# Generalizable equivariant diffusion models for non-Abelian lattice gauge theory

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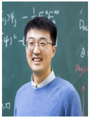

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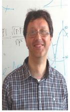

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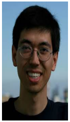

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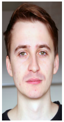

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Diffusion models applications on LFT in recent years

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# Diffusion models

DMs are a class of generative AI which learn distributions from data.

- Relies on a stochastic process to learn the *score function*
- Related to Stochastic Quantization Wang, Aarts, Zhou 2309.17082

Forward process (Data to noise) ⟶

⟵ Backward process (Noise to data)

$$\dot{\mathbf{x}}(t) = \frac{1}{2}\underbrace{\mathbf{K}[\mathbf{x}(t), t]}_{\text{drift}} + \underbrace{g(t)\boldsymbol{\eta}(t)}_{\text{noise}}, \quad 0 \le t \le T$$

- Initial conditions determined by $\mathbf{x}_0 \sim p_0(\mathbf{x}_0)$

# Diffusion models

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Forward process (Data to noise) $\longrightarrow$

$\longleftarrow$ Backward process (Noise to data)

$$\dot{\mathbf{x}}(t) = \frac{1}{2}\mathbf{K}[\mathbf{x}(t), t] - g^2(t)\underbrace{\nabla \log p_t(\mathbf{x})}_{\text{score function}} + g(t)\boldsymbol{\eta}(t),$$

- Initial conditions sampled from a simple prior, eg Gaussian
- Process starts at $t = T$ and flows backwards to $t = 0$

# Score matching

- Processes described by a time-dependent distribution

$$p_t(x) = \int \mathrm{d}x_0 \, p_t(x|x_0) p_0(x_0)$$

- The score is not known; approximate it with a time-dependent model $s_\theta(x, t) \approx \nabla \log p_t(x)$
- Train using a Fisher objective Hyvärinen 2005

$$\mathcal{L}_\theta = \frac{1}{2} \int_0^T \mathrm{d}t \, \mathbb{E}_{p_t(x)} \left[ \sigma^2(t) \| s_\theta(x, t) - \nabla \log p_t(x) \|^2 \right]$$

- Skipping some step, the above relation can be made tractable

$$\begin{aligned} \mathcal{L}_\theta &= \frac{1}{2} \int_0^T \mathrm{d}t \, \mathbb{E}_{p_t(x)} \left[ \| \sigma(t) s_\theta(x, t) + \frac{x_t - x_0}{\sigma(t)} \|^2 \right] \\ &= \frac{1}{2} \int_0^T \mathrm{d}t \, \mathbb{E}_{p_t(x)} \left[ \| \sigma(t) s_\theta(x, t) + \eta(t) \|^2 \right] \end{aligned}$$

# Stochastic Quantization

- In SQ, evolve random field configurations according to Langevin equation in fictitious time $t$ Parisi, Wu 1980

$$\frac{\mathrm{d}\phi(x,\tau)}{\mathrm{d}\tau} = -\frac{\partial S[\phi(x,\tau)]}{\partial \phi(x,\tau)} + \sqrt{2}\,\eta(x,\tau), \quad \eta \sim \mathcal{N}(0,1)$$

- At $\tau \to \infty$, recover probability distribution, $p(\phi) \propto e^{-S[\phi]}$
- Compare with the reverse process of a diffusion model (no drift term)

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} = -g^2(t)\nabla_\phi \log p_t(\phi) + g(t)\eta(x,t)$$

- At $t = 0$, the model score learns the drift in SQ,

$$\nabla_\phi \log p_0(\phi) = -\nabla_\phi S[\phi]$$

# Non-Abelian stochastic processes

- For applications to LGT, diffusion process needs to be adapted to group manifold geometry

- Stochastic dynamics known from stochastic quantization

$$U'_{x,\mu} = \exp\left[ i \sum_{a=1} T^a \left( \epsilon K^a_{x,\mu} + \sqrt{2\epsilon}\eta^a_{x,\mu} \right) \right] U_{x,\mu}$$

- Drift term $K^a_{x,\mu}(U) = -D^a_{x,\mu} S_E(U)$ and $\eta^a_{x,\mu} \sim \mathcal{N}(0,1)$

- Process will equilibrate to action, eg, Wilson for $SU(N)$

$$Z = \int DU \, e^{-S_E(U)}, \qquad S_E(U) = \frac{\beta}{N_c} \sum_{x,\mu<\nu} \mathrm{Re}\,\mathrm{Tr}\left[\mathbb{I} - P_{\mu\nu}\right]$$

# Non-Abelian diffusion models

- Define group-preserving forward process as solution to Stratonovich SDE

$$dU_{x,\mu} = i \sum_a T^a \left[K^a_{x,\mu}(U)\, dt + g(t) dW^a_{x,\mu}\right] \circ U_{x,\mu}$$

- Equivalently to flat space case

$$K^a_{x,\mu}(U) \to K^a_{x,\mu}(U) - g^2(t) D^a_{x,\mu} \log p_t(U)$$

  with time running backward $t = T \to 0$.
- The initial conditions of the reverse process are sampled from the Haar uniform.

# Loss function - Score matching

- Approximate score function by neural network $s^a_{\theta;x,\mu}(U,t)$, minimizing

$$\int_0^T \mathrm{d}t \underset{\substack{p_0(U^{(0)}) \\ p_{0t}(U^{(t)}|U^{(0)})}}{\mathbb{E}} \left[ \sum_{x,\mu,a} \left( s^a_{\theta;x,\mu}(U^{(t)},t) - D^a_{x,\mu} \ln p_{0t}(U^{(t)}|U^{(0)}) \right)^2 \right]$$

- Consider forward process with zero drift $K^a_{x,\mu} = 0$,

$$U_{x,\mu} = \exp\left[ i\sigma(t) \sum_a T^a \eta^a_{x,\mu} \right] U_{x,\mu}, \quad \sigma^2(t) = \int_0^t ds\, g^2(s)$$

- Disregard contributions from multiple wrappings

$$p_{0t}(U^{(t)}|U^{(0)}) \approx p(\eta) \propto \exp\left[ -\frac{1}{2} \sum_{a,x,\mu} (\eta^a_{x,\mu})^2 \right]$$

- Tractable loss function

$$\int_0^T \mathrm{d}t \underset{\substack{p_0(U^{(0)}) \\ p_{0t}(U^{(t)}|U^{(0)})}}{\mathbb{E}} \left[ \sum_{x,\mu,a} \left( s^a_{\theta;x,\mu}(U^{(t)},t) + \frac{\eta^a_{x,\mu}}{\sigma(t)} \right)^2 \right]$$

- Process interpolates gauge invariant objects, prior and target distributions
- The score model itself has to respect gauge equivariance
- *Lattice Convolutional Neural Networks* (L-CNNs) can express arbitrary gauge invariant and equivariant functions

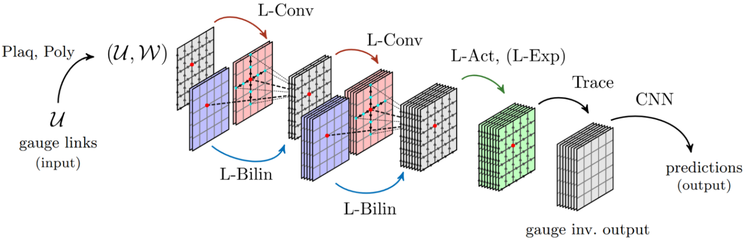



Figure: M. Favoni, A. Ipp, D.I. Müller, D. Schuh, Phys. Rev. Lett. **128**, 3 (2022)

# DMs for LFT

- Diffusion models are intended to generate field configurations.
- To do so, they need to be trained on a high-quality dataset
- What's the advantage?
- Extrapolate to bigger lattices
- Extrapolate to different couplings $\rightarrow$ Metropolis-adjusted annealed Langevin

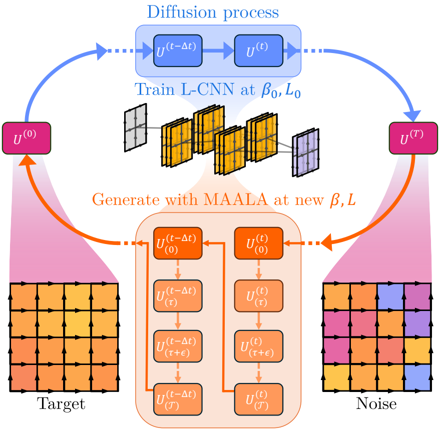
# Metropolis-adjusted Annealed Langevin

- After training at $\beta_0$, the model can be employed at different $\beta$
- Solve SDE using *score rescaling* to generalize in $\beta$

$$U^t_{\tau+\epsilon} = \exp\left[i\left(\epsilon\frac{\beta}{\beta_0}\hat{s}_\theta(U,t)+\sqrt{2\epsilon}\hat{\eta}\right)\right]U^t_\tau$$

- Include accept reject w.r.t. target action

$$p_{\text{acc}} = \min\left\{1, \frac{p(\widetilde{U}^{(t)}_{(\tau)})}{p(U^{(t)}_{(\tau)})}\frac{q(U^{(t)}_{(\tau)}|\widetilde{U}^{(t)}_{(\tau)})}{q(\widetilde{U}^{(t)}_{(\tau)}|U^{(t)}_{(\tau)})}\right\}$$

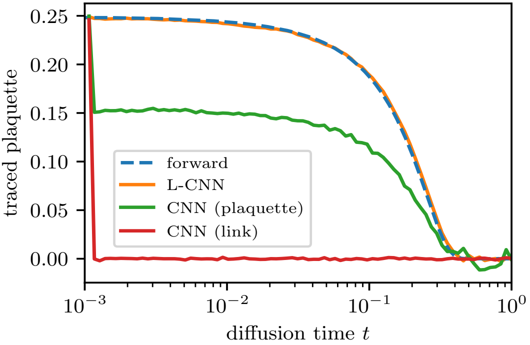


# Numerical setup

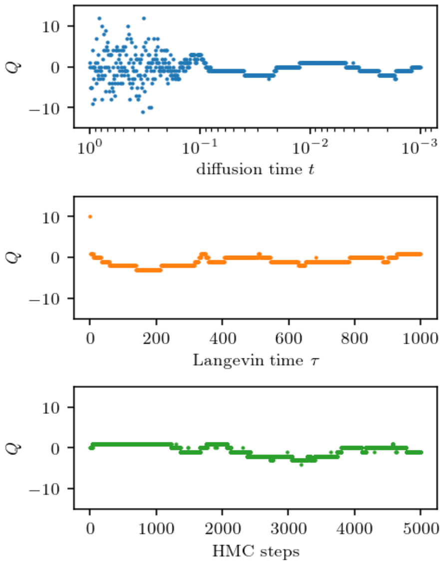
- We consider $U(2)$ and $SU(2)$ in two dimensions
- Train using 100k HMC-generated data at $\beta_0 = 2$, $L = 16$
- Employ at range of values $2 \leq \beta \leq 18$, and $L = 16, 32, 64$
- Wilson loops $W_{\ell\times\ell}$ and topological charge/susc. ($U(2)$ only)
- In strong coupling limit, $\langle W_{\ell\times\ell}\rangle \to 0$ and $\langle \chi_{\text{top}}\rangle \to \frac{1}{12}$

# Comparison with standard CNNs

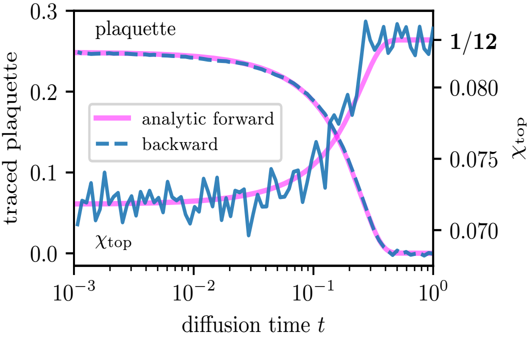
- Naive link implementation on standard CNNs fail
- CNNs with invariant representations struggle to fully capture target
- L-CNNs manage to follow analytical expectations
- Minimal corrections from the Metropolis step



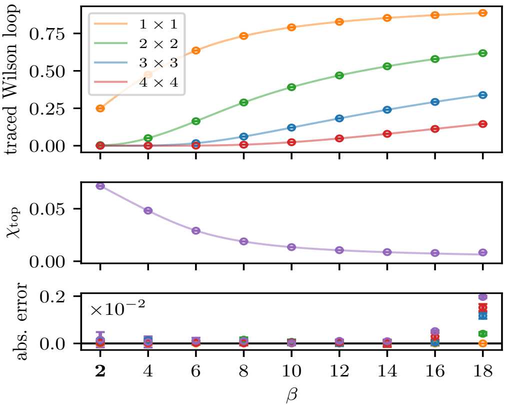
- Evolution of topological charge $Q$ for one field configuration at $\beta = 14, L = 16$
- **MAALA** explores many topological vacua in the early stages of the de-noising process
- Standard **SQ** and **HMC** might remain trapped in a few topological sectors.



- Observables interpolate between target and strong coupling values
- Forward process solved analytically using character expansions
- Time dependence $\exp(-C_2(t)\sigma(t))$
- Excellent agreement with de-noising process



- $W_{\ell\times\ell}$ and $\chi_{top}$ in $U(2)$
- Trained at $\beta_0 = 2$, generalize in $\beta$
- Extrapolation breaks down at $\beta \sim 16$
- However, it covered a large range of couplings



# Detailed comparison $U(2)$

Table: Numerical results for U(2) for larger Wilson loops and the topological susceptibility at $L = 16$, $32$ and $64$ and three separate inverse couplings $\beta$. The DM was trained on $\beta = 2$, $L = 16$ (highlighted). For $L = 32$ and $L = 64$ only $1000$ samples were generated.

| $U(2)$ | | $2 \times 2$ | $3 \times 3$ | $4 \times 4$ | $\chi_{\text{top}}$ |
|---|---|---|---|---|---|
| $\boldsymbol{\beta = 2}$ | $\boldsymbol{L = 16}$ | $0.00381(7)$ | $1.3(7) \cdot 10^{-4}$ | $-3(9) \cdot 10^{-5}$ | $0.0716(3)$ |
| | $L = 32$ | $0.0038(1)$ | $-1(1) \cdot 10^{-4}$ | $0(1) \cdot 10^{-4}$ | $0.070(1)$ |
| | $L = 64$ | $0.00378(6)$ | $2(6) \cdot 10^{-5}$ | $5(7) \cdot 10^{-5}$ | $0.072(1)$ |
| | exact | $0.003835$ | $3.660 \cdot 10^{-6}$ | $2.163 \cdot 10^{-10}$ | $0.071802$ |
| $\beta = 10$ | $L = 16$ | $0.39106(9)$ | $0.1209(1)$ | $0.0234(1)$ | $0.01345(8)$ |
| | $L = 32$ | $0.3909(2)$ | $0.1210(2)$ | $0.0236(2)$ | $0.0137(2)$ |
| | $L = 64$ | $0.39108(7)$ | $0.12102(9)$ | $0.02335(8)$ | $0.0135(2)$ |
| | exact | $0.390989$ | $0.120884$ | $0.023370$ | $0.013442$ |
| $\beta = 18$ | $L = 16$ | $0.61824(7)$ | $0.3383(1)$ | $0.1450(1)$ | $0.00837(5)$ |
| | $L = 32$ | $0.6184(1)$ | $0.3390(2)$ | $0.1459(2)$ | $0.0084(1)$ |
| | $L = 64$ | $0.6184(1)$ | $0.3390(2)$ | $0.1460(2)$ | $0.0084(1)$ |
| | exact | $0.618647$ | $0.339427$ | $0.146478$ | $0.006399$ |

# Detailed comparison $SU(2)$

Table: Numerical results for SU(2) calculations on $L = 16$, $32$ and $64$ lattices for Wilson loops at several inverse couplings $\beta$. The DM was trained on $\beta = 2$, $L = 16$.

| $SU(2)$ | | $1 \times 1$ | $2 \times 2$ | $3 \times 3$ | $4 \times 4$ |
|---|---|---|---|---|---|
| $\boldsymbol{\beta = 2}$ | $\boldsymbol{L = 16}$ | **0.4333(2)** | **0.0357(3)** | **0.0006(3)** | $-0.0003(3)$ |
| | $L = 32$ | 0.4333(4) | 0.0349(5) | 0.0014(5) | $-0.0001(5)$ |
| | $L = 64$ | 0.4333(2) | 0.0351(3) | 0.0002(3) | 0.0004(2) |
| | exact | 0.433127 | 0.035194 | 0.000536 | $1.534 \cdot 10^{-6}$ |
| $\beta = 10$ | $L = 16$ | 0.85420(7) | 0.5325(3) | 0.2421(5) | 0.0807(5) |
| | $L = 32$ | 0.8541(1) | 0.5326(4) | 0.2422(8) | 0.0808(8) |
| | $L = 64$ | 0.85420(5) | 0.5323(2) | 0.2421(4) | 0.0805(4) |
| | exact | 0.854185 | 0.532364 | 0.242086 | 0.080322 |
| $\beta = 18$ | $L = 16$ | 0.91793(4) | 0.7097(2) | 0.4621(4) | 0.2533(6) |
| | $L = 32$ | 0.91782(7) | 0.7096(3) | 0.4620(7) | 0.253(1) |
| | $L = 64$ | 0.91792(3) | 0.7099(2) | 0.4628(4) | 0.2545(5) |
| | exact | 0.917894 | 0.709854 | 0.462520 | 0.253909 |

# Summary & Outlook

- Diffusion models offer a new approach for ensemble generation in LFT
- Coupled with gauge equivariant architectures (L-CNNs), successfully sample non-Abelian LGTs
- Score rescaling enables single trained models to generalize across wide range of couplings
- Scaling to 4D SU(3) theories with large volumes (see also work by Komijani, Marinkovic, Turgut [2605.06134])
- Extend to include fermionic fields and test critical scaling

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Thank you for listening!