Flow-based density of states for complex actions

arXiv:2203.01243*

Julian Urban
ITP Heidelberg

*in collaboration with Jan M. Pawlowski

Flow-based density of states for complex actions

arXiv:2203.01243*

Julian Urban
ITP Heidelberg

*in collaboration with Jan M. Pawlowski

Complex actions

- Finite density, topological terms, spin / mass imbalance, real-time physics, ...
- Standard importance sampling not applicable
- Direct reweighting often becomes prohibitively expensive
- Complex Langevin, Lefschetz thimbles, contour deformation, dual formulations, Taylor expansion, analytic continuation, density of states, ...

Complex actions

- This talk: imaginary coupling constant

$$S(\phi) = S_r(\phi) + \mathrm{i}hX(\phi)$$

- Partition function

$$Z = \int \mathcal{D}\phi \, e^{-S_r(\phi) - \mathrm{i}hX(\phi)}$$

- Observables

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, e^{-S_r(\phi) - \mathrm{i}hX(\phi)} \mathcal{O}(\phi)$$

Flow-based density of states for complex actions

arXiv:2203.01243*

Julian Urban
ITP Heidelberg

*in collaboration with Jan M. Pawlowski

Density of states

- Slices with constant imaginary part of the action

$$\rho(c) = \int \mathcal{D}\phi \, e^{-S_r(\phi)} \delta(X(\phi) - c)$$

- Partition function and observables become one-dimensional integrals

$$Z = \int \mathrm{d}c \, \rho(c) \, e^{-\mathrm{i}hc}$$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathrm{d}c \, \rho(c) \, e^{-\mathrm{i}hc} \, \mathcal{O}(c)$$

Density of states

- Replace δ-distribution with Gaussian of finite width

$$\int \mathrm{d}c\, e^{-\frac{P}{2}(c-a)^2} = \sqrt{\frac{2\pi}{P}} \equiv \mathcal{N}$$

- Width-dependent density of states

$$\rho_P(c) = \int \mathcal{D}\phi\, e^{-S_{c,P}(\phi)}$$

$$S_{c,P}(\phi) = S_r(\phi) + \frac{P}{2}(c - X(\phi))^2 + \log \mathcal{N}$$

- Exactness retained at the cost of a residual average phase factor, tractable for sufficiently large *P*

Density of states

- Direct computation infeasible with standard methods
- Reconstruction up to normalization by measuring derivative of logarithm and numerical integration

$$
\begin{aligned}
\frac{\partial \log \rho_P(c)}{\partial c} &= \frac{1}{\rho_P(c)} \frac{\partial \rho_P(c)}{\partial c} \\
&= \frac{\int \mathcal{D}\phi \, e^{-S_{c,P}(\phi)} (-P(c - X(\phi)))}{\int \mathcal{D}\phi \, e^{-S_{c,P}(\phi)}} \\
&= \big\langle -P(c - X(\phi)) \big\rangle_{\phi \sim e^{-S_{c,P}(\phi)}}
\end{aligned}
$$

Flow-based density of states for complex actions

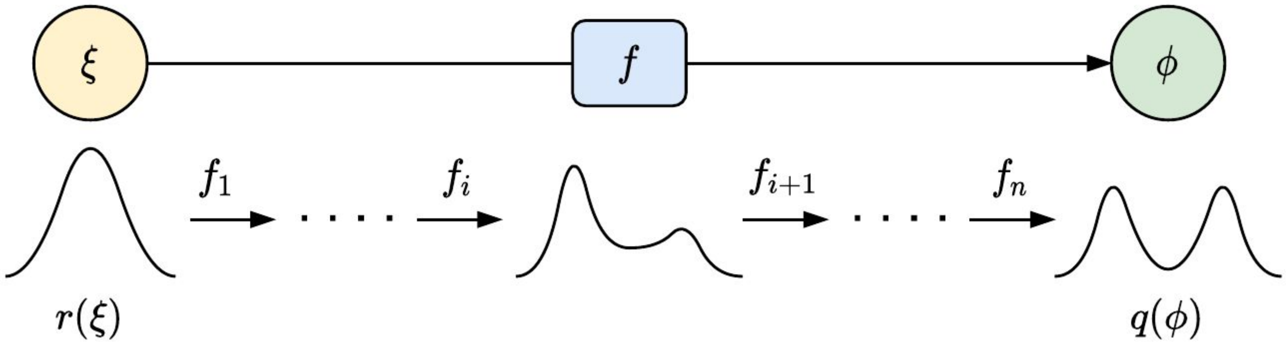
arXiv:2203.01243*

Julian Urban
ITP Heidelberg

*in collaboration with Jan M. Pawlowski

Normalizing flows

- Generative machine learning approach to sampling and density estimation via change-of-variables



- Tractable probability of generated configurations

$$q(\phi) = r(\xi) \left| \det \left(\frac{\partial f}{\partial \xi} \right) \right|^{-1}$$

Normalizing flows

- Potential solution to ergodicity issues like critical slowing-down and topological freezing

- Direct computation of thermodynamic observables purely from model samples

$$Z = \int \mathcal{D}\phi \, q(\phi) \frac{e^{-S(\phi)}}{q(\phi)} = \left\langle e^{-S(\phi) - \log q(\phi)} \right\rangle_{\phi \sim q(\phi)}$$

➔ "variationally optimized reweighting"

Flow-based density of states for complex actions

arXiv:2203.01243*

Julian Urban
ITP Heidelberg

*in collaboration with Jan M. Pawlowski

Flow-based DoS for complex actions

- Direct computation of DoS instead of reconstruction

$$\rho_P(c) = \int \mathcal{D}\phi\, q(\phi) \frac{e^{-S_{c,P}(\phi)}}{q(\phi)}$$
$$= \left\langle e^{-S_{c,P}(\phi) - \log q(\phi)} \right\rangle_{\phi \sim q(\phi)}$$

- Efficient representation via conditional flow + offset

$$\phi(\xi|c) = f_c(\xi) + \bar{\phi}(c) \quad \text{with} \quad X(\bar{\phi}(c)) = c$$

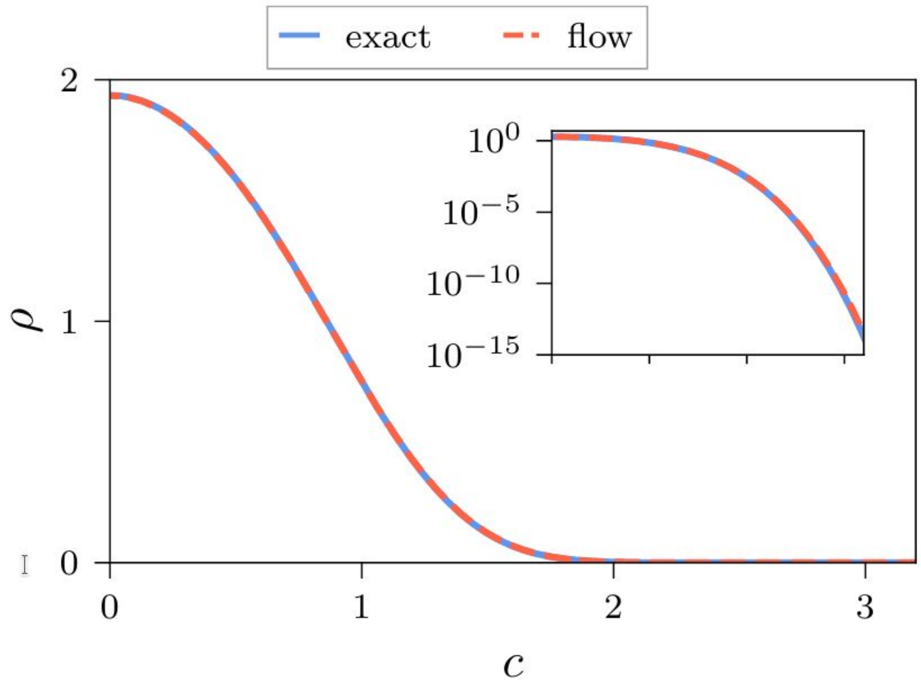
$$\rho_P(c) = \left\langle e^{-S_{c,P}(\phi) - \log q_c(\phi)} \right\rangle_{\phi \sim q_c(\phi)}$$

Numerical demonstration

- Two-component real scalar field theory in $d = 0,1,2$
- O(2) symmetry broken by imaginary magnetic field
- Simple, but non-trivial test due to Lee-Yang zeroes
- Reweighting and complex Langevin can be shown to fail
- Interesting physics: toy model for quark-meson model

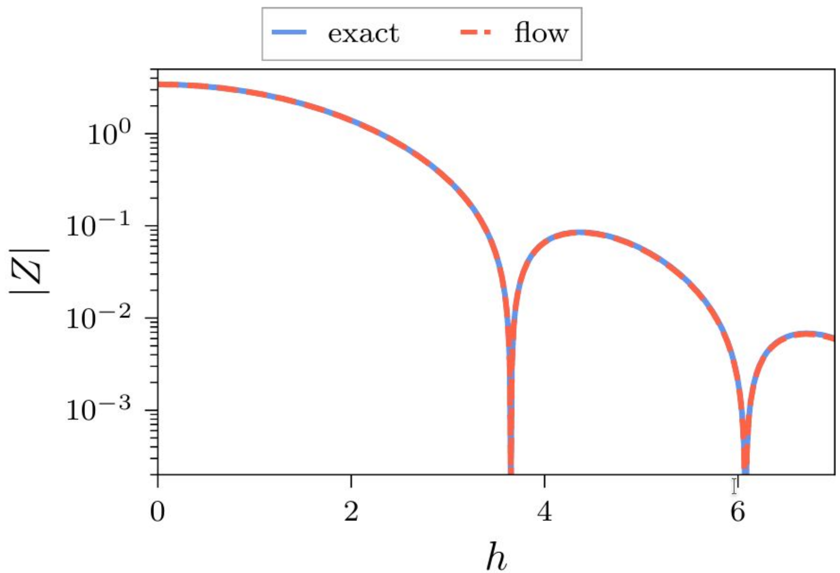
Exactly solvable case: *d* = 0

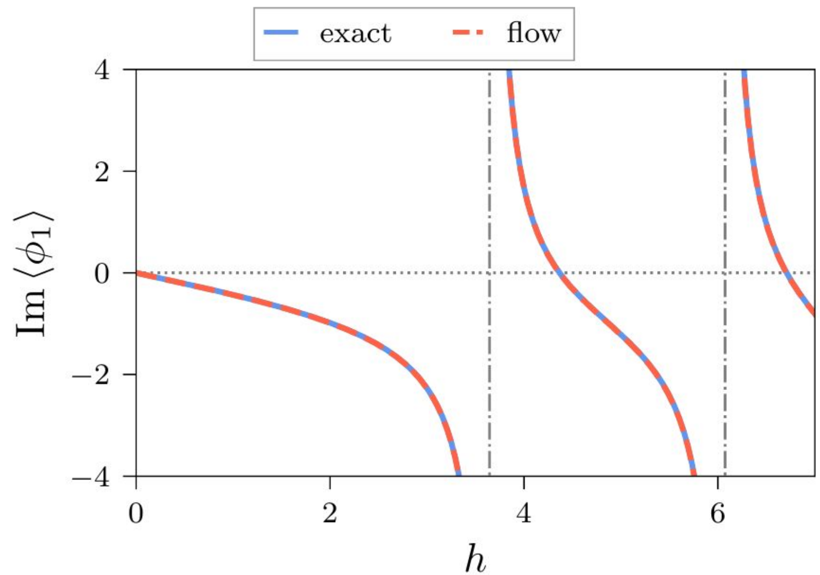
$$S(\phi) = \frac{m^2}{2}\left(\phi_1^2 + \phi_2^2\right) + \frac{\lambda}{4}\left(\phi_1^2 + \phi_2^2\right)^2 + \mathrm{i}h\phi_1$$



Exactly solvable case: $d = 0$

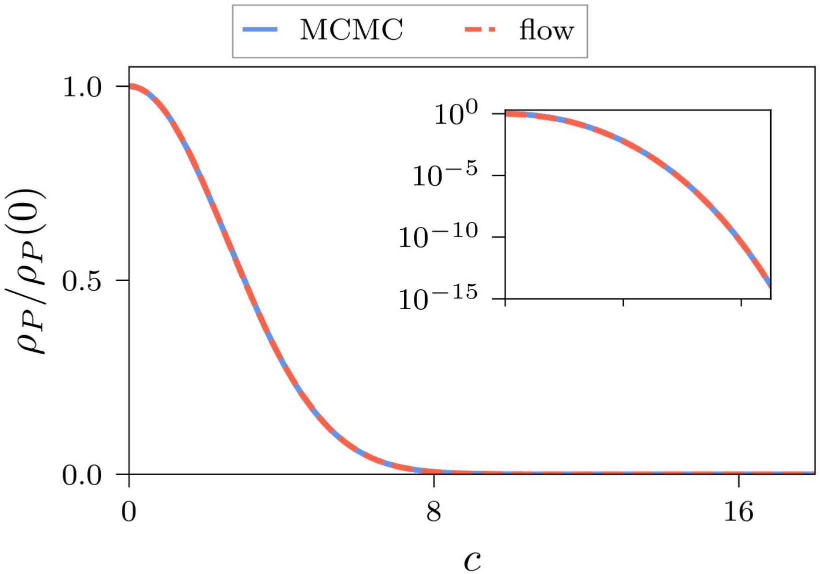
$$S(\phi) = \frac{m^2}{2}\left(\phi_1^2 + \phi_2^2\right) + \frac{\lambda}{4}\left(\phi_1^2 + \phi_2^2\right)^2 + \mathrm{i}h\phi_1$$

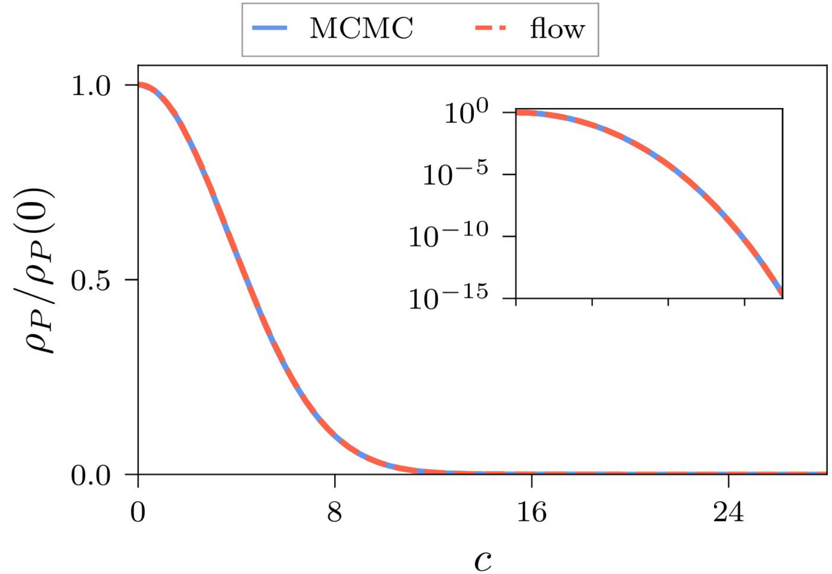




d = 1,2 with L = 8,4

$$S(\phi) = \sum_{n \in \Lambda} \left(\frac{1}{2} \sum_{\mu=1}^{d} |\phi(n) - \phi(n+\hat{\mu})|^2 + \frac{m^2}{2} |\phi(n)|^2 + \frac{\lambda}{4} |\phi(n)|^4 + \mathrm{i} h \phi_1(n) \right)$$





Potential (dis)advantages

+

- Avoids reconstruction by numerical integration
- Allows direct computation of DoS at arbitrary points
- Access to overall normalization constant
- No MCMC, just "embarrassingly parallel" sampling

–

- Additional up-front cost of training
- High-quality models not guaranteed

But: both approaches are complementary, not competitive!

Outlook

- Demonstrate feasibility on not-so-tiny lattices
- Investigate & compare computational cost, scaling
- Quark-meson model, heavy-dense QCD, θ-terms
- Solve ergodicity issues in theories with real actions

Thank you!