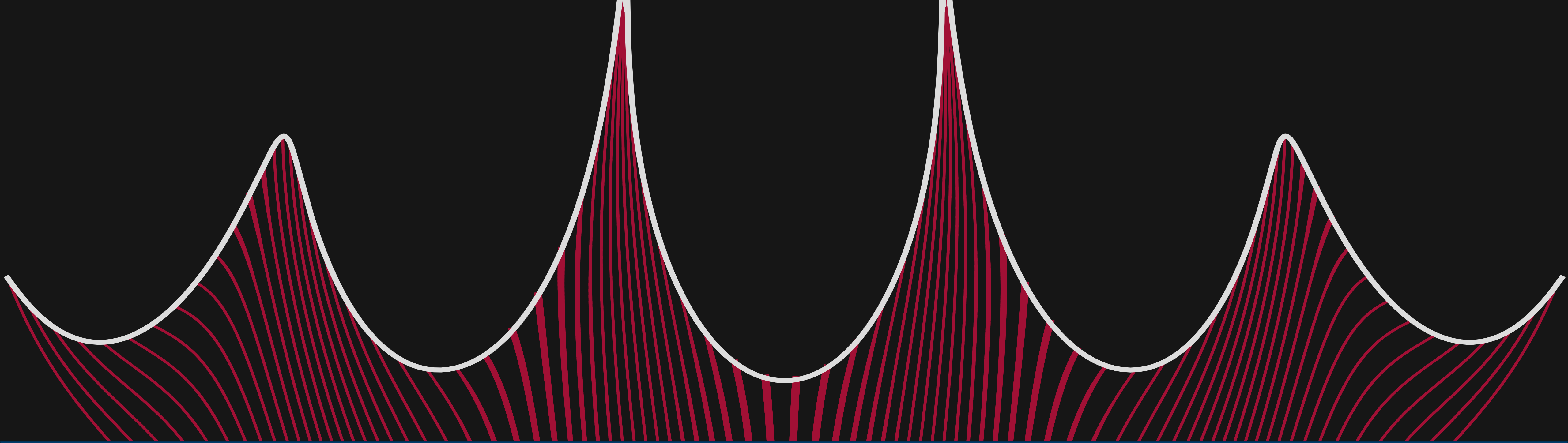

USING MACHINE LEARNING TO ALLEVIATE THE SIGN PROBLEM IN THE HUBBARD MODEL

ECT* WORKSHOP *MACHINE LEARNING FOR HIGH ENERGY PHYSICS, ON AND OFF THE LATTICE*, **09.30.2021**

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

MY PARTNERS IN CRIME . . .

Jan-Lukas Wynen

Marcel Rodekamp

Christoph Gäntgen

Evan Berkowitz

Shout outs also go to:
Chelsea John, Stefan Krieg, Timo Lähde, Johann Ostmeyer, Estela Suarez, Carsten Urbach

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 $S[\phi] = S_\mathrm{R}[\phi] + iS_\mathrm{I}[\phi]$ then $\mathbb{P}[\phi]\mathcal{D}[\phi] \notin [0, \infty)$

Question: How do we interpret such "Probabilities"?

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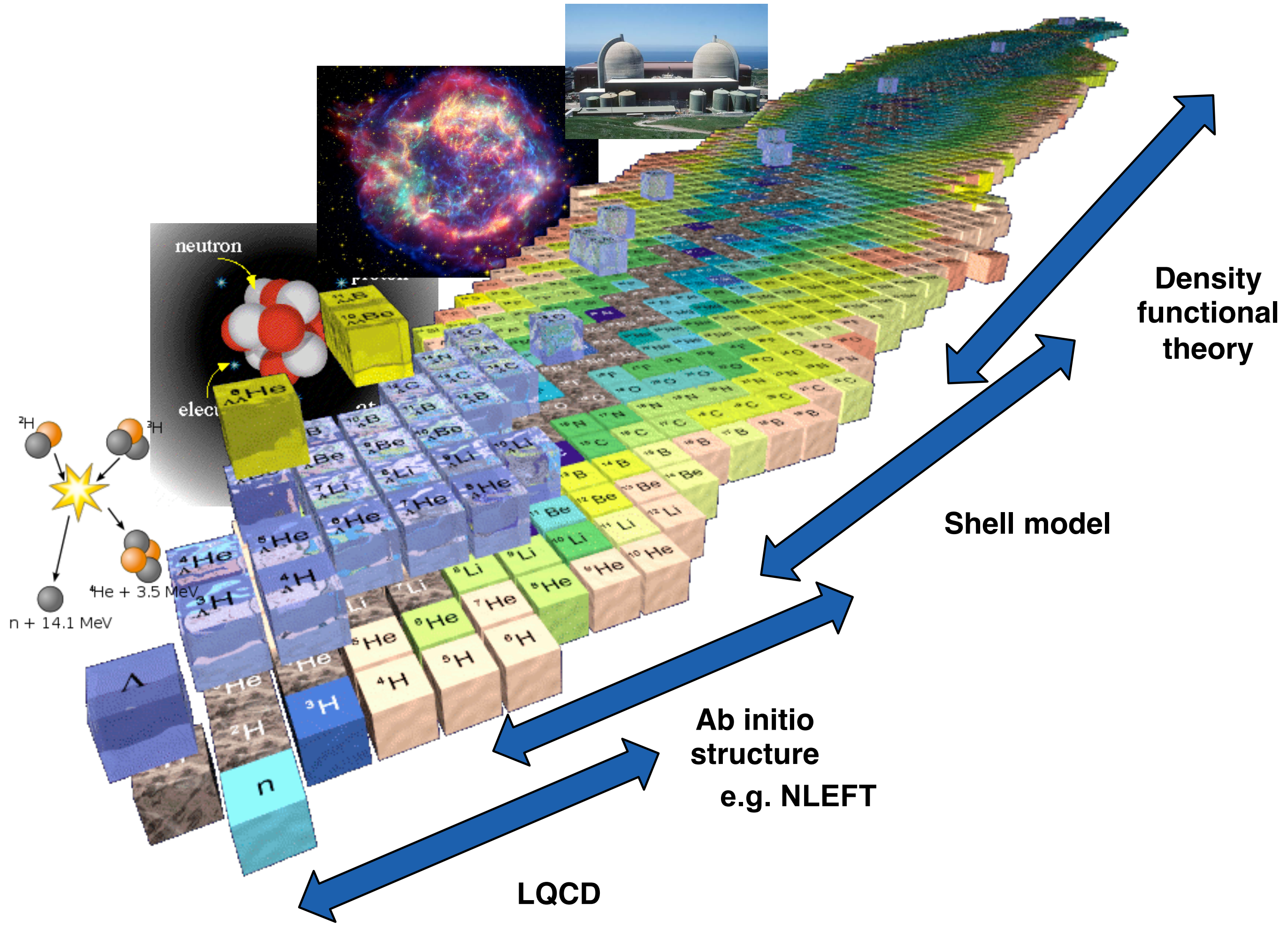
"Complex Phase sign problem"

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
- . . . and others . . .

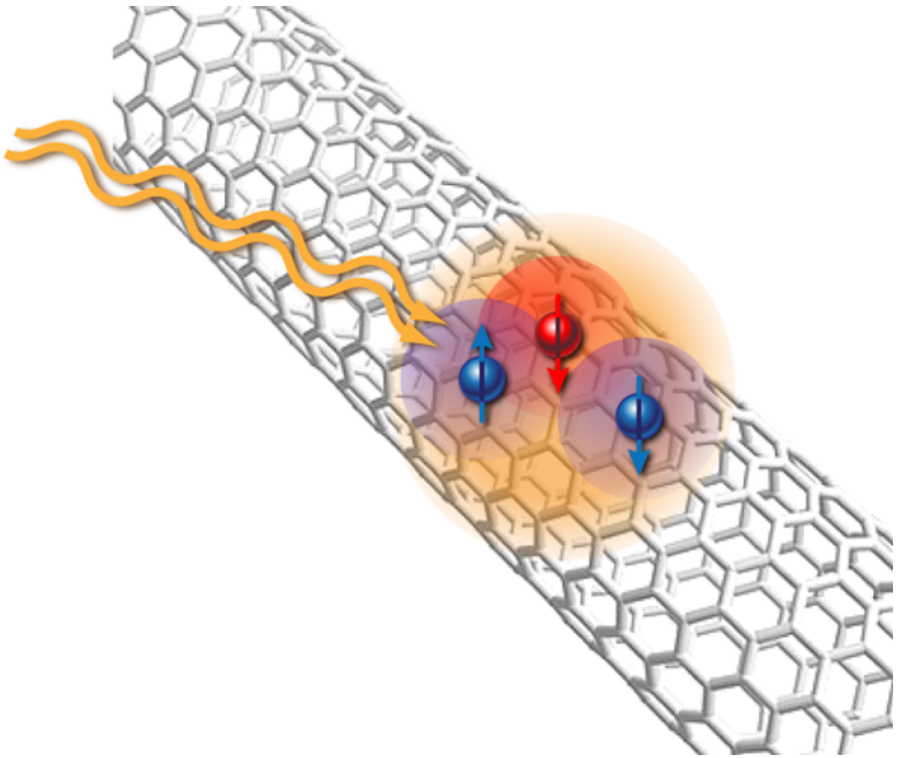


Sign problem shows up in the *most interesting problems in particle & nuclear physics!!*

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

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

- High density strongly correlated electrons
- Doped systems
  - Electron chemical potential
- Non-bipartite systems (geometry)



PATH INTEGRAL FOR THE HUBBARD MODEL

Introducing the Hamiltonian

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

$$n_x = a_x^\dagger a_x \qquad \tilde{n}_x = b_x^\dagger b_x$$

see eg., Negele & Orland, ***Quantum Many-particle Systems*** (1988)
Brower et al., [arXiv:1204.5424] PoS **LATTICE2011** (2011) 056

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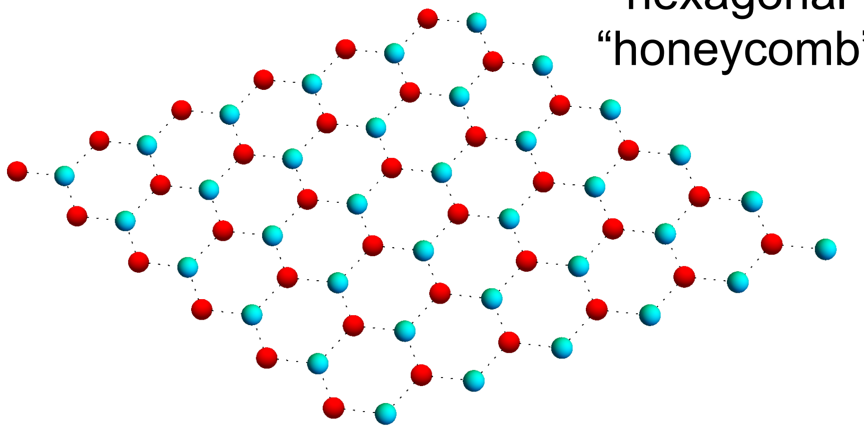
BOTH CHEMICAL POTENTIAL AND TYPE OF THE LATTICE CAN INFLUENCE THE SIGN PROBLEM

$$\mu \neq 0$$

bipartite lattice

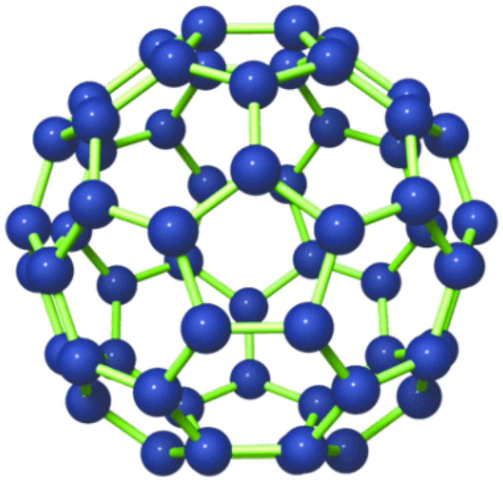


hexagonal
“honeycomb”

special feature of bipartite lattice:

$$M[-\phi, -\kappa, \mu = 0] = M^{\dagger}[\phi, \kappa, \mu = 0]$$

non-bipartite lattice



C60
“soccer ball”

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

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- Re-weighting
  - Bad with small statistical power

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      - see eg, J. Dragos, **TL**, et al. arXiv:1902.03254

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Holomorphic flow (Lefschetz Thimbles)
The subject of this talk. . .

Kanazawa & Tanizaki [arXiv:1412.2802]

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

LEFSCHETZ THIMBLE PRIMER 101

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

$$\int_{\phi\in\mathbb{R}^N} \mathscr{D}[\phi]e^{-S[\phi]}$$

flow equations

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

- critical points $\nabla S[\phi_{cr}] = 0$
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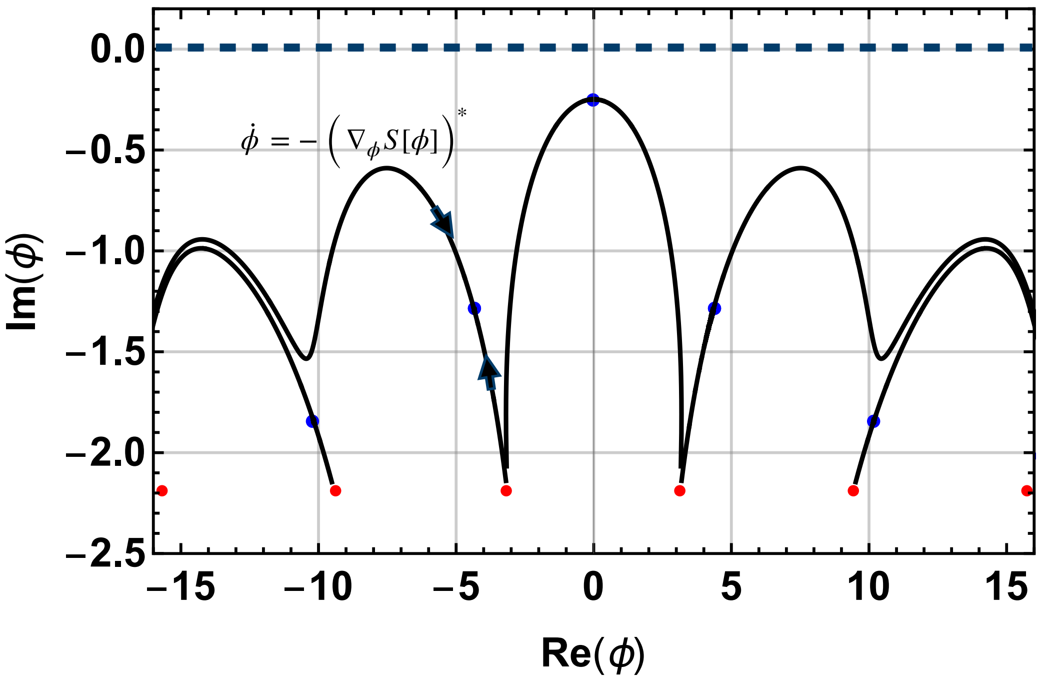

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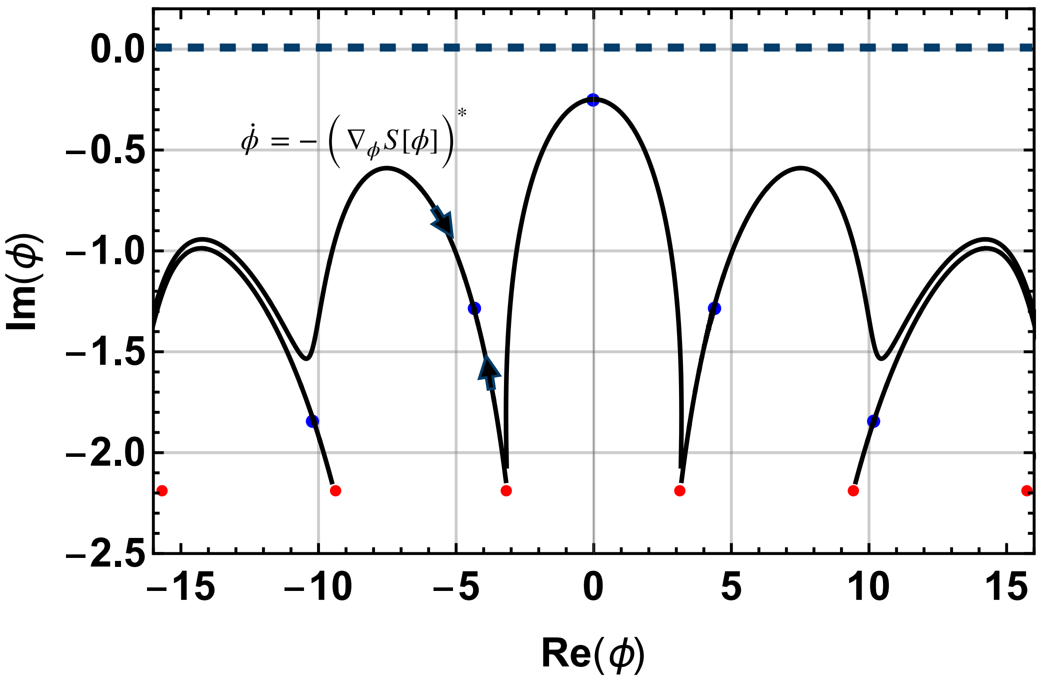

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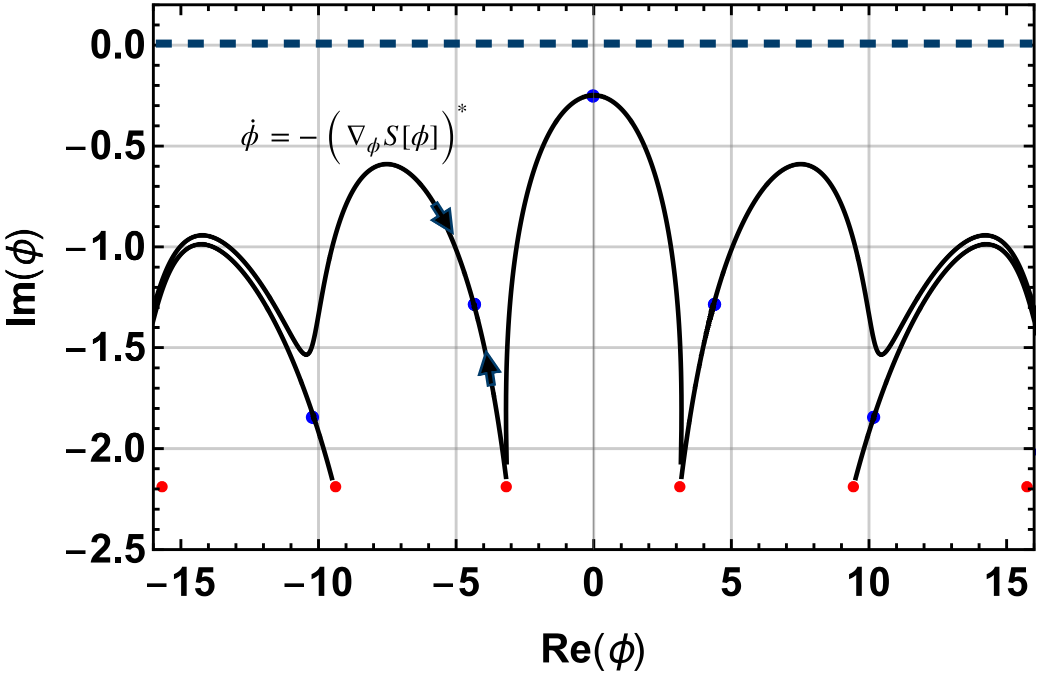

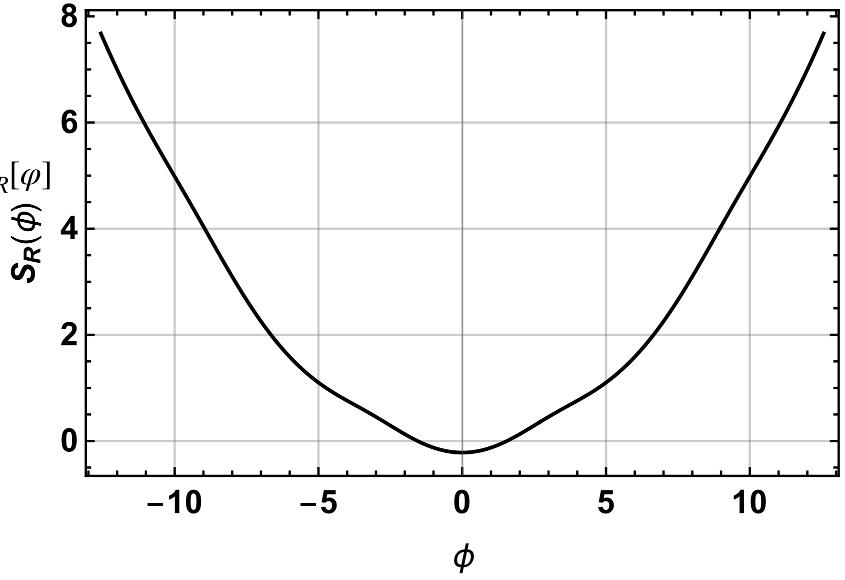

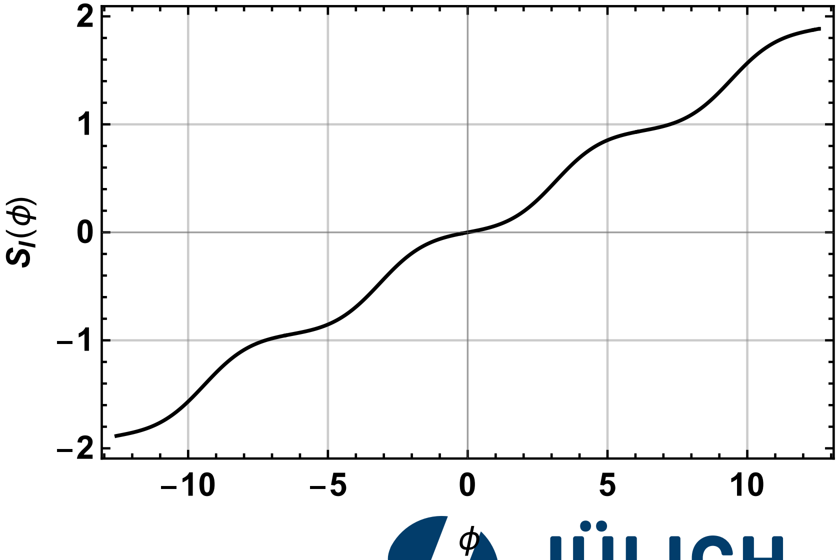

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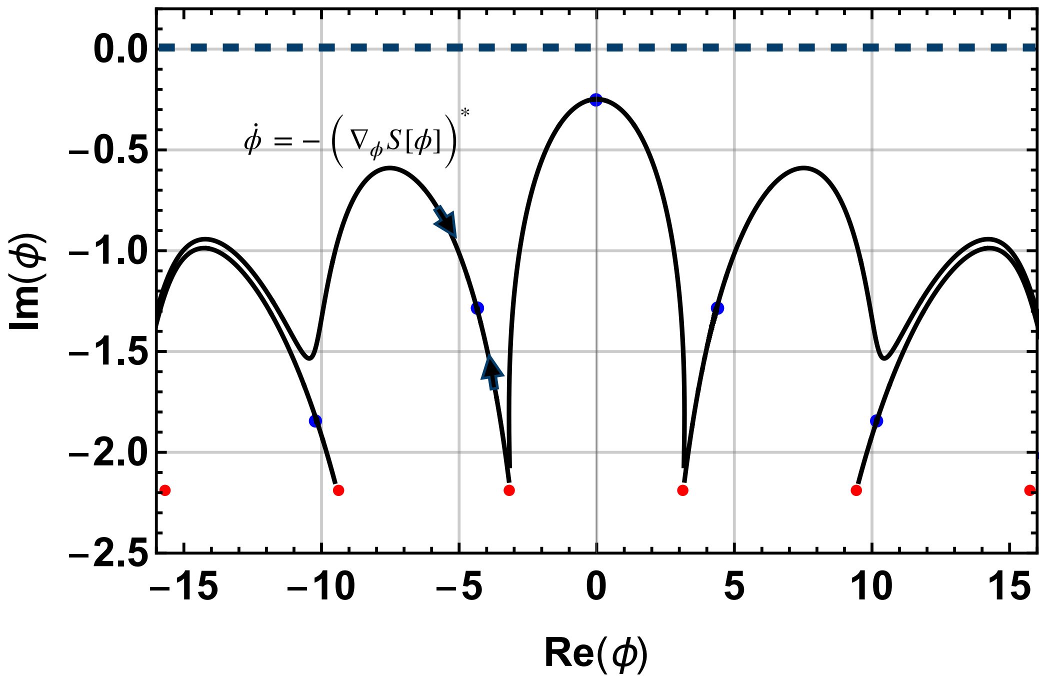

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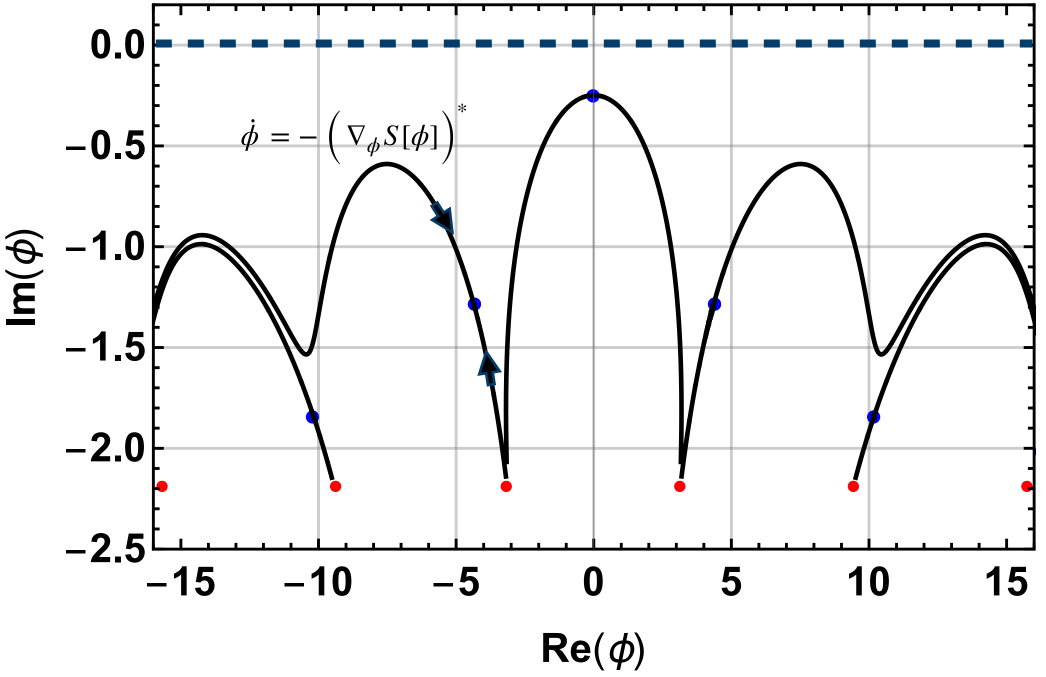

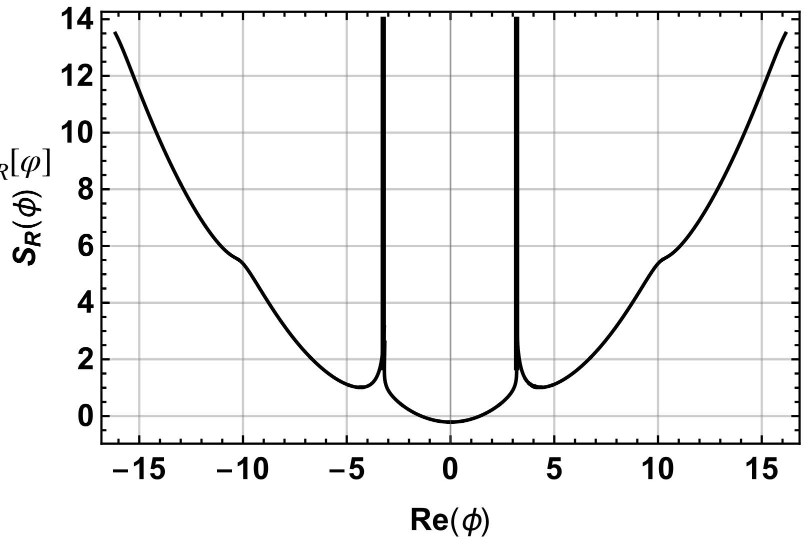

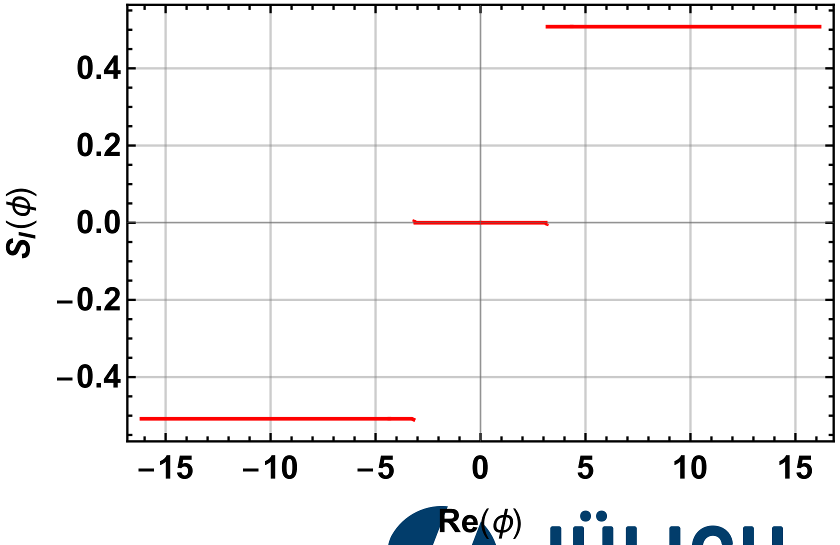

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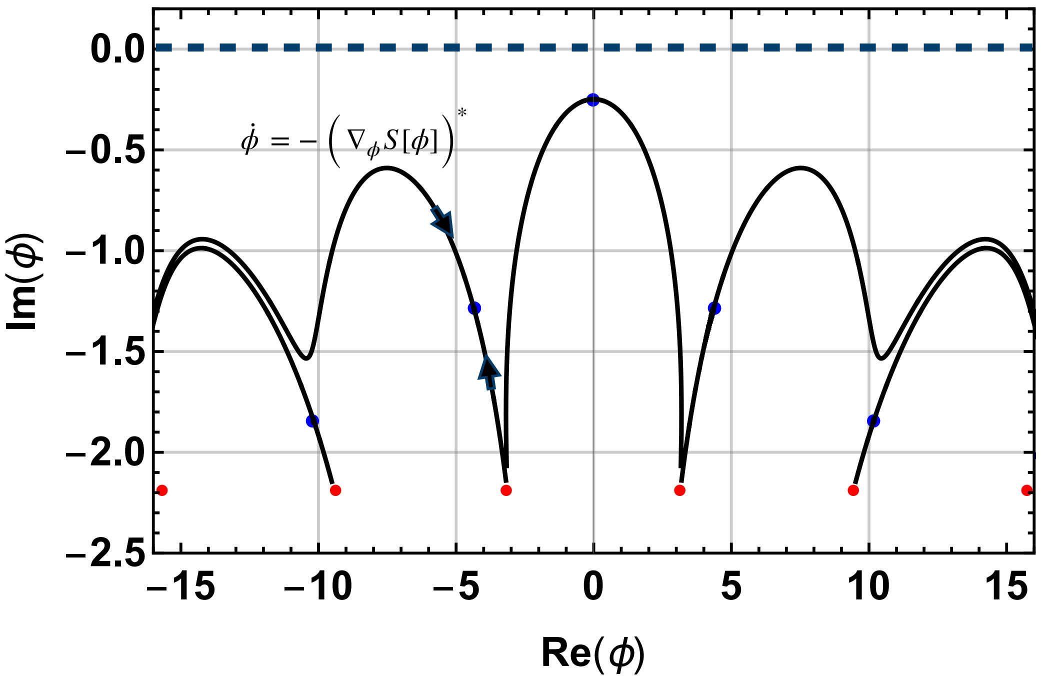
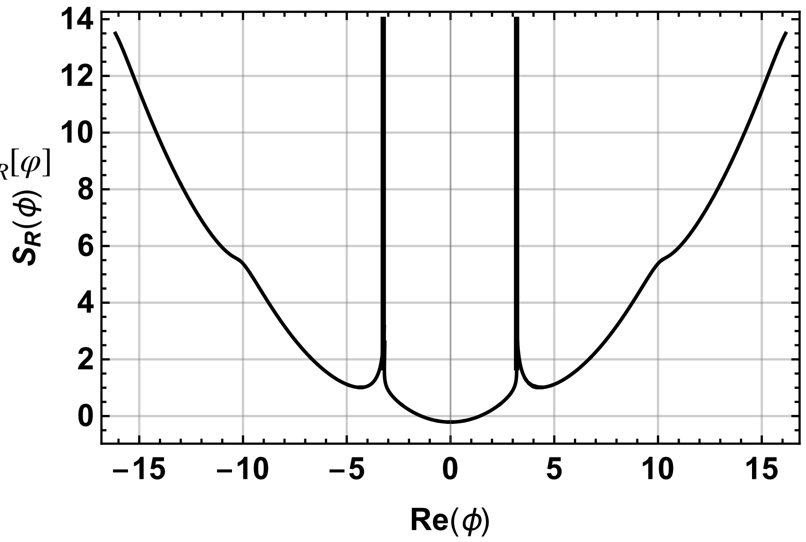
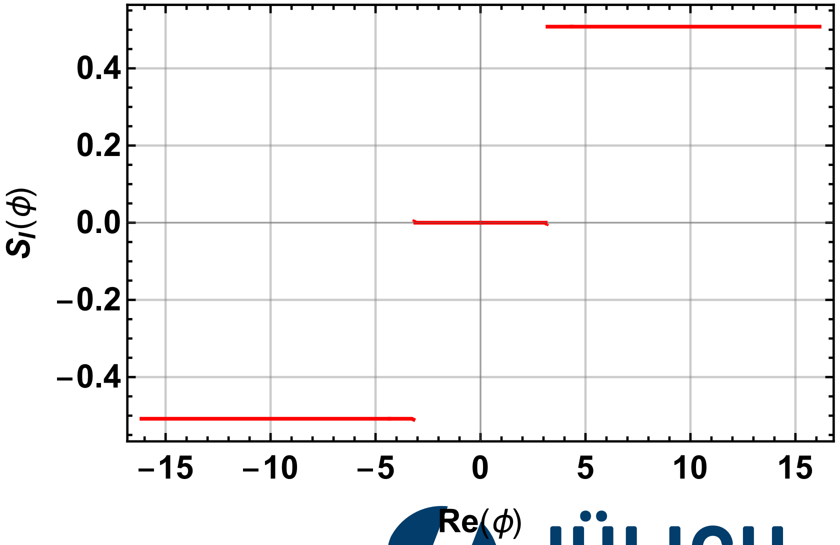


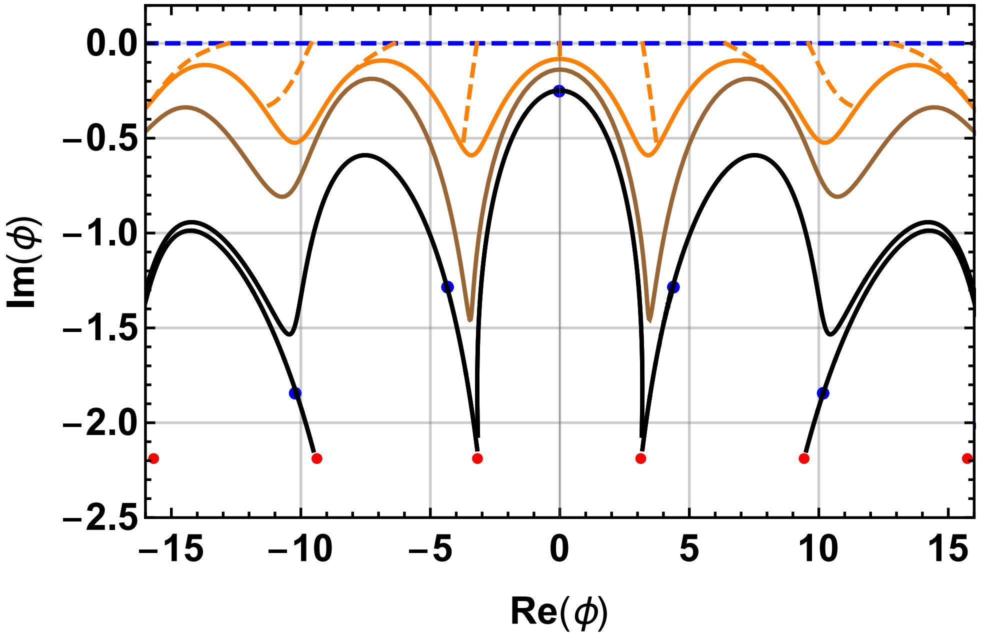




But we don't know *a priori* where these thimbles are!

BUT WE CAN APPROXIMATE THIMBLES BY FLOWING FROM REAL PLANE

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



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

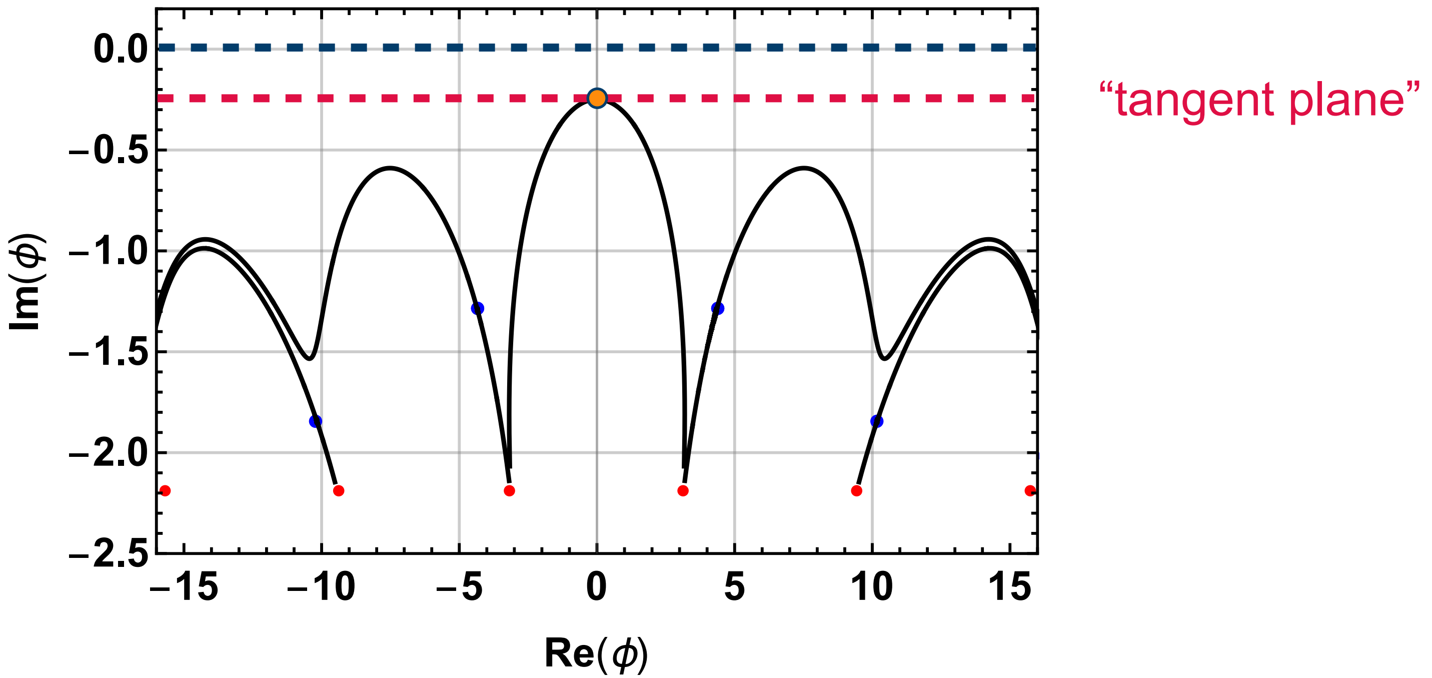
"Generalized Thimble" approach

Nishimura & Shimasaki, 1703.09409

Alexandru et al., 1512.08764

THE SIMPLEST "FLOW"

Constant contour deformation



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HOW DO WE SAMPLE FROM THE MANIFOLDS?

Integration on manifolds → 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

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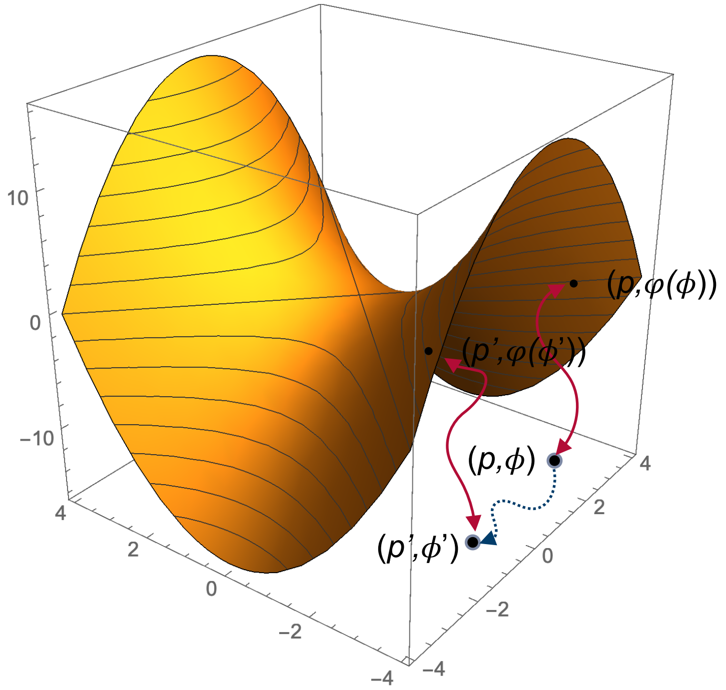
HMC WITH HOLOMORPHIC FLOW

- 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 $\mathbb{P}_{a/r} = \min\left(1, \frac{e^{-p'^2/2 - \mathrm{Re}S_{eff}[\varphi(\phi')]}}{e^{-p^2/2 - \mathrm{Re}S_{eff}[\varphi(\phi)]}}\right)$
- Reversible, satisfies detailed balance



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

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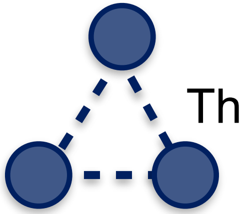
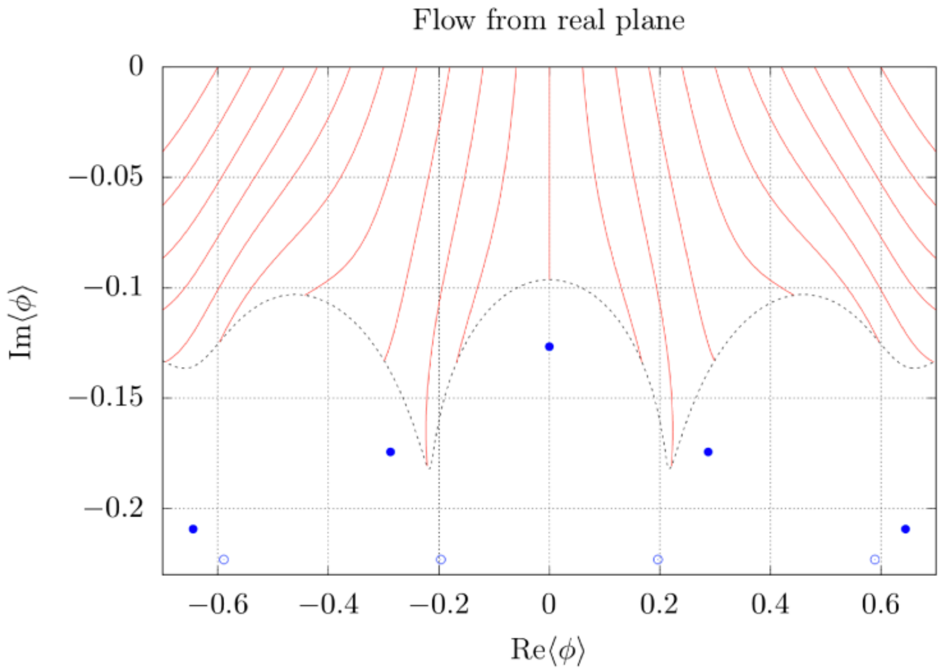
FLOWING THE ACTION



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



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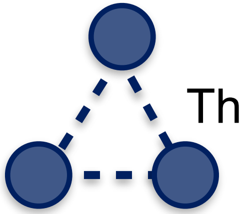

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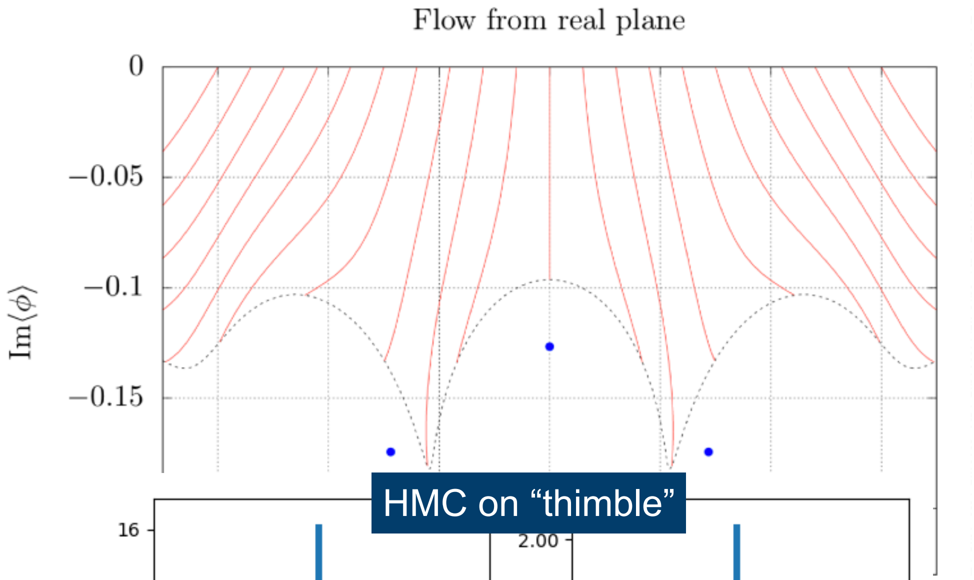
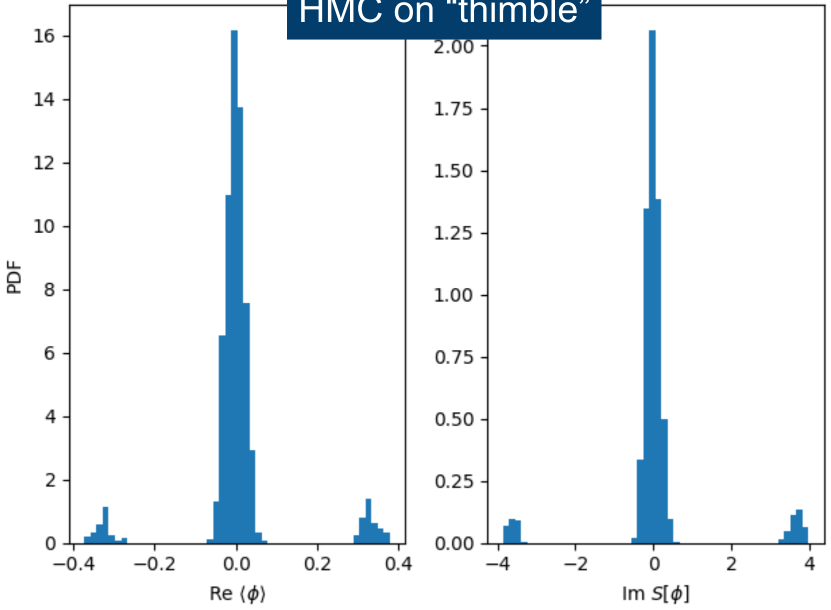


HMC on “thimble”



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FLOWING THE ACTION

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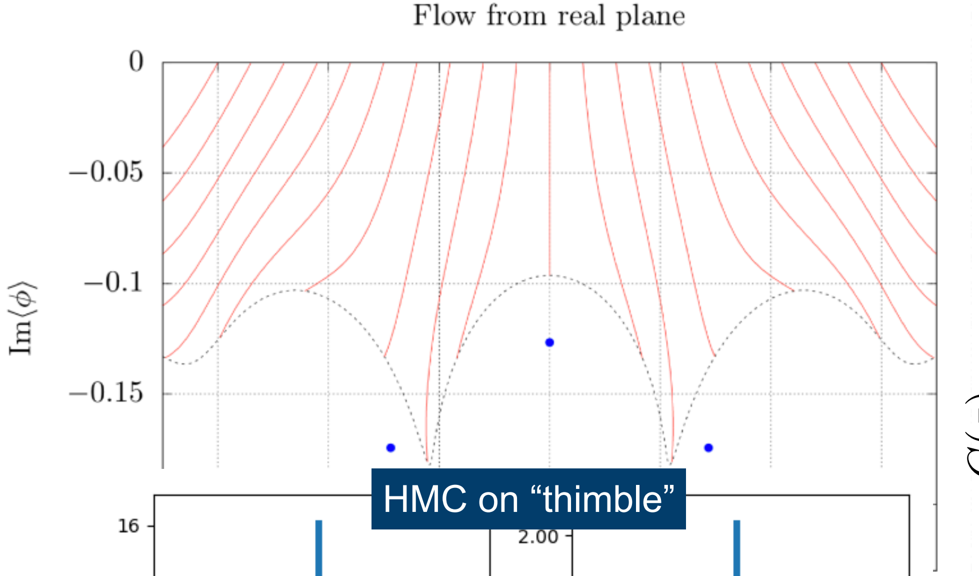
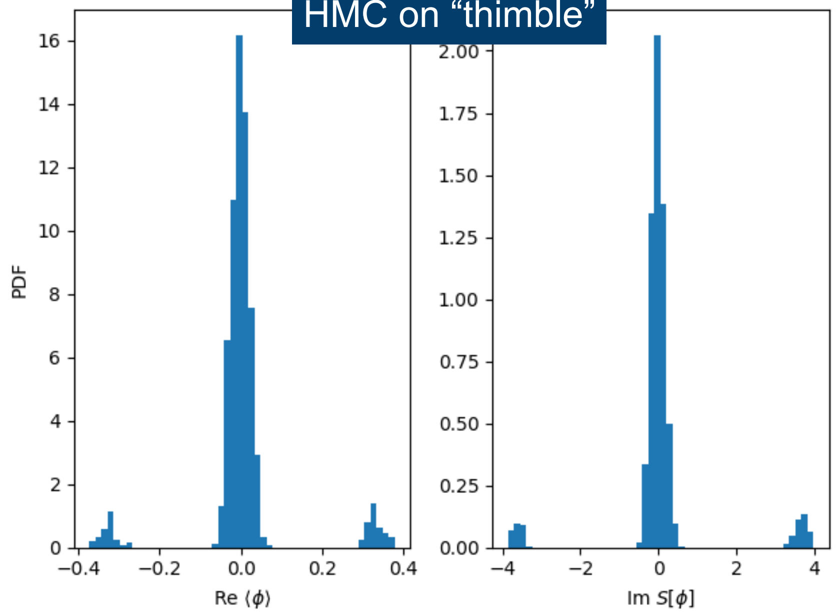
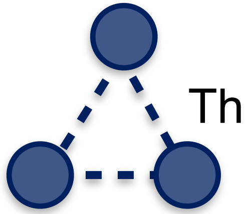


HMC on “thimble”

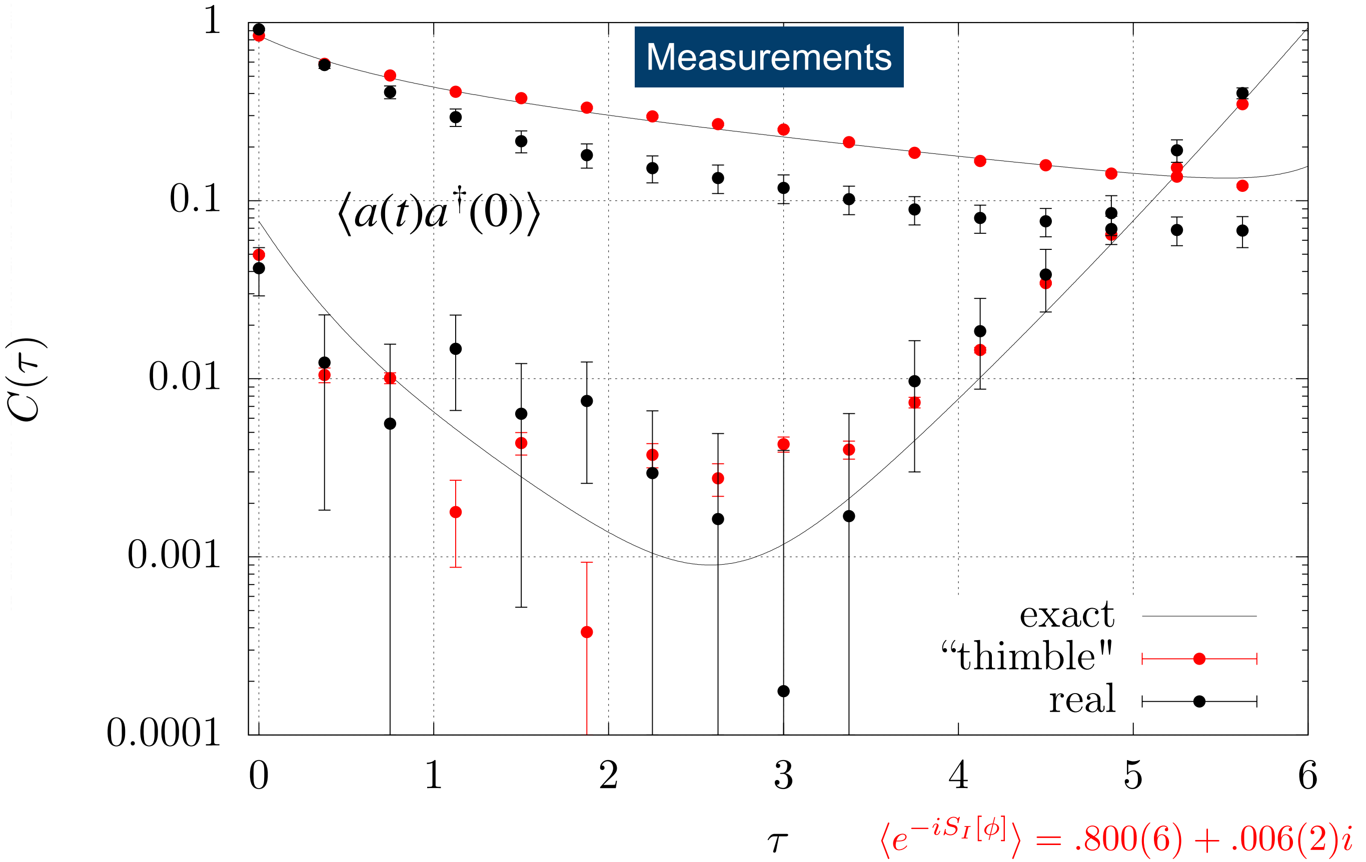




Three-site problem

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

Measurements



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

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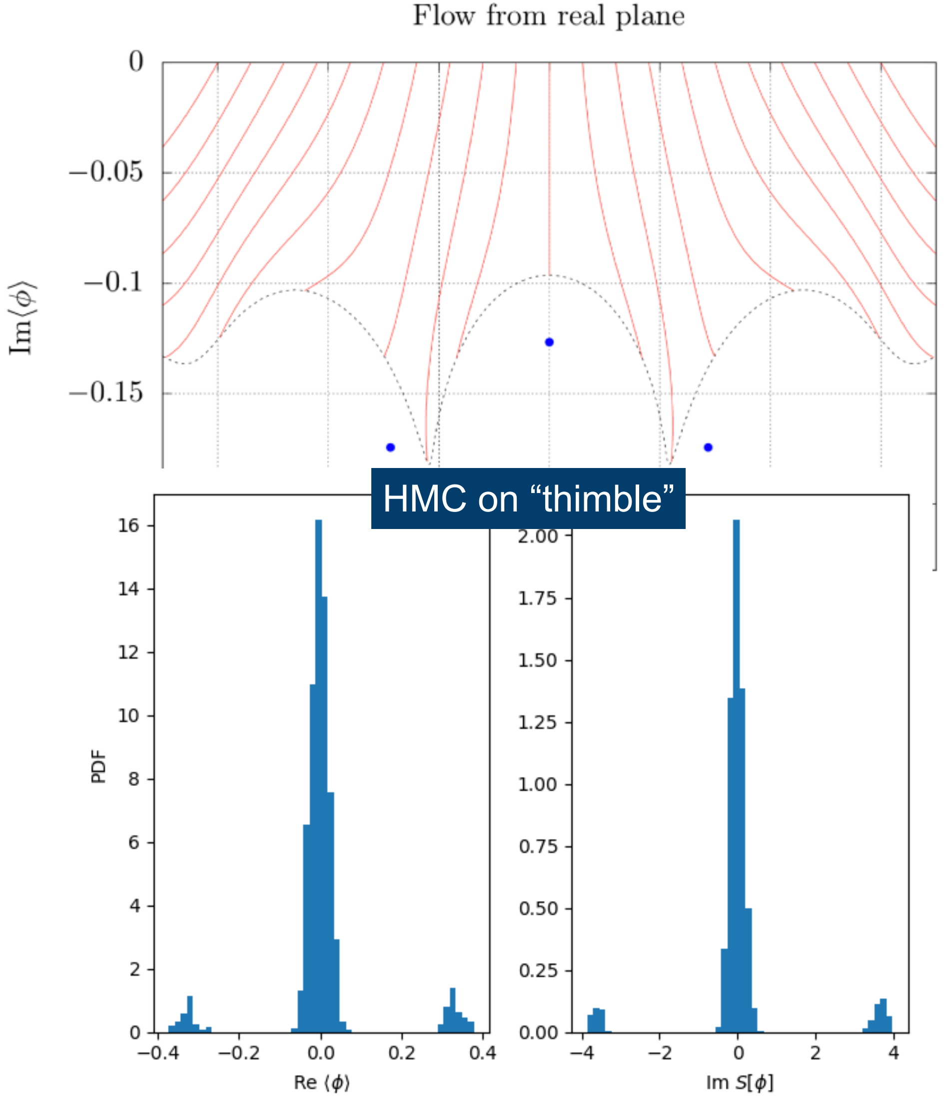
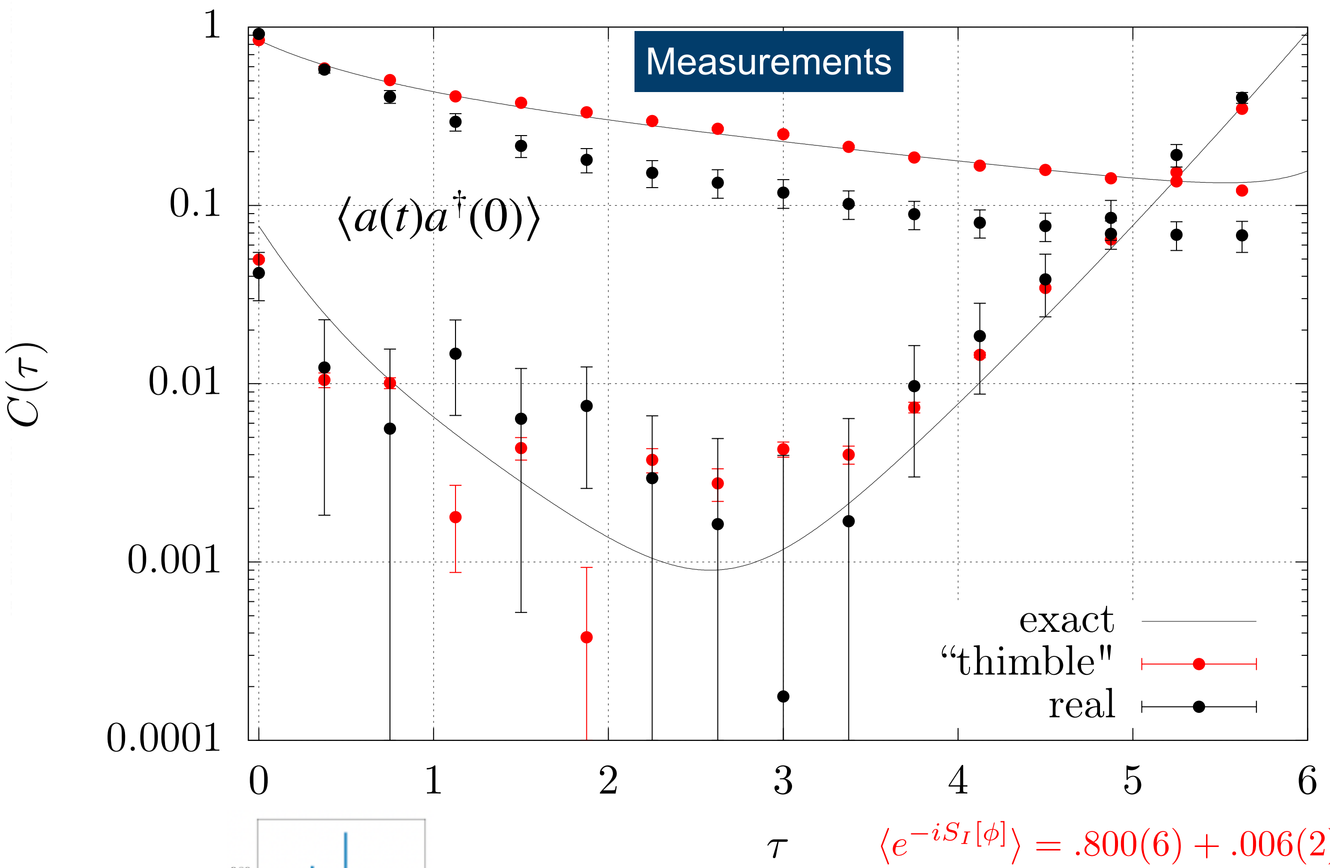
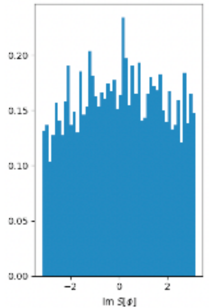




$\langle e^{-iS_I[\phi]}\rangle = .800(6) + .006(2)i$



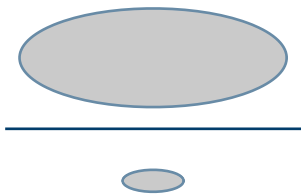
$\langle e^{-iS_I[\phi]}\rangle = .049(6) + .008(6)i$

UNFORTUNATELY, THIS “SOLUTION” IS NOT VIABLE NUMERICALLY

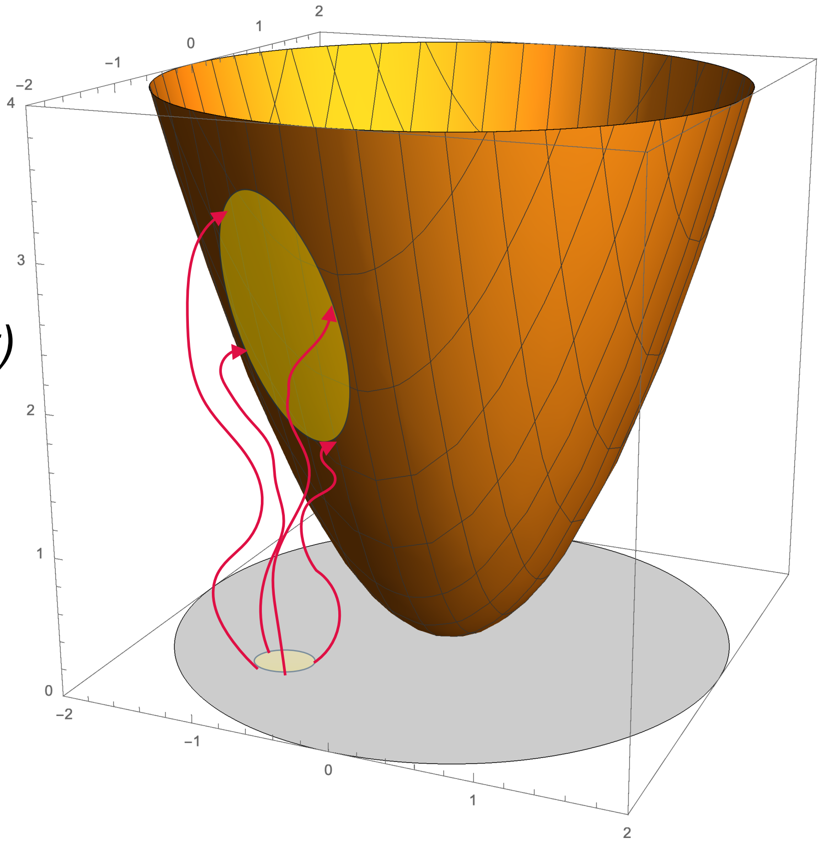
“No free lunch theorem”

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

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



= det *J(t)*



- Flowing of fields is not cheap
- Calculation of Jacobian due to flow is extremely time consuming!
    - At every step of the flow integration, must compute a dense matrix!

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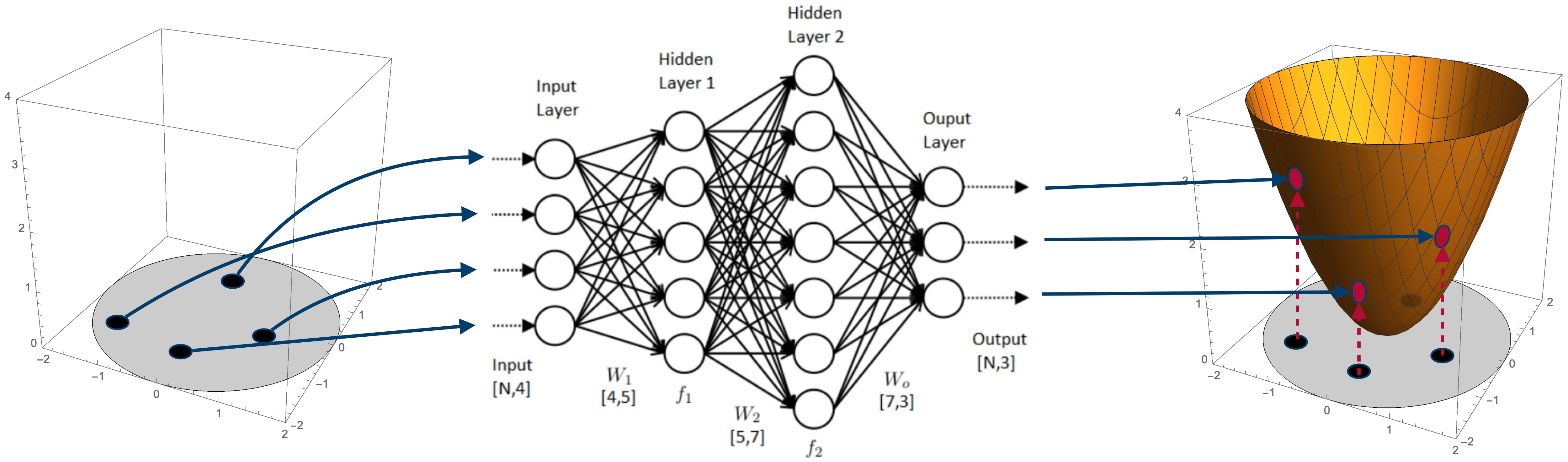
MACHINE LEARNING TO THE RESCUE!

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



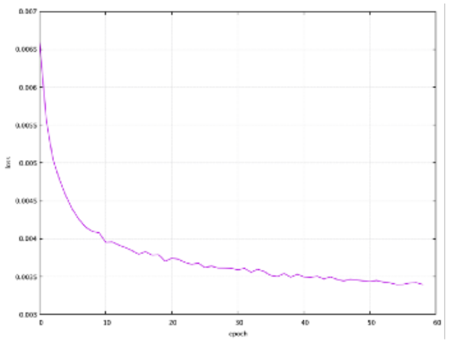
“learnifolds”

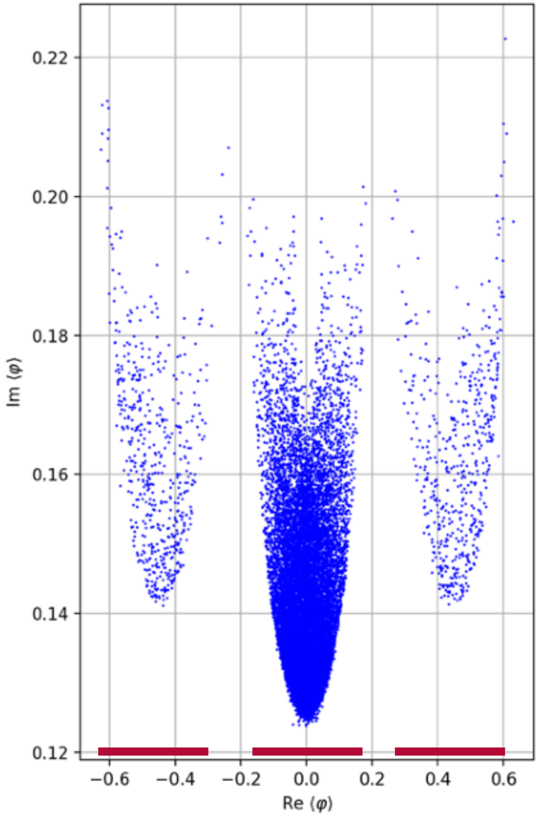
Alexandru et al., [arXiv:1709.01971] Phys.Rev. **D96** (2017) 094505

TRAINING THE NETWORK

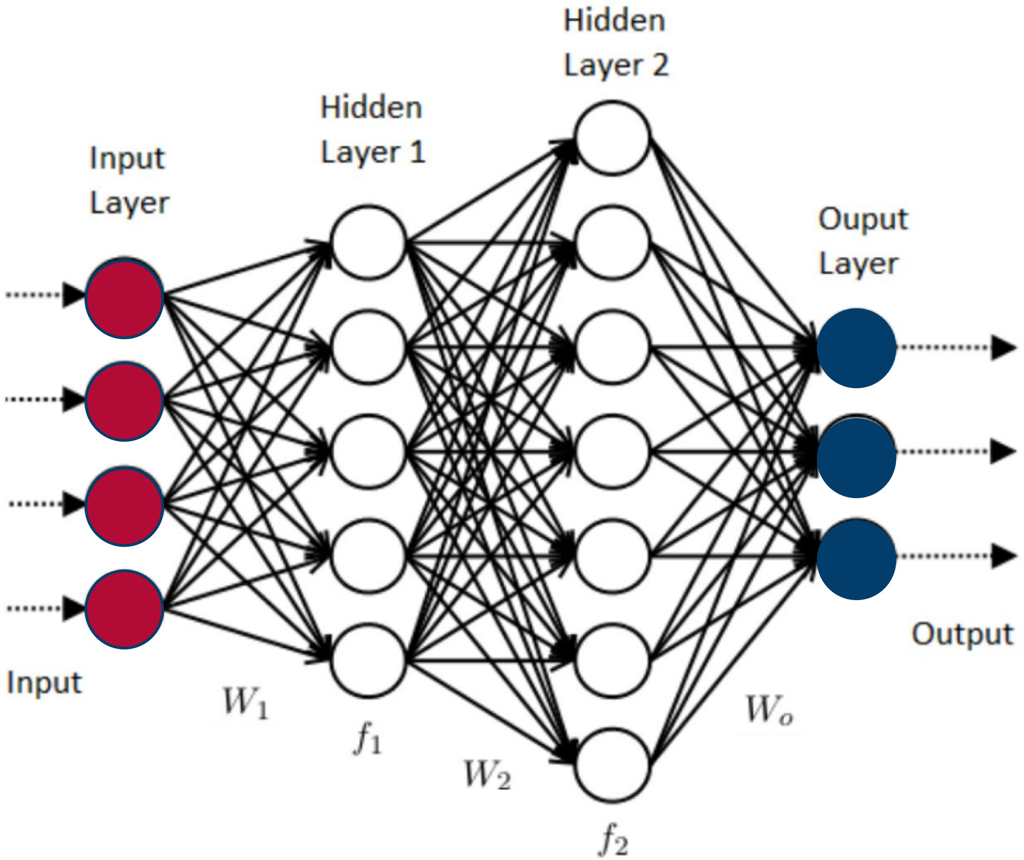
Trying to get a computer to do what you want. . .

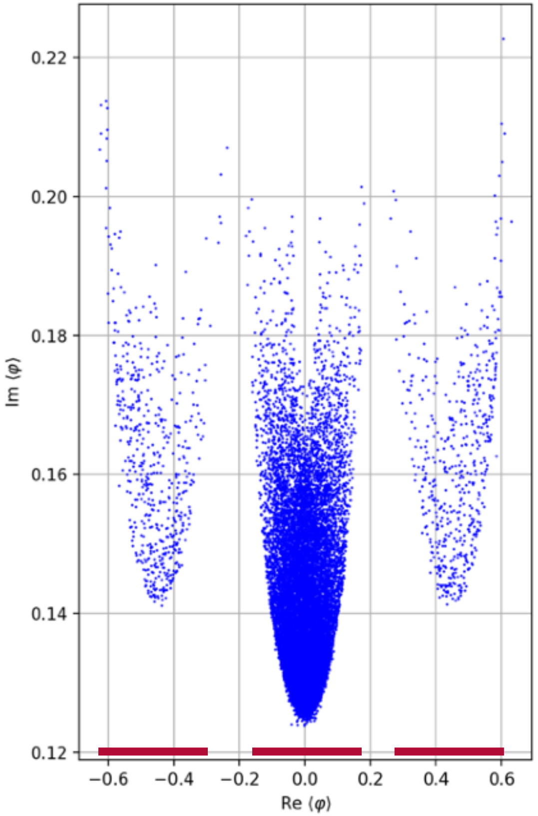
Single dense layer
“softmax” activation





training data





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

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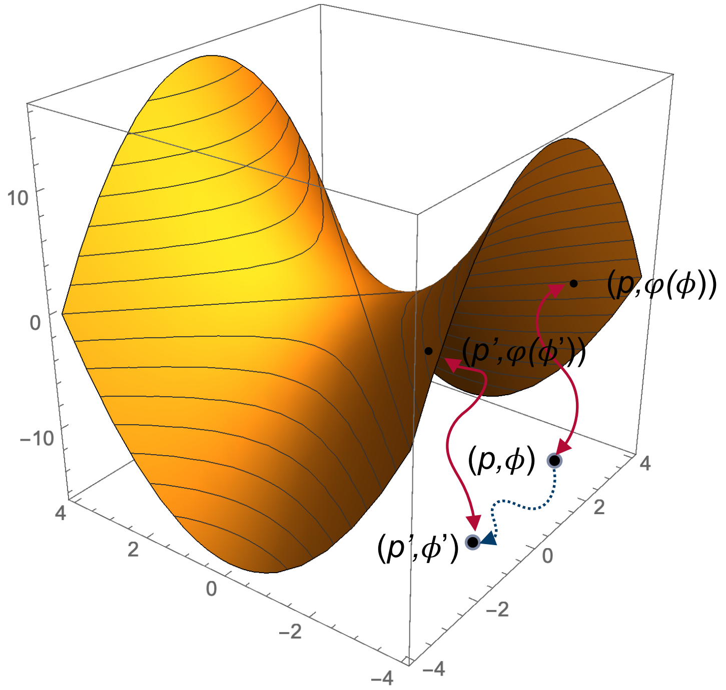
HMC WITH NEURAL NETWORKS

- 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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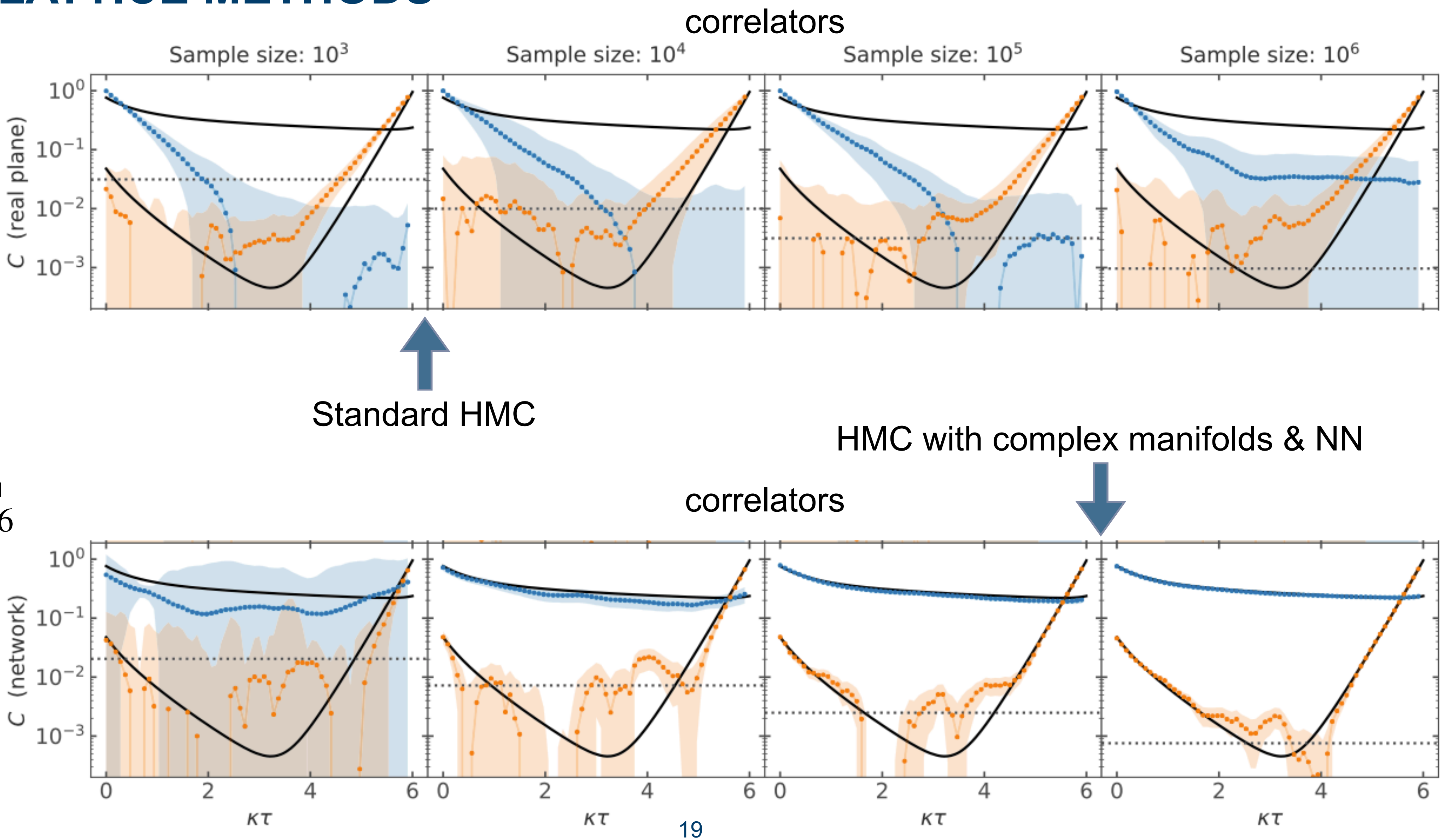
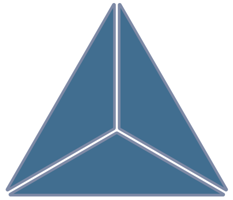
WE CAN NOW SIMULATE SYSTEMS THAT WERE NOT POSSIBLE BEFORE WITH LATTICE METHODS





tetrahedron
$U = 3 \quad \beta = 6$

J.-L. Wynen, **TL**, et al.,[arXiv:2006.11221] Phys.Rev.B **103** (2021) 125153

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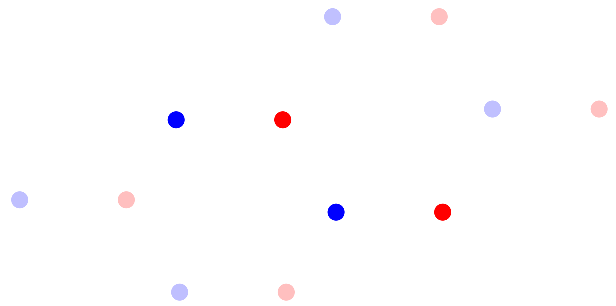
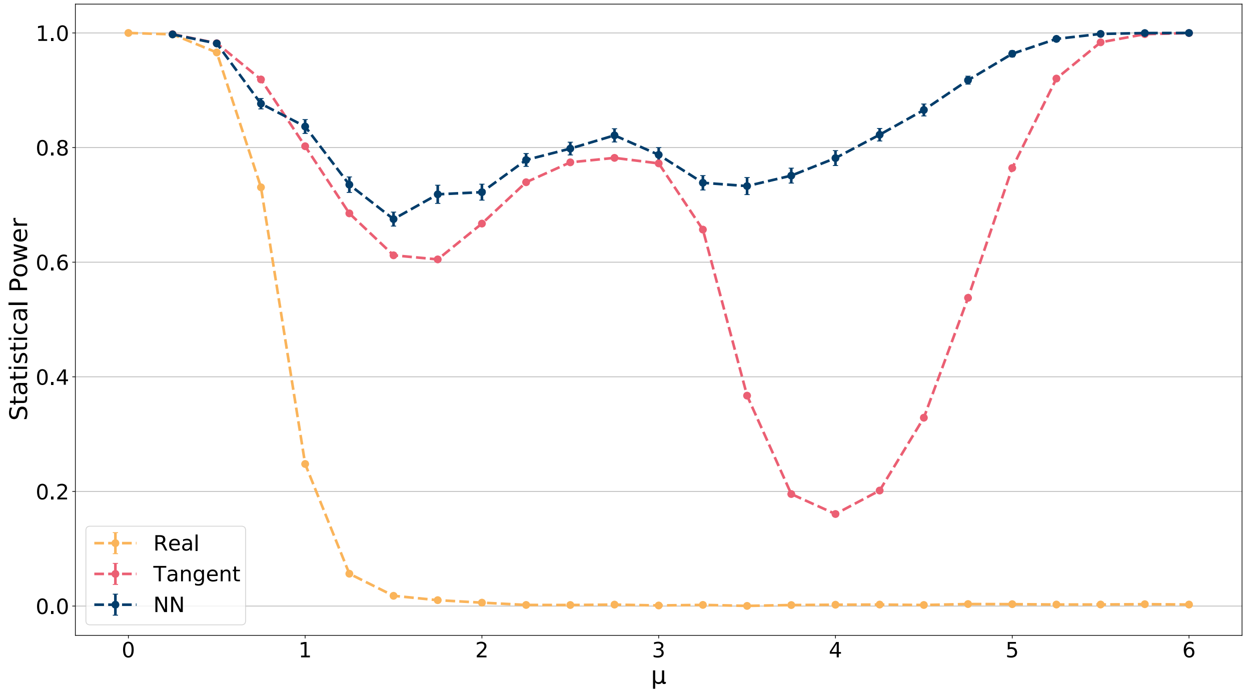
CALCULATIONS WITH NON-ZERO CHEMICAL POTENTIAL

4 sites honeycomb lattice





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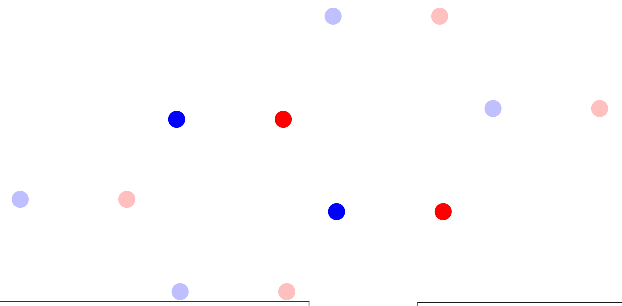
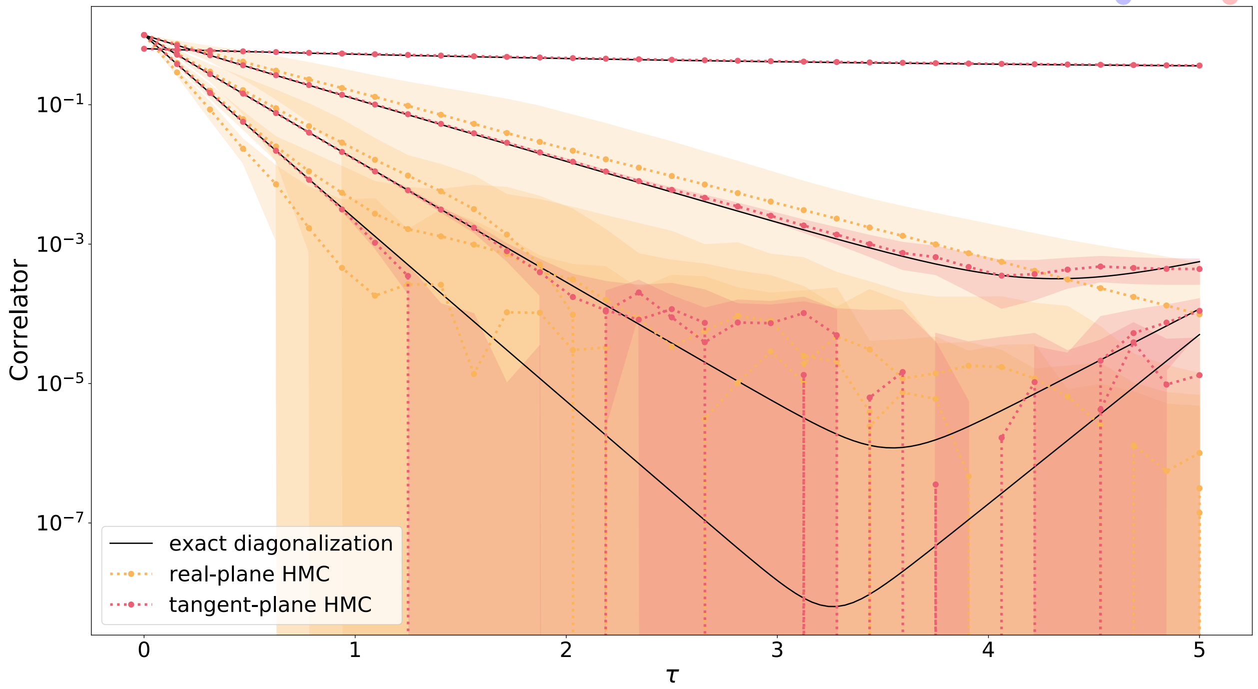
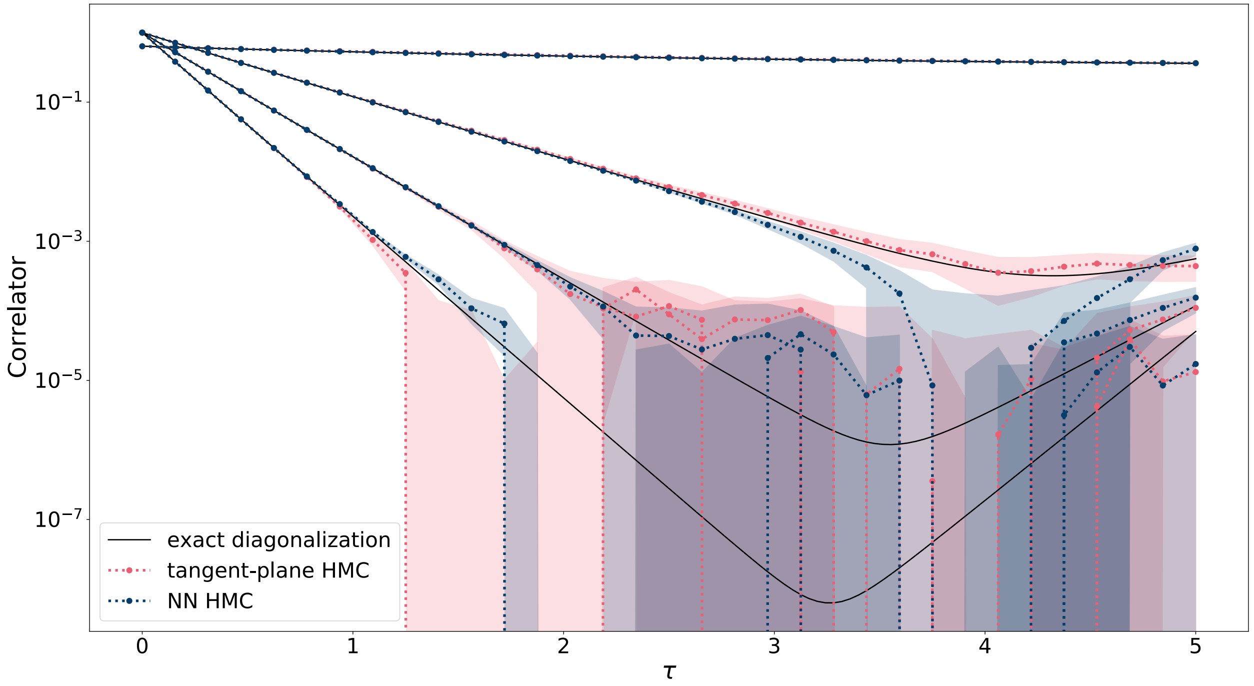
SINGLE PARTICLE CORRELATORS

4 sites honeycomb lattice





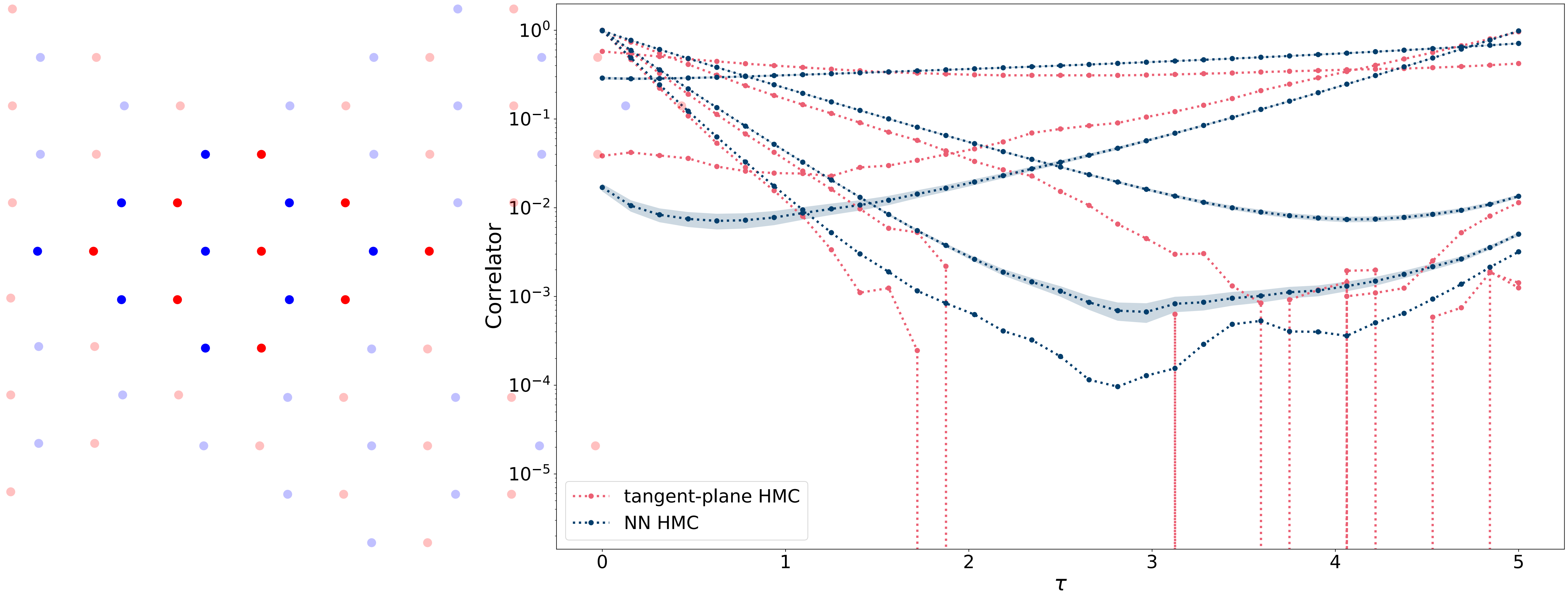


$$U = 2,\ \mu = 4,\ \beta = 5,\ N_t = 32$$

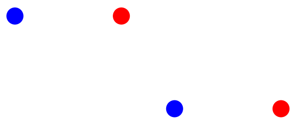
OUR BENCHMARK RESULTS GIVE US CONFIDENCE TO GO TO BIGGER SYSTEMS

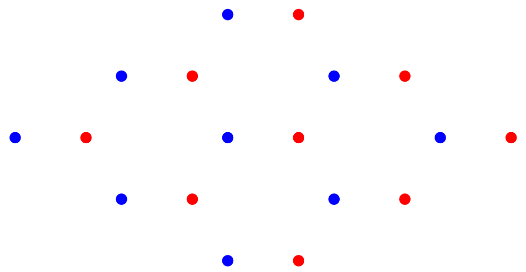
18 sites Honeycomb lattice

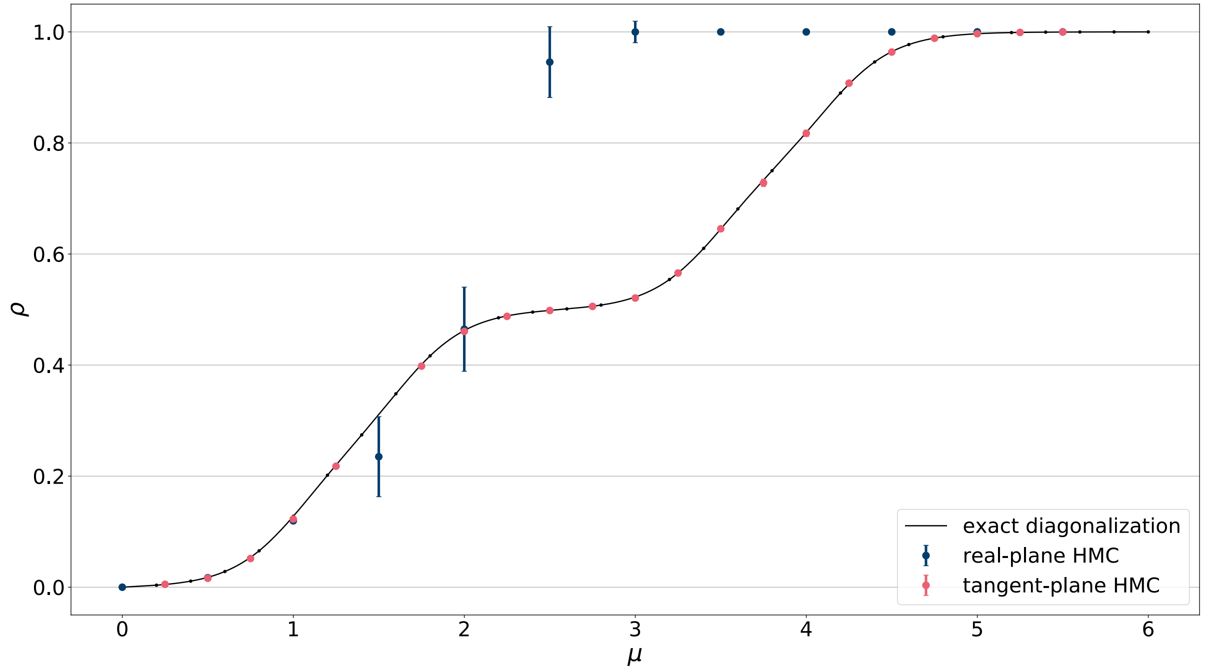
$$U = 2,\ \mu = 2,\ \beta = 5,\ N_t = 32$$

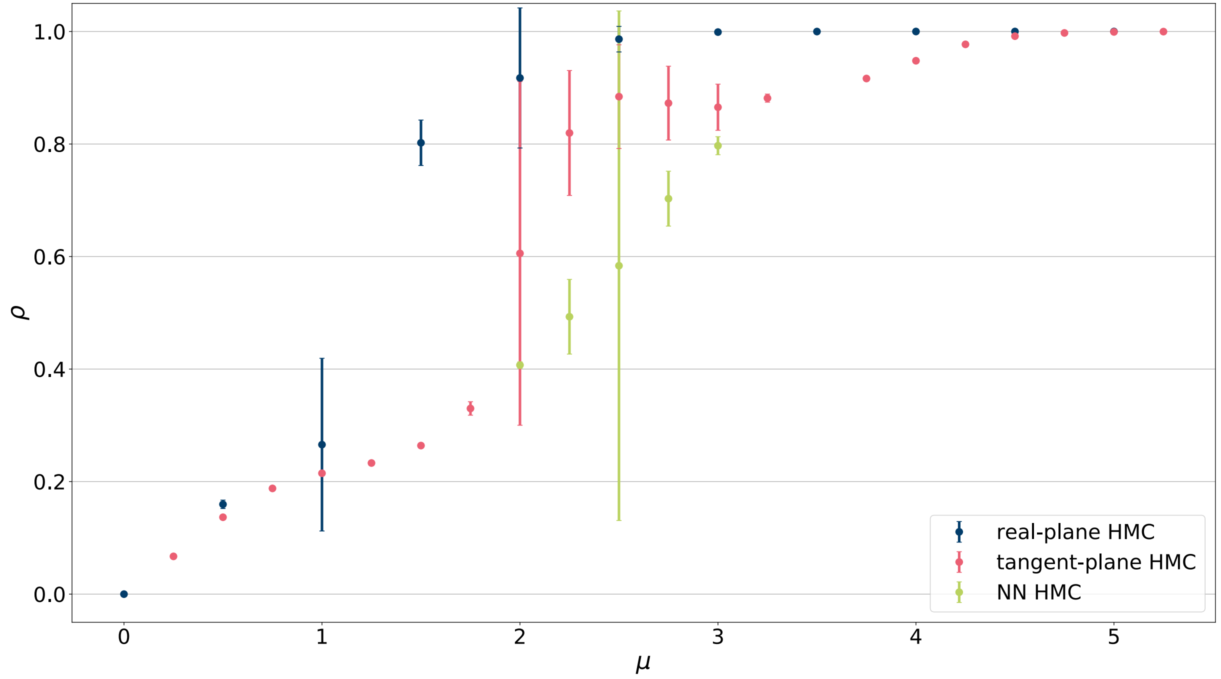


CHARGE DENSITY AS A FUNCTION OF CHEMICAL POTENTIAL









$$U = 2,\ \beta = 5$$

C. Gäntgen et al., in preparation

COMING BACK TO THE ISSUE OF $\det(J)$

Complex-valued neural network (CVNN)

- Current transformation has $\Phi_r \to \Phi_r + i\mathbb{NN}(\Phi_r)$
  - mitigates ergodicity issues, but. . .
  - $\det(J) = \det\left(1 + J_{\mathbb{NN}}\right) = \det\left(1 + \prod_{i \in \text{layers}} j^i_{\mathbb{NN}}\right)$
  - scales $\propto \mathcal{O}(V^3)$

see A. Alexandru et al. [arXiv:1604.00956] Phys.Rev. **D93** (2016) 094514, for an alternative example of dealing with Jacobians

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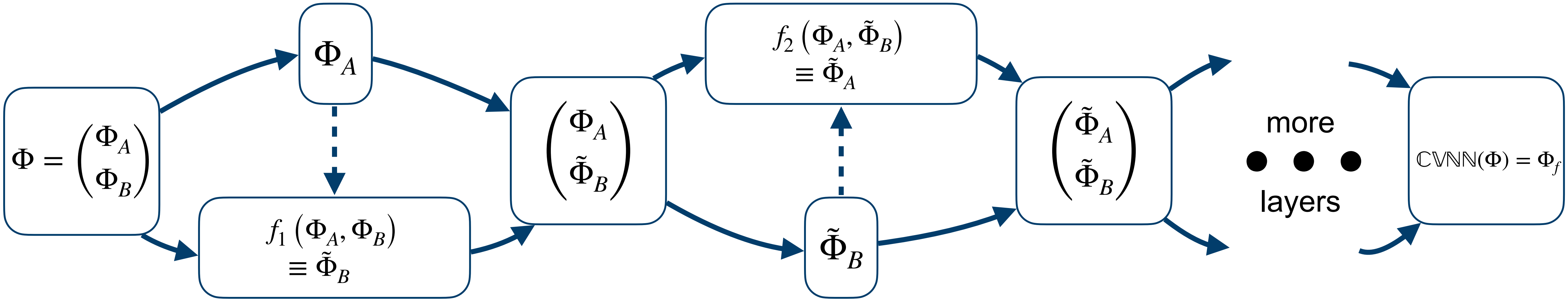
  - scales $\propto \mathcal{O}(V^3)$

- Instead consider $\Phi \to \mathbb{CVNN}(\Phi)$ where $\Phi \in \mathbb{C}$ and $\mathbb{CVNN}(\Phi) \in \mathbb{C}$
  - flow modestly from tangent plane to mitigate ergodicity issues (sufficient??)
  - $\det(J) = \det\left(J_{\mathbb{CVNN}}\right) = \det\left(\prod_{i\in\text{layers}} j^i_{\mathbb{CVNN}}\right)$
  - Affine coupling layer provides scaling $\propto \mathcal{O}(V)$

see A. Alexandru et al. [arXiv:1604.00956] Phys.Rev. **D93** (2016) 094514, for an alternative example of dealing with Jacobians

AFFINE COUPLING LAYERS

We only vary half of our inputs per layer:



Albergo et al., [arXiv:1904.12072] Phys.Rev.D **100** (2019) 034515

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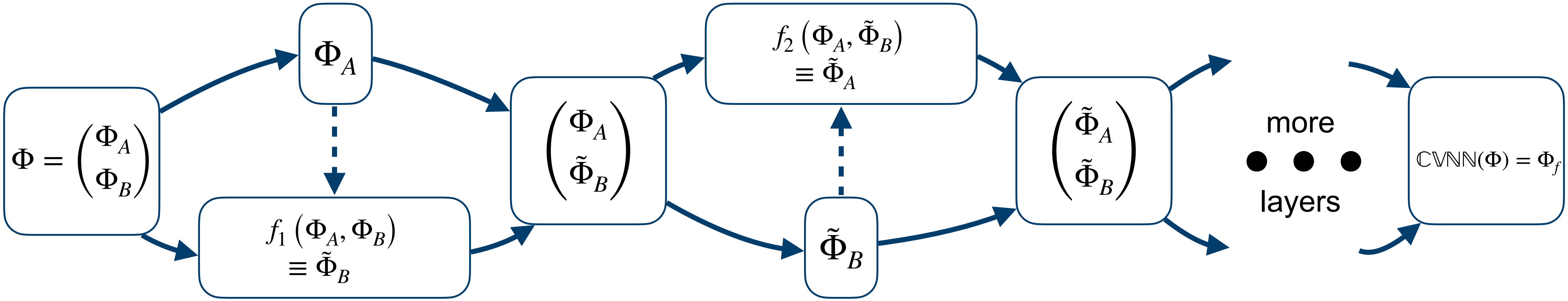

Calculation of Jacobian:

$$\begin{pmatrix} \mathbb{1} & 0 \\ \frac{df_1(\Phi_A, \Phi_B)}{d\Phi_A} & \frac{df_1(\Phi_A, \Phi_B)}{d\Phi_B} \end{pmatrix} \times \begin{pmatrix} \frac{df_2(\Phi_A, \tilde{\Phi}_B)}{d\Phi_A} & \frac{df_2(\Phi_A, \tilde{\Phi}_B)}{d\tilde{\Phi}_B} \\ 0 & \mathbb{1} \end{pmatrix} \times \bullet\bullet\bullet = J_{\mathbb{CVNN}}$$

Albergo et al., [arXiv:1904.12072] Phys.Rev.D **100** (2019) 034515

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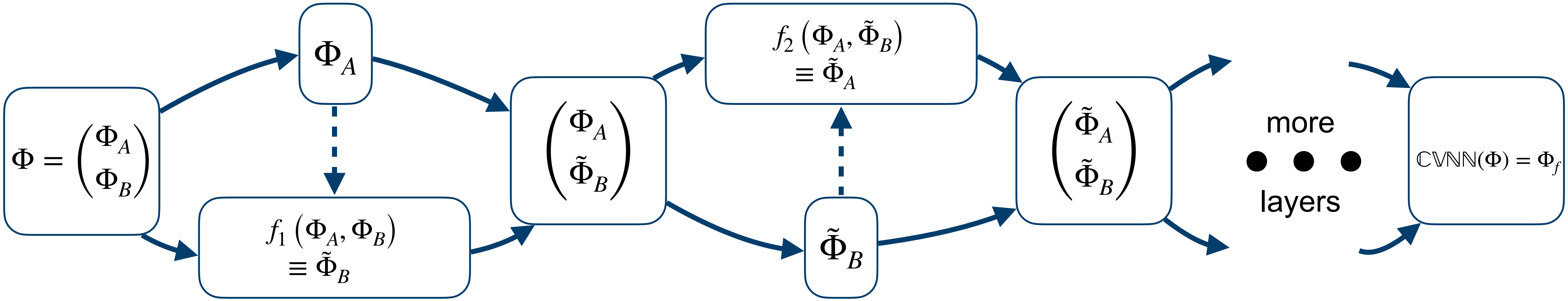

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Calculation of $\det J$: $\det\left(J_{\mathbb{CVNN}}\right) = \prod_{i \in \text{layers}} \det j^i_{\mathbb{CVNN}} = \prod j^i_{dd} \propto \mathcal{O}(V) \times$ (# of layers)

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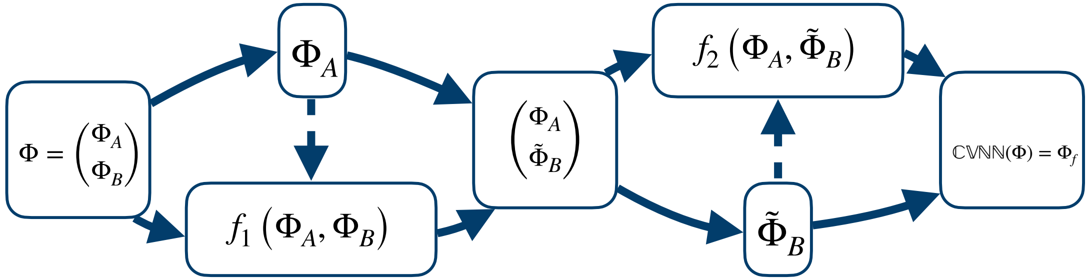
Albergo et al., [arXiv:1904.12072] Phys.Rev.D **100** (2019) 034515

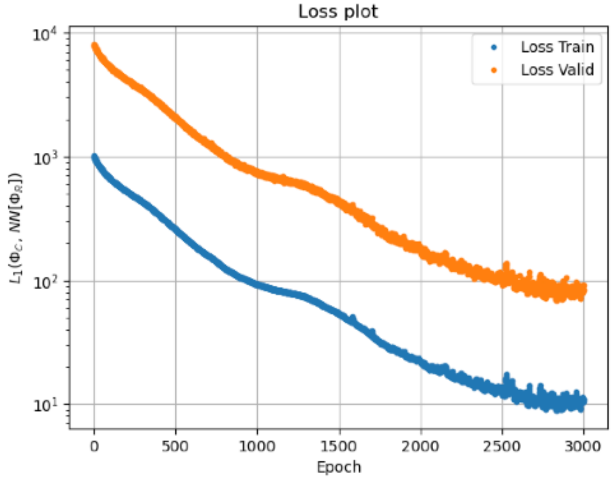
OUR INITIAL RESULTS WITH CVNN ARE VERY PROMISING!

Two sites problem

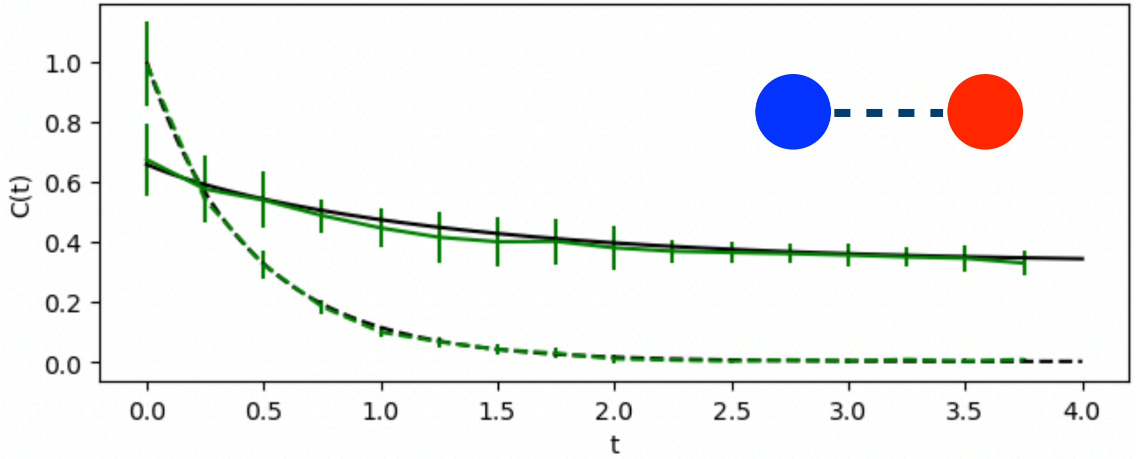
Two affine layers

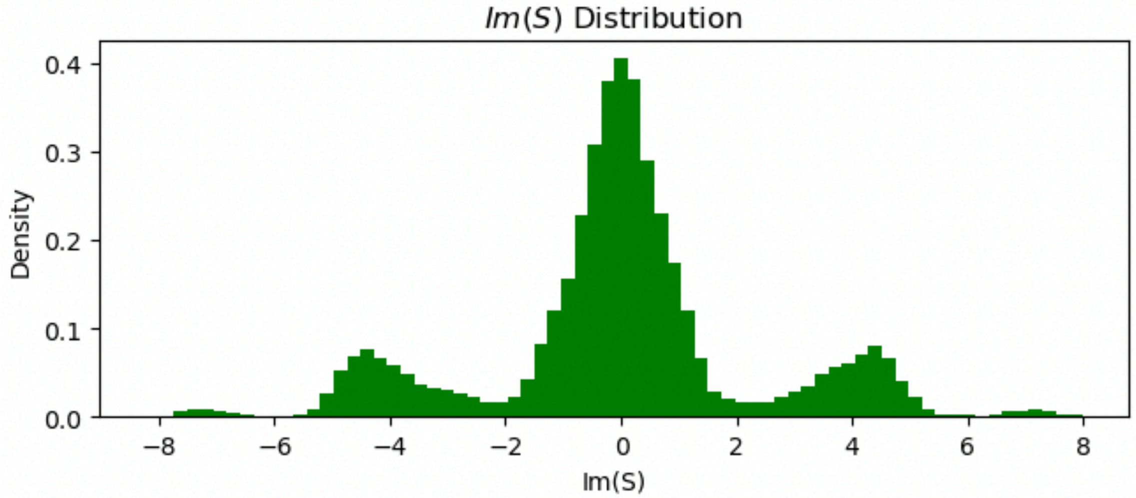


Training data was flowed from tangent plane



$U = 2,\ \mu = 2,\ \beta = 4,\ N_t = 16$





M. Rodekamp et al., in preparation

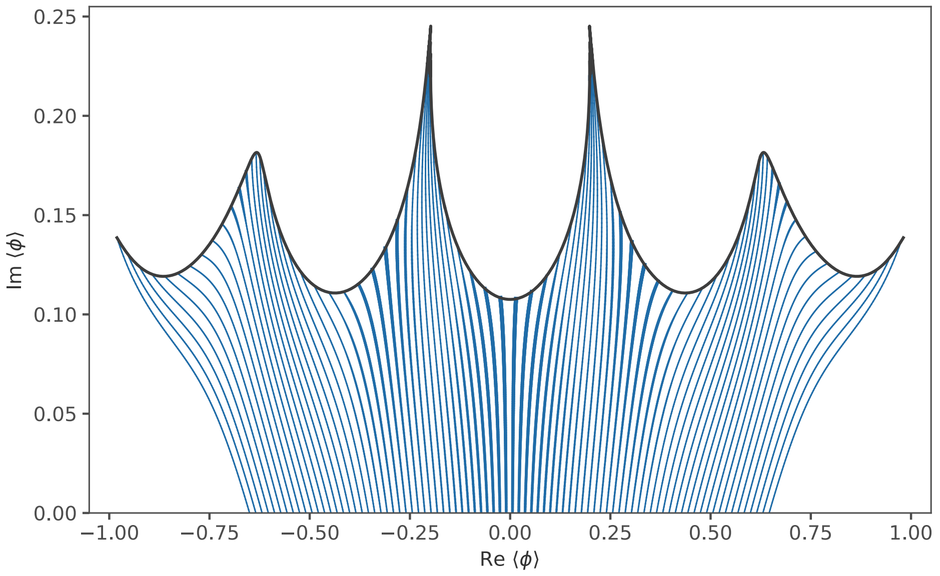
CONCLUSIONS

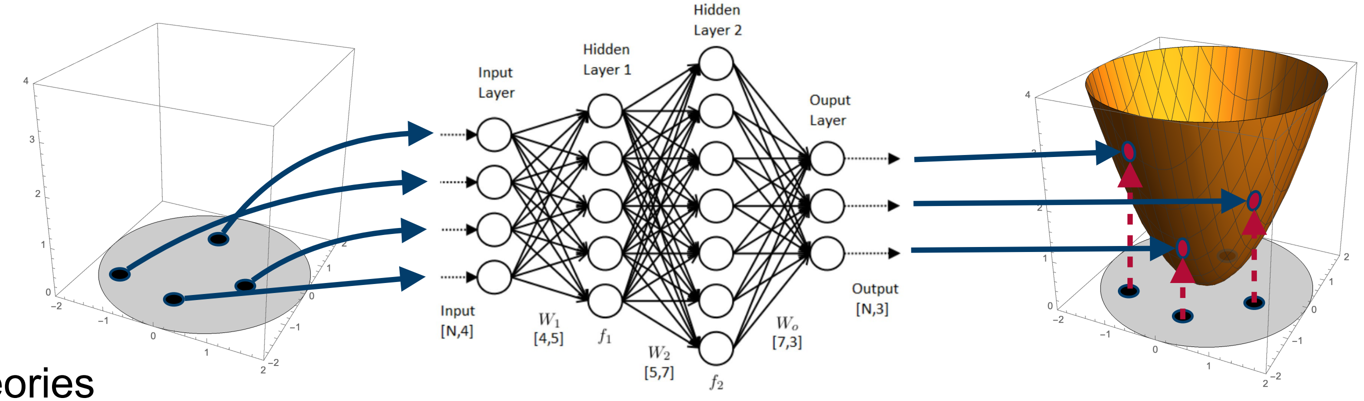
- Hubbard model sign problem can be alleviated
  - by holomorphic flow
  - calculation of Jacobian prohibitive (numerically)

- Used NN to train location of manifolds
  - Fast/efficient interpolation routine
  - With CVNN, $\det J$ scales as $\mathcal{O}(V)$!

- Found success in simple systems, moving now to larger systems
  - C20, C60
  - doped graphene/tubes

- Ultimate goal: apply holomorphic flow to lattice gauge theories
  - Fermions, fermions, fermions!





Thank you!