A novel gauge-equivariant neural network architecture for preconditioners in lattice QCD

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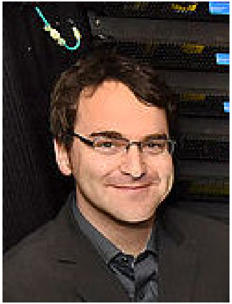

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Background

Problem statement

Bigger picture

- Lattice QCD calculations are expensive
- One of the most expensive parts is solving the Dirac equation
- Preconditioners can accelerate this

Preconditioners

- State of the art:
  algebraic multigrid (AMG)
- But AMG needs costly setup
- Can this setup be avoided?
- **Goal**: Preconditioner competitive with AMG, but with very little (or even no) setup

Status quo

Previous work

- Exploratory studies with different kinds of Machine Learning models [1,2]
- Multigrid coarse grid solver and smoother were reformulated in a learnable way [3]
- Prolongation and restriction operators were translated into ML language [4]

Shortcomings

- Focus on preconditioning the high modes
- expensive AMG setup is still needed
- no generalization to unseen configurations

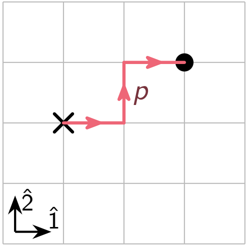
[1] S. Calì et al., PRD **107**, 034508 (2023)
[2] Y. Sun et al., arXiv:2509.10378 [hep-lat] (2025)
[3] C. Lehner and T. Wettig, PRD **108**, 034503 (2023)
[4] C. Lehner and T. Wettig, PRD **110**, 034517 (2024)

Gauge equivariance

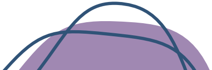
- Gauge-equivariant transport of information between adjacent lattice sites:
  hop operator

$$H_{p_i}\varphi(x) = U^{\dagger}_{p_i}(x - \hat{p}_i)\varphi(x - \hat{p}_i)$$

- Combining multiple hops leads to **parallel transports** T_p along a path p
- weighted linear combinations of parallel transports are gauge-equivariant



$T_p = H_1 H_2 H_1$



Machine Learning

Network Architecture

Dense linear (L) layer

- n spin-color fields $\varphi \in \mathbb{C}^{L_x \times L_y \times L_z \times L_t \times N_c \times N_s}$
- build m linear combinations of the input fields, with spin matrices $W_{ij} \in \mathbb{C}^{N_s \times N_s}$ as weights:

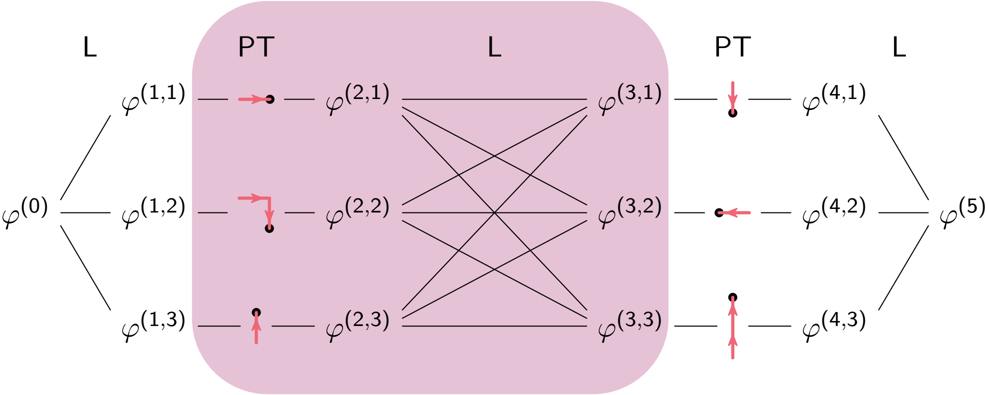
$$\psi_i(x) \stackrel{\mathrm{L}}{=} \sum_{j=1}^{n} W_{ij} \varphi_j(x)$$

Parallel Transport (PT) layer

- n spin-color fields $\varphi \in \mathbb{C}^{L_x \times L_y \times L_z \times L_t \times N_c \times N_s}$
- apply a different parallel transport $p^{(i)}$ to every input field:

$$\psi_i(x) \stackrel{\mathrm{PT}}{=} T_{p^{(i)}} \varphi_i(x)$$

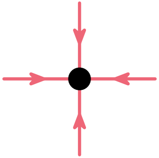
Network Architecture



Choice of PT paths

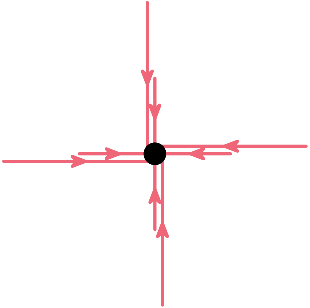
- **1-hop paths**:

$$P = \left\{ H_p | p \in \{\pm 1, \pm 2, \pm 3, \pm 4\} \right\}$$



- **long straight paths**:

$$P = \left\{ H_p^n | p \in \{\pm 1, \pm 2, \pm 3, \pm 4\}, \; n \in \{2^0, 2^1, \dots, {}^{L_p}/_2\} \right\}$$



Choice of PT paths

- **1-hop paths**:

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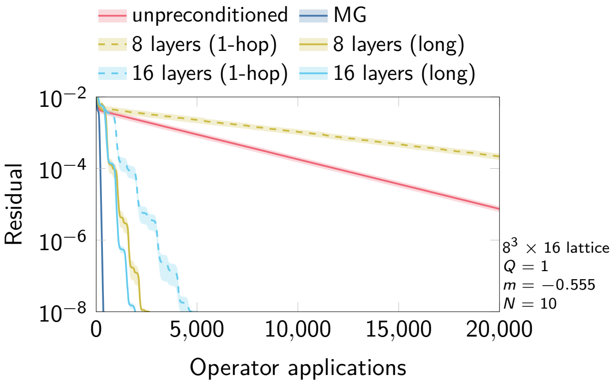
- **long straight paths**:

$$P = \left\{ H_p^n | p \in \{\pm 1, \pm 2, \pm 3, \pm 4\}, \\ n \in \{2^0, 2^1, \dots, L_p/2\} \right\}$$



Score function

- **Standard choice**:

$$C = \|MD\varphi - \varphi\|^2$$

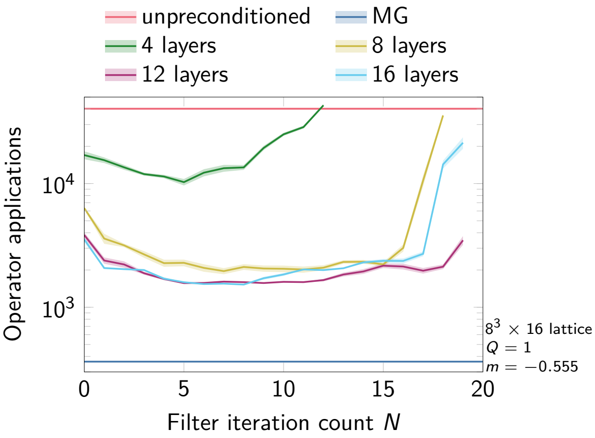
with random field φ

- **Filtered cost function**:

$$C = \|MD\tilde{\varphi} - \tilde{\varphi}\|^2$$

where $\tilde{\varphi}$ is obtained through N iterations of GMRES for $D\varphi = 0$ with random initial guess

$\Rightarrow$ Stronger emphasis on the low modes!



Results

Gauge configurations

$8^3 \times 16$ ensemble[1]:

- Wilson action
- quenched, heat bath
- Wilson-clover Dirac operator
- configurations with topological charge $|Q| \in \{0, 1, 2\}$

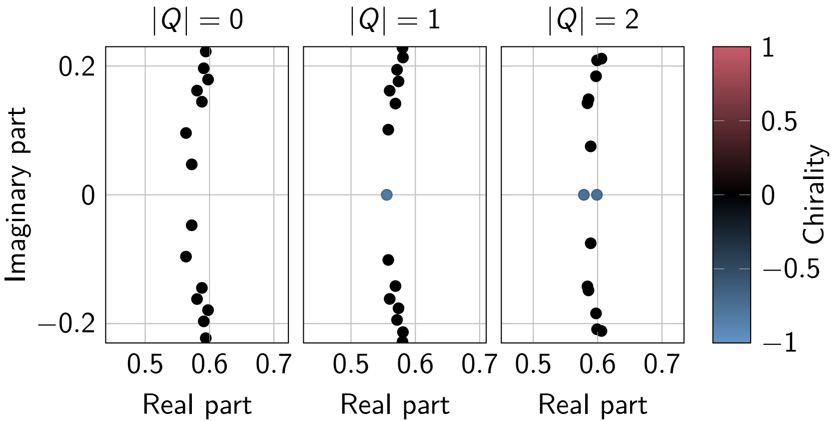
$16^3 \times 32$ ensemble[2]:

- Wilson action
- quenched, HMC
- Wilson-clover Dirac operator
- configurations with topological charge $|Q| \in \{0, 4\}$

[1] doi.org/10.5281/zenodo.15018324
[2] doi.org/10.5281/zenodo.17494829

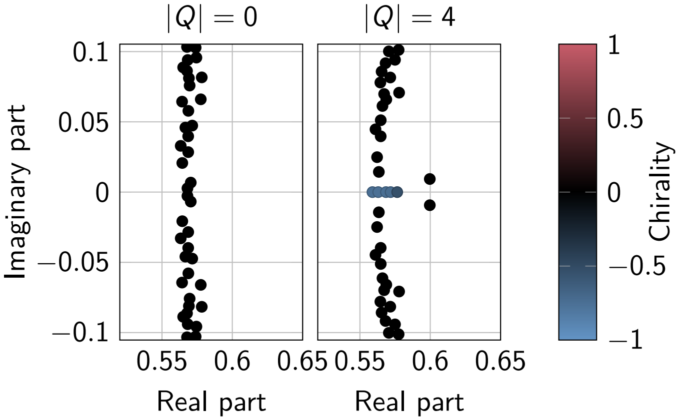
Gauge configurations

$8^3 \times 16$ lattice

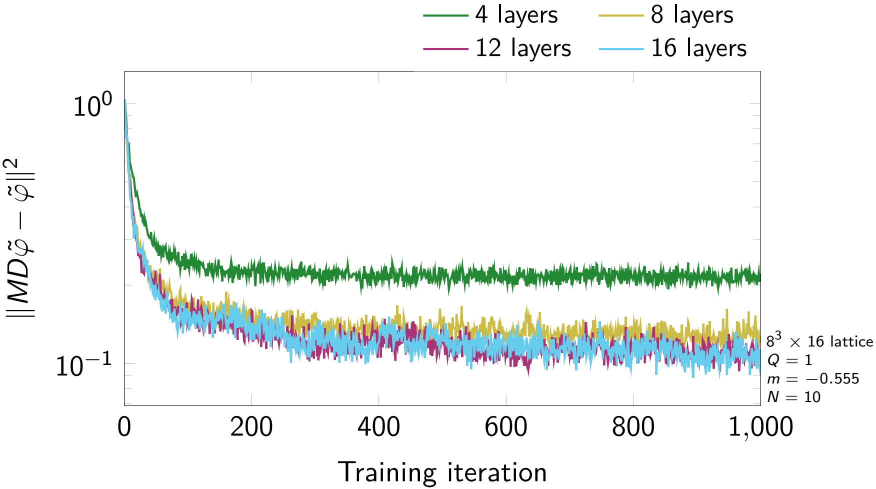


Gauge configurations

$16^3 \times 32$ lattice

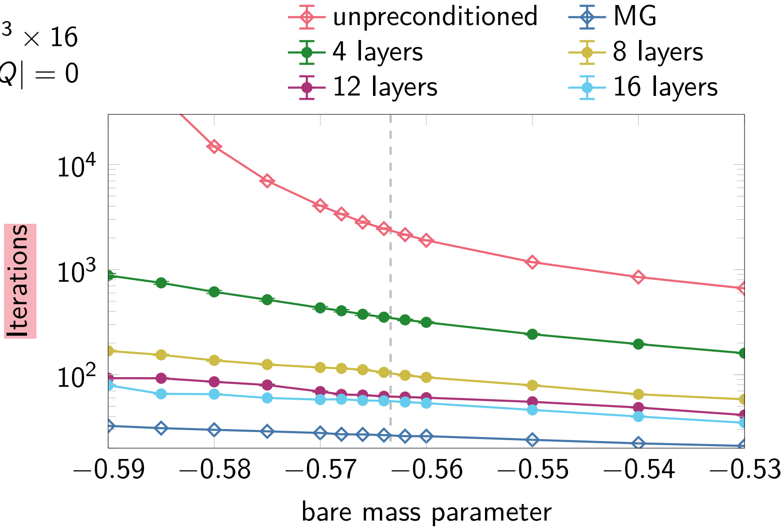


Training cost



Iteration count gain?

$8^3 \times 16$
$|Q| = 0$

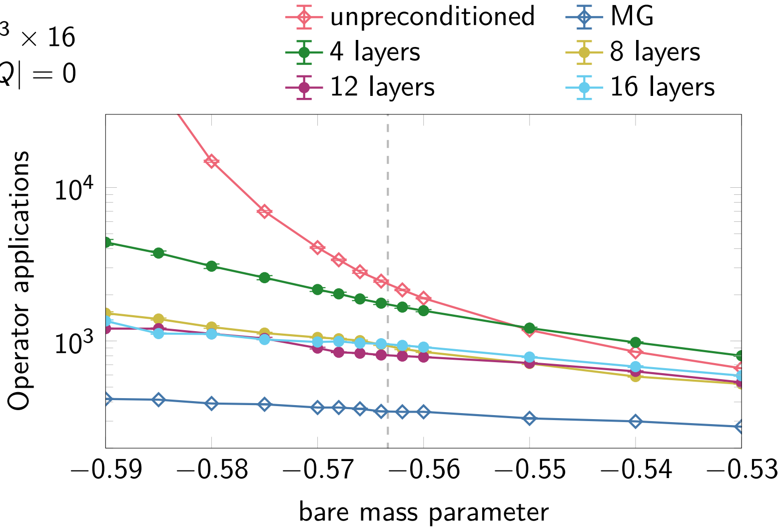


Critical slowing down

$8^3 \times 16$
$|Q| = 0$

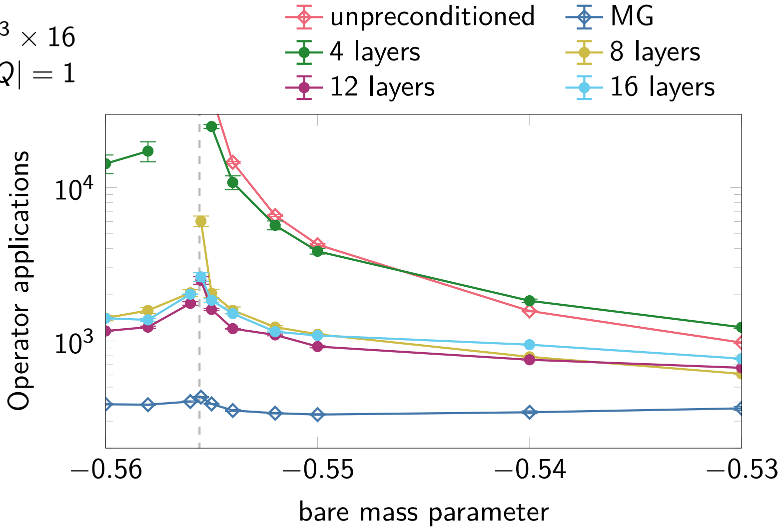
applications of:

- D_{fine}
- PT layer



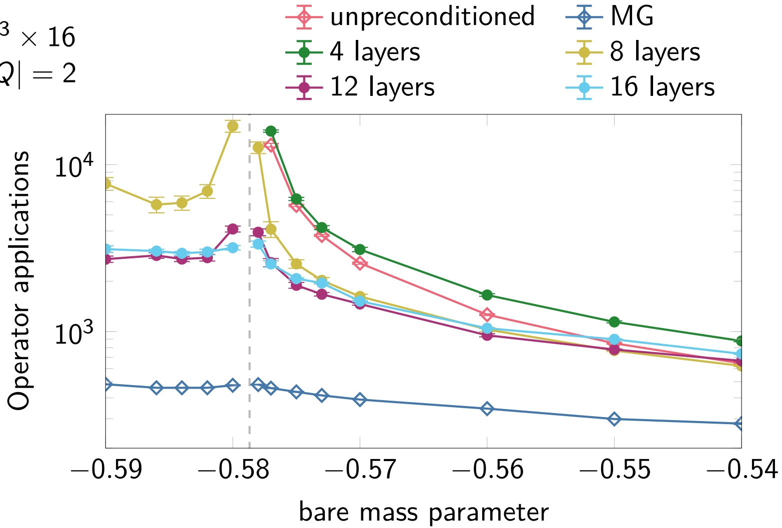
Critical slowing down

$8^3 \times 16$
$|Q| = 1$



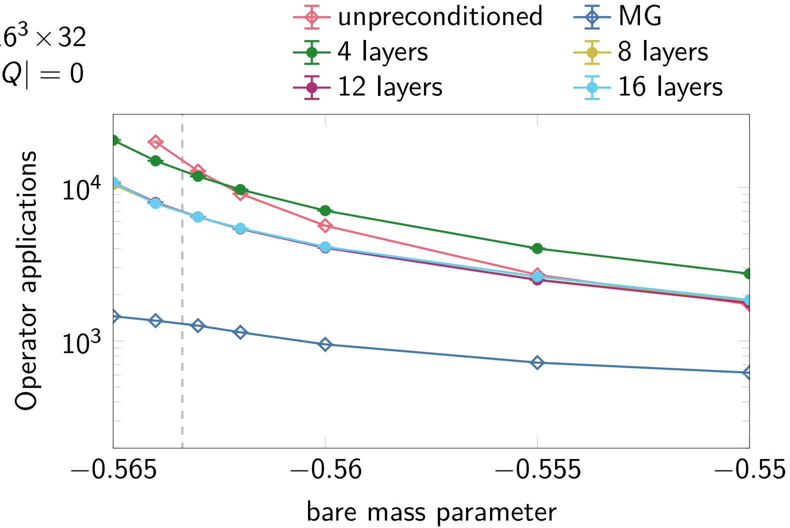
Critical slowing down

$8^3 \times 16$
$|Q| = 2$



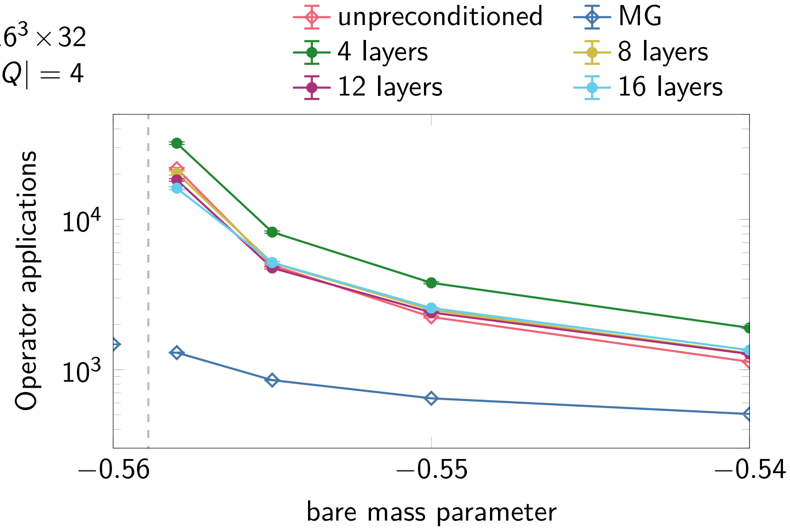
Critical slowing down

$16^3 \times 32$
$|Q| = 0$



Critical slowing down

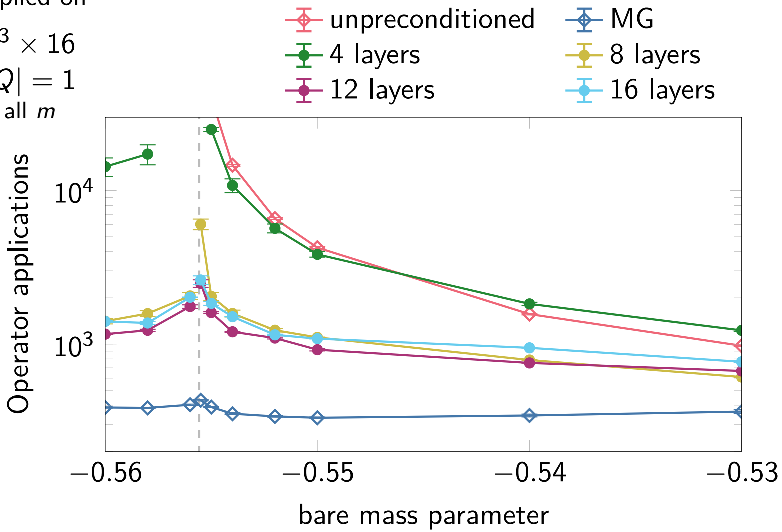
$16^3 \times 32$
$|Q| = 4$



Transfer

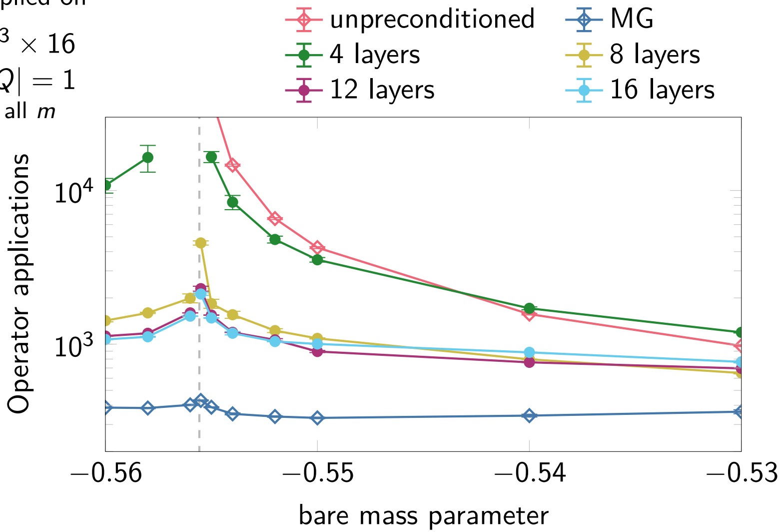
trained and
applied on

$8^3 \times 16$
$|Q| = 1$
all m



Transfer

trained on		applied on
$8^3 \times 16$		$8^3 \times 16$
$\lvert Q\rvert = 0$	$\rightarrow$	$\lvert Q\rvert = 1$
$m = -0.56$		all m



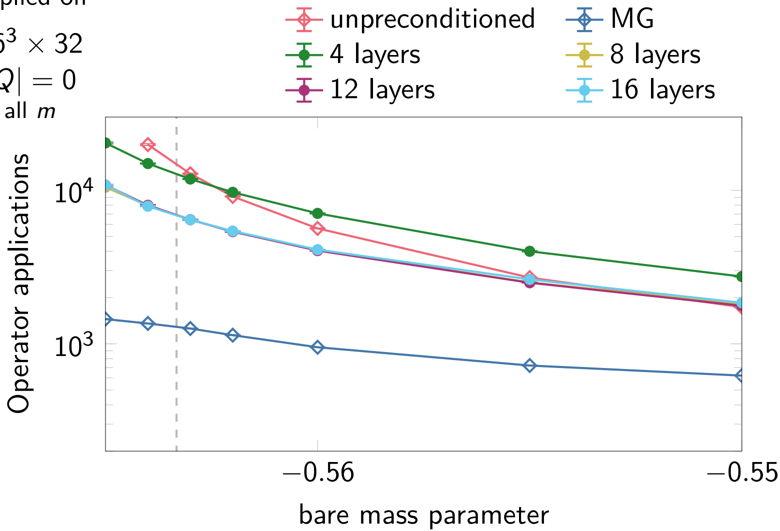
Transfer

trained and applied on

$16^3 \times 32$

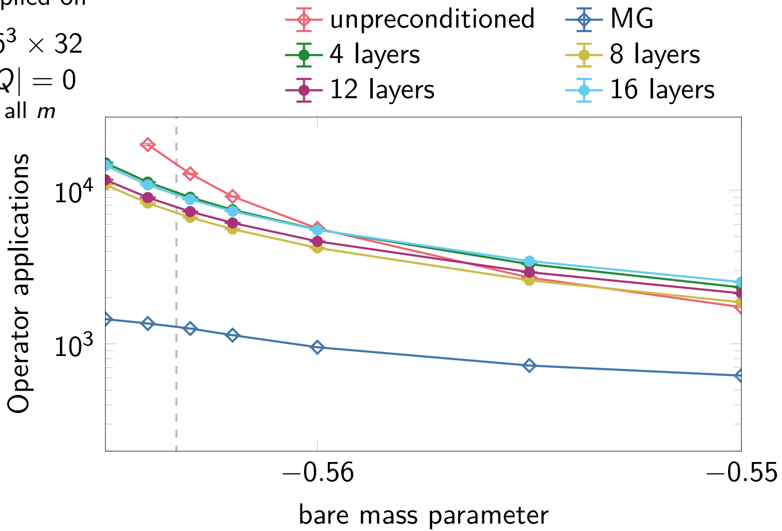
$|Q| = 0$

all m



Transfer

trained on		applied on
$8^3 \times 16$		$16^3 \times 32$
$\lvert Q\rvert = 0$	$\rightarrow$	$\lvert Q\rvert = 0$
$m = -0.56$		all m



Conclusion

Conclusion

Goals

- ☑ Build a preconditioner using ML that mitigates critical slowing down
- ☑ Transfer to unseen configurations without retraining
  $\rightarrow$ No costly setup
- ☒ Handle topological modes nicely

Next steps

- Understand why the architecture fails for topological modes
  - First study easier systems like Laplace operator or Schwinger model
  - Identify what is problematic about topological modes
- Explore models to generate representative near-null space vectors economically

Slides and code: simon-pfahler.github.io