LATTICE 2024
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UNIVERSITÄT BONN
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TRA MATTER
TRANSDISCIPLINARY RESEARCH AREA

HISKP

Simulating the Hubbard Model with Normalizing Flows

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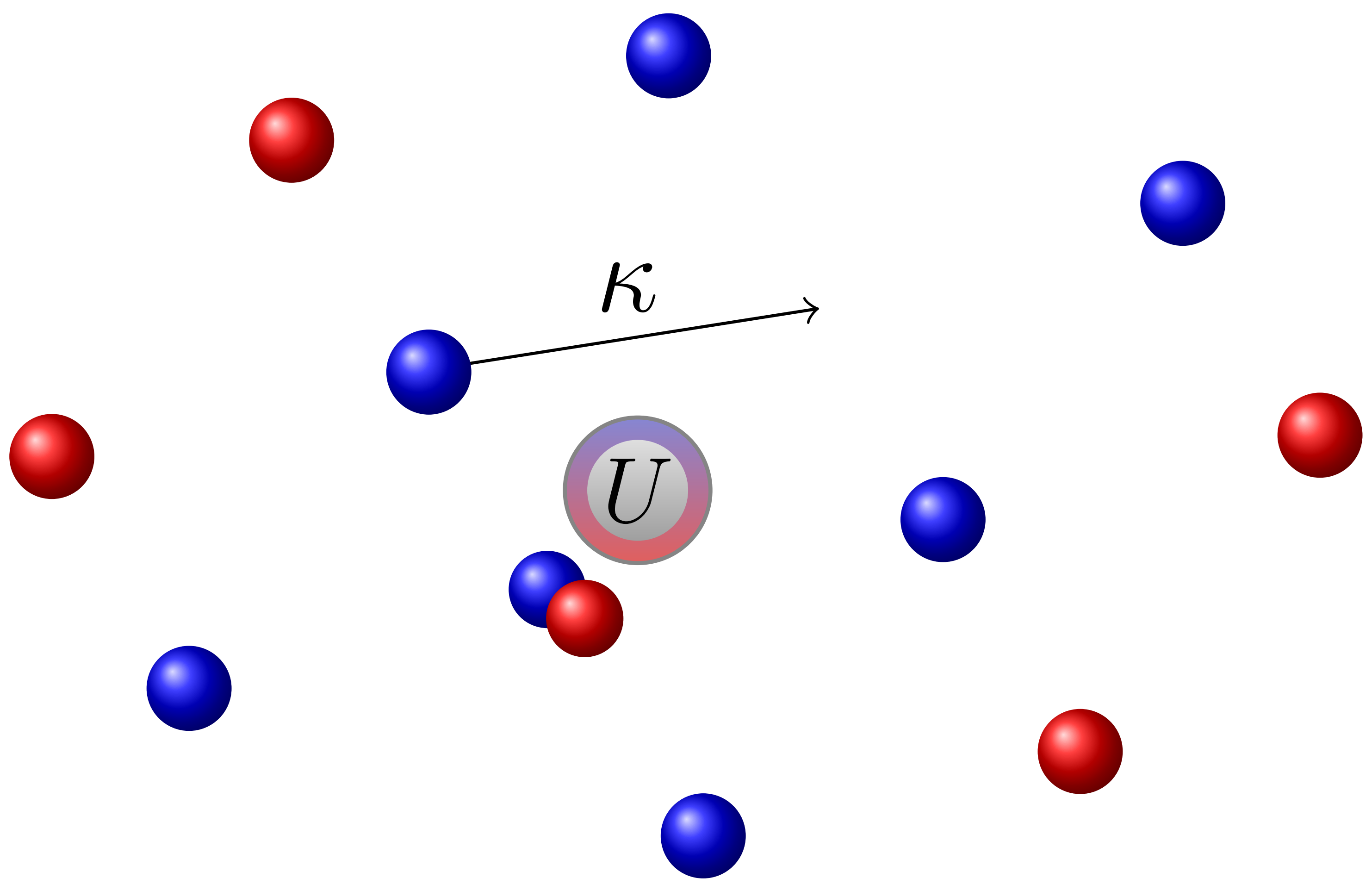
Hubbard Model

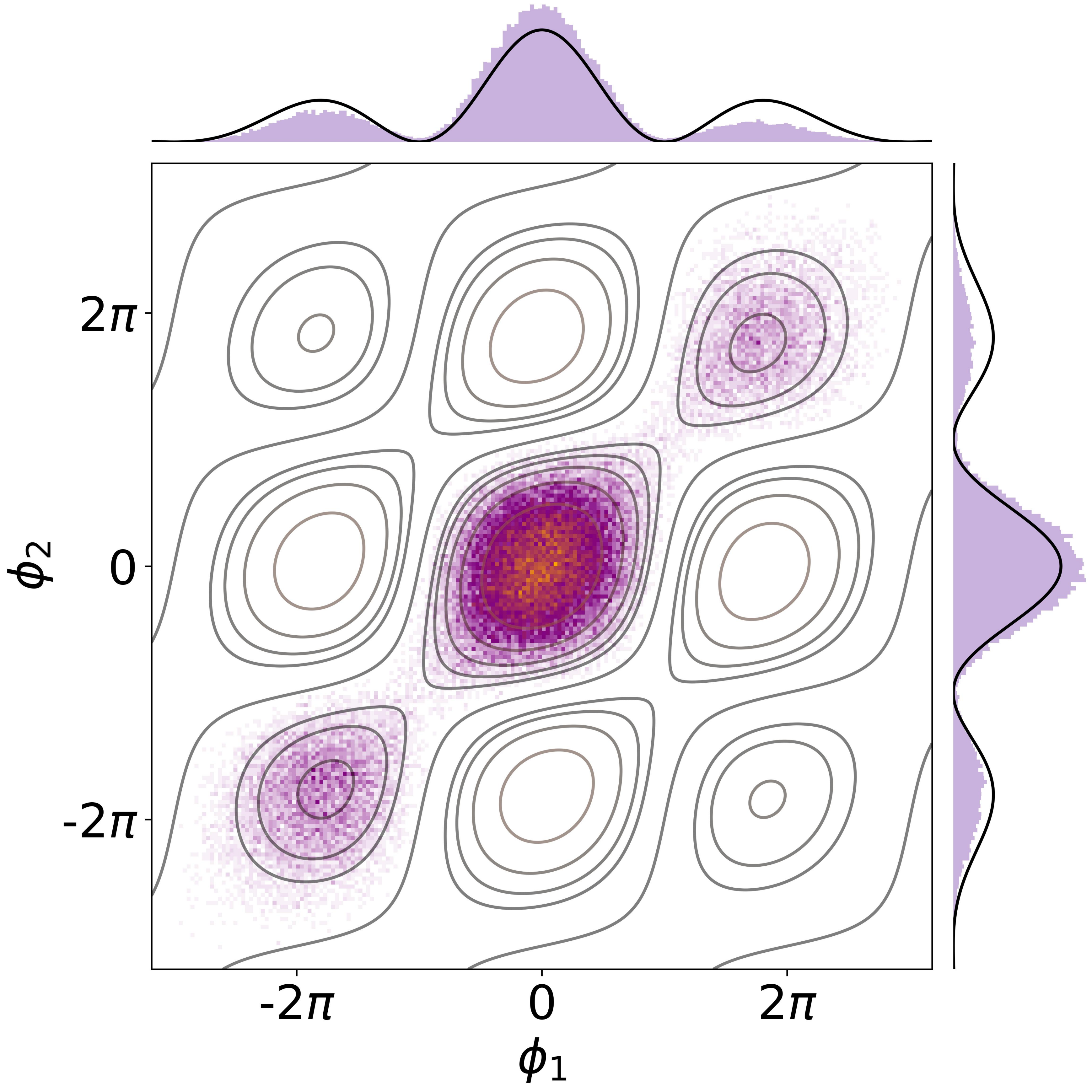
$$H = -\kappa \underbrace{\sum_{\langle x,y \rangle} (a^\dagger_{x,\uparrow} a_{y,\uparrow} + a^\dagger_{x,\downarrow} a_{y,\downarrow})}_{\text{tight−binding}} - \underbrace{\frac{U}{2} \sum_x (n_{x,\uparrow} - n_{x,\downarrow})^2}_{\text{on−site interaction}}$$

- Used to describe carbon nanomaterial, e.g. graphene
- Apply Hubbard-Stratanovich transformation to describe the system with bosonic auxiliary fields ϕ

$$S = \frac{1}{2\tilde{U}} \sum_{x,t} \phi^2_{x,t} - \log\det M[\phi] - \log\det M[-\phi]$$



Current Issues with HMC



$N_x = 2,\ N_t = 1,\ \epsilon = 0.1,\ a = 99.8\ \%$

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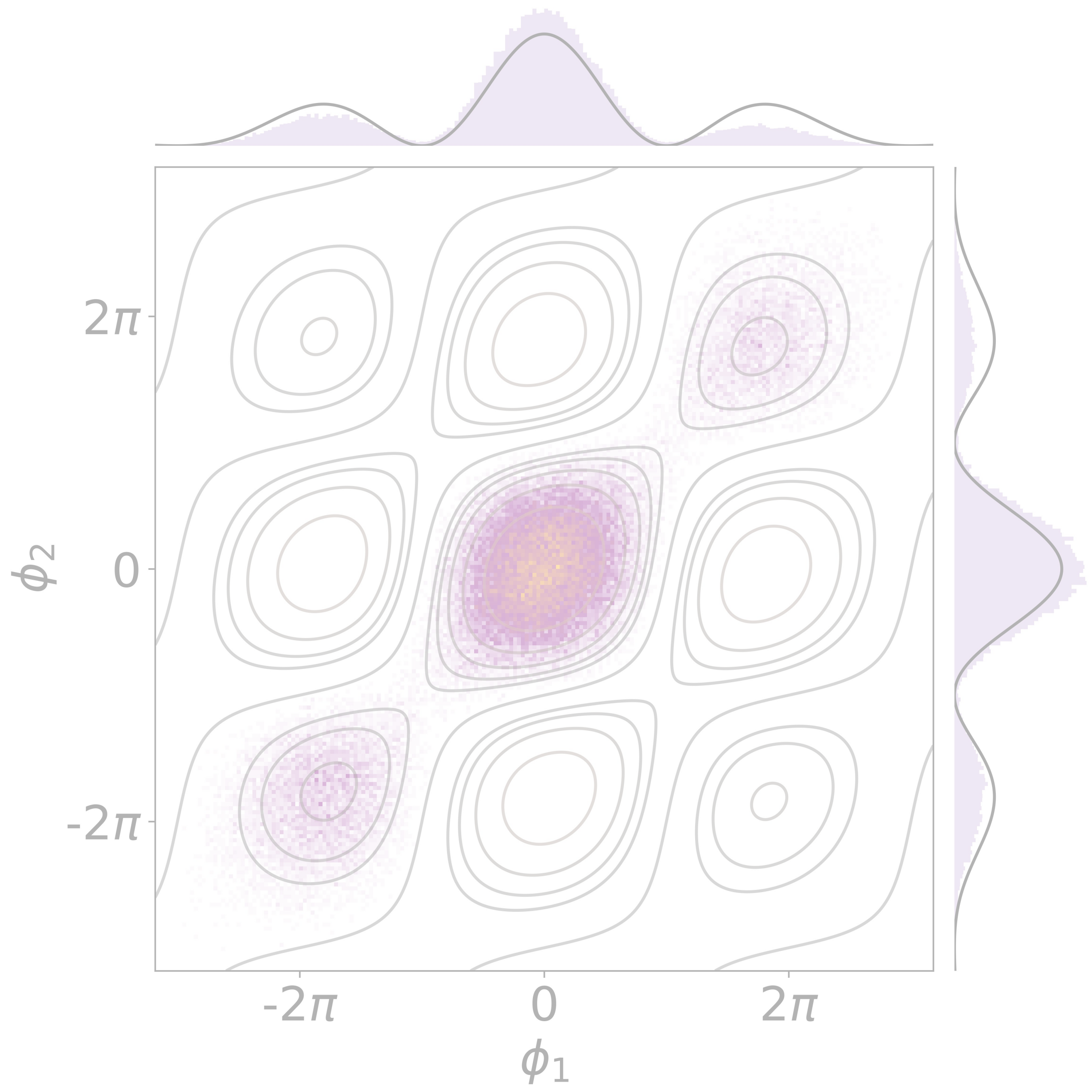

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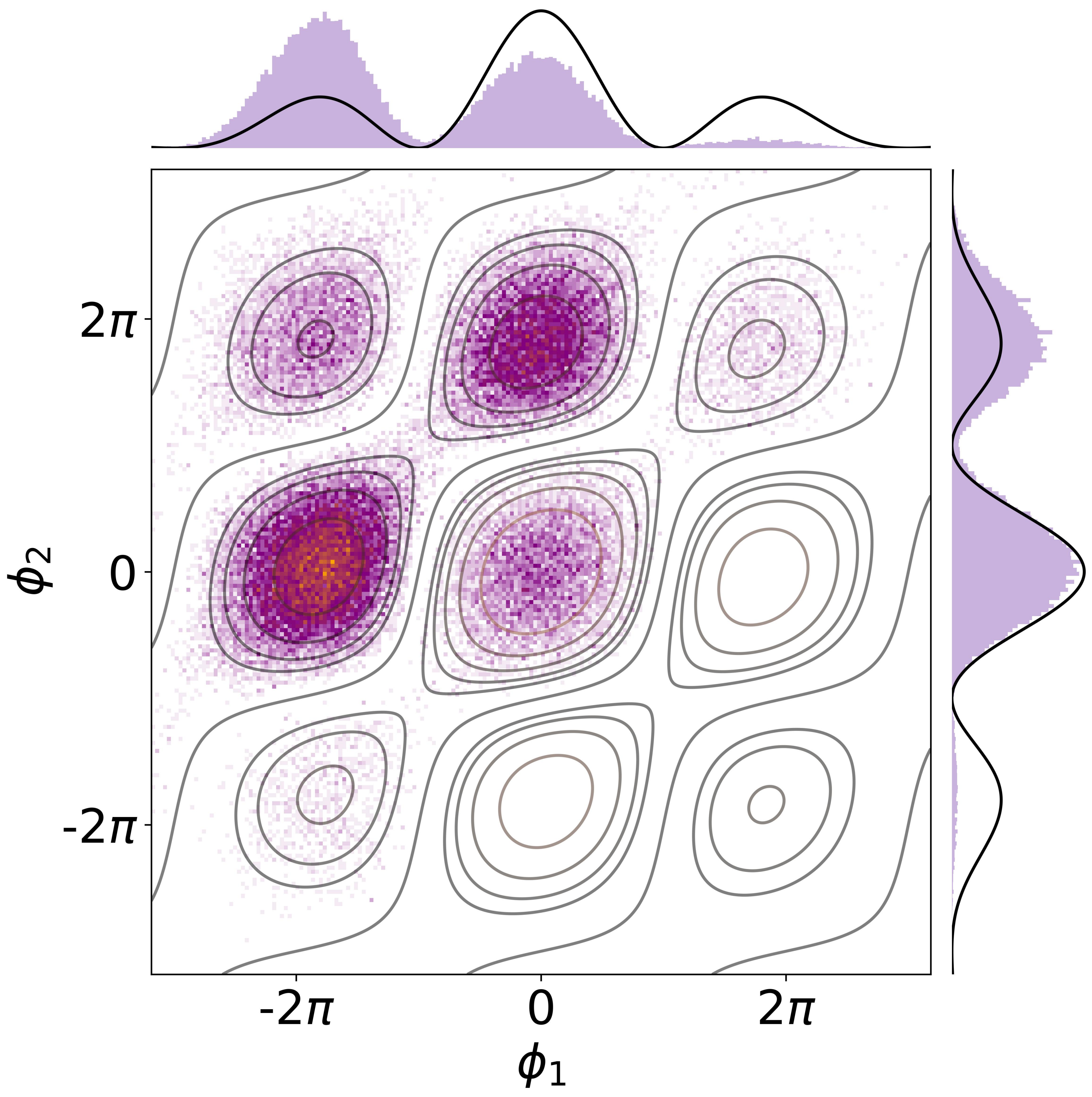

$N_x = 2,\ N_t = 1,\ \epsilon = 0.5,\ a = 96.5\ \%$

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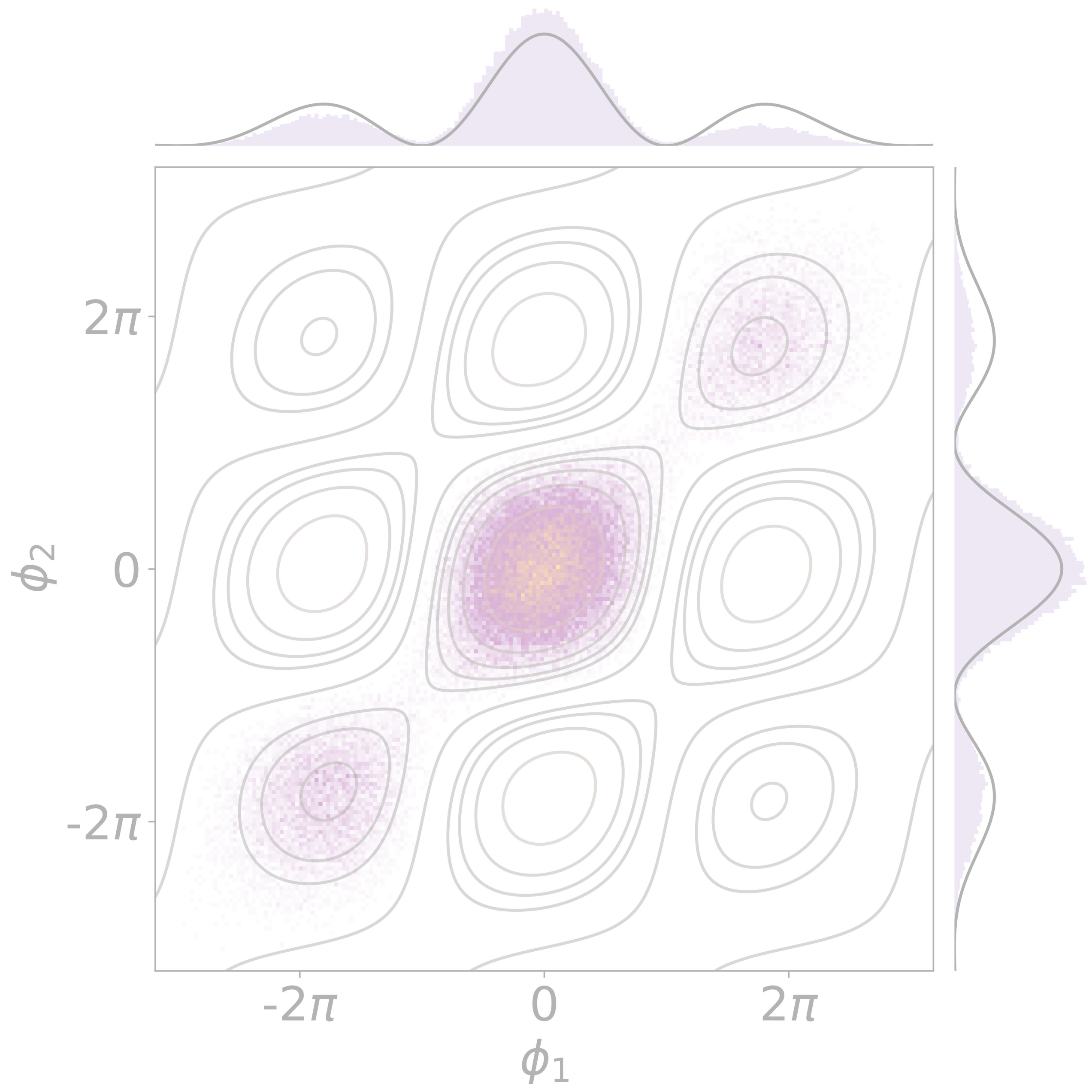

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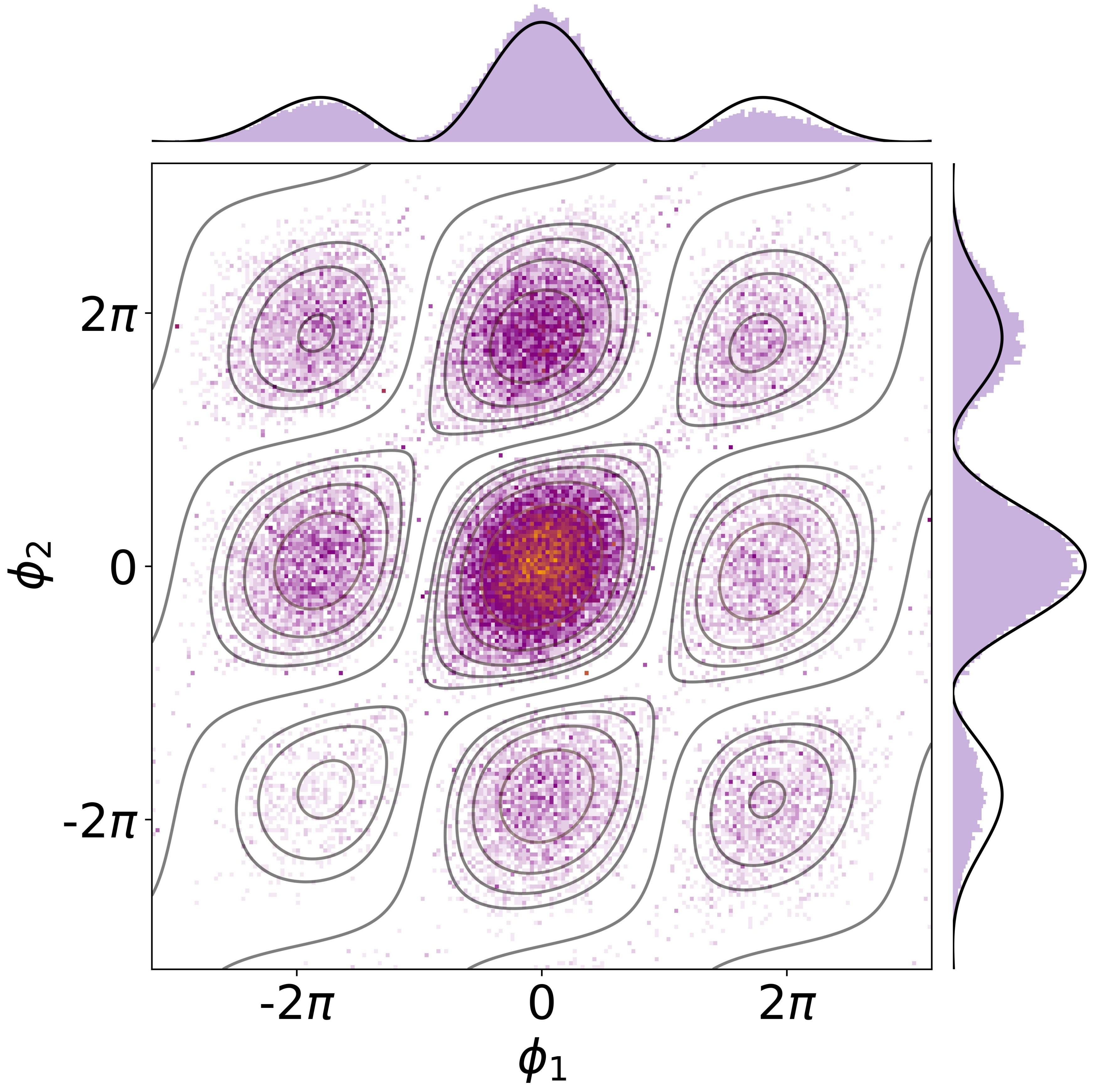
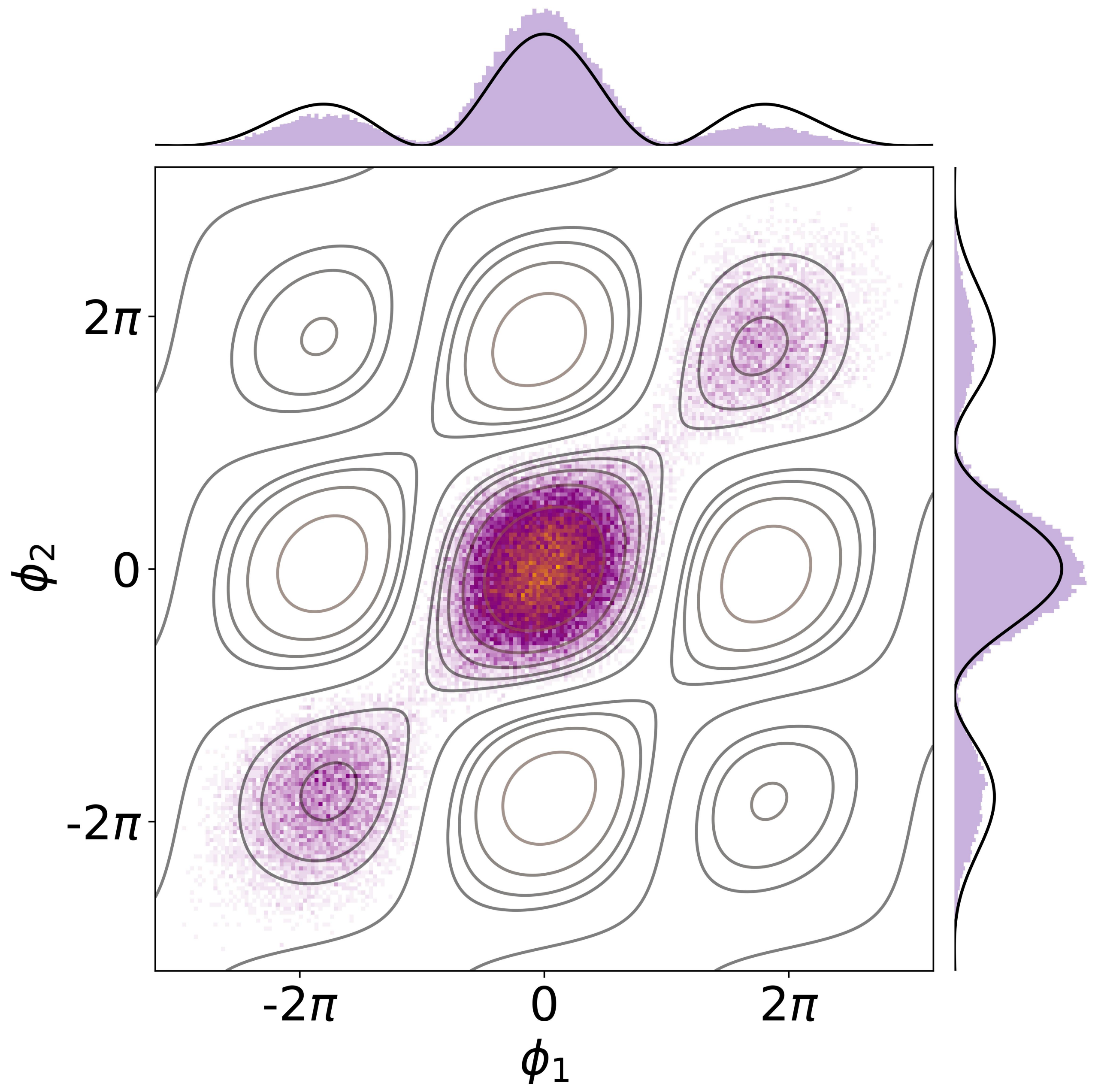


$N_x = 2,\ N_t = 1,\ \epsilon = 1.0,\ a = 87.2\,\%$

Current Issues with HMC



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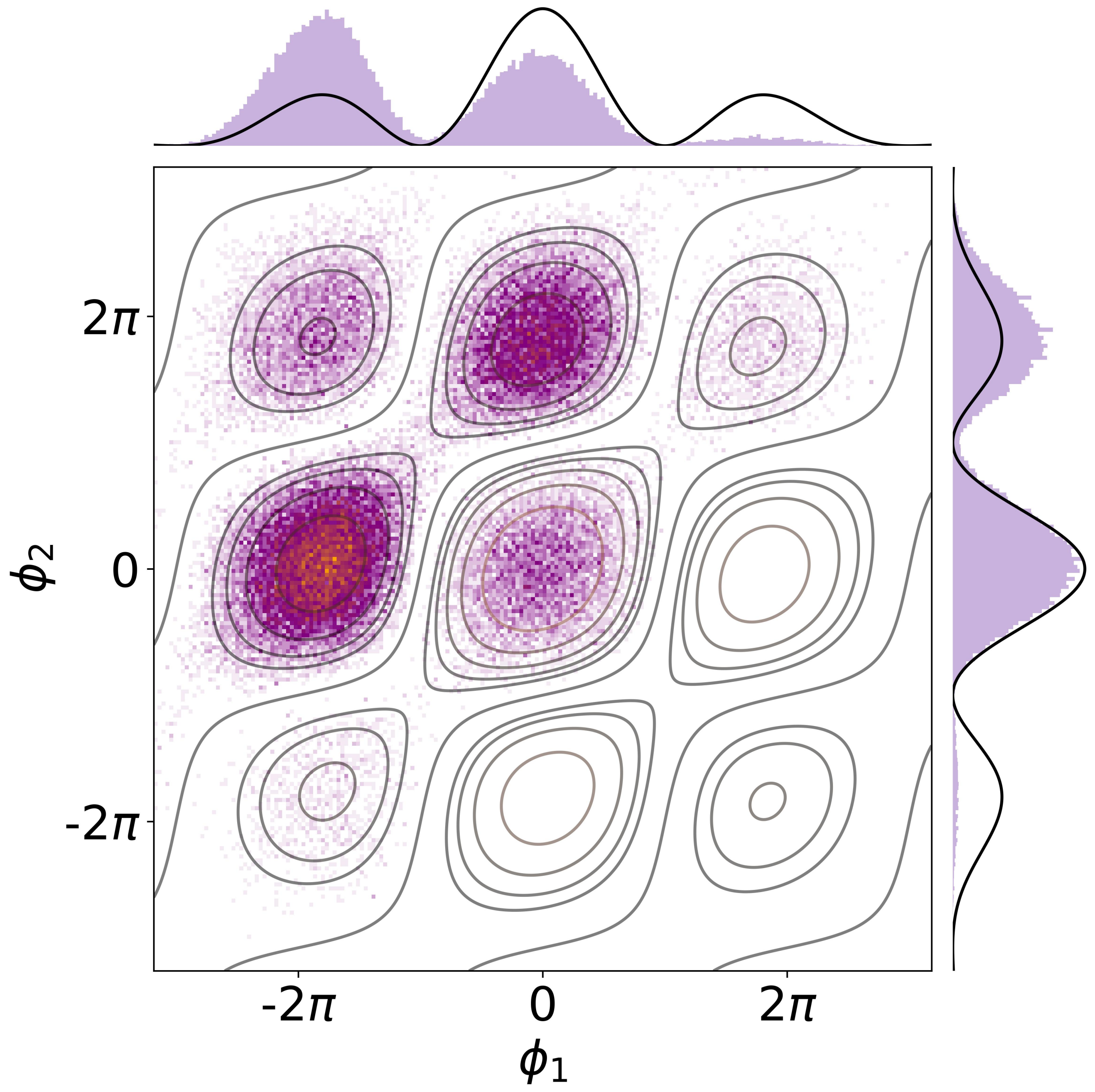

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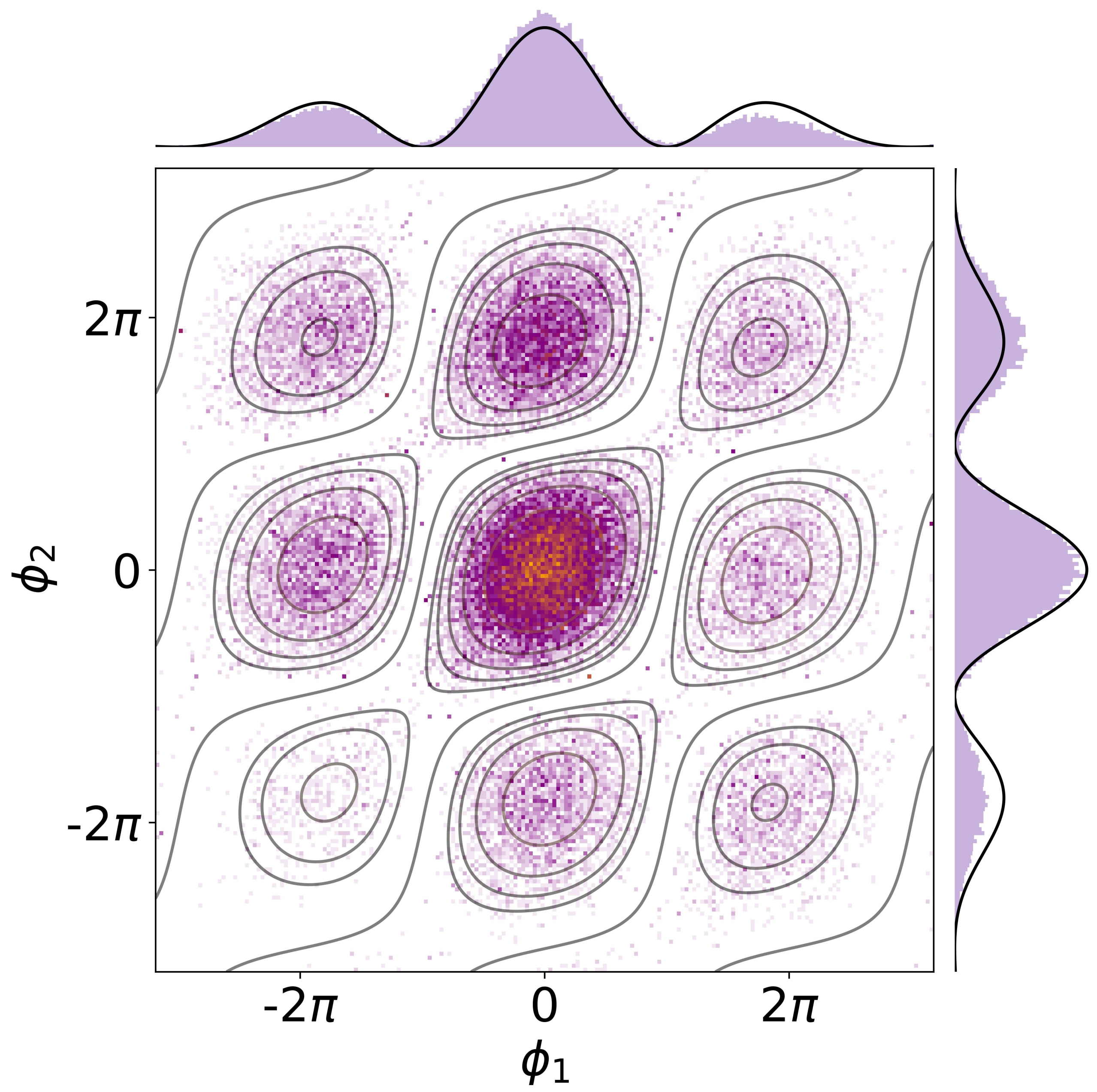

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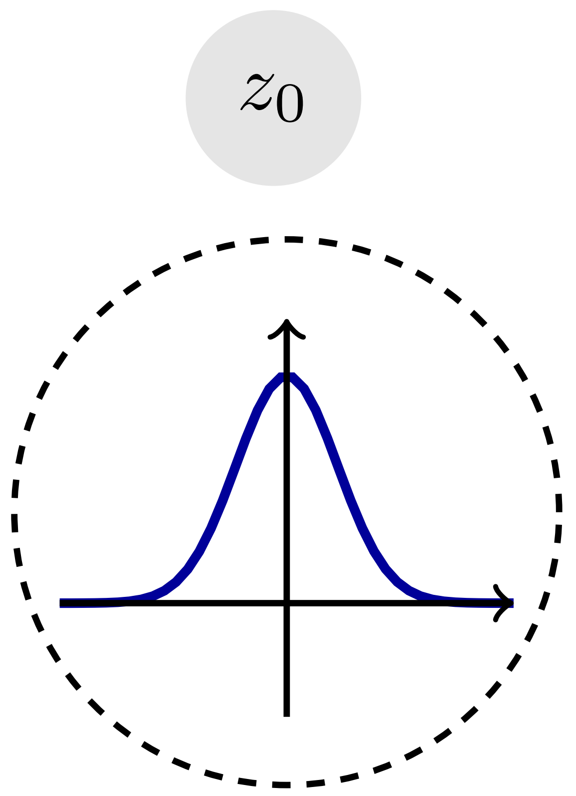
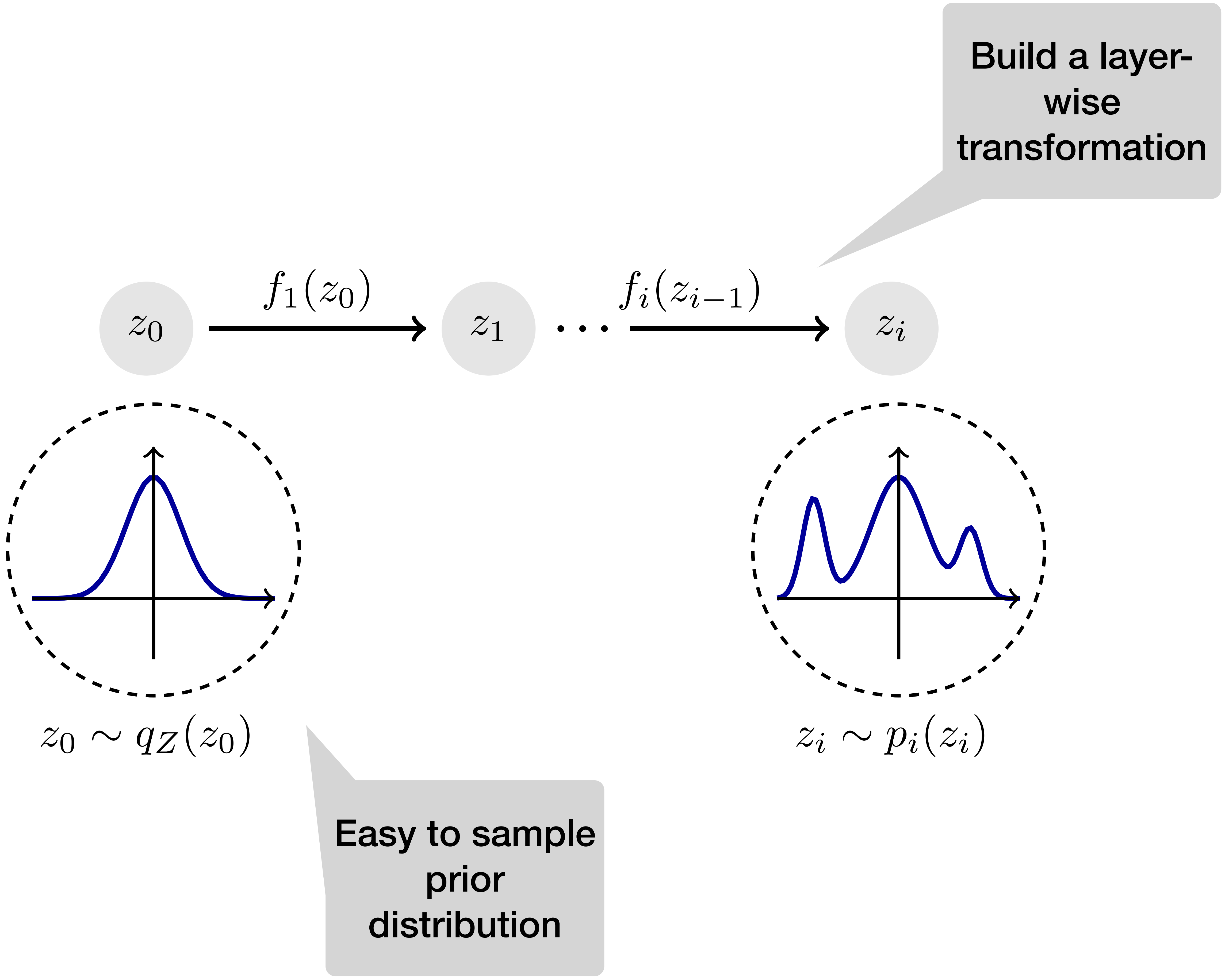
Normalizing Flows



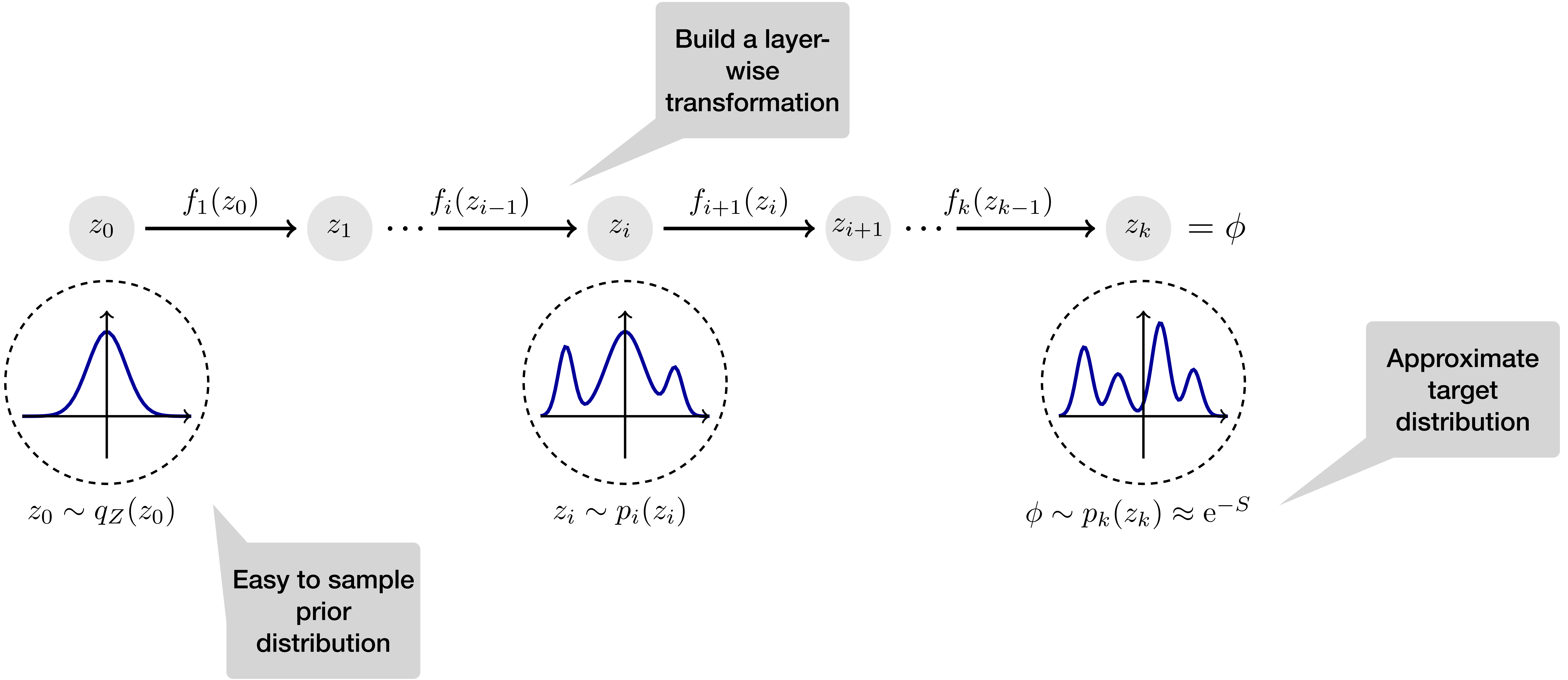
$z_0 \sim q_Z(z_0)$

Easy to sample prior distribution

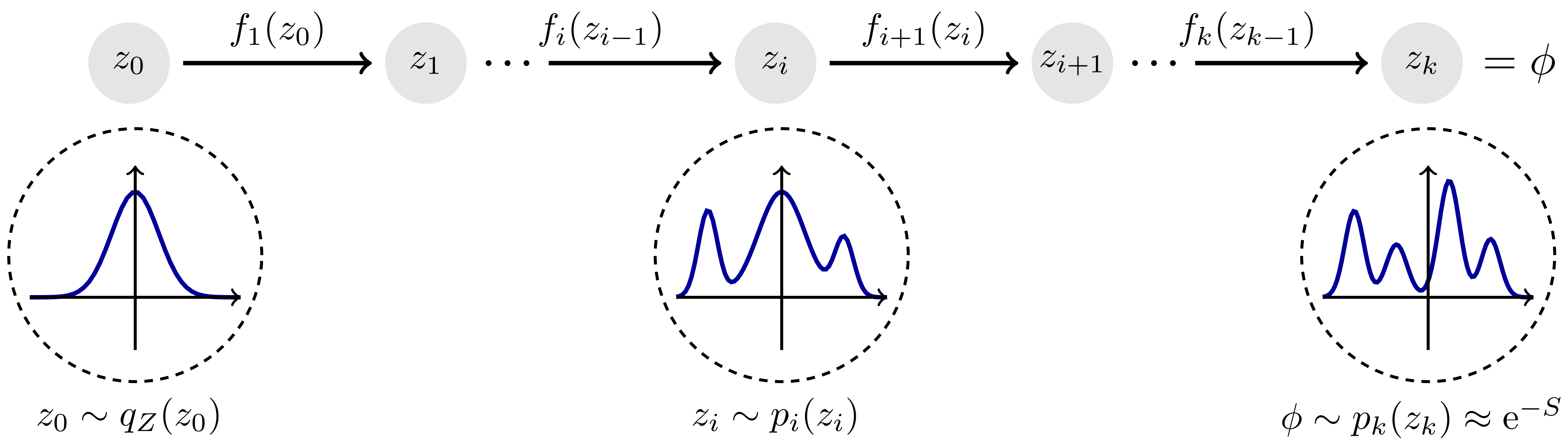
Normalizing Flows



Normalizing Flows



Normalizing Flows



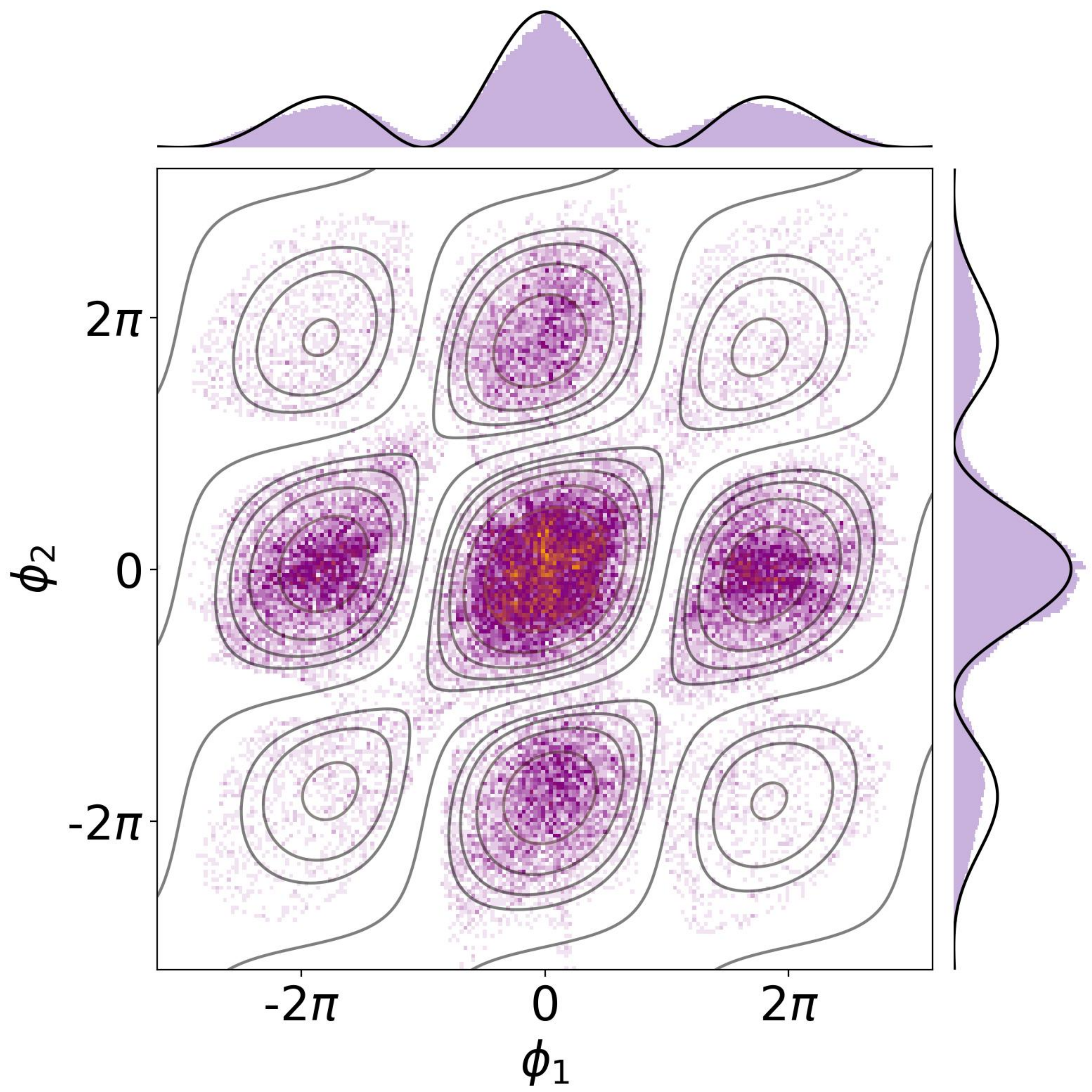
<u>Advantages</u>

- Embarrassingly parallel sampling
- Independent and identically distributed (i.i.d) samples -> small autocorrelation times
- Correctly normalized distribution → estimation of thermodynamic observables

Already been applied to :

- 3+1D LQCD
  Abbot, et al., 2024
- Fermionic lattice field theories
  Albergo, et al., 2021
- Thermodynamic observables
  Nicoli, et. al., 2020
- ϕ^4-Theory
  Albergo, et al., 2019
- …

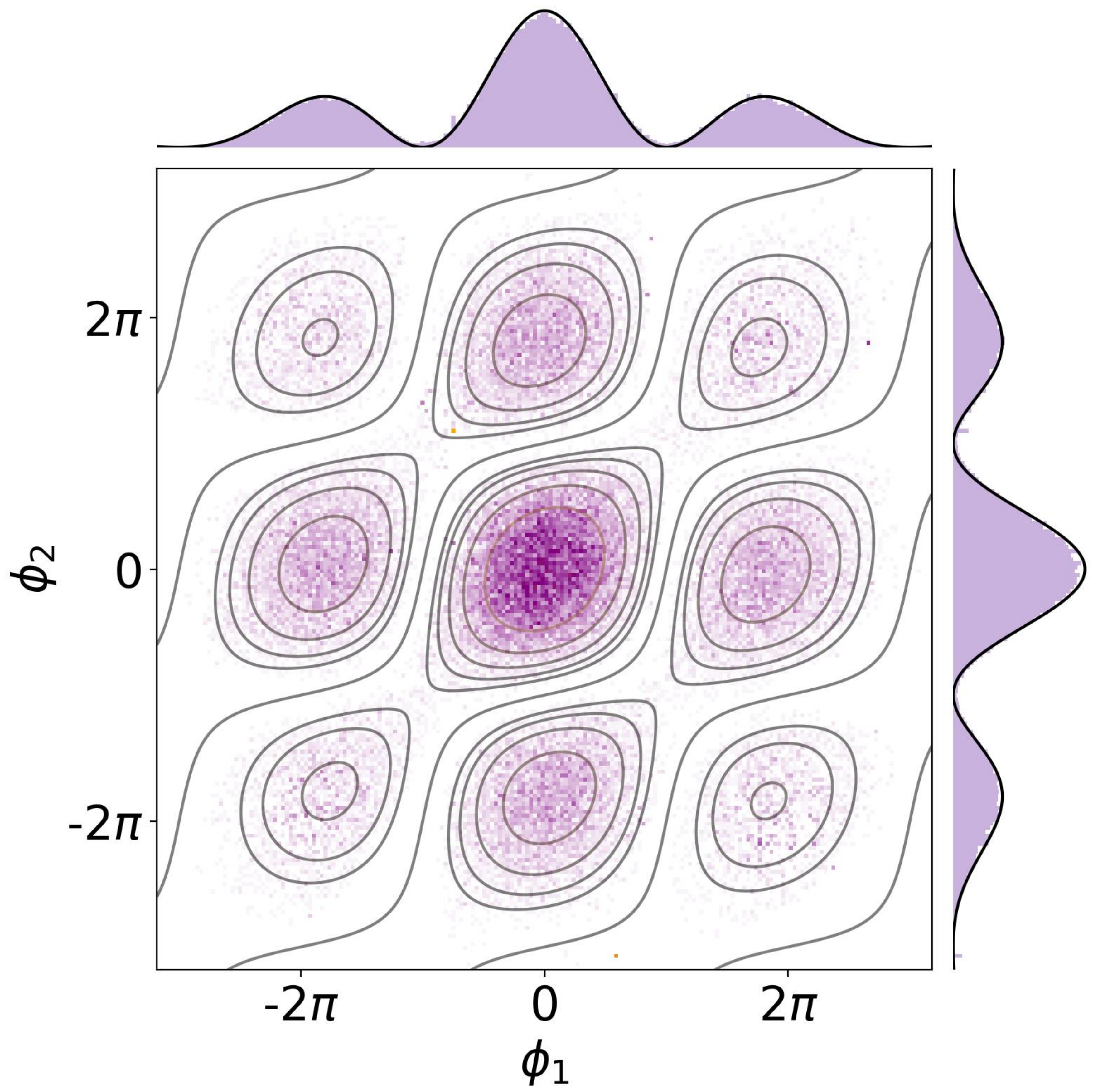
Result: Hubbard Model with Normalizing Flows



$N_x = 2,\ N_t = 1$

70.1% effective sampling size

Result: Hubbard Model with Normalizing Flows



$N_x = 2,\ N_t = 1$

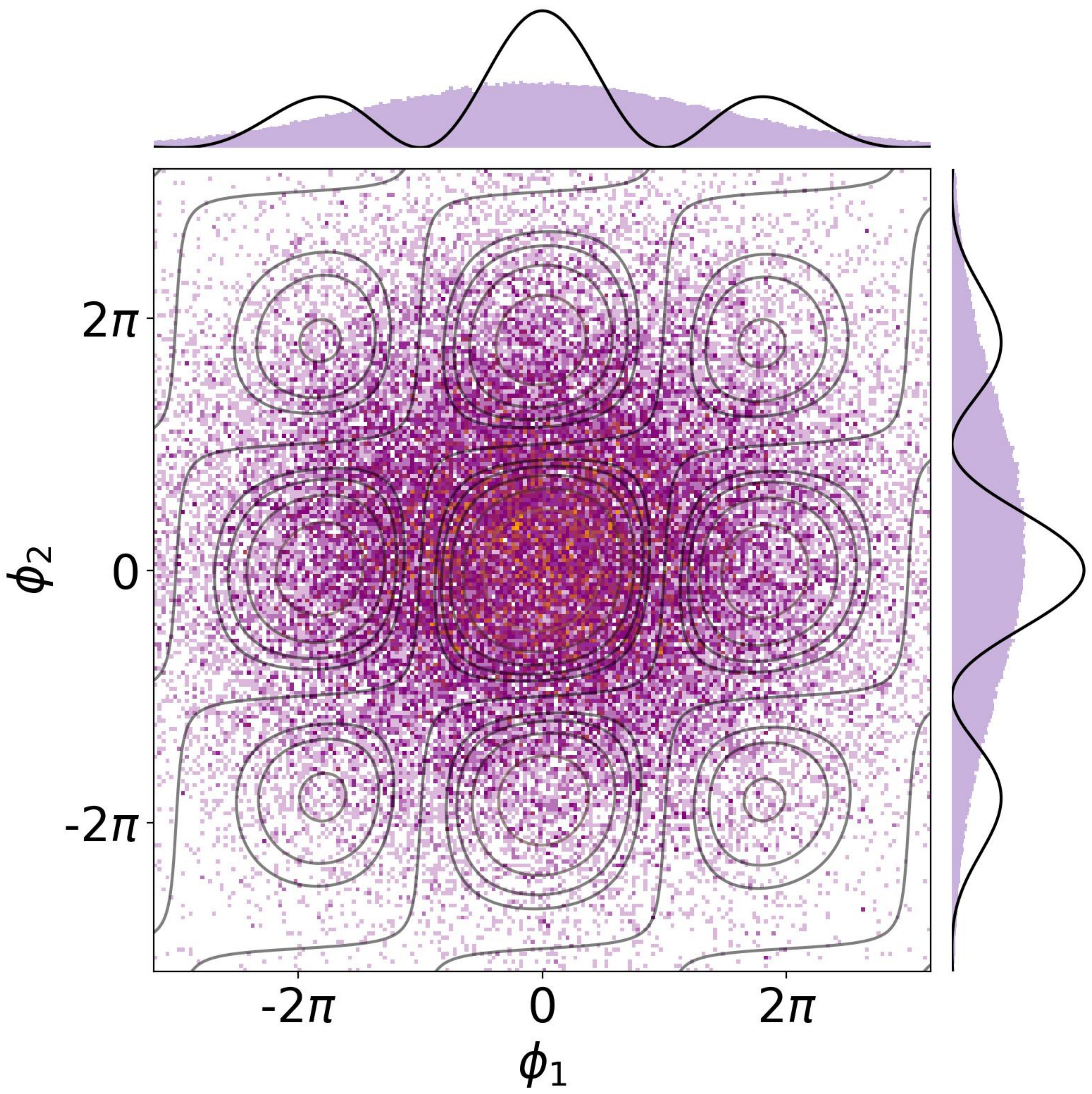
70.1% effective sampling size

74.2% acceptance rate

$\tau = 1.19 \pm 0.04$

$\tau_{\mathrm{HMC}} = 443 \pm 136$

Result: Hubbard Model with Normalizing Flows

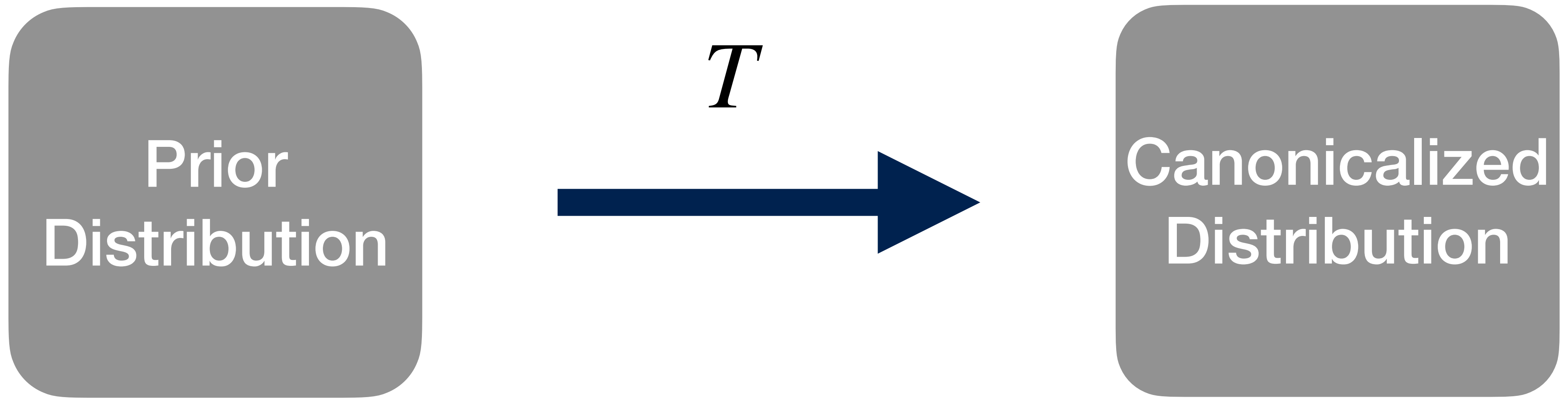


$N_x = 2,\ N_t = 2$

Equivariant Normalizing Flows

Prior
Distribution

Equivariant Normalizing Flows



Equivariant Normalizing Flows

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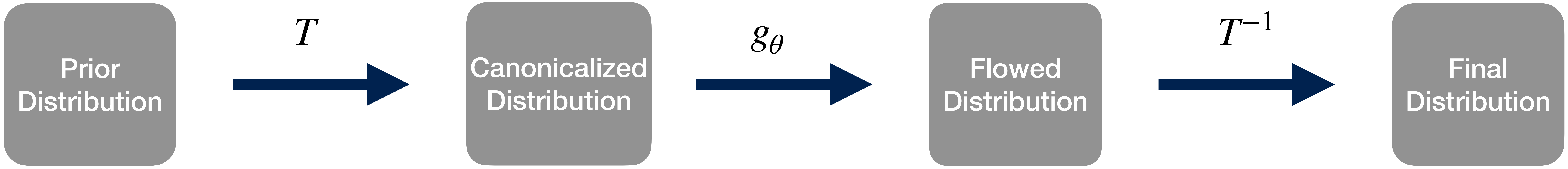

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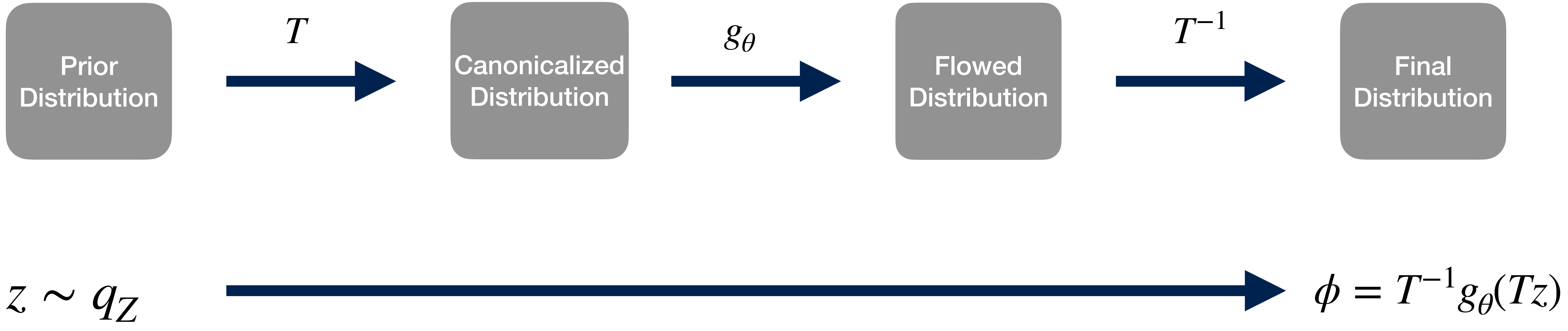
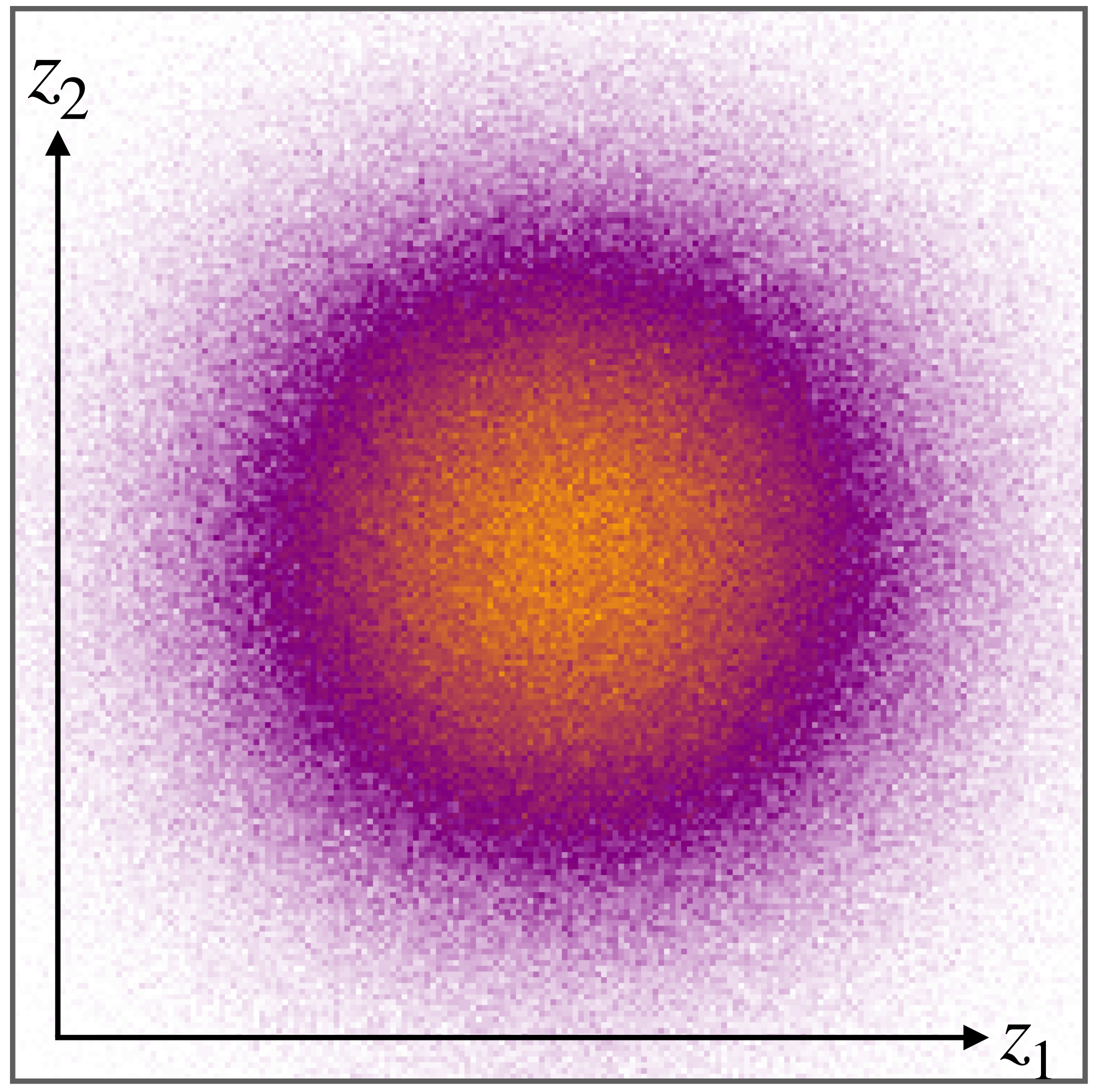


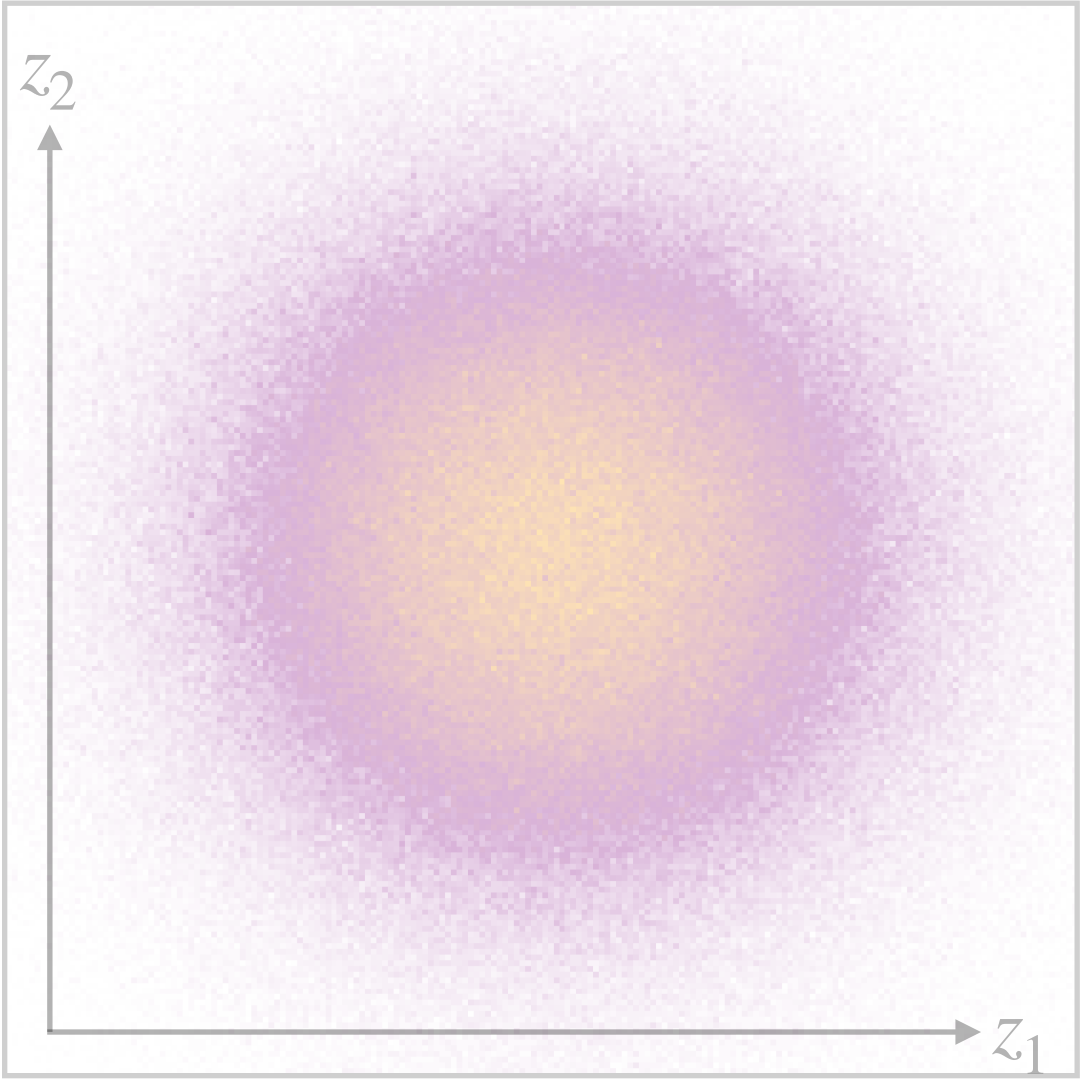
See also: J. Köhler et al., 2020, D. Boyda et al., 2021

Equivariant Normalizing Flows



Prior distribution

Equivariant Normalizing Flows



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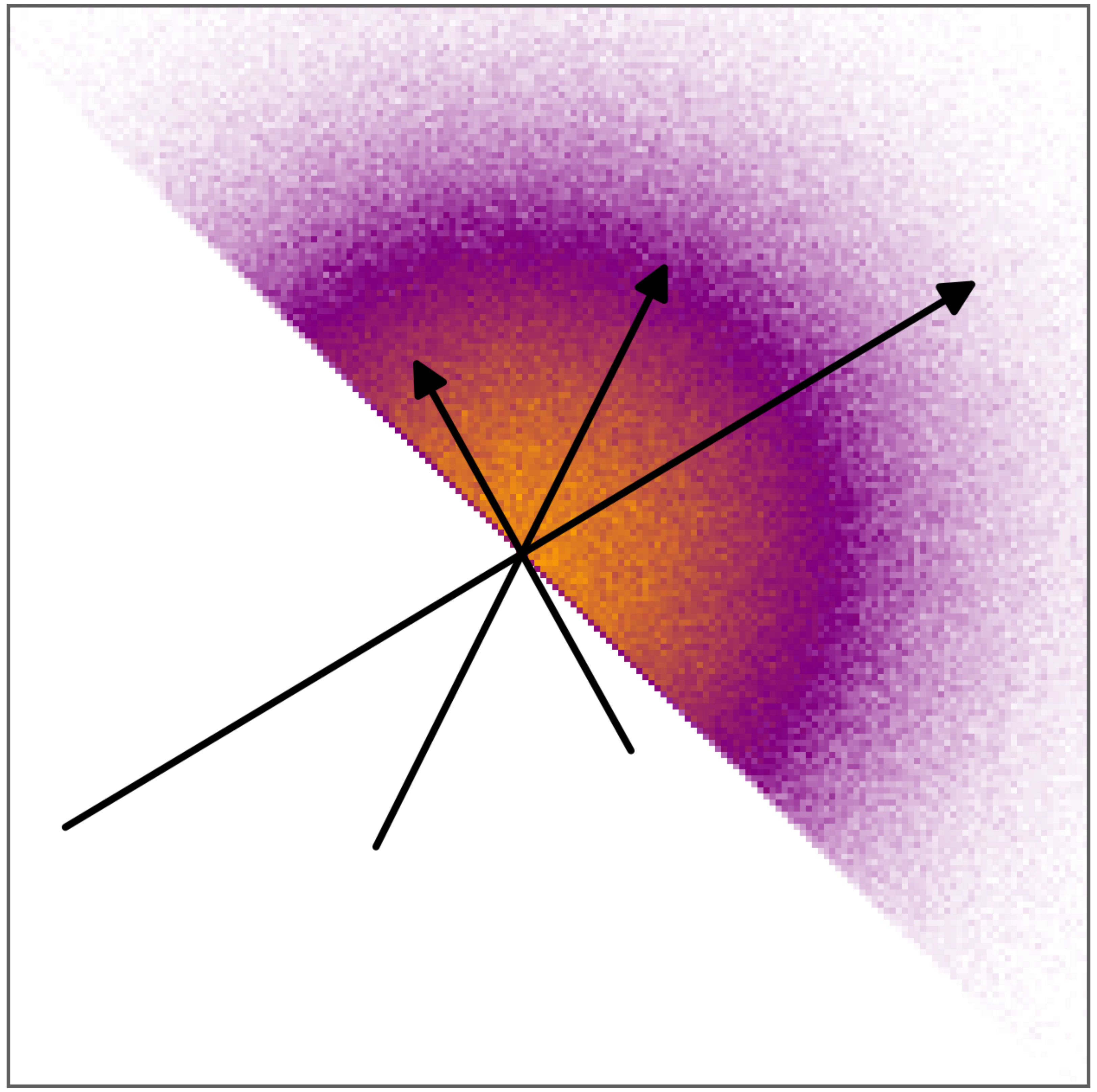
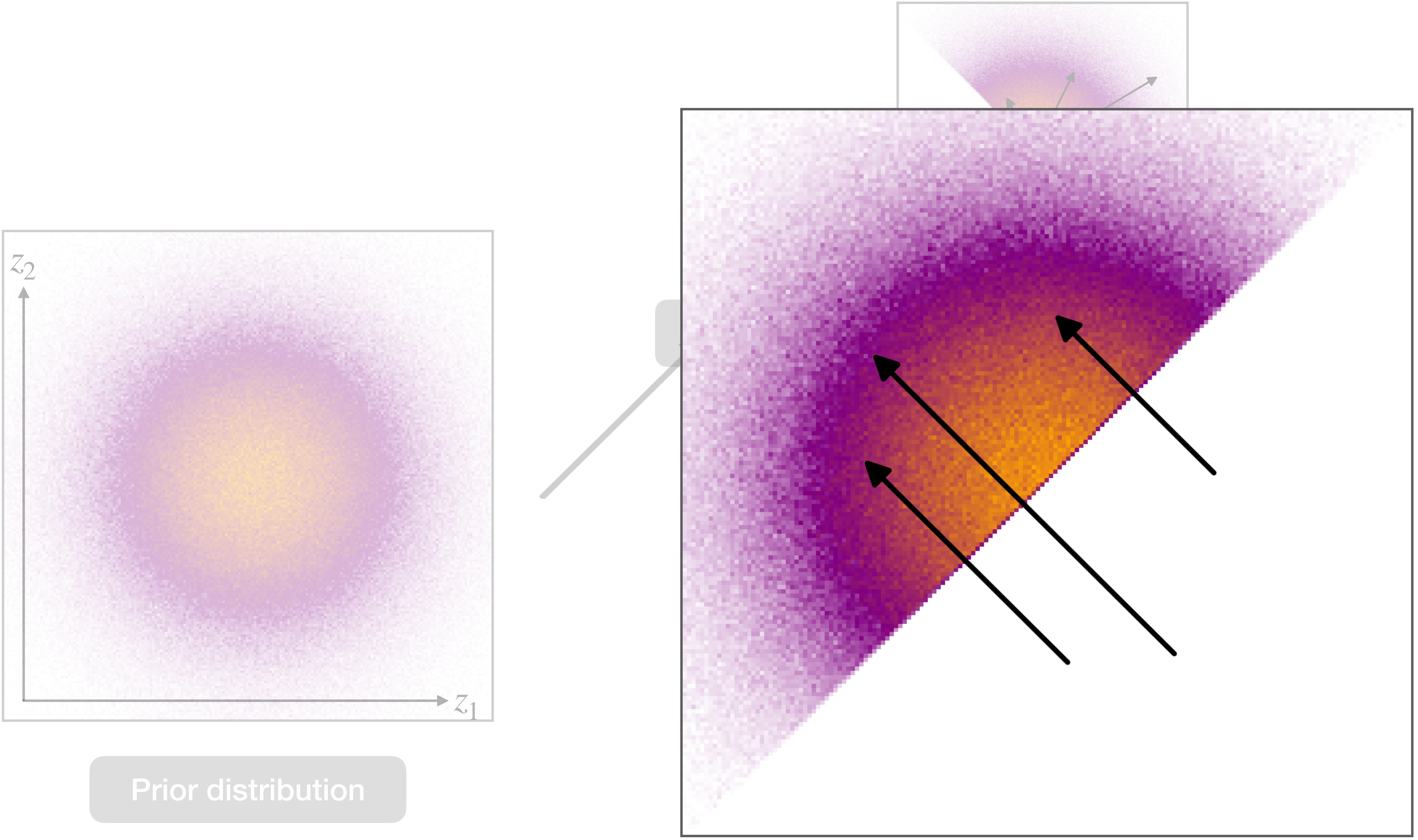


Z_2 Symmetry

$$z \to \begin{cases} z & \text{if } z_1 + z_2 \geq 0 \\ -z & \text{else} \end{cases}$$

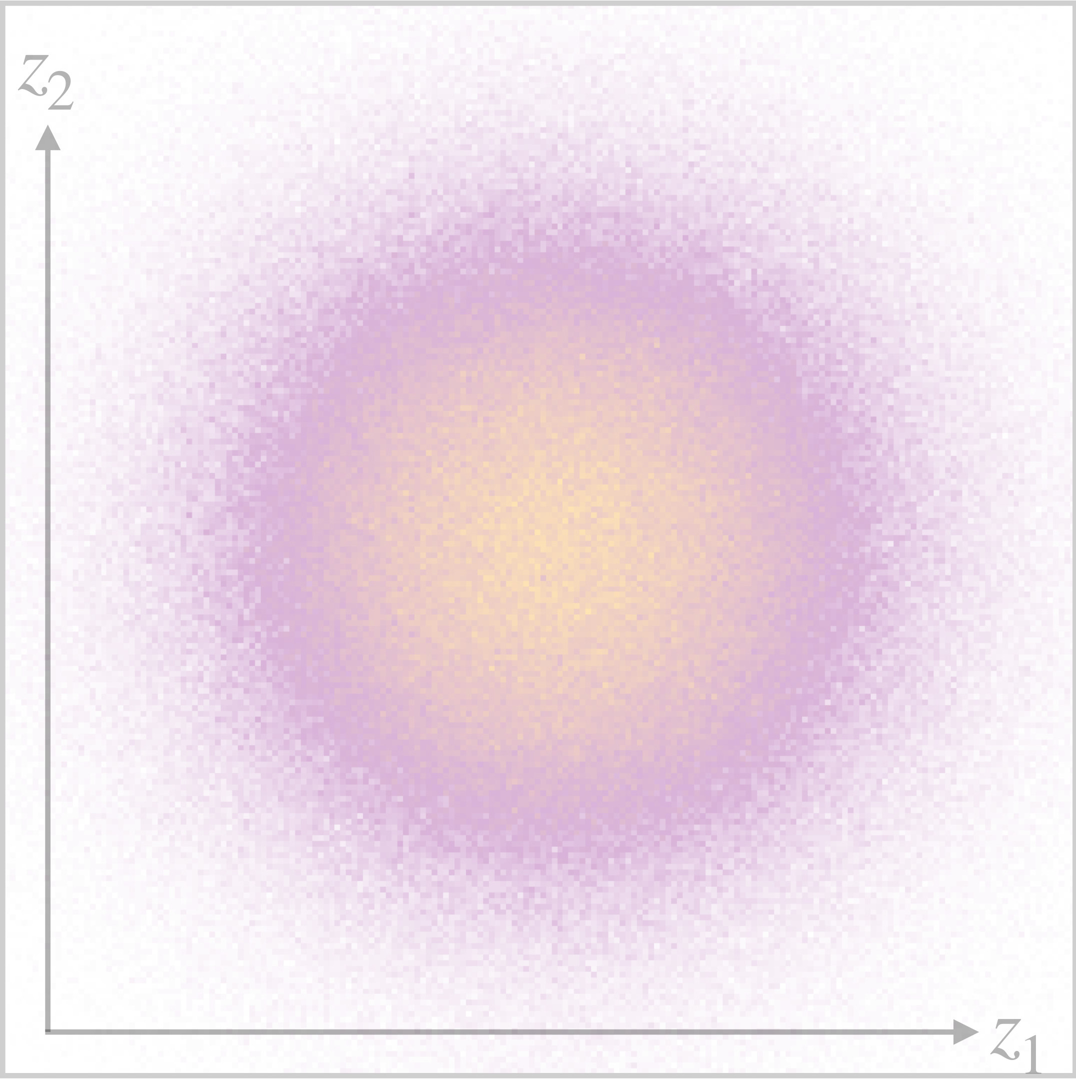
Equivariant Normalizing Flows



Spacetime Symmetry

$$(z_1, z_2) \to \begin{cases} (z_1, z_2) & \text{if } z_1 - z_2 \leq 0 \\ (z_2, z_1) & \text{else} \end{cases}$$

Equivariant Normalizing Flows



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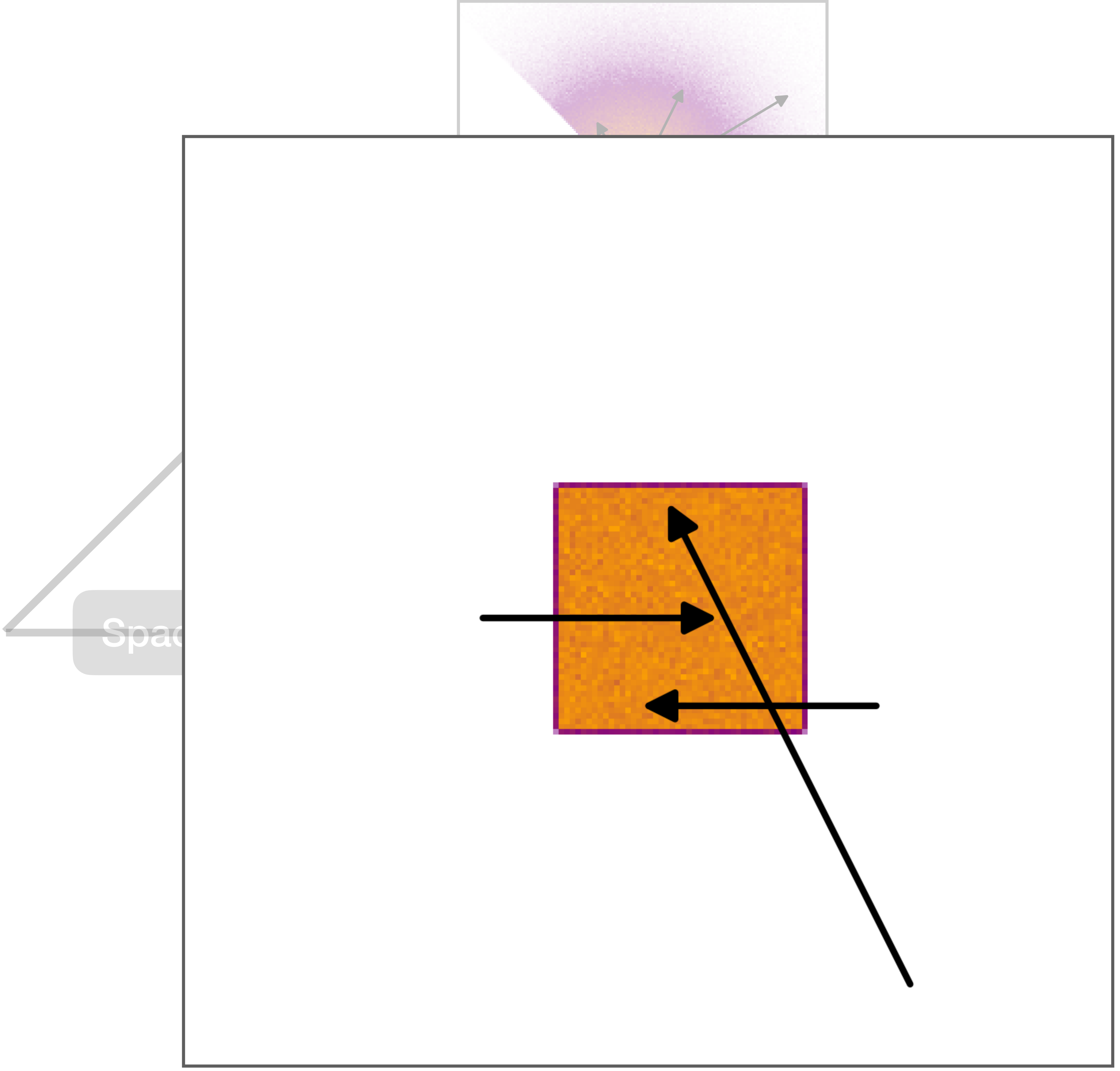
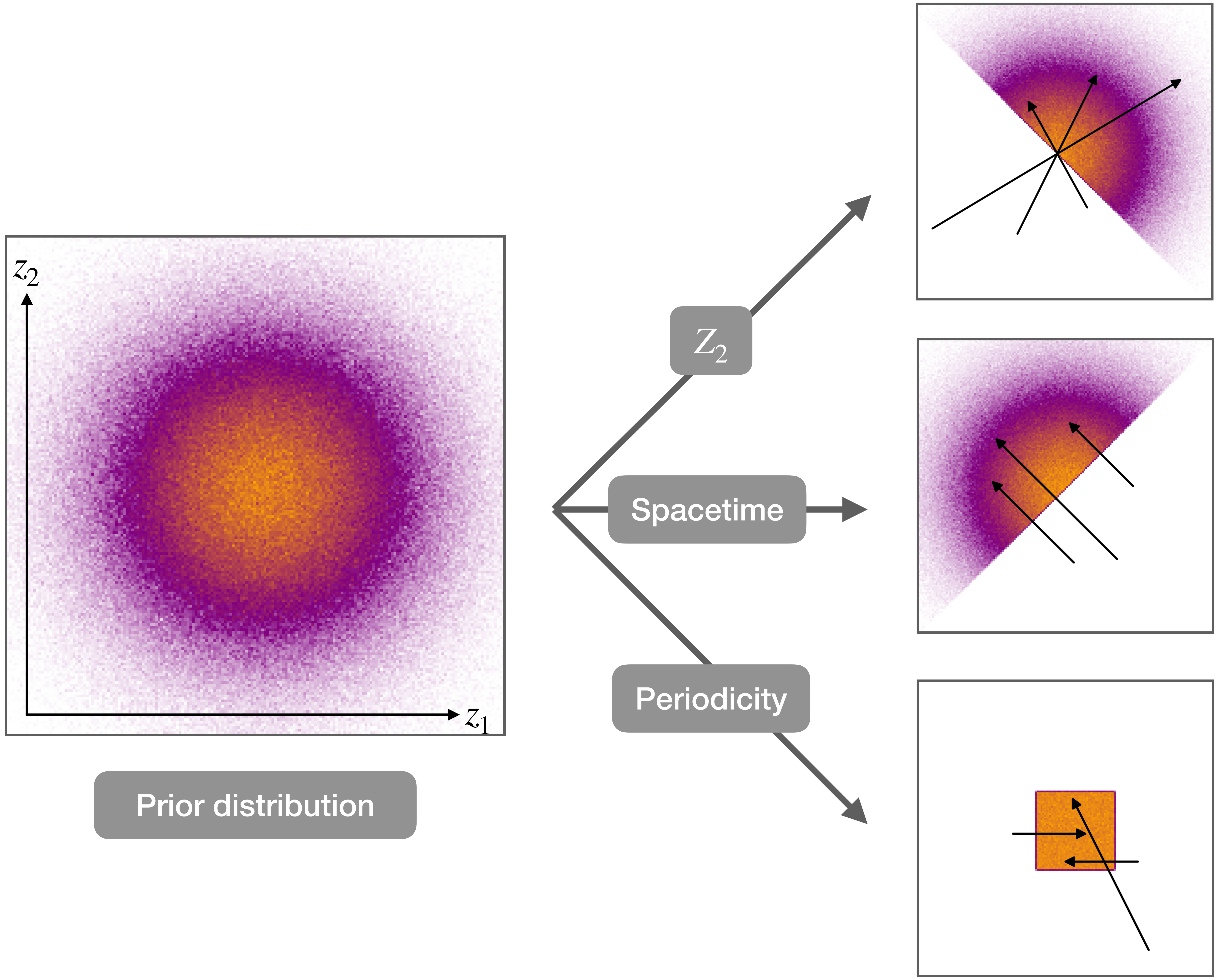


Periodicity Symmetry

$$z \rightarrow z - 2\pi \cdot \text{round}\left(\frac{z}{2\pi}\right)$$

Equivariant Normalizing Flows



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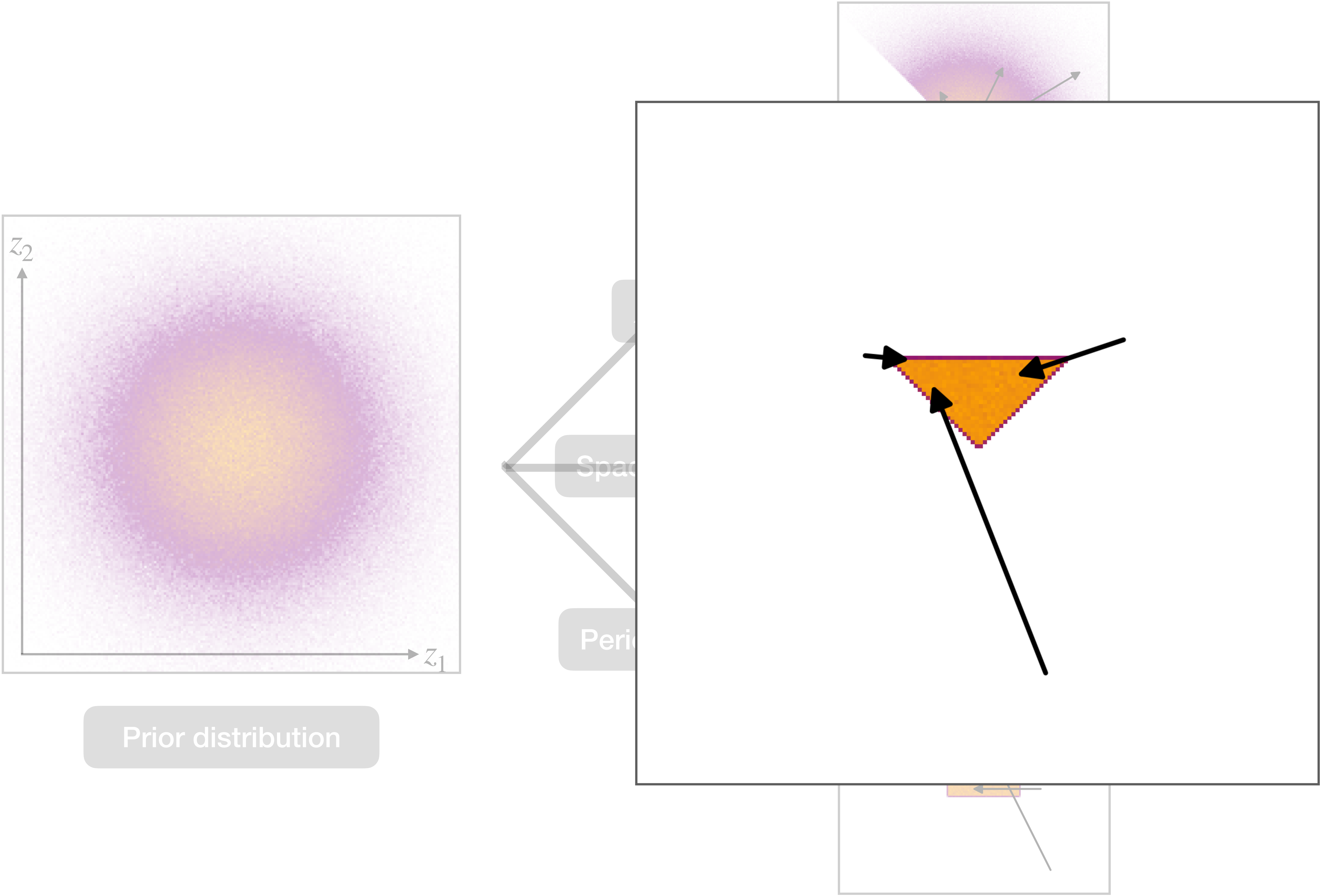

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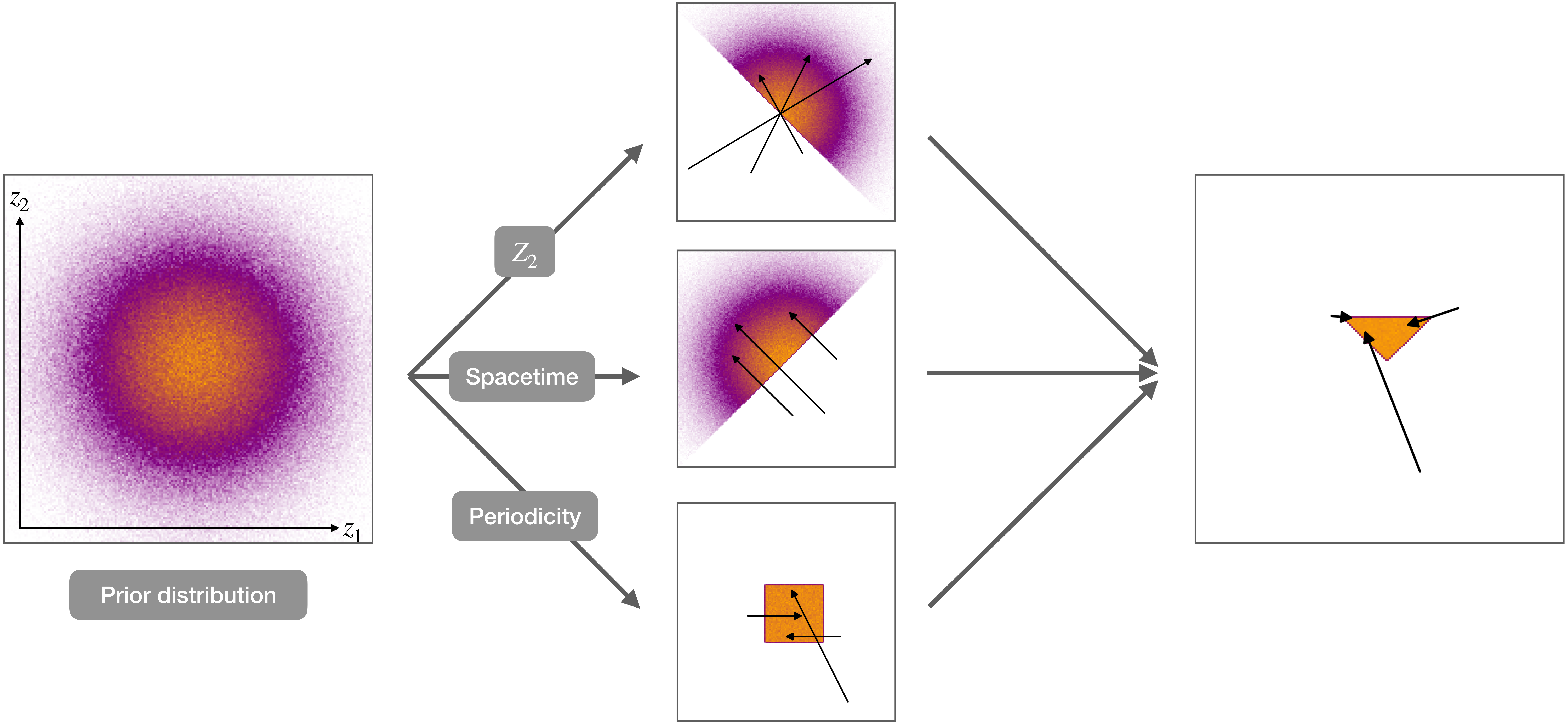
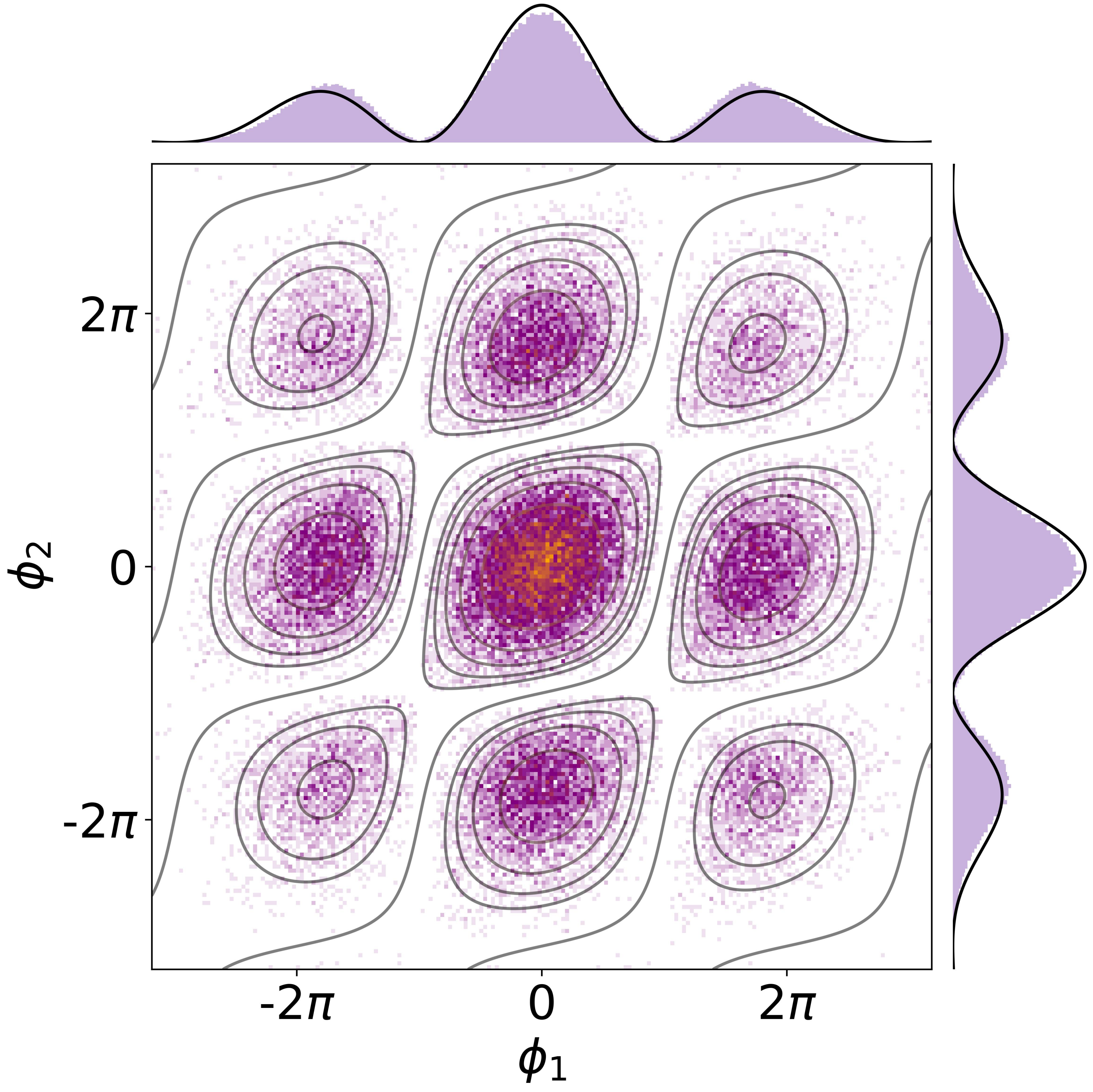


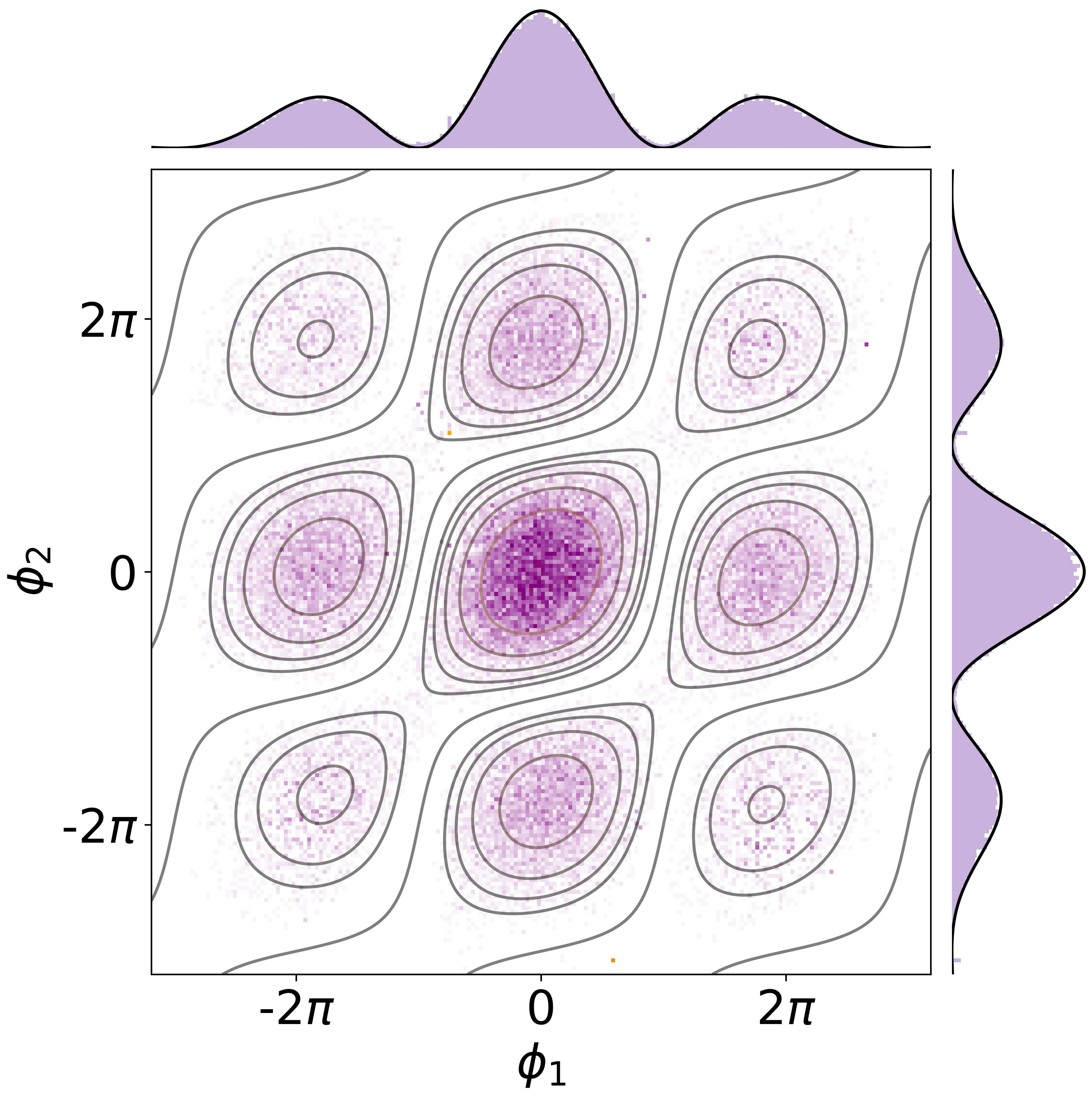
Results: Equivariant Flow



$N_x = 2,\ N_t = 1$

92.3% effective sampling size

Results: Reweighted Equivariant Flow



$N_x = 2,\ N_t = 1$

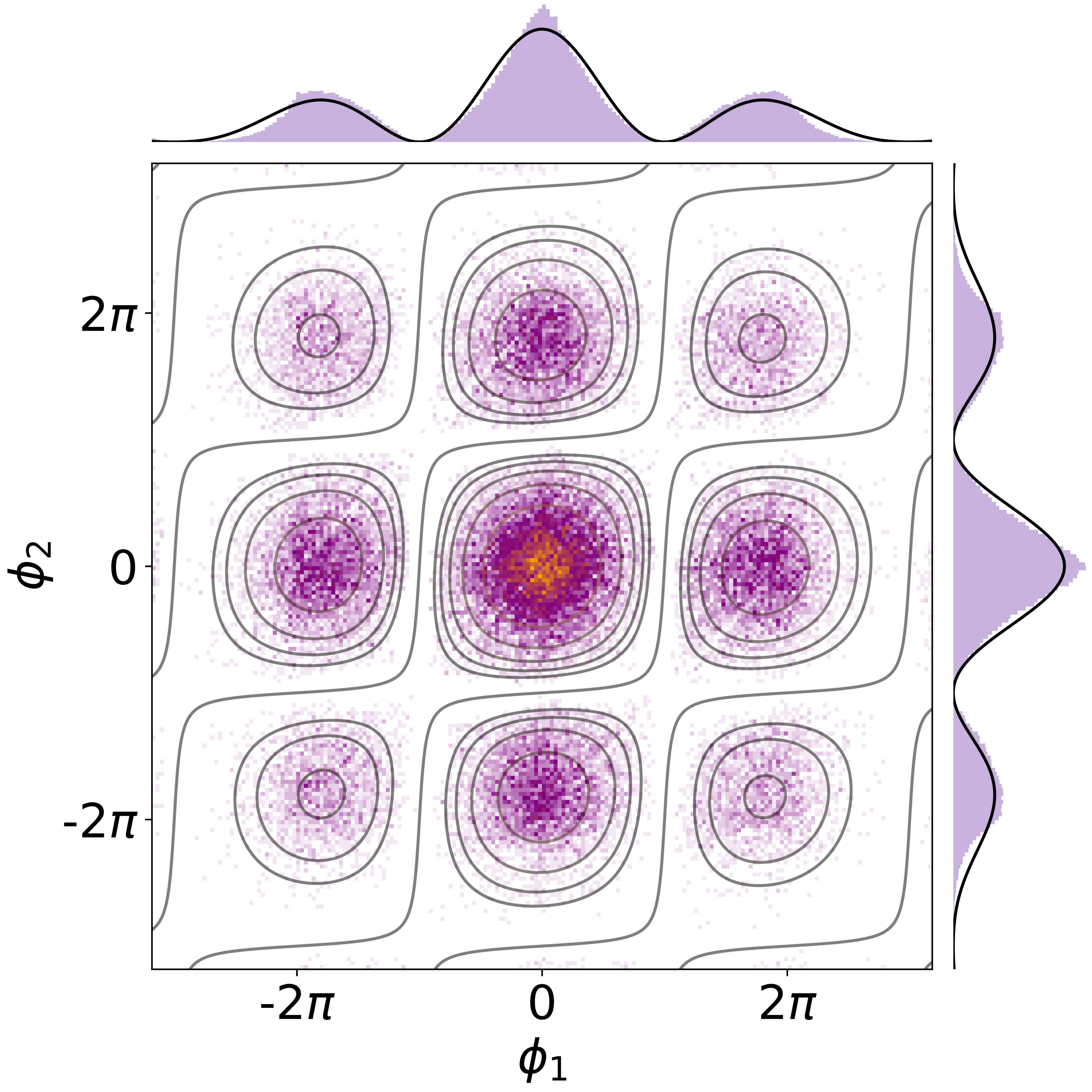
92.3% effective sampling size

84.8% acceptance rate

$\tau = 0.72 \pm 0.02$

$\tau_{\mathrm{HMC}} = 443 \pm 136$

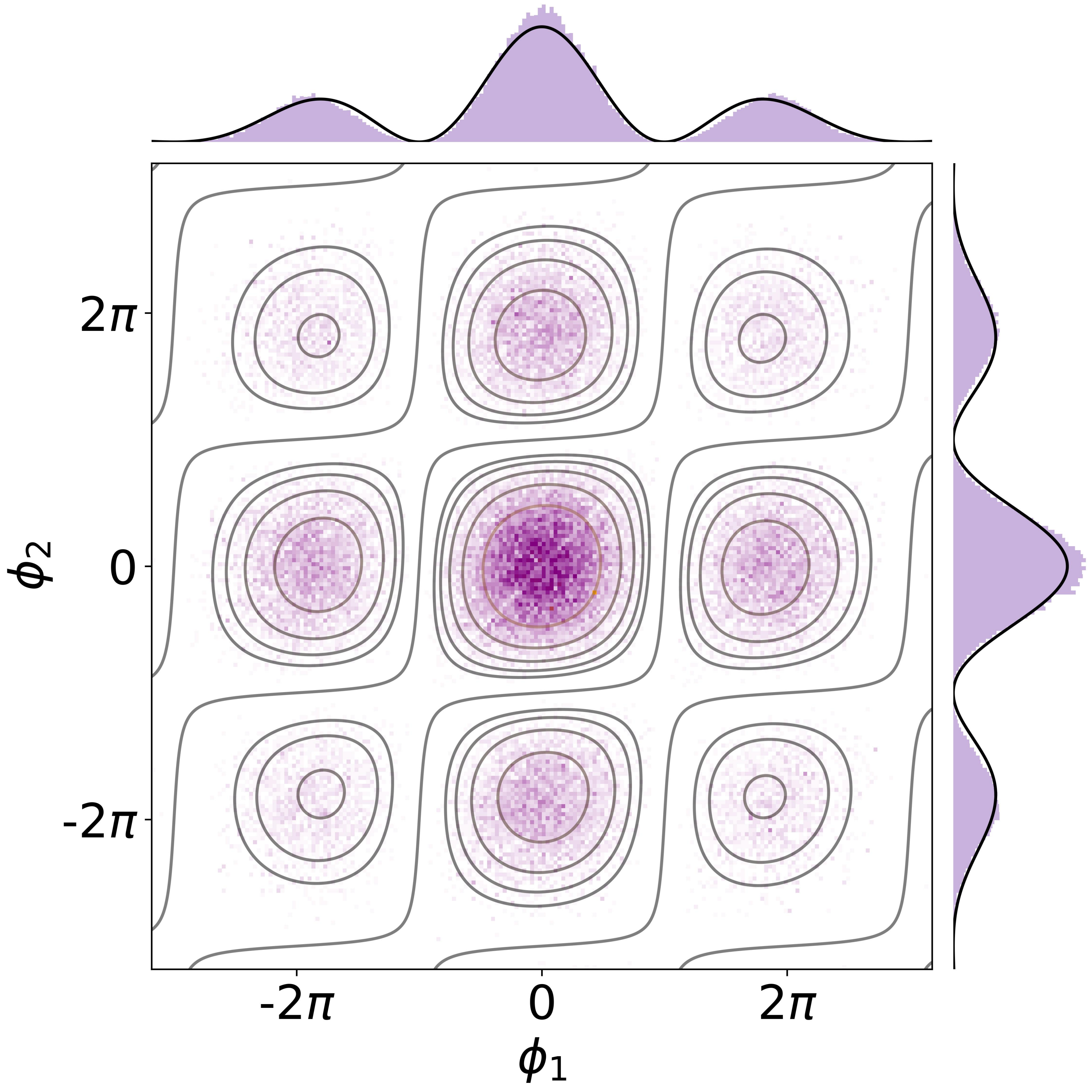
Results: Equivariant Flow



$N_x = 2,\ N_t = 2$

73.9% effective sampling size

Results: Reweighted Equivariant Flow



$N_x = 2,\ N_t = 2$

73.9% effective sampling size

69.4% acceptance rate

$\tau = 1.19 \pm 0.04$

Summary and Outlook

- For the first time, applied normalizing flows to the Hubbard model
- Incorporated symmetries in the architecture
- Correctly reproduced distributions for small lattices

Outlook

- Reach larger lattices
- Calculate further observables, e.g. correlators

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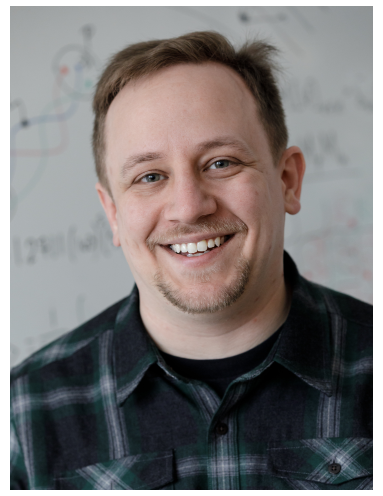
In collaboration with


Janik Kreit


Evan Berkowitz


Lena Funcke


Thomas Luu


Kim Nicoli


Marcel Rodekamp

Poster session: Janik Kreit, Tuesday 17:15

Backup Slides

The Hubbard Action

The Hubbard action in the spin basis reads

$$S = \frac{1}{2\tilde{U}} \sum_{x,t} \phi_{x,t}^2 - \log \det M[\phi] - \log \det M[-\phi],$$

and in the particle-hole basis

$$S = \frac{1}{2\tilde{U}} \sum_{x,t} \phi_{x,t}^2 - \log \det M[i\phi] - \log \det M[-i\phi]\,.$$

The fermion matrix M reads

$$M^e[\phi]_{x't',xt} = \delta_{x',x}\delta_{t',t} - [e^h]_{x',x} e^{\phi_{xt}} B_{t'} \delta_{t',t+1}, \qquad M^d[\phi]_{x't',xt} = \left(\delta_{x',x} - h_{x',x}\right)\delta_{t',t} - e^{\phi_{xt}} \delta_{x',x} B_{t'} \delta_{t',t+1},$$

with the hopping matrix h and $B_t = \begin{cases} -1 & \text{if } t = 0 \\ +1 & \text{else} \end{cases}$ incorporating the anti-periodic boundary conditions in time direction.

Real NVP

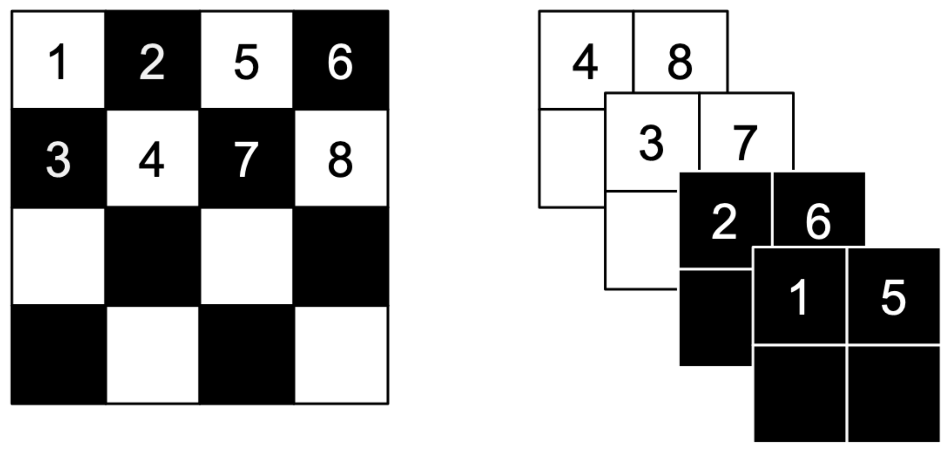
The **RealNVP** architecture:

Block Transformation

$y^l = (y^l_u, y^l_d)\,,\ \ y^l \in \mathbb{R}^{|\Lambda|}$

$$\begin{cases} y_u^{l+1} = y_u^l \\ y_d^{l+1} = y_d^l \cdot \mathrm{e}^{s(y_u^l)} + m(y_u^l) \end{cases} \xrightarrow{\text{Trivially Invertible}} \begin{cases} y_u^l = y_u^{l+1} \\ y_d^l = (y_d^{l+1} - m(y_u^{l+1}))\mathrm{e}^{-s(y_u^{l+1})} \end{cases}$$

Splitting



Checkerboard Masking

Tractable Jacobian Det

$$\mathbf{J}_g = \begin{bmatrix} 1 & 0 \\ \star & \mathrm{e}^{-s} \end{bmatrix}$$

Training the Flow

- We train the normalizing flow using the Reverse-KL divergence

$$\mathrm{KL}(q_\theta || p) = \int \mathscr{D}[\phi] q_\theta(\phi) \ln \left(\frac{q_\theta(\phi)}{p(\phi)} \right) = \beta(F_q - F)$$

- Ignoring the irrelevant (and unknown) constant F, the loss reads

$$\beta F_q = \mathbb{E}_{z \sim q_Z} \left[S(g_\theta(z)) - \ln \left| \frac{\mathrm{d}g_\theta}{\mathrm{d}z} \right| (z) + \ln q_Z(z) \right]$$

Neural Importance Sampling (NIS)

1. We define the unnormalized importance weights $\tilde{w}(\phi) = \dfrac{\tilde{p}(\phi)}{q_\theta(\phi)} = \dfrac{\exp(-S(\phi))}{q_\theta(\phi)}$
2. We estimate the partition function $Z = \int \mathrm{D}[\phi]\, q_\theta(\phi)\, \tilde{w}(\phi) \approx \hat{Z} = \dfrac{1}{N} \sum_{i=1}^{N} \tilde{w}(\phi_i)$
3. From which we have direct access to the free energy $\hat{F} = -T\ \ln \hat{Z}$
4. And other thermodynamic observables like pressure $p = -\dfrac{F}{V}$ and entropy $H = \beta(-F + U)$

NMCMC: Neural Markov Chain Monte Carlo

Standard **MCMC** updates a system configuration by proposing a new candidate configuration following the evolution of the chain

Configurations are thus accepted based on accept/reject algorithm

In **NMCMC** the idea is to take ne candidates drawn from the trained sampler $q(s)$

$$\longrightarrow \quad \min\left(1, \frac{p_0(s\,|\,s')\,p(s')}{p_0(s'\,|\,s)\,p(s)}\right) = \min\left(1, \frac{q(s)\ \exp(-\beta H(s'))}{q(s')\ \exp(-\beta H(s))}\right)$$

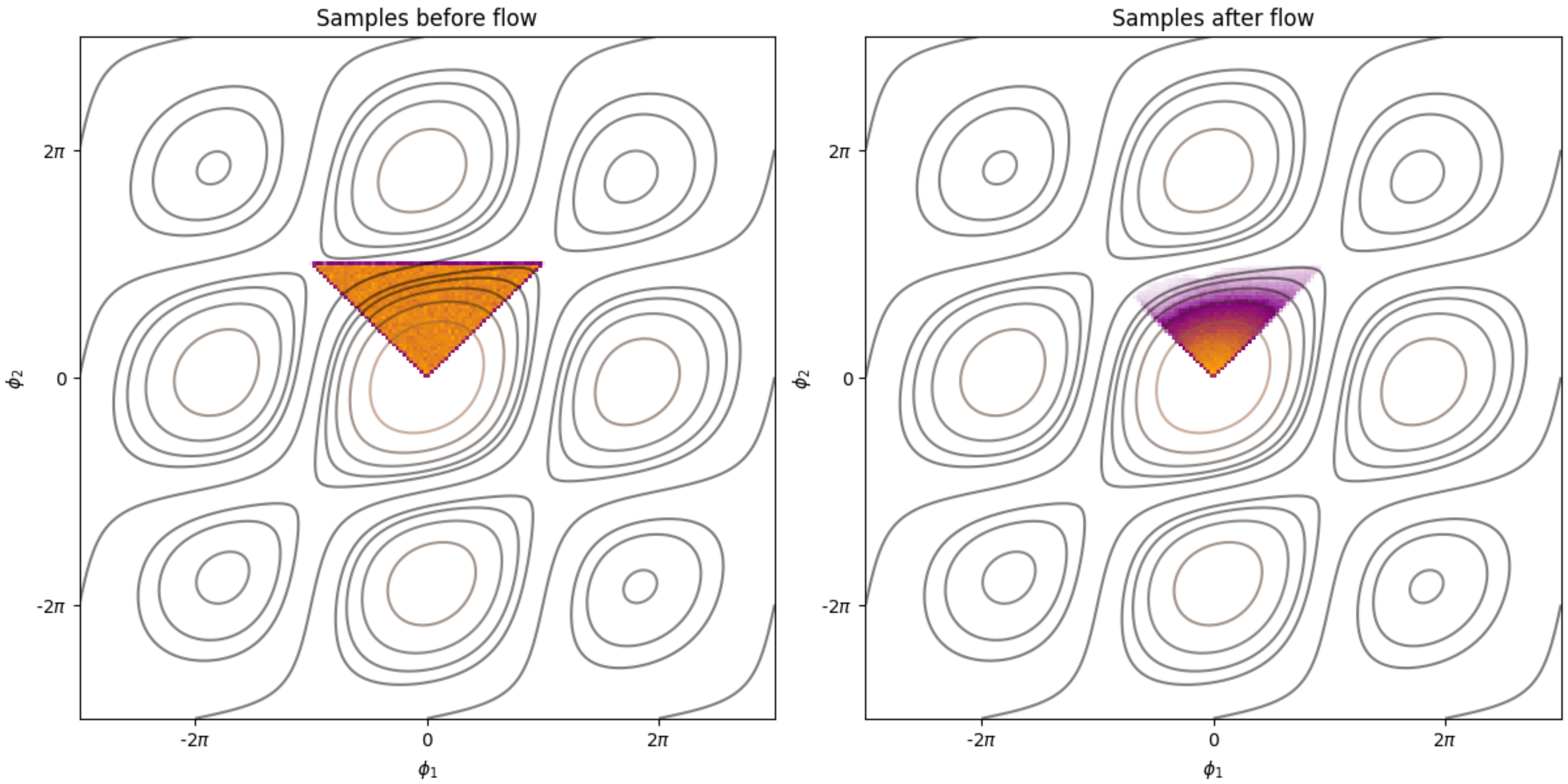
Low dependence between new candidates and previous elements in the chain.

This leads to:

- Efficient and parallel sampling
- New estimates have very small autocorrelation time

See also: M. S. Albergo et al., 2019

Equivariant Flow Output



$N_x = 2,\ N_t = 1$

Outlook: Larger Lattice Sizes

Current lattice sizes for the honeycomb lattice:

- HMC: $2 \times 21 \times 21$ sites
- Exact diagonalization: $2 \times 3 \times 3$ sites
- Tensor networks, e.g. PEPS: $2 \times 15 \times 15$ sites

See also: J. Ostmeyer, Lattice 2022

Comparison

	HMC	Fermionic PEPS	Exact Diagonalization	Normalizing Flows
Lattice Size	L ≲ 100	L ≲ 15	L ≲ 3	L ≲ 2 (for now)
Sign problem	Yes	No	No	Yes
Performance	GPU-intensive	RAM-intensive	CPU-intensive	GPU-intensive
Excited States	Few lowest, expensive	Some specific, instabilities	Yes	Few lowest, expensive

See also: J. Ostmeyer, Lattice 2022