Equivariant Normalizing Flows for the Hubbard Model

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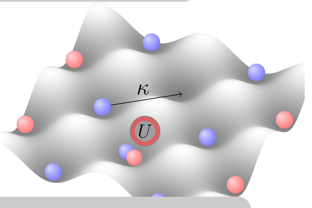
Introduction — Hubbard Model

- Model for electron-electron interaction on lattice [1] e.g. graphene
- Fermionic Hamiltonian:

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

- Lattice size: N_x **spatial** and N_t **temporal** points
- Parameters: Hopping κ, on-site interaction U
- Integrate out fermions:



Fermion fields — Hubbard-Stratonovich transformation → Auxiliary scalar fields

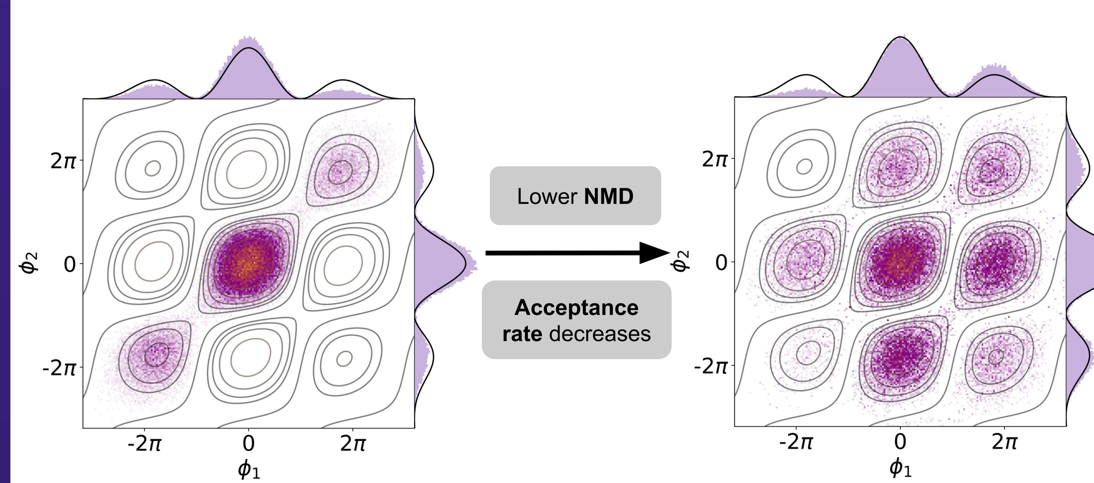
- Bosonic action:

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

- Parameters: Rescaled interaction strength $\tilde{U}$, fermion matrix M
- Symmetries:
  - Action: **Z_2 & space-time translation**
  - Fermion matrix: **2π translation**

Ergodicity Problems

- **Potential barriers**: Challenging to tunnel through



- Solid lines: Strong-coupling limit, exact for $N_x = 2$ and $N_t = 1$
- Sampler: Hamiltonian Monte Carlo (HMC)
- Ergodicity problems: Alleviated with **lower NMD**
- Downside: **Decreased acceptance rate**

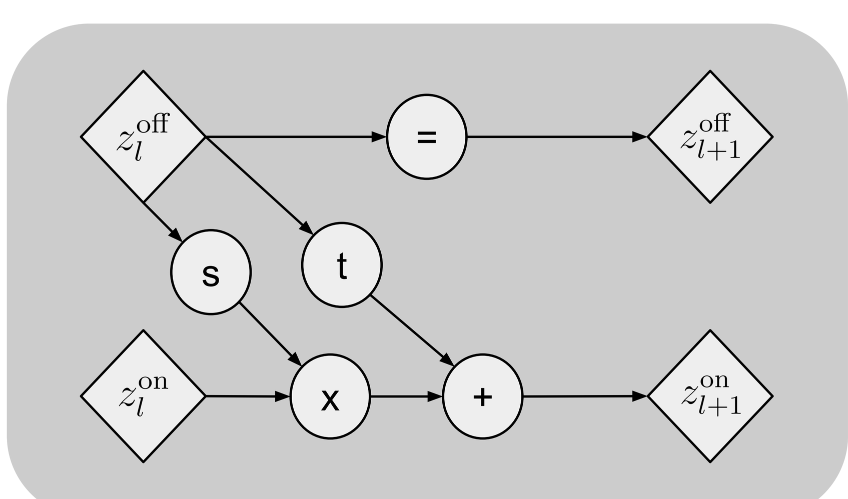
Normalizing Flows[2]

- Flow from **Gaussian distribution** q_Z to **target distribution** q_θ

$$z_0 \xrightarrow{g_1(z_0)} z_1 \cdots z_{N-1} \xrightarrow{g_N(z_{N-1})} z_n = \phi$$

$z \sim q_Z(z)$ → Normalizing Flow → $\phi \sim q_\theta(\phi)$

- Single layer l of **Real NVP** architecture $\quad z_l \xrightarrow{g_{l+1}(z_l)} z_{l+1}$



- Layer computation: alter only **on part** of z_l

$$z_l = (z_l^{\text{on}}, z_l^{\text{off}}) \qquad z_l^{\text{on}} \in R^k,\ z_l^{\text{off}} \in R^{D-k} \qquad 0 < k < D$$

z_l → (z_l^{on}, z_l^{off}) → Coupling layer l → $z_{l+1}^{\text{on}} = z_l^{\text{on}} \odot \exp\left(s(z_l^{\text{off}})\right) + t(z_l^{\text{off}})$, $z_{l+1}^{\text{off}} = z_l^{\text{off}}$ → z_{l+1}

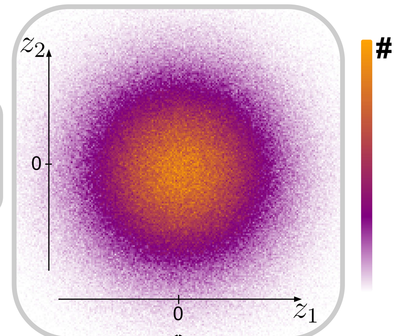
- Minimize: **KL divergence** for target distribution $p = \frac{1}{Z} e^{-S}$

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

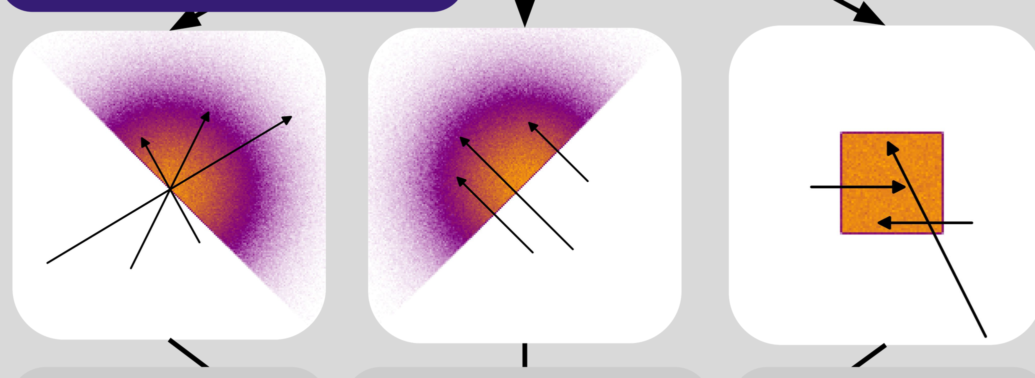
Method — Equivariant Layers

Prior gaussian distribution $z \sim q_Z = \mathcal{N}(0, \tilde{U})$

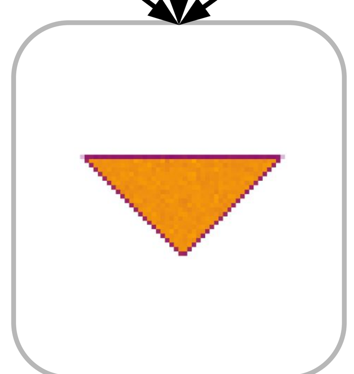
$N_x = 2$, $N_t = 1$



Symmetry transformations

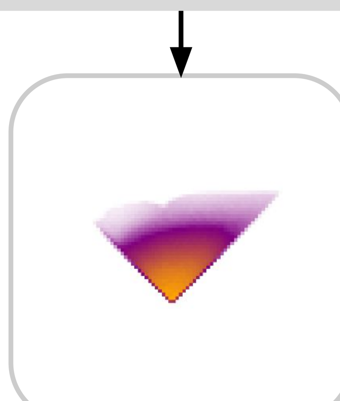


Z_2 symmetry	Space translation	Periodicity
$z \to \begin{cases} z & \text{if } z_1 + z_2 \geq 0 \\ -z & \text{else}\end{cases}$	$(z_1, z_2) \to \begin{cases}(z_1, z_2) & \text{if } z_1 - z_2 \leq 0 \\ (z_2, z_1) & \text{else}\end{cases}$	$z_{xt} \to z_{xt} - 2\pi \cdot k$, $k = \text{round}\left(\frac{z_{xt}}{2\pi}\right)$



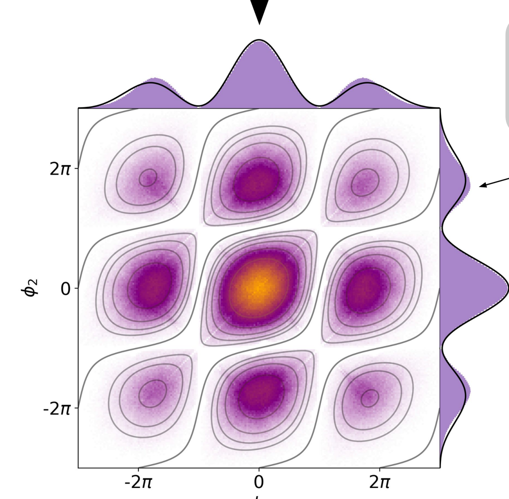
Normalizing Flow

Not allowed to flow outside "triangle" $\qquad \phi = g_\theta(z)$

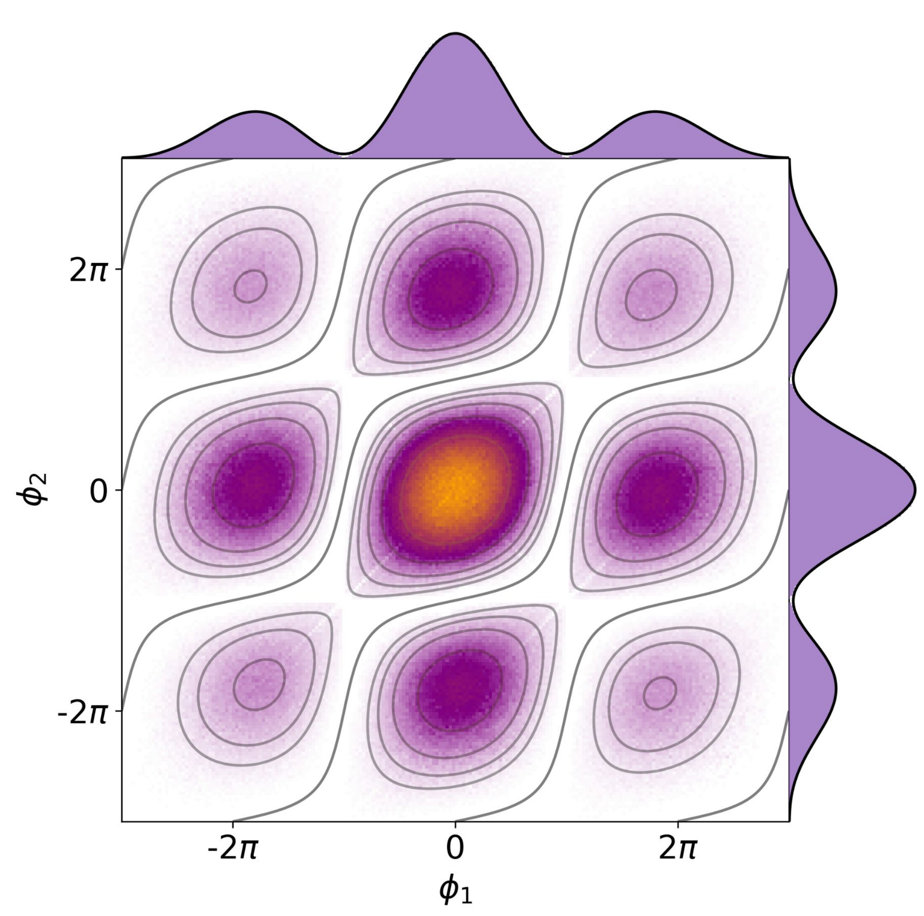


Inverse symmetry transformations

Z_2 symmetry | Space translation | Periodicity

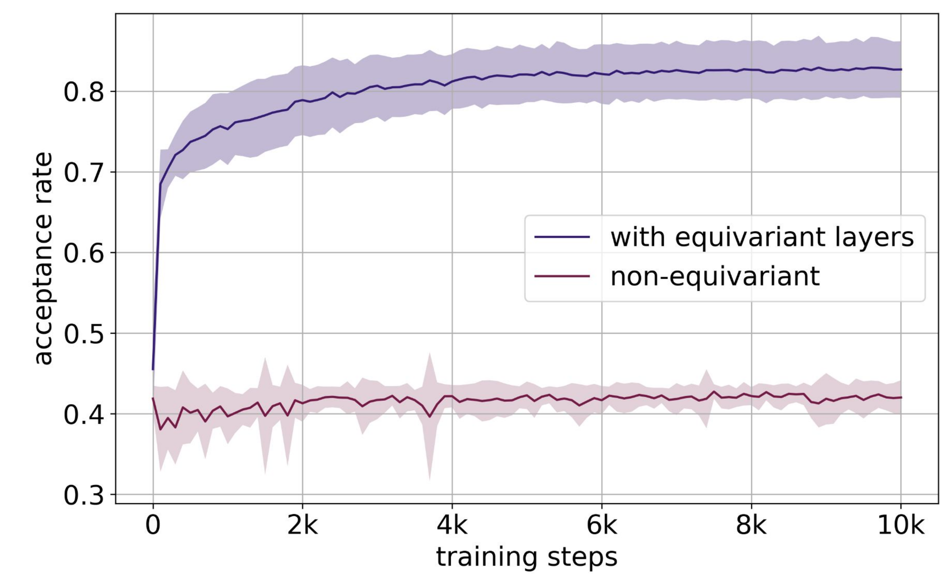


Reweighting — Acceptance rate: 87%

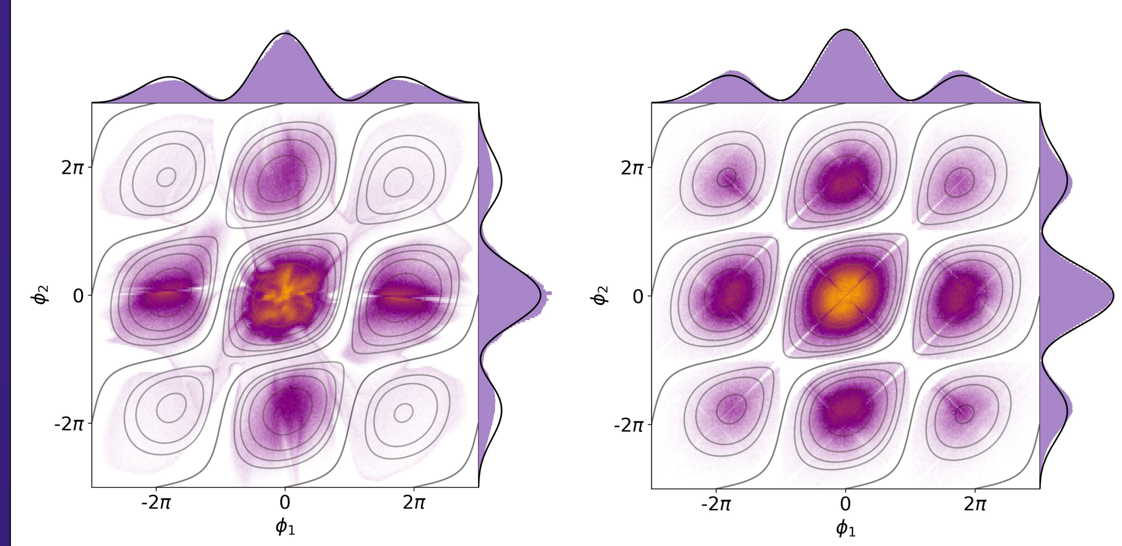


Results — Comparison

Equivariant layers **speed up** training![3]



- Method:
  - 20 equivariant & 20 non-equivariant models trained
  - **Mean** and **standard deviation** of **acceptance rate** shown
- Non-equivariant: Comparable acceptance rates after 500k training steps
- Equivariant layers: Computational overhead less than 10%

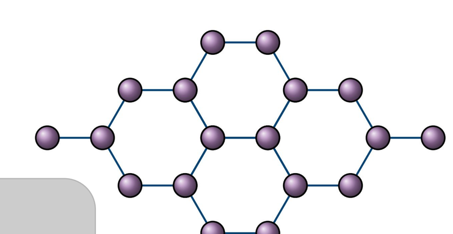


Non-equivariant	Equivariant
Acceptance rate: 75%	Acceptance rate: 85%
Training time: 25h	Training time: 16min

Summary

- **Embarrassingly parallel sampling** with normalizing flows [2]
- **First time** using normalizing flows for Hubbard Model
- **Speed up training** with equivariant layers
- **Implementation of symmetries** is advantage compared to HMC
- **High acceptance rates** across large range of hyperparameters

Outlook



- **Graphene** sized lattices [4]
- **Honeycomb** lattices in 2+1D
- **Chemical potential**
- Various **observables**, e.g. correlators

References

[1] J. Wynen et al.,"Avoiding Ergodicity Problems in Lattice Discretizations of the Hubbard Model", PRB **100**, 075141 (2019)

[2] D. Rezende, S. Mohamed, "Variational Inference with Normalizing Flows", PMLR **37**, 1530-1538 (2015)

[3] G. Kanwar et al., "Equivariant flow-based sampling for lattice gauge theory", PRL **125**, 121601 (2020)

[4] M. Rodekamp et al., "Mitigating the Hubbard Sign Problem with Complex-Valued Neural Networks", PRB **106**, 125139 (2022)