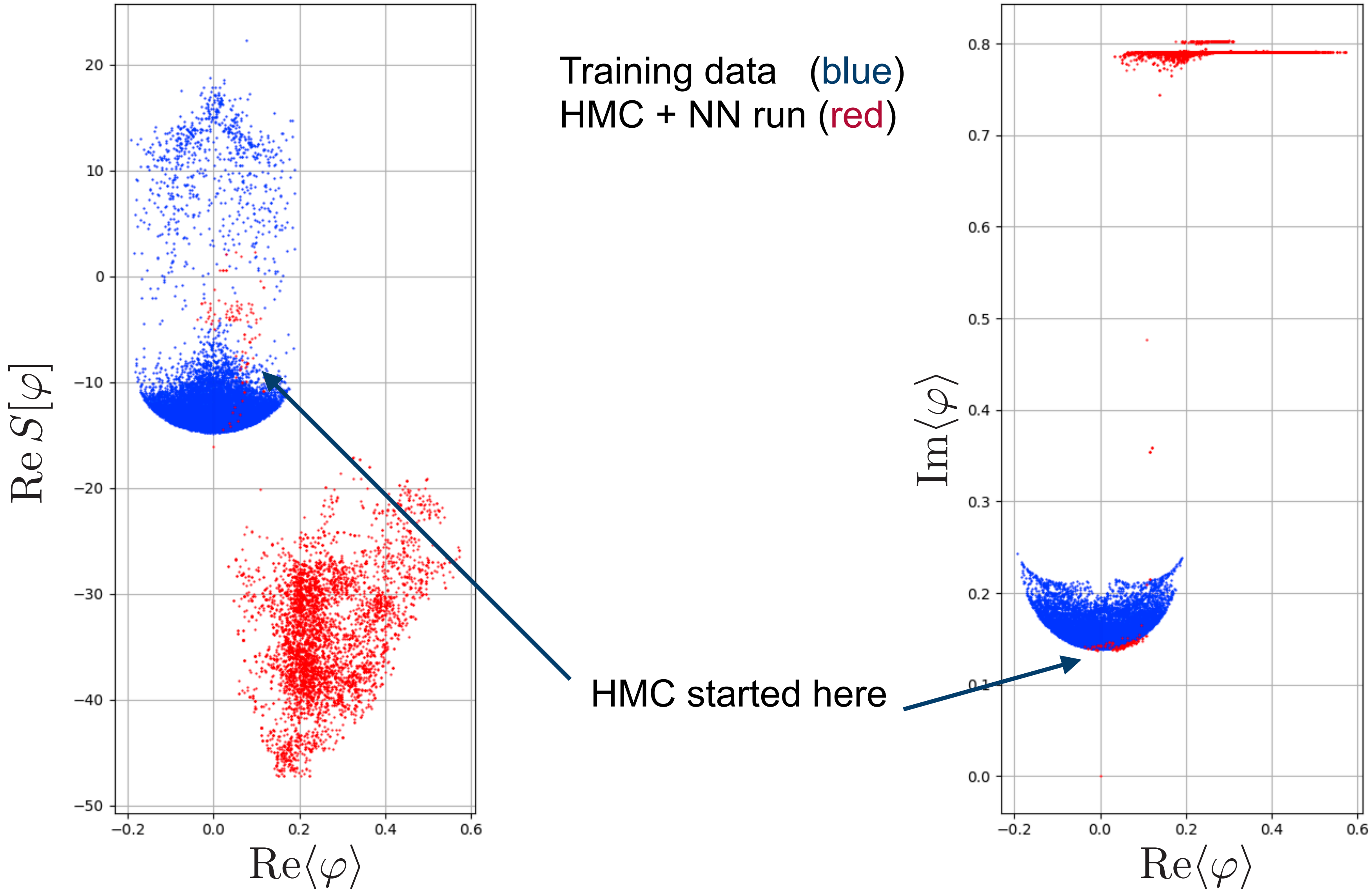

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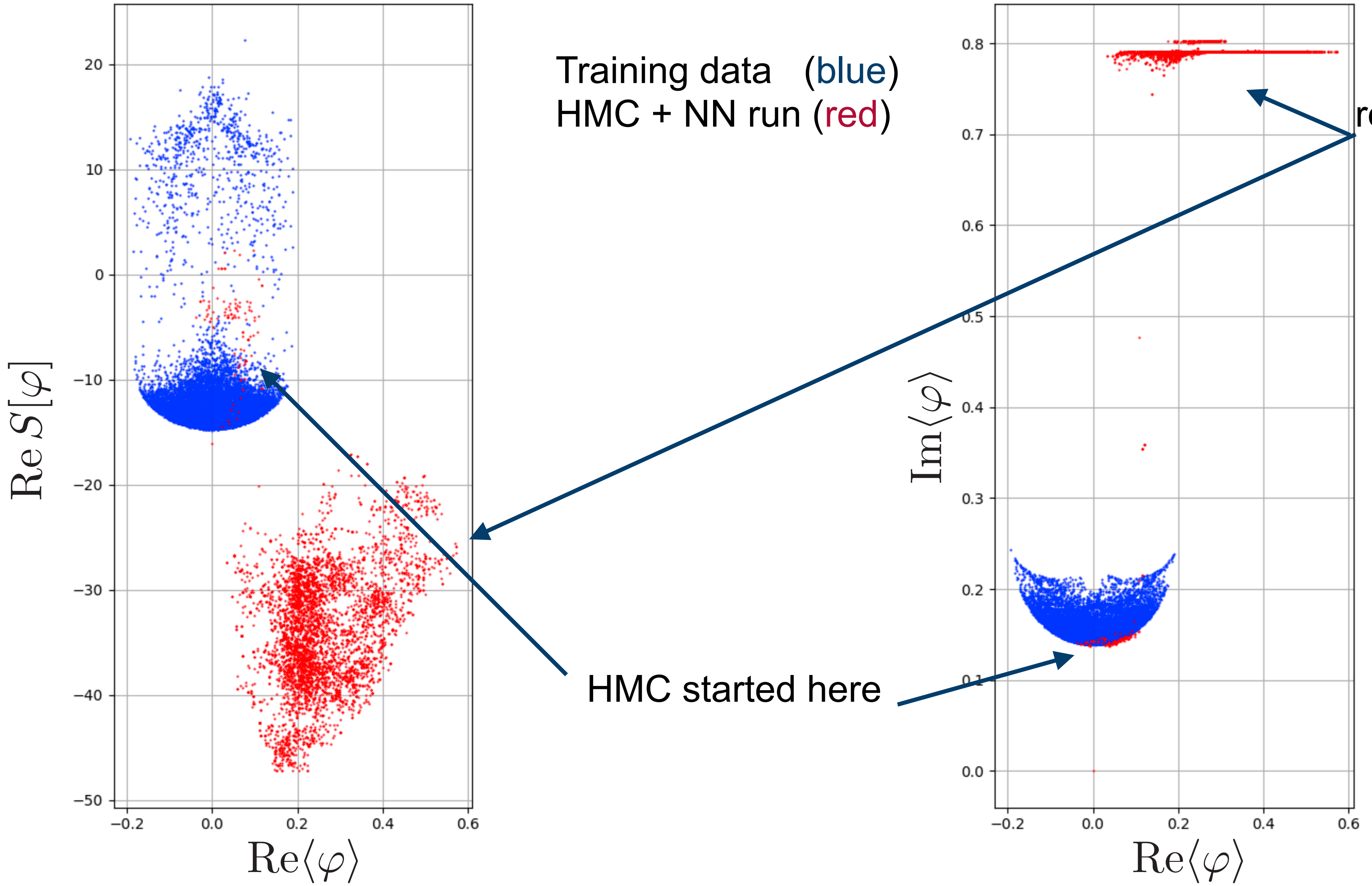

Training data (blue)
HMC + NN run (red)

HMC pushed configurations to a region well outside the training set

HMC started here

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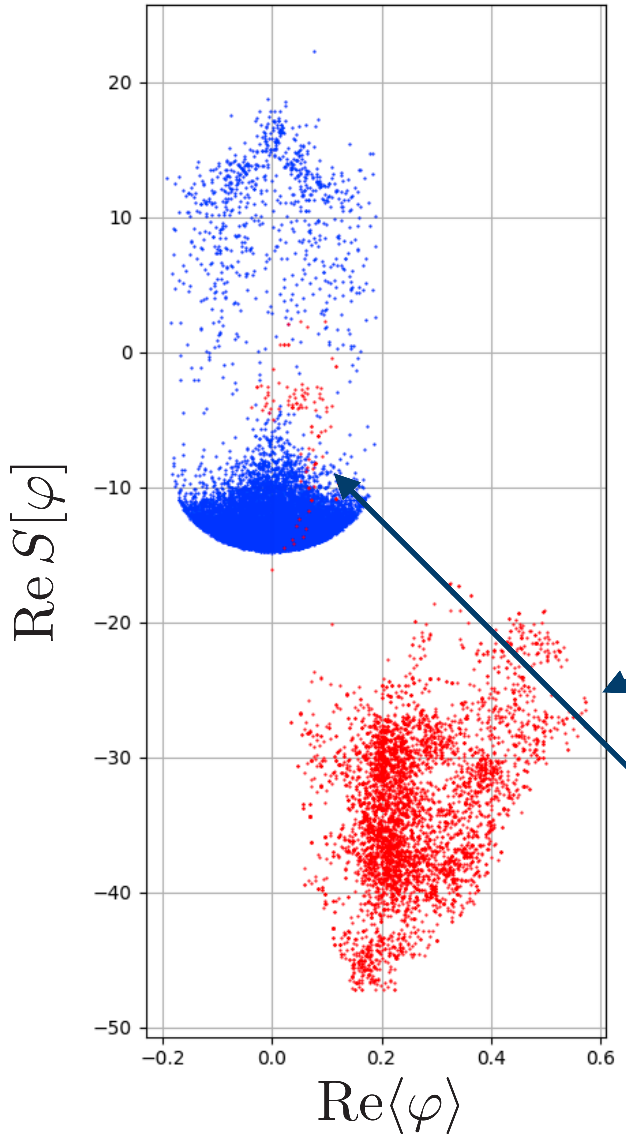
Lessons learned so far. . .



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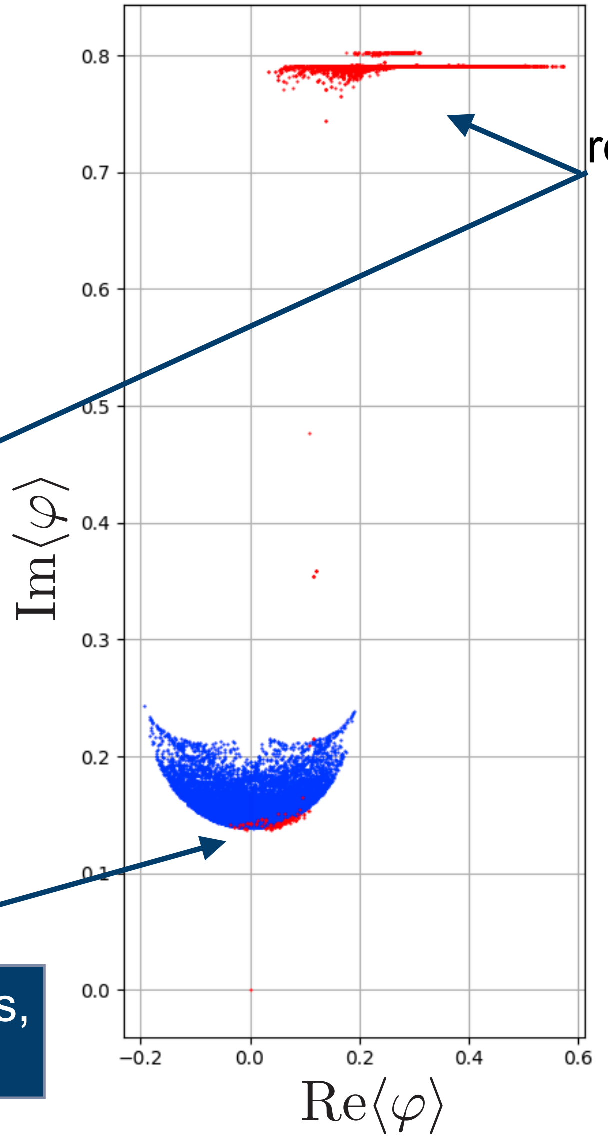

HMC pushed configurations to a region well outside the training set

HMC started here

When HMC + NN fails, it fails spectacularly!

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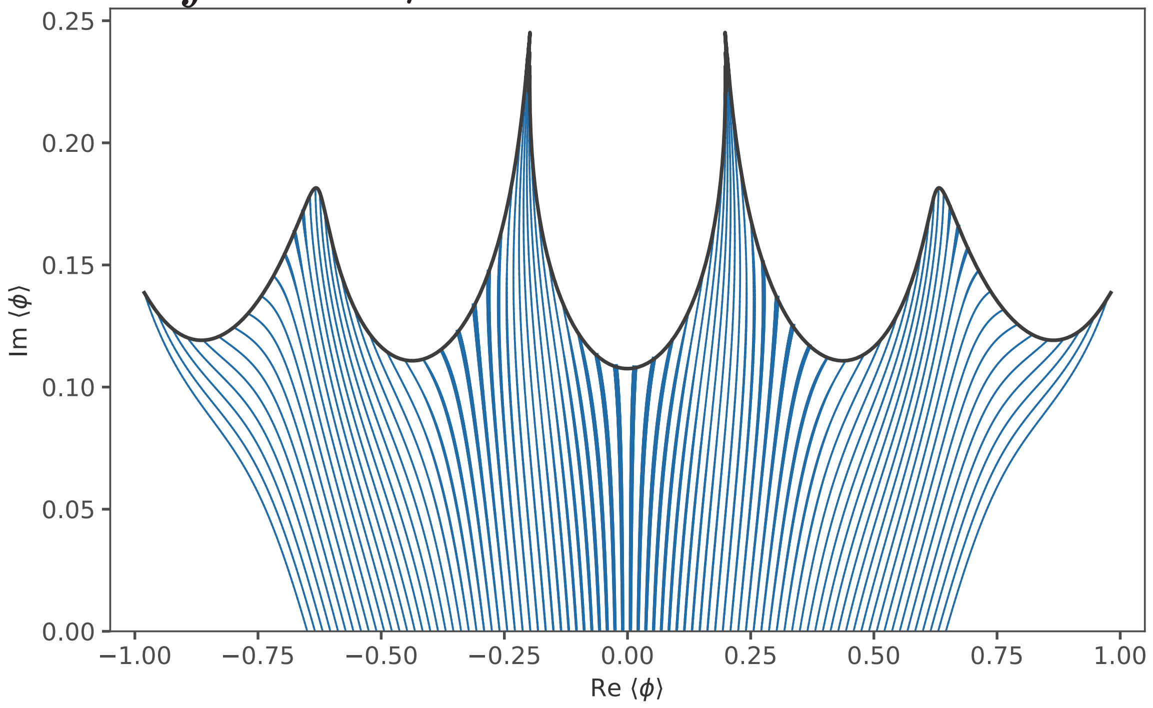
THE GOAL IS TO *ALLEVIATE* THE SIGN PROBLEM, NOT *SOLVE* IT!

Lessons learned so far. . .

$$T_f = 1/2$$



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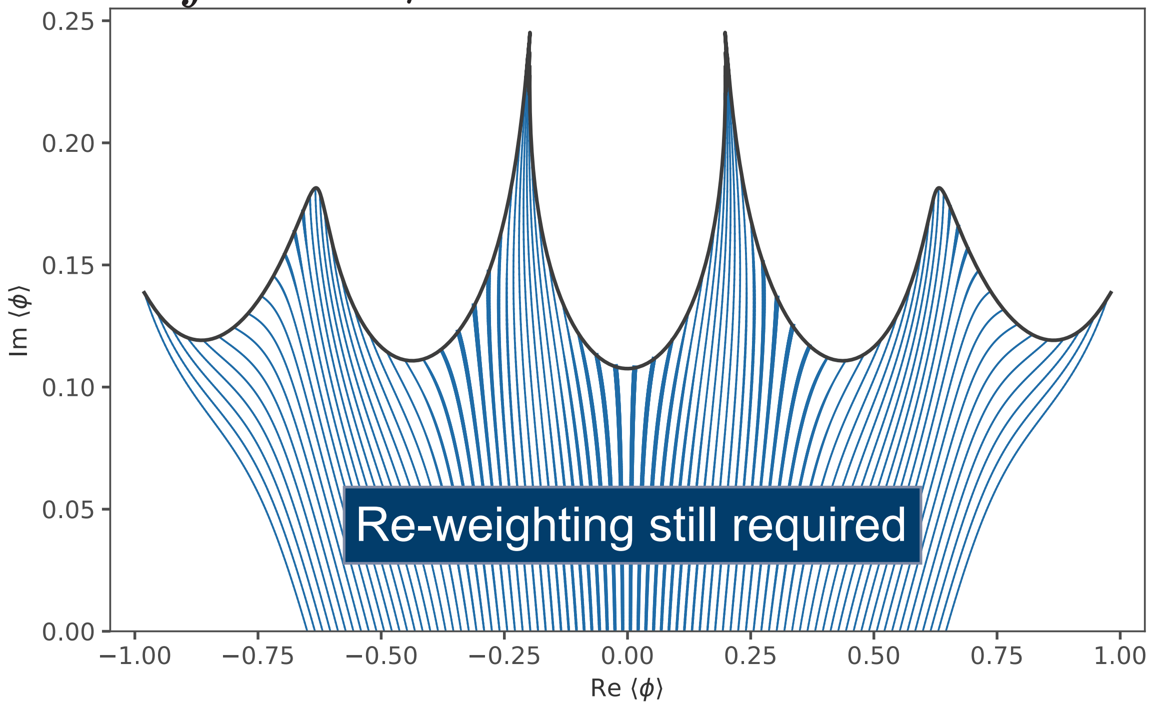

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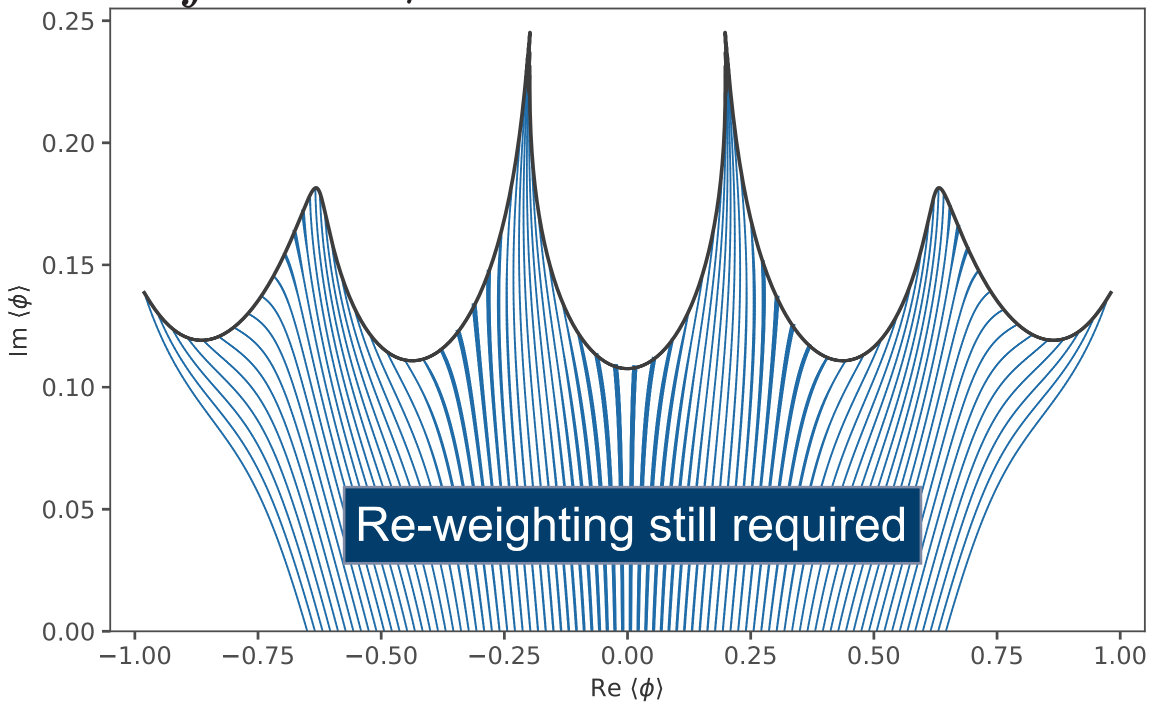
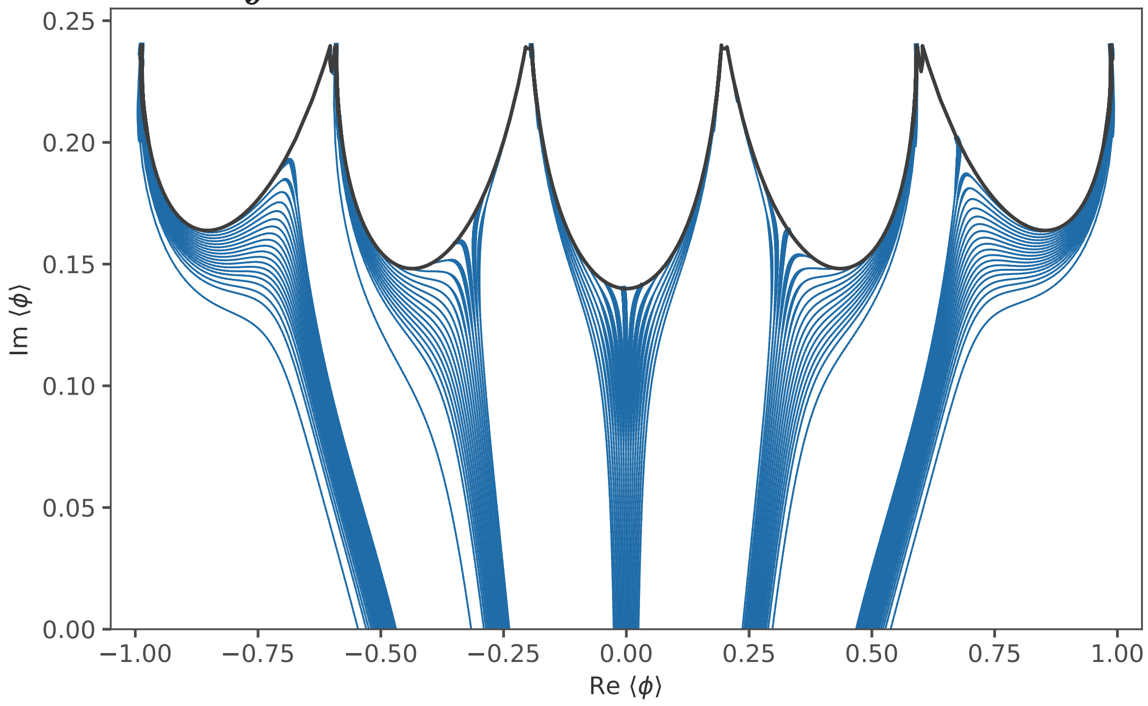


$T_f = 1$



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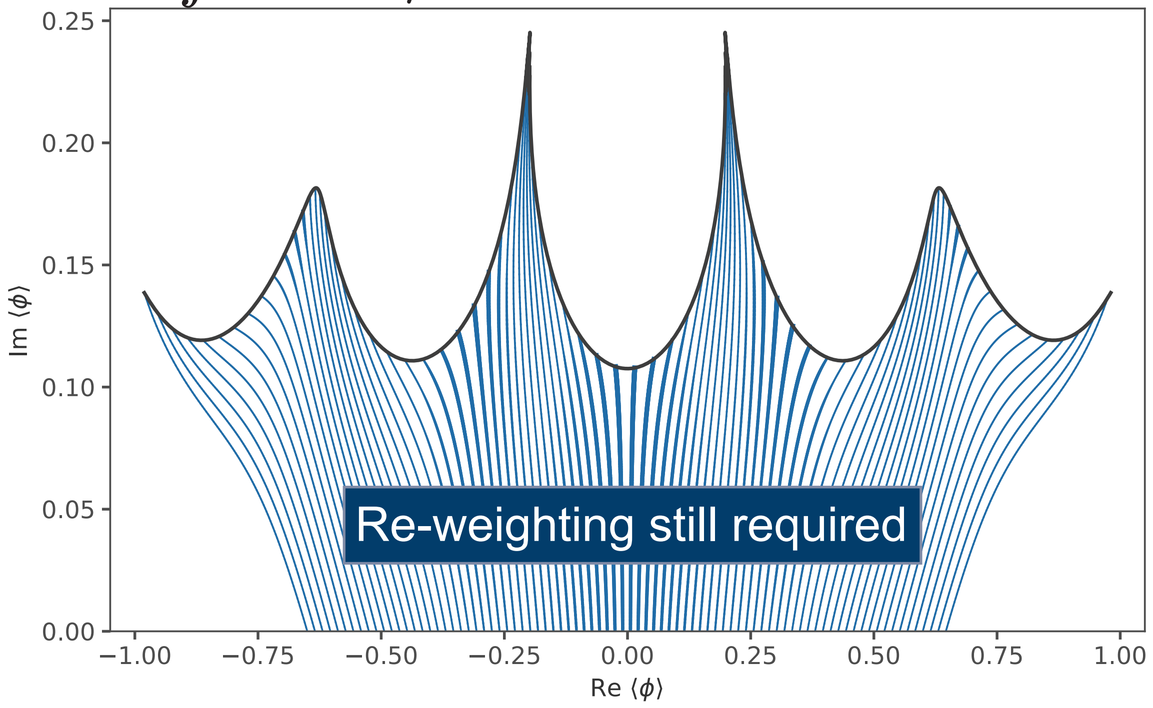

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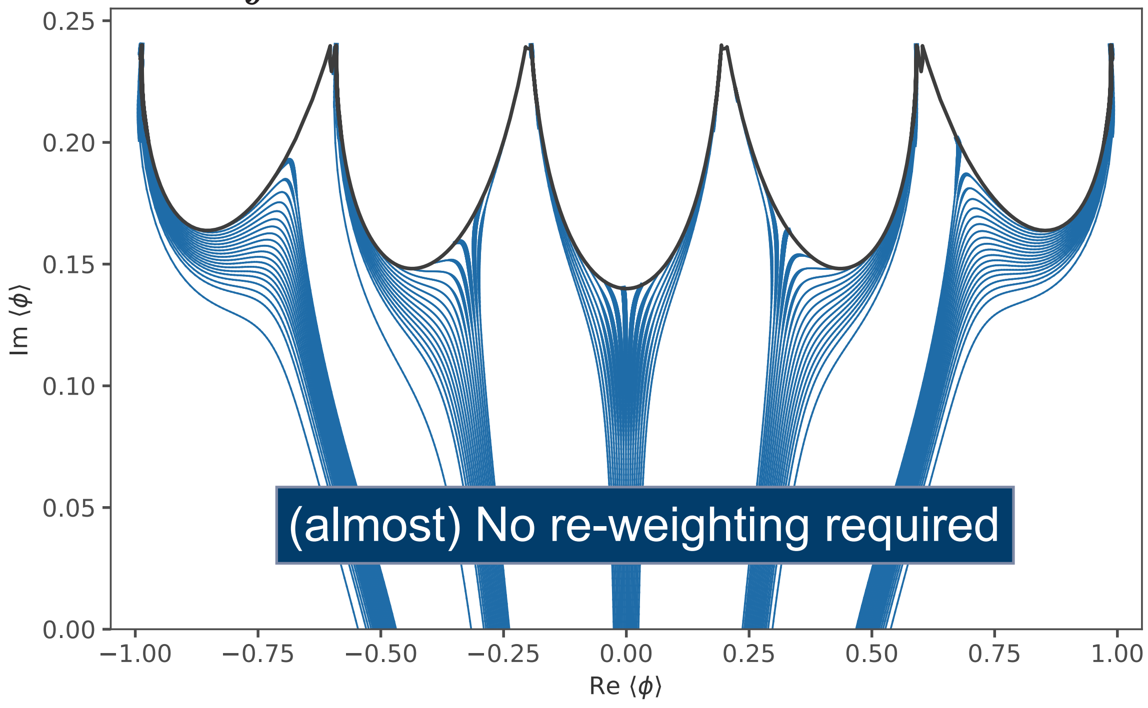

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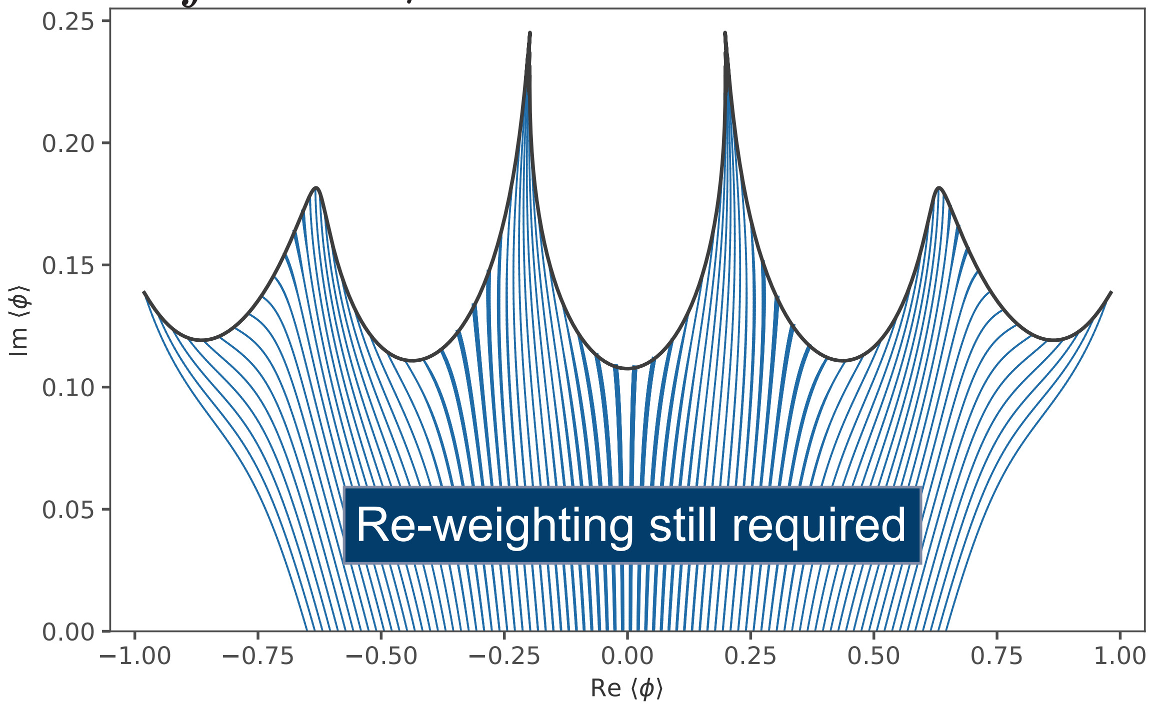
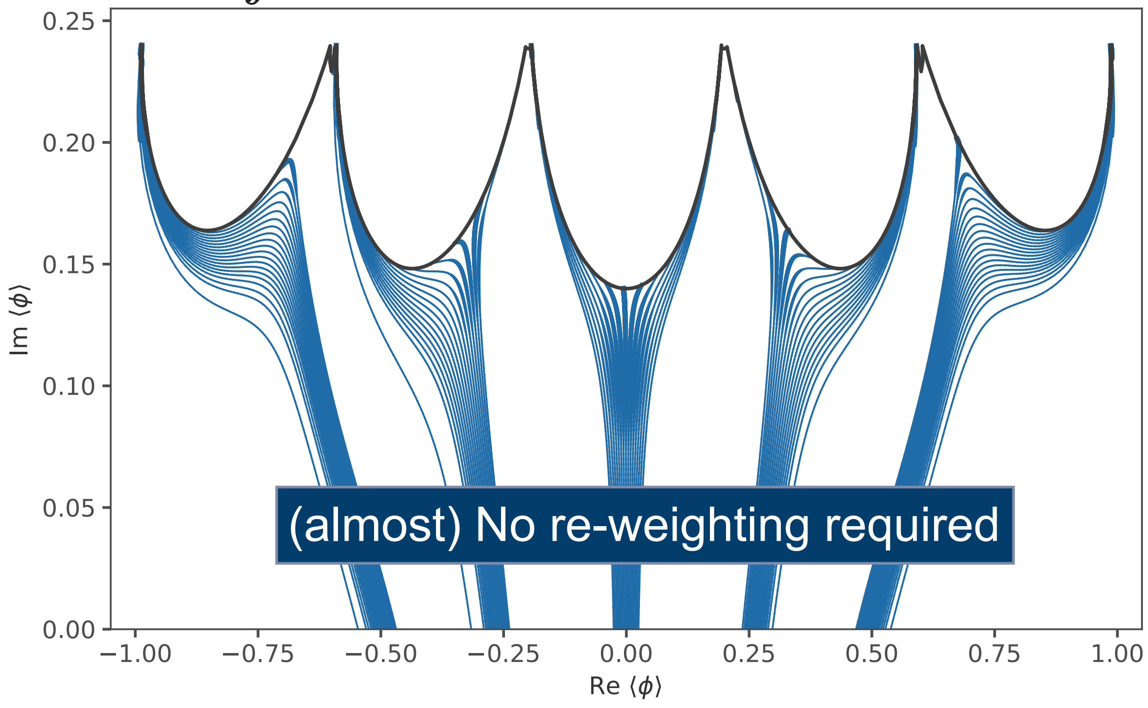


Re-weighting still required

$T_f = 1$

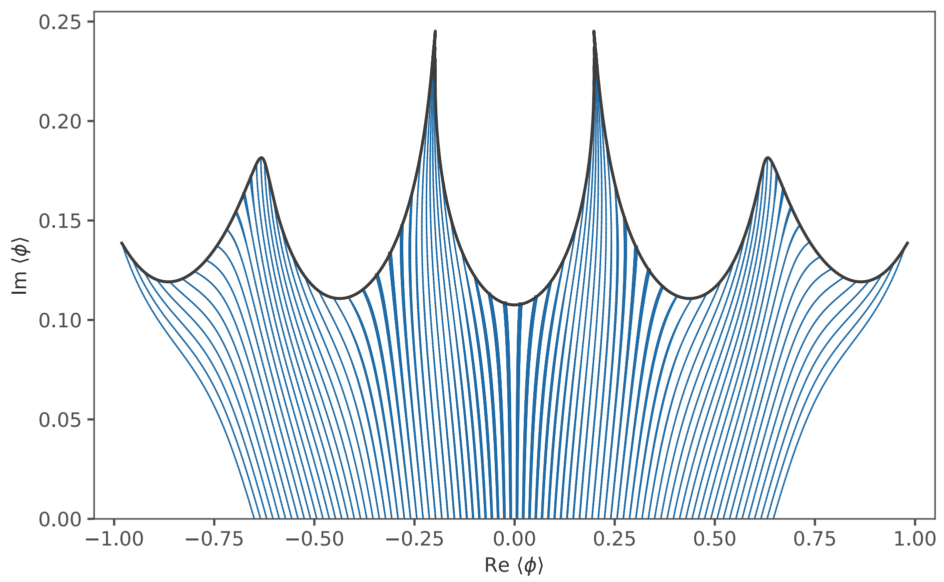


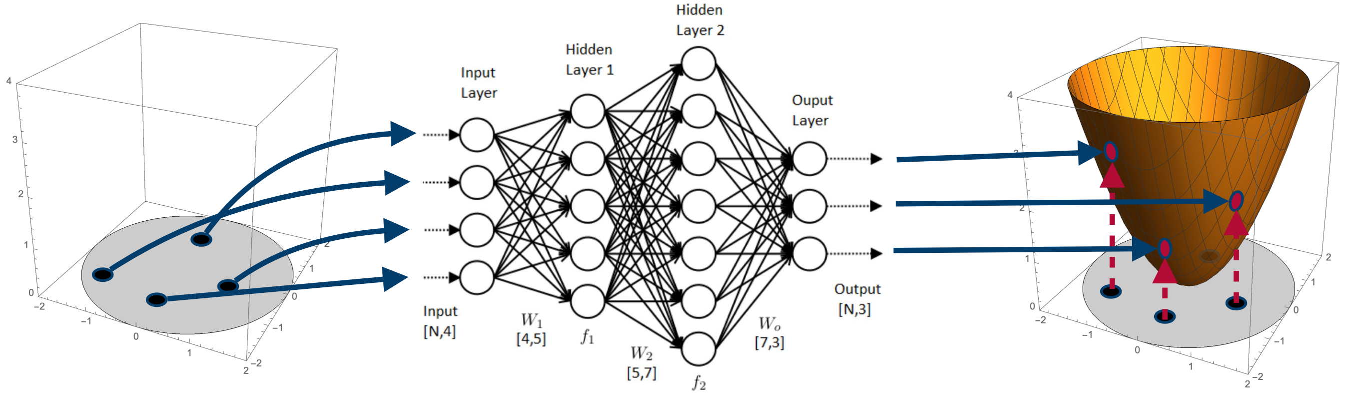
(almost) No re-weighting required

But!!! Numerically very difficult for HMC+NN to stay on the thimble

CONCLUSIONS

- Sign problem can be alleviated
  - by holomorphic flow
  - calculation of Jacobian prohibitive (numerically)
- Used NN to train location of manifolds, i.e.. ML
  - Fast/efficient interpolation routine
  - Calculation of Jacobian much faster
- Found success in simple systems, but. . .
  - Still understanding limits of ML
  - Bias/limitation of training data
- Go to larger systems, like C20, C60, doped tubes
- Ultimate goal: apply holomorphic flow to lattice gauge theories





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Thank you!

FLOW EQUATIONS

$$\phi_i = x_i + i y_i$$

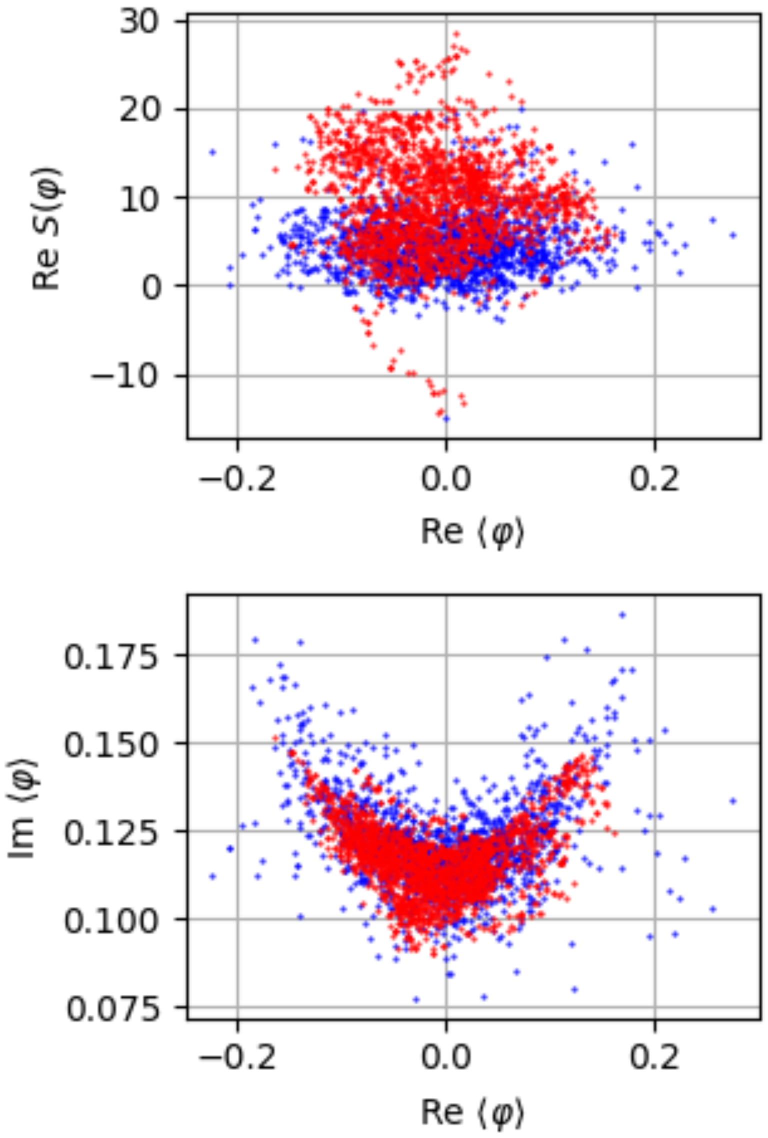
$$\dot{\phi} = -\left(\nabla_\phi S[\phi]\right)^* \implies$$

$$\frac{dx_i}{dt} = -\frac{\partial S_R}{\partial x_i} = -\frac{\partial S_I}{\partial y_i},$$

$$\frac{dy_i}{dt} = -\frac{\partial S_R}{\partial y_i} = \frac{\partial S_I}{\partial x_i}.$$

Gradient flow (heat equation)

EoM (constant of motion)



30
20
10
0
−10
Re $S(\varphi)$
−0.2
0.0
0.2
Re $\langle\varphi\rangle$
0.175
0.150
0.125
0.100
0.075
Im $\langle\varphi\rangle$
−0.2
0.0
0.2
Re $\langle\varphi\rangle$