

Normalising flows for all-orders QED corrections in lattice quantum field theory

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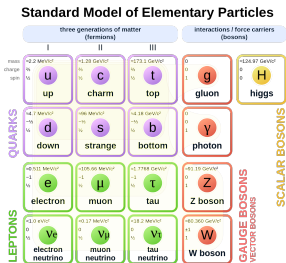


Precision tests

- **Precision tests** of the Standard Model: theory and experiment
- **Low energy**: Many interesting observables [Flavour Lattice Averaging Group (NHT)]
- **My work**: Decays of pions/kaons/neutrons, neutron EDM
→ to explain baryon asymmetry/dark matter
- Control of QCD + QED for **percent-level precision**



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Unknown

Experiment PSI/ESS/Fermilab

Theory prediction

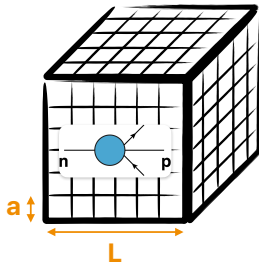
Lattice QCD+QED

- Simulate quantum field theory with action $S_{\text{QCD+QED}}$

$$\underbrace{\langle \mathcal{O} \rangle_{\text{QCD+QED}}}_{\text{Decay process, ...}} = \int_{\text{fields}} \mathcal{O} \frac{e^{-S_{\text{QCD+QED}}}}{Z_{\text{QCD+QED}}} = \int_{\text{fields}} \mathcal{O} p_{\text{QCD+QED}}$$

- In essence: Sampling problem from $p_{\text{QCD+QED}} \sim e^{-S_{\text{QCD+QED}}}$
- Traditionally: Monte Carlo. **Machine learning** can help
- **Discretise** theory and spacetime on grid of **finite extent**

- ★ **Discretisation:** a
- ★ **Finite volume:** L
- ★ **Physics:** $L \rightarrow \infty, a \rightarrow 0, \dots$



- How to determine the expectation value $\langle \mathcal{O} \rangle_{\text{QCD+QED}}$?

1. Fixed-order e^2 : **Expansion** around QCD ($e^2 \sim 0.09$) [RM123 13]

$$\langle \mathcal{O} \rangle_{\text{QCD+QED}} \approx \langle \mathcal{O} \rangle_{\text{QCD}} + e^2 \langle \delta \mathcal{O} \rangle_{\text{QCD}}$$

Standard for most calculations **but** more challenging operator:
difficult for full e^2 answer [RC* 25] **and e.g. neutron decays** [Gorchtein et al. 23]

2. **All-orders** approach: Fully sample QCD+QED [BMW 15; RC* 25]
but difficult because **unphysical noise** to remove
3. Our work: **Normalising flows** for **all-orders** QED at **reduced variance**

Normalising flows

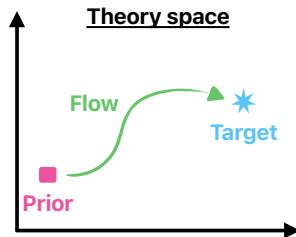
- Normalising flows have received much attention in the lattice community: Transform between distributions
- First step: Consider **scalar QED**: charged scalar fields ϕ , photons A_μ
- Action in scalar QED: $S_0(\phi, A) + S_{\text{int}}(\phi, A; e)$
- Start: **Uncoupled prior** ($e = 0$)

$$p_0(\phi, A) = \frac{1}{Z_0} e^{-S_0(\phi, A)}$$

Benefit: Gaussian, easy to sample

- Goal: **Coupled target** (all orders in e)

$$p_e(\phi, A) = \frac{1}{Z_e} e^{-S_0(\phi, A) - S_{\text{int}}(\phi, A; e)} \longrightarrow \langle \mathcal{O} \rangle_e = \int \mathcal{O} p_e(\phi, A)$$



Normalising flows

- Define the normalising flow f transforming field configurations

$$f : (\phi, A) \mapsto (\phi', A')$$

- The new fields follow the distribution

$$q(\phi', A') = p_0(\phi, A) |\det J_f|^{-1}$$

- Goal:** Optimise flow to get q close to the **target** p_e

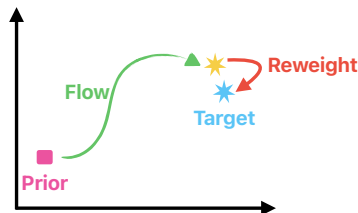
- In practice:** no flow is perfect

- Reweight** for unbiased estimators:

$$w \propto p_e/q$$

- Target observables:

$$\langle \mathcal{O} \rangle_e = \langle \mathcal{O}(\phi', A') w \rangle_0$$

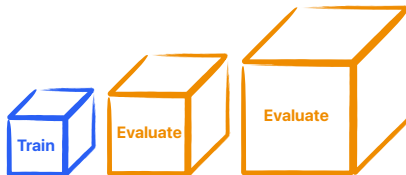


Normalising flows

- We consider two kinds of flows: **Machine learned** and linear
- Residual-flow architecture [Chen et al. 19] (to be further explored)

$$f: \phi' = \phi + \varepsilon b_{\phi}(\phi, A) \quad A' = A + \varepsilon b_A^L(\phi, A)$$

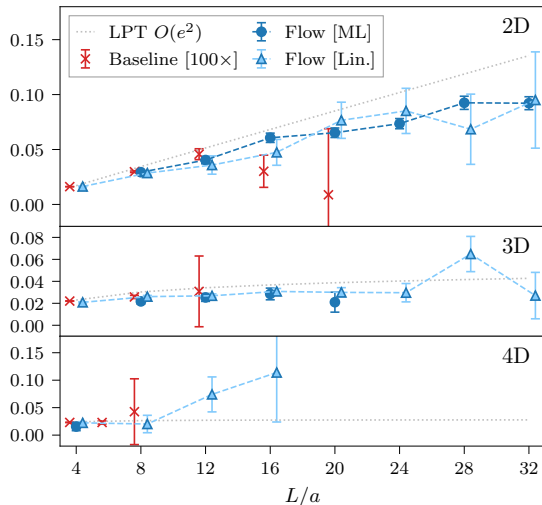
- b_{ϕ}/b_A^L : UNets to capture short- and long-range features
- **Feature I**: Observable-independent flow training to full action automatically reduces unwanted and unphysical noise
- **Feature II**: Volume transfer to larger lattices



Numerical results

Methods: **Flows** (ML/Linear); **Baseline** (all-orders stochastic)

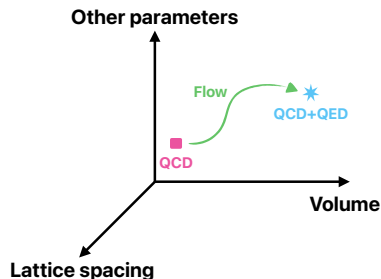
$a \Delta m$



- Mass shift: $a \Delta m$
- Clear **hierarchy** in variance
- **Good volume transfer** of trained models: **baseline too noisy**
- Improvement comes from reweighting factors
- Comparison to **lattice perturbation theory**: Flows resolve e^4

Conclusions and outlook

- Proof-of-concept study: Lattice **scalar QED** with normalising flows
- **Uncoupled** ($e = 0$) $\xrightarrow{\text{flow}}$ **all-orders in e**
- **Observable-independent** flow: **Volume transfer** and **variance reduction**
- Future questions:
 - * **Fixed** simulation parameters here:
Can we learn the dependence?
 - * **QCD/Fermion theories**: How well do flows perform? Reuse QCD distributions
 - * Many applications of normalising flows, e.g. **neutron physics** at PSI, ESS, ...



Fysikaktuellt

- Fysikersamfundet magazine: Articles etc.
- If you have an idea about a particle-physics article:

Come and talk to me in the coffee break!

Email: nils.hermansson-truedsson@ed.ac.uk



Backup

Scalar QED

- We consider **scalar QED**: charged scalars ϕ , photons A_μ

$$S(\phi, A; e) = S_0(\phi) + S_A(A) + S_{\text{int}}(\phi, A; e)$$

- The actions take the form [\[Davoudi et al. 18\]](#)

$$S_A(A) = -\frac{1}{2} A_\mu(x) \delta^2 A_\mu(x) \quad \leftarrow \text{Feynman gauge}$$

$$\delta^2 = \frac{1}{a^2} \sum_{\mu} (\tau_{\mu} + \tau_{-\mu} - 2)$$

$$S_0(\phi) + S_{\text{int}}(\phi, A; e) = \sum_x \phi^\dagger(x) \Delta \phi(x)$$

$$\Delta = m_0^2 + \frac{1}{a^2} \sum_{\mu} \left(2 - e^{ieaA_\mu} \tau_{\mu} - \tau_{-\mu} e^{-ieaA_\mu} \right) = \Delta_0 + \sum_{n=1}^{\infty} e^n \Delta^{(n)}$$

- For finite-volume QED, we use **QED_L** but methodology generalises

Normalising flows: Linear

- The scalar QED Lagrangian is very simple at order e

$$\mathcal{S}_{\text{int}}^{(1)}(\phi, A) = \sum_{x, \mu} A_{\mu}(x) j_{\mu}(x) = \sum_{x, \mu} A_{\mu}(x) \frac{2}{a} \text{Im}[\phi^{\dagger}(x) \tau_{\mu} \phi(x)]$$

- Can define an analytic **linear** flow matching the target at leading order

$$\phi'^{\text{Lin.}}(x) = \phi(x), \quad A'_{\mu}{}^{\text{Lin.}}(x) = A_{\mu}(x) + e P_{\text{QED}_L} [(\delta^2)^{-1} j_{\mu}(x)]$$

- Jacobian of the linear flow has

$$\det J^{\text{Lin.}} = 1$$

- This would not directly generalise to fermionic theories, but it lets us test a cheap but imperfect flow

Normalising flows: Machine learned

- Our flow f transforms to the distribution q

$$\log q(\phi', A') = -S_0(\phi) - S_A(A) - \log \det J_f - \log Z_0$$

- The target density is

$$\log p_e(\phi, A) = -S_0(\phi) - S_A(A) - S_{\text{int}}(\phi, A; e) - \log Z_e$$

- Optimised with Kullback-Leibler divergence + path gradients [\[Vaitl et al. 22\]](#)

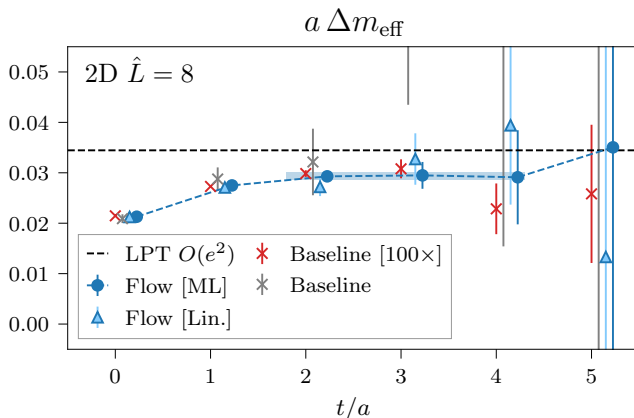
$$\mathcal{L}_{kl} = \langle \log q(\phi', A') - \log p_e(\phi', A') - \log(Z_e/Z_0) \rangle_0$$

- Jacobian evaluated through

$$\log \det J = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \text{Tr} [J^k]$$

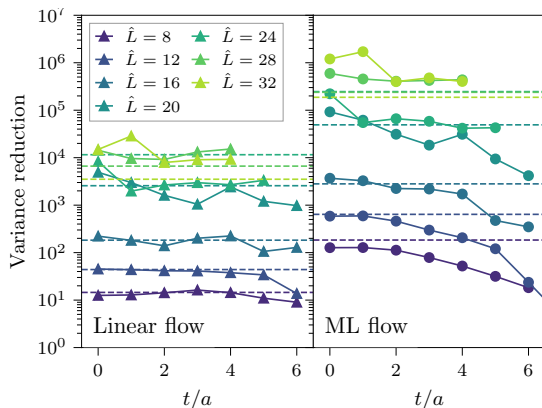
- We use UNets, convolutional networks, 1 hidden layer, 32 channels

Numerical results: Effective mass shift



- Compare flows and baseline: 10^5 samples
- Clear [hierarchy](#) in variance
- At 100 times more statistics, baseline becomes comparable to flows
- In comparison to LPT: Resolves e^4 dependence

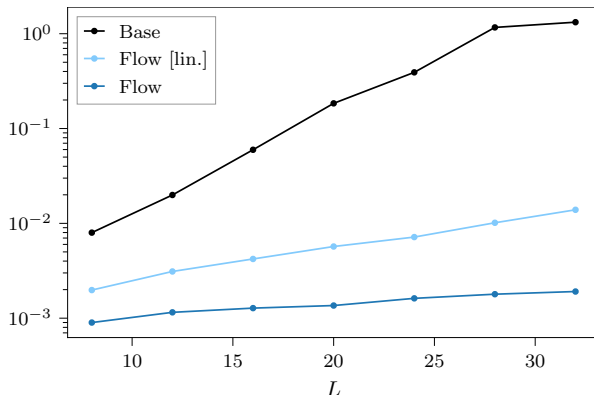
Numerical results



- Where does the **improvement** originate?
- Variance in **correlation function ratio** relative to baseline
- Dashed horizontal lines: Improvement in: **$\log Z_e/Z_0$**
- This is what governs the variance improvement, before the dip

$$\hat{w}(\phi', A') = \frac{e^{-S_0(\phi', A') - S_{\text{int}}(\phi', A'; e)}}{e^{-S_0(\phi, A)}} |\det J_f|$$

Numerical results



- Error in ratio $C_e(t)/C_0(t) \approx \frac{A_e}{A_0} e^{-\Delta m_e t} + \dots$

$$C_e(t) = \frac{1}{\hat{L}^{N_d-1}} \sum_{\mathbf{x}} \langle \phi(t, \mathbf{0}) \phi^\dagger(0, \mathbf{0}) \rangle_e, \quad C_0(t) = \frac{1}{\hat{L}^{N_d-1}} \sum_{\mathbf{x}} \langle \phi(t, \mathbf{0}) \phi^\dagger(0, \mathbf{0}) \rangle_0$$

Lattice perturbation theory

- Compare to lattice perturbation theory at fixed order e^2

[Davoudi et al. 19; Bijnens, NHT, Jüttner, Portelli et al. 19]

$$\delta_{e^2} C_e(t) = \frac{1}{T} \sum_{p_0} \frac{\Sigma(p_0, \mathbf{0})}{(\hat{p}_0^2 + m^2)^2} e^{ip_0 t}$$

- Calculate as an FFT
- One-loop self energy (exactly or with VEGAS Monte Carlo [Lepage 77/20])

$$\Sigma(p) = \frac{e^2}{TL^{N_d-1}} \sum_{k_0} \sum_{\mathbf{k} \neq \mathbf{0}} \left\{ \frac{N_d - 1 + \cos(ap_0)}{\hat{k}^2} - \frac{\widehat{2p - k}^2}{\hat{k}^2 (\widehat{p - k}^2 + m_0^2)} \right\}$$

