Probing techniques for disconnected quark loop estimation in Lattice QCD

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QCD: theory of the strong interaction

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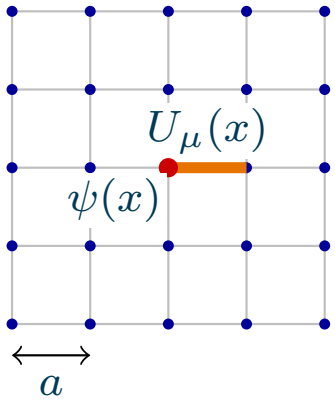

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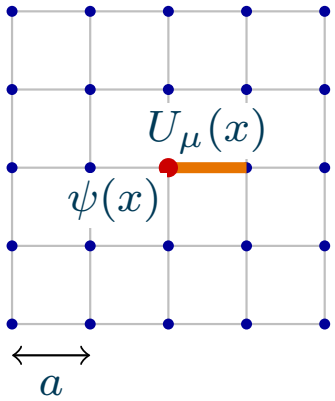

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4D lattice, N_{sites} sites: Dirac operator $D \longrightarrow$ sparse Dirac matrix

The Wilson–Dirac matrix

$$(D_W\psi)(x) = \left(m_0 + \frac{4}{a}\right)\psi(x)$$
$$- \frac{1}{2a}\sum_{\mu=0}^{3}\Big[(I_4 - \gamma_\mu)\otimes U_\mu(x)\,\psi(x+\hat{\mu}) + (I_4+\gamma_\mu)\otimes U_\mu^\dagger(x-\hat{\mu})\,\psi(x-\hat{\mu})\Big]$$

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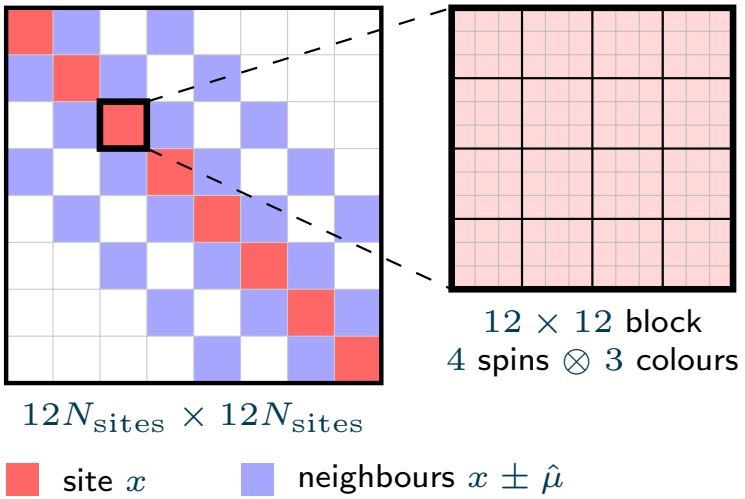

E250: 192×96^3 sites

$\Rightarrow \sim 2 \cdot 10^9$ unknowns

Operators

Lattice calculations: $\mathrm{Tr}[B(t)\, D^{-1}(t,t')]$

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Focus of this work: $t = t'$, $B(t) \in \{\Gamma_5(t),\, \Gamma_\mu(t)\}$

$$\Gamma(t) = I_{L^3} \otimes \gamma \otimes I_3, \qquad \gamma = \begin{cases} \gamma_5 & \text{pseudoscalar density} \\ \gamma_\mu & \text{vector current} \end{cases}$$

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Solution: stochastic trace estimation, e.g. the Hutchinson estimator.

Hutchinson method

Given $D \in \mathbb{C}^{n \times n}$ and random vectors $x^{(i)} \in \mathbb{R}^n, x_j : \mathbb{E}[x_j] = 0, \mathbb{E}[\bar{x}_j x_k] = \delta_{jk}$

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Hutchinson estimator*:

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Probing

$$\boxed{\mathbb{V}[x^\dagger A x] = \tfrac{1}{2}\|\mathrm{offdiag}(A + A^T)\|_F^2} \qquad (\mathbb{Z}_2 \text{ noise})$$

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- Couplings between sites at distance $\leq d$ do not contribute to $\mathbb{V}$

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Example: 4×4 grid (open boundaries)

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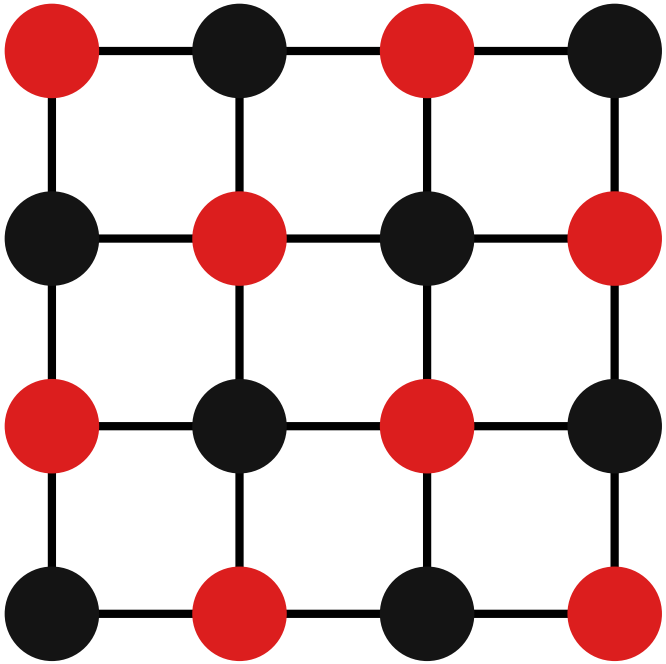

$d = 1$: 2 colors

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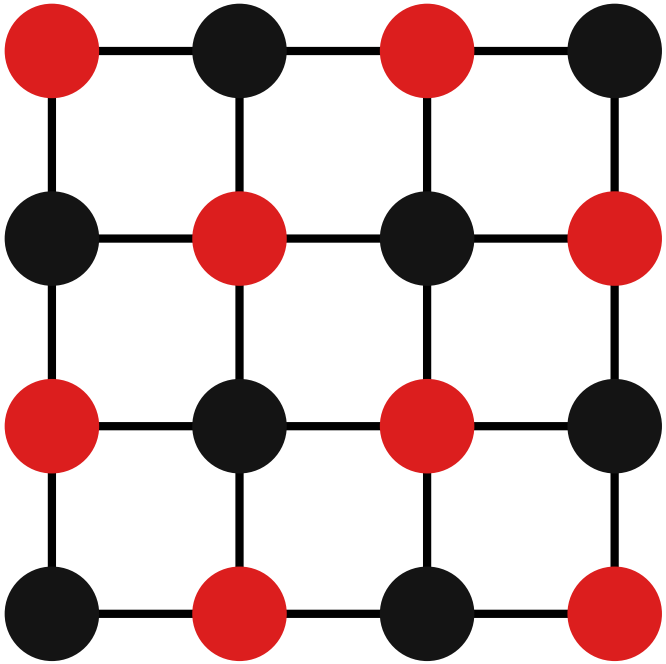

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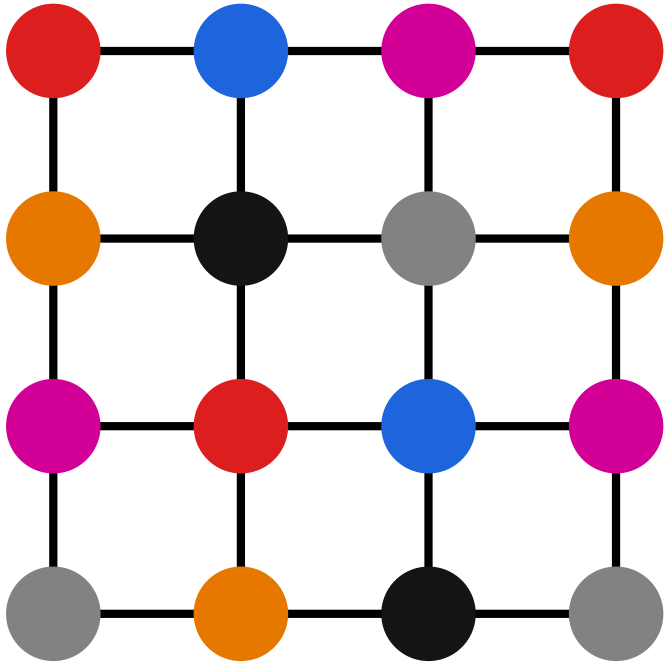

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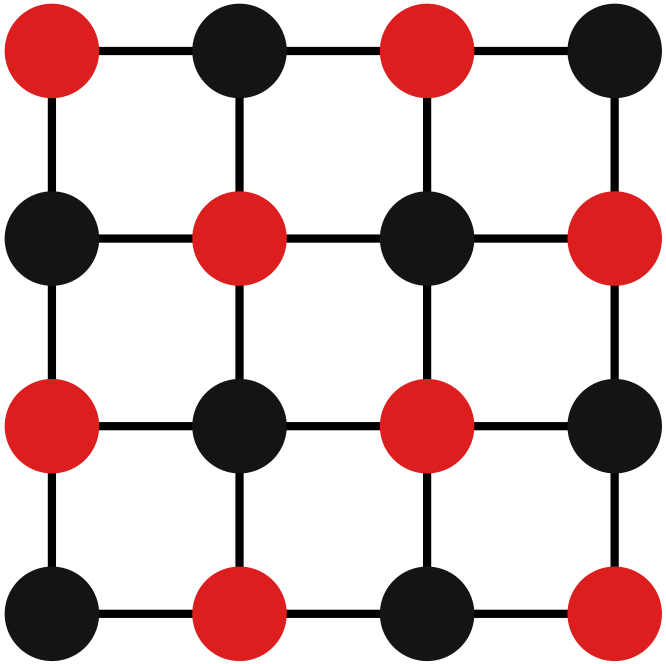

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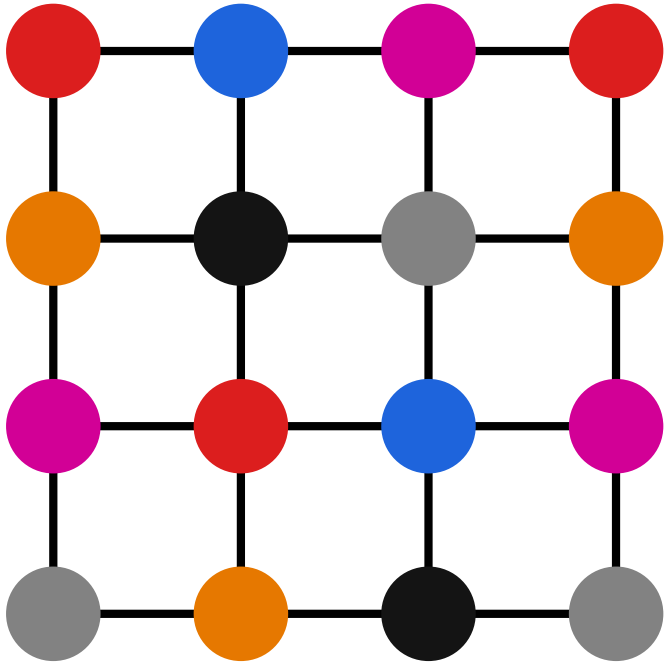

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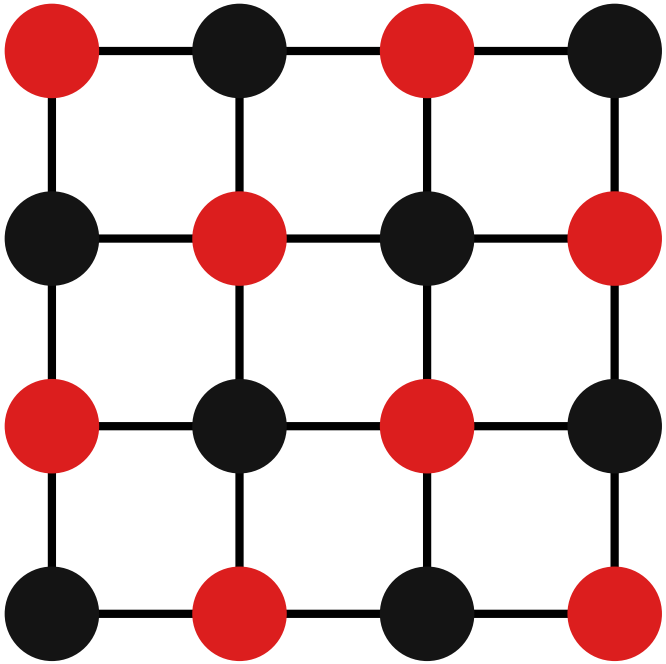

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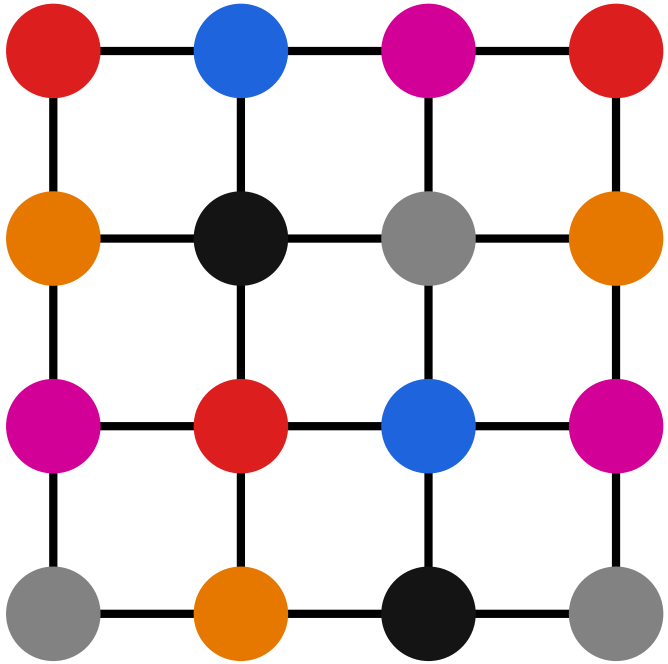

$d = 2$: 6 colors

$$v_2 = [0 \ \pm 1 \ 0 \ \pm 1 \ \pm 1 \ 0 \ \pm 1 \ 0 \ 0 \ \pm 1 \ 0 \ \pm 1 \ \pm 1 \ 0 \ \pm 1 \ 0]$$

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Full dilution $N_d = 12$: one vector per spin-color component.

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Probing + dilution estimator

$$\mathrm{Tr}\left[\Gamma(t)\, D^{-1}(t,t)\right] \approx \frac{1}{N} \sum_{k=1}^{N} \sum_{c=1}^{s} \sum_{l=1}^{N_d} \left(v_{c,l}^{(k)}\right)^{\dagger} \Gamma(t)\, D^{-1}(t,t)\, v_{c,l}^{(k)}$$

Total number of solves: $N_{\text{solve}} = s \cdot N_d \cdot N$

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Hierarchical coloring of the lattice [†] $\longrightarrow$ reuse of previous computation.

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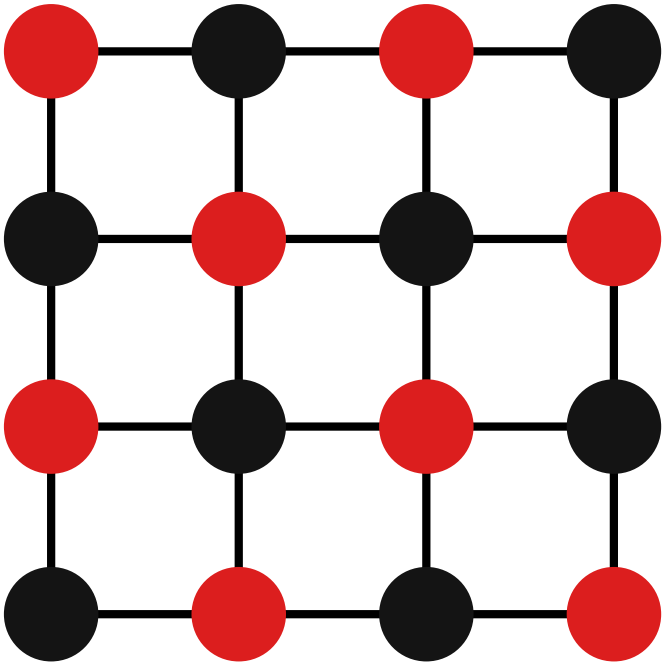

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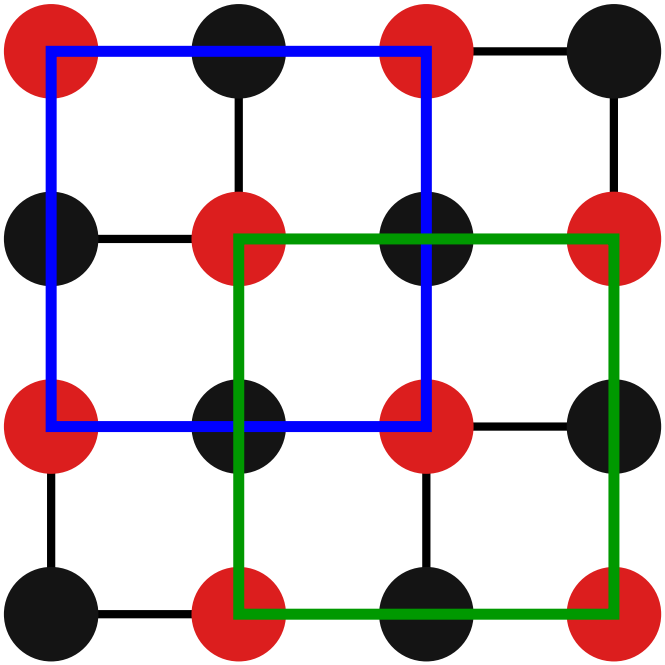

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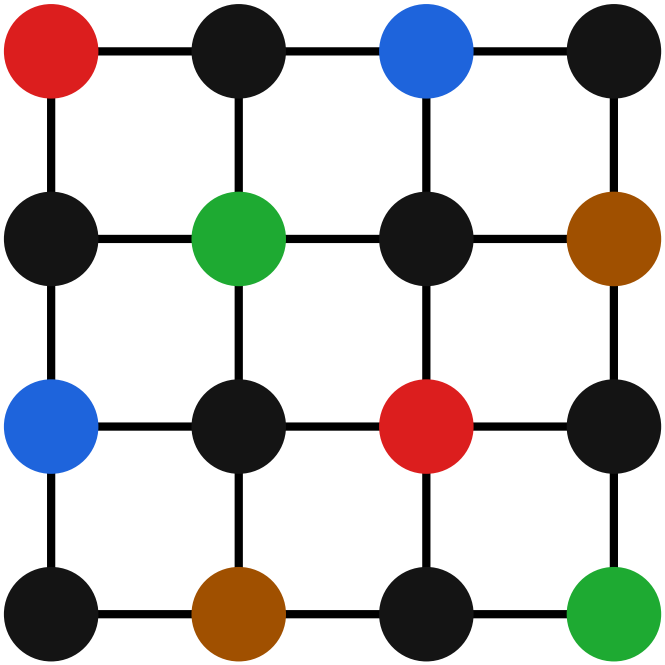

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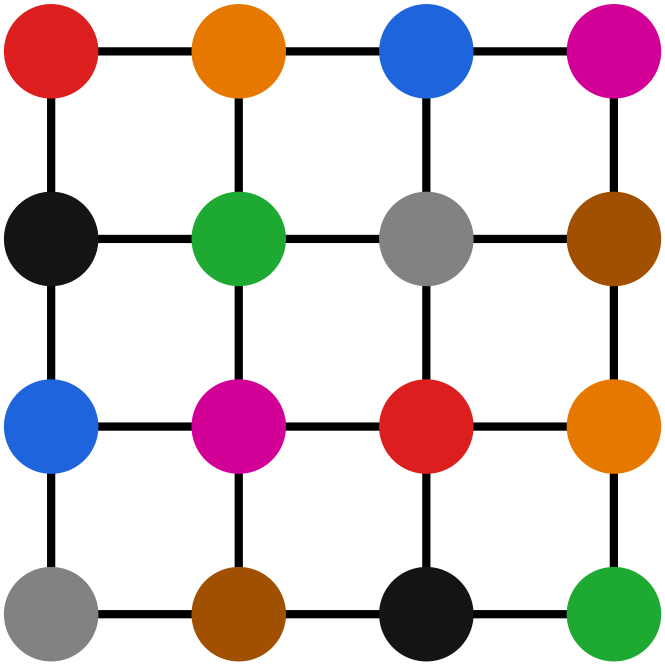

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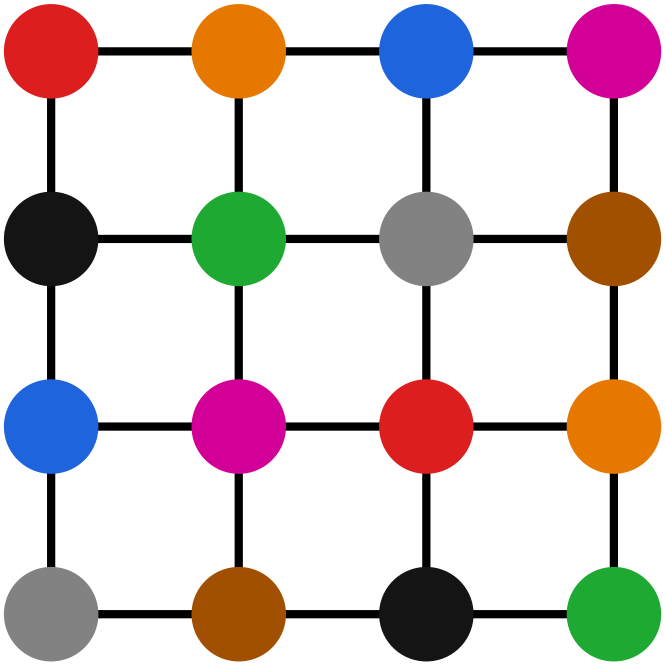

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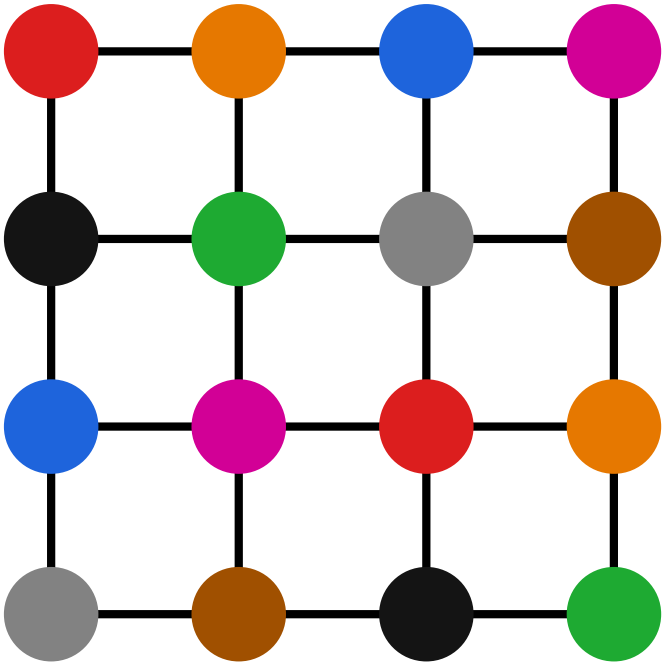

$$s = 2^{n_D(k-1)+1}$$

- **Large number of colors!**

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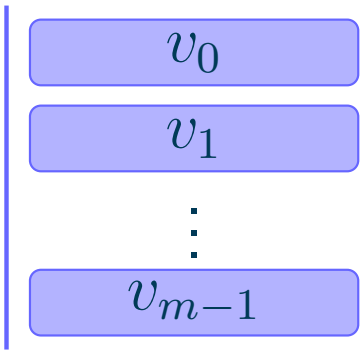
Hierarchical Probing: Nesting property

Level $k-1$

$d = 2^{k-2}$

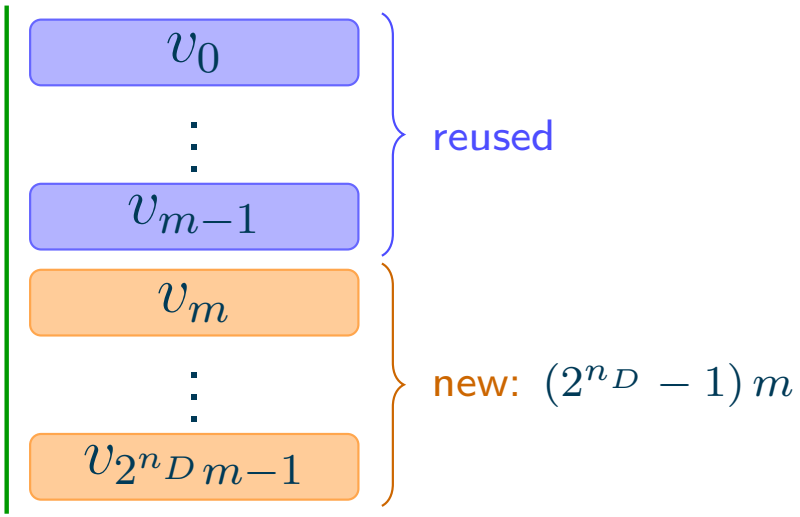


$m = 2^{n_D(k-2)+1}$ colors

$\subset$

Level k

$d = 2^{k-1}$



$2^{n_D} m = 2^{n_D(k-1)+1}$ colors

Multiplier-Based Coloring

Coloring function

Given a lattice site $x = (x_1, \ldots, x_{n_D})$:

$$\mathsf{col}(x) = \left(\sum_{i=1}^{n_D} \sigma_i \, x_i \right) \bmod \; s$$

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Input

- Lattice dimensions
- Boundary conditions
- Coloring distance d

exhaustive search →

Output

- $\sigma_1, \ldots, \sigma_{n_D}$
- s

Multiplier-based coloring

d	s			$s^{(HP)}$
	IV – 32^3	D450 – 64^3	E250 – 96^3	
1	2	2	2	2
2	10	8	8	16
3	16	16	12	–
4	32	32	32	128
5	88	64	48	–
6	128	128	96	–
7	176	152	144	–
8	272	256	288	1024

Table: Number of colors s for the multiplier-based coloring on the spatial time slices ($n_D = 3$) of the CLS ensembles D450 (128×64^3) and E250 (192×96^3), and of the 64×32^3 configuration. $s^{(HP)}$ is only defined for d a power of two.

Numerical setup

Observable: $\mathrm{Tr}[\Gamma(t)\, D^{-1}(t,t)]$ on time slice $t = 0$

- solver: DDαAMG
- full spin-colour dilution ($N_d = 12$)

Lattice	$T \times L^3$
IV	64×32^3
D450	128×64^3
E250	192×96^3

Comparison at fixed budget N

At fixed budget, each noise vector costs s solves

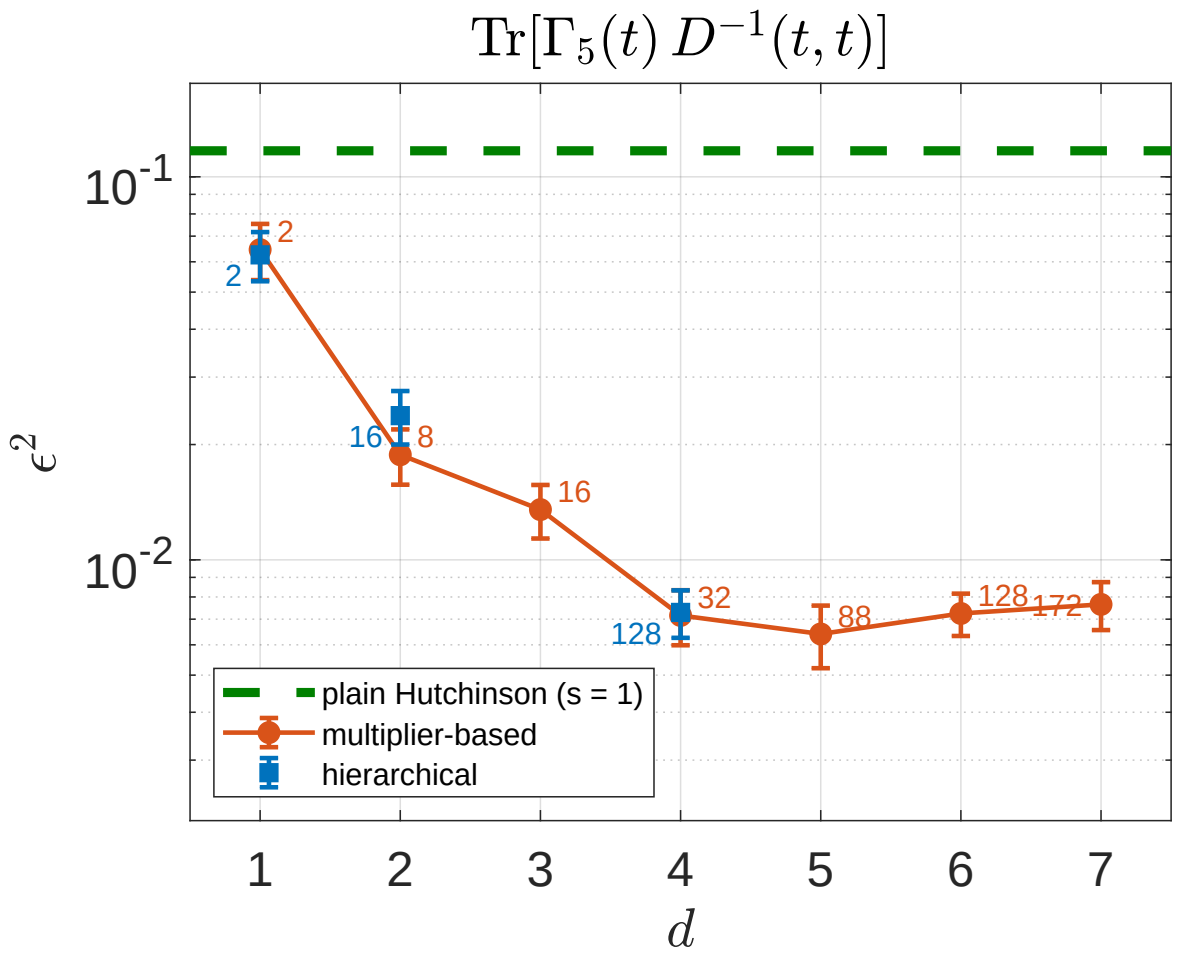
(per dilution component; the common factor N_d is omitted)

$$\epsilon^2 = \frac{s\, V(s)}{N}$$

Numerical results - IV

$m_\pi \approx 295\,\mathrm{MeV}$
$a \approx 0.071\,\mathrm{fm}$

$$\epsilon^2 = \frac{s\,V(s)}{N}$$

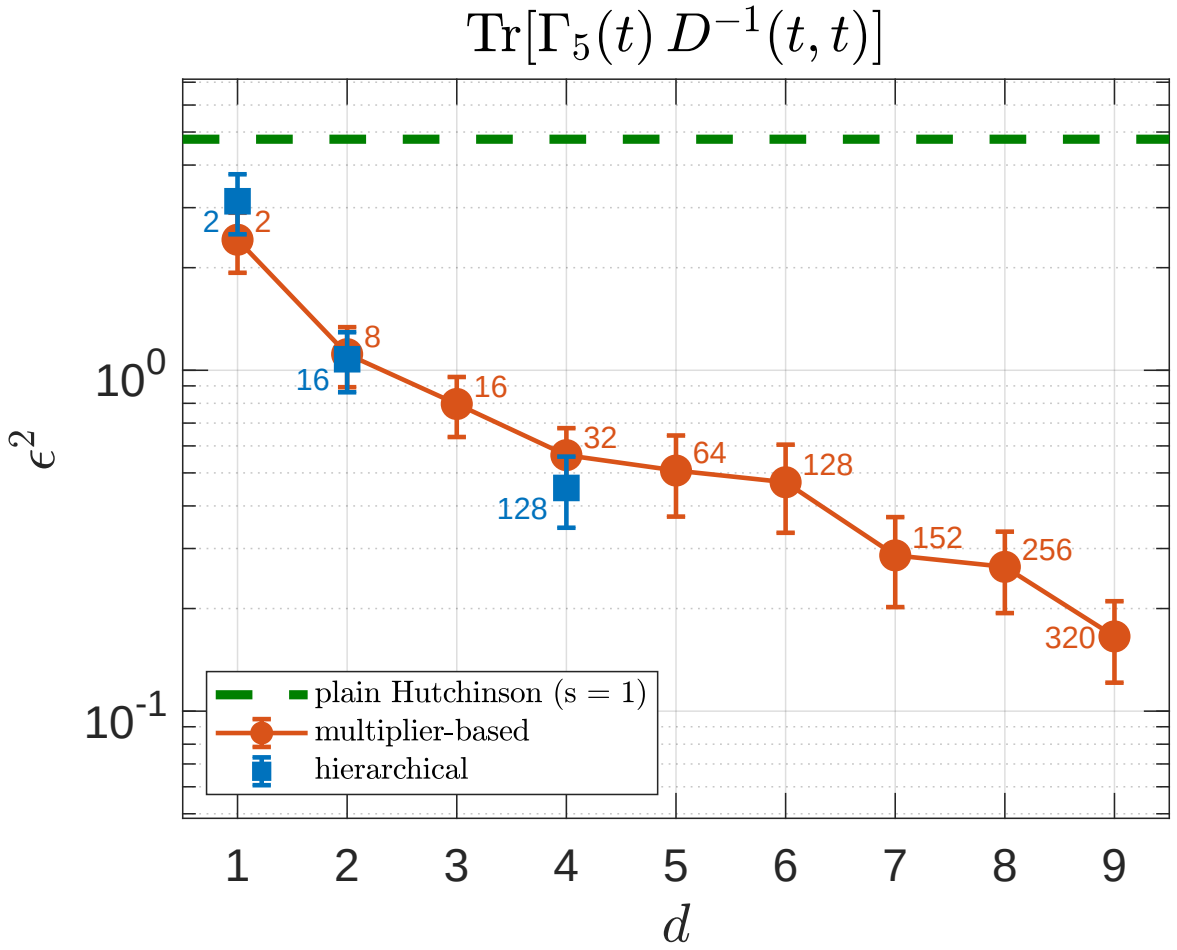


$d{=}3$: intermediate lower ϵ^2 | $s{=}8, 32$ ($d{=}2, 4$) matches HP at $s{=}16, 128$

Numerical results - D450

$m_\pi \approx 220\,\mathrm{MeV}$
$a \approx 0.075\,\mathrm{fm}$

$$\epsilon^2 = \frac{s\,V(s)}{N}$$

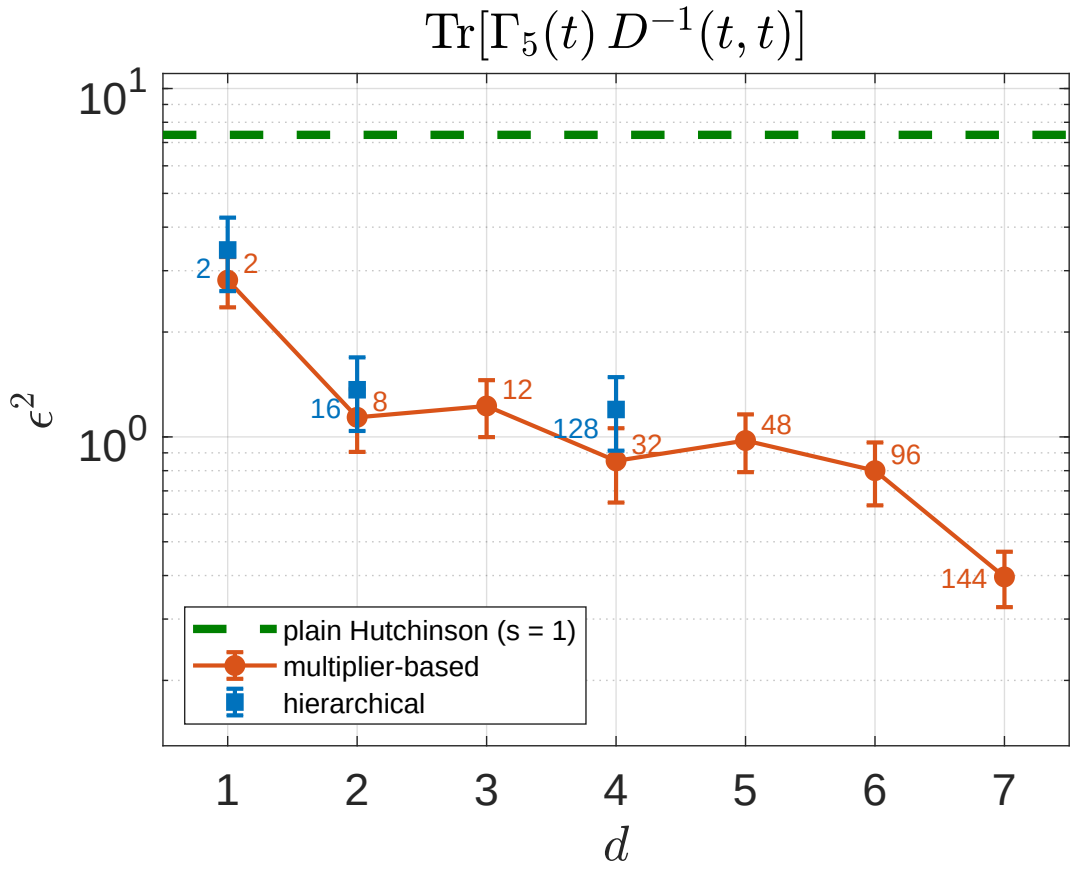


s=320: below every HP point

Numerical results - E250

$m_\pi \approx 135\,\mathrm{MeV}$
$a \approx 0.064\,\mathrm{fm}$

$$\epsilon^2 = \frac{s\,V(s)}{N}$$

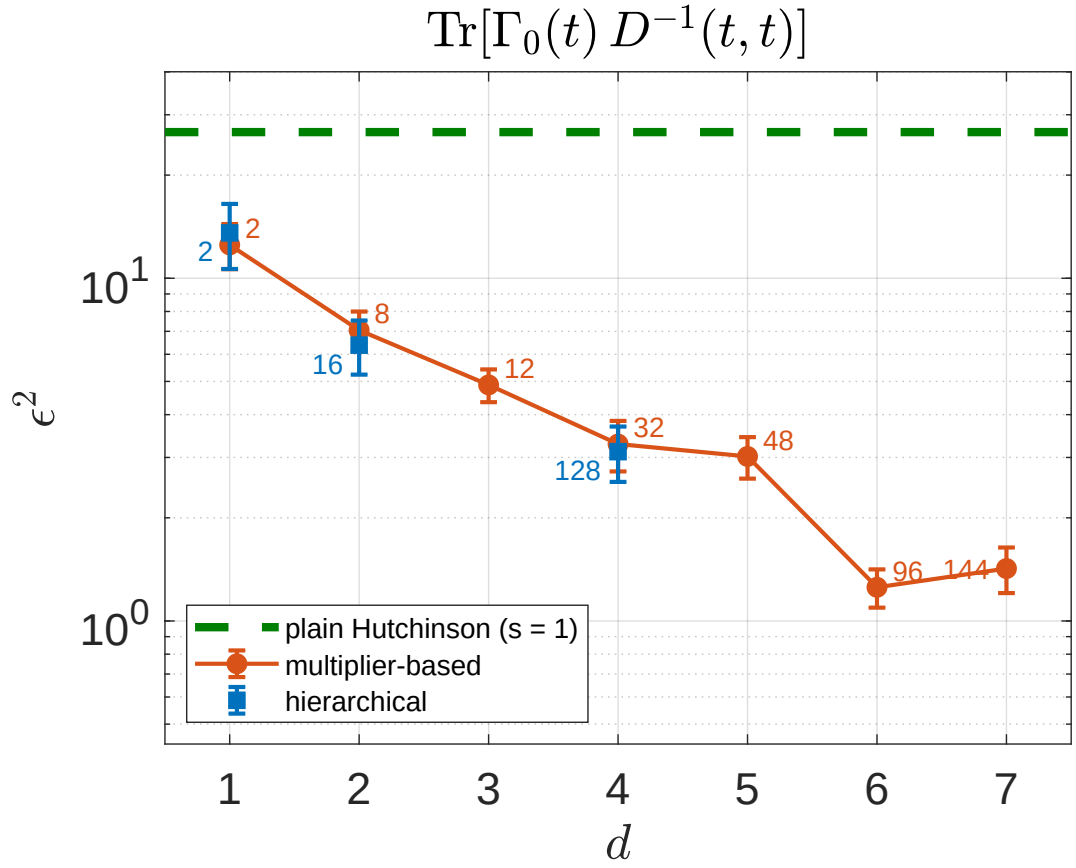


s=144: $\sim$3$\times$ below HP at s=128

Numerical results - E250

$m_\pi \approx 135\,\mathrm{MeV}$
$a \approx 0.064\,\mathrm{fm}$

$$\epsilon^2 = \frac{s\,V(s)}{N}$$



s=96, 144: $\sim$3$\times$ below HP at s=128

Conclusions and outlook

Multiplier-based coloring for $\mathrm{Tr}[\Gamma(t)\, D^{-1}(t,t)]$

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Multiplier-based coloring for $\mathrm{Tr}[\Gamma(t)\, D^{-1}(t,t)]$

- works for *any* distance d, not only powers of two
- fewer colors than hierarchical probing at comparable d
- variance reduction at equal cost on IV, D450 and E250

Thank you for your attention!

Questions?

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