# Multilevel strategies for full-QCD simulations

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## Multilevel basics: Local sampling

Parisi, Petronzio & Rapuano '83; ML & Weisz '01

Consider pure gauge theory

$$\langle \mathrm{tr}\{W\} \rangle \propto \mathrm{e}^{-\sigma A}$$

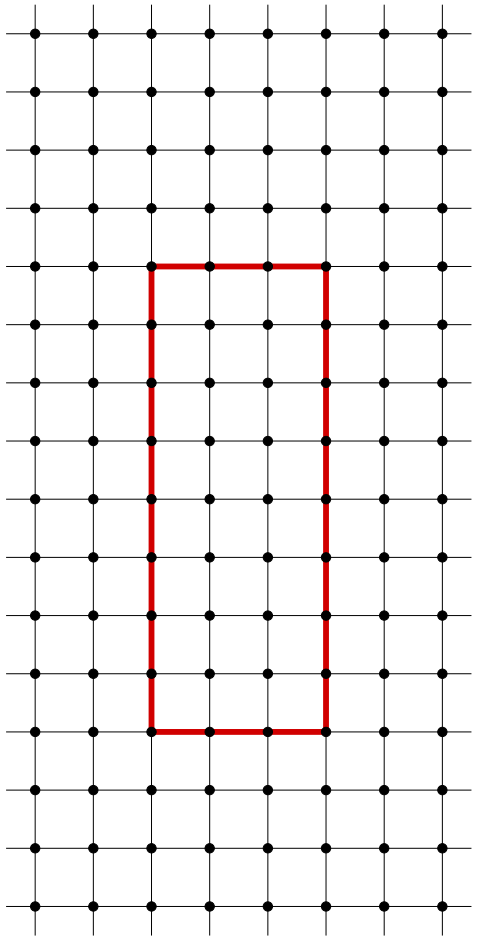
$\Rightarrow$ need $N \propto \mathrm{e}^{2\sigma A}$ measurements

Factorization

- Division of the lattice in *independent* domains
- Factorization of the observable

$$\mathrm{tr}\{W\} = \sqcup_{\alpha\beta} \sqcap_{\beta\alpha}$$

$\Rightarrow$ May sample $\sqcup_{\alpha\beta}$ and $\sqcap_{\beta\alpha}$ independently



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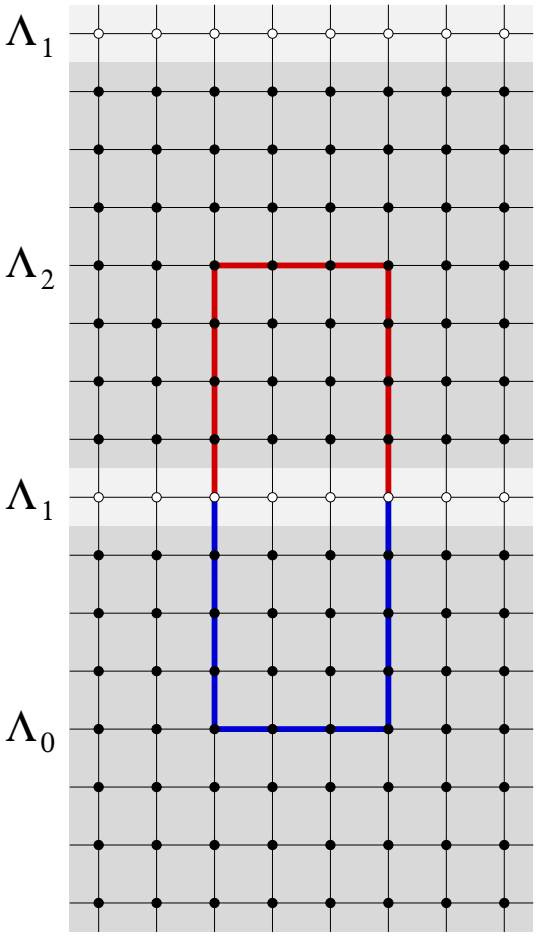


## 2-level update cycle

- ⋆ $n_0$ global updates, followed by
- ⋆ $n_1$ domain updates & measurement of $\langle \sqcup_{\alpha\beta} \rangle_{\Lambda_0}$ and $\langle \sqcap_{\beta\alpha} \rangle_{\Lambda_2}$

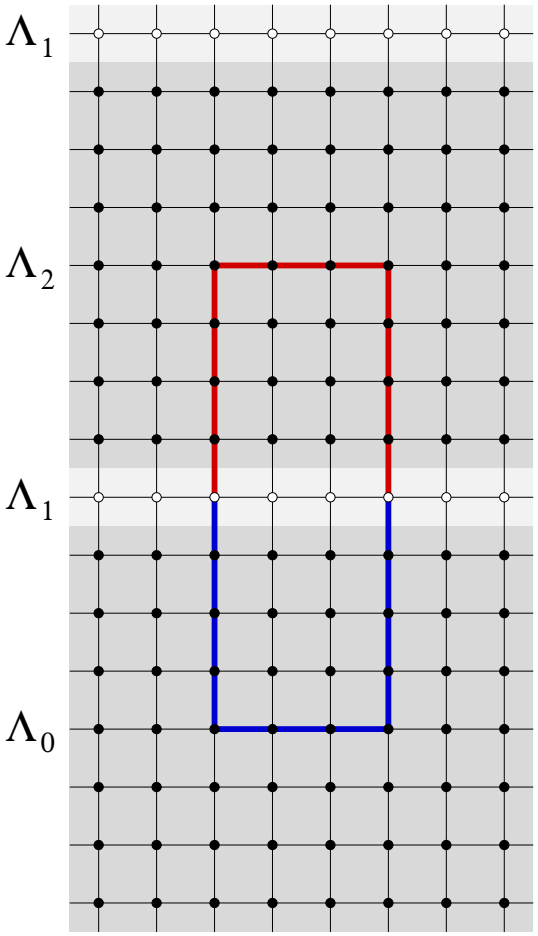
Up to statistical errors

$$\big\langle \mathrm{tr}\{W\} \big\rangle = \big\langle \langle \sqcup_{\alpha\beta} \rangle_{\Lambda_0} \langle \sqcap_{\beta\alpha} \rangle_{\Lambda_2} \big\rangle_{\mathrm{cycles}}$$

$\Rightarrow$ In each cycle, $S/N = \mathrm{O}(1)$ if

$$n_1 \propto \mathrm{e}^{\sigma A}$$

$\Rightarrow$ Exponential acceleration!

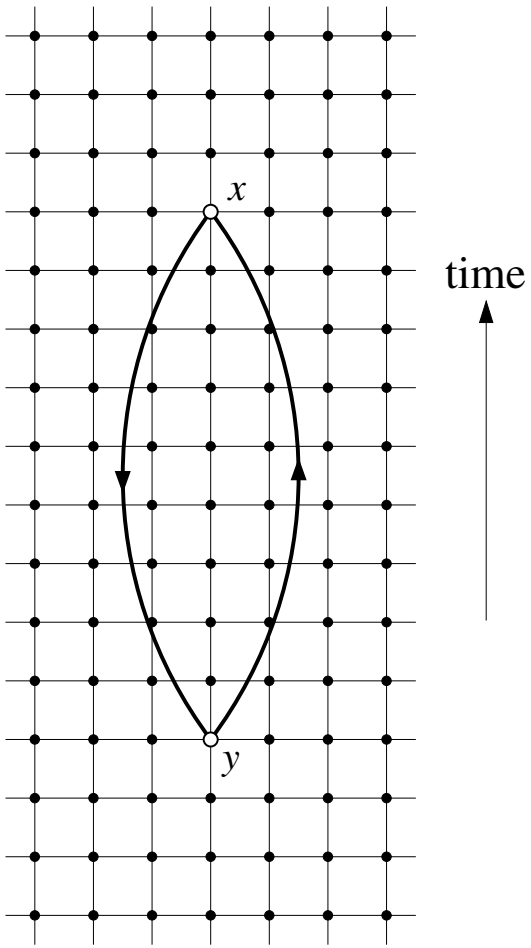


## Multilevel in full QCD?

After integrating over the quark fields

- Quark-line diagrams do not factorize
- Nor does the integration measure

But not all is lost ...



## Multiboson representation – a very old idea

ML '94; Boriçi & de Forcrand '95; Borelli et al. '96

Choose a real polynomial $P_N$ of even degree $N$ such that

$$\det D \simeq \det\{P_N(D)\}^{-1}$$

$$= \prod_{k=1}^{N/2} |\det(D - z_k)|^{-2}$$

The corresponding pseudo-fermion action

$$S_{\mathrm{mb}} = \sum_k \|(D - z_k)\phi_k\|^2$$

is local

$\Rightarrow$ QCD functional integral factorizes, but ...

## A better strategy

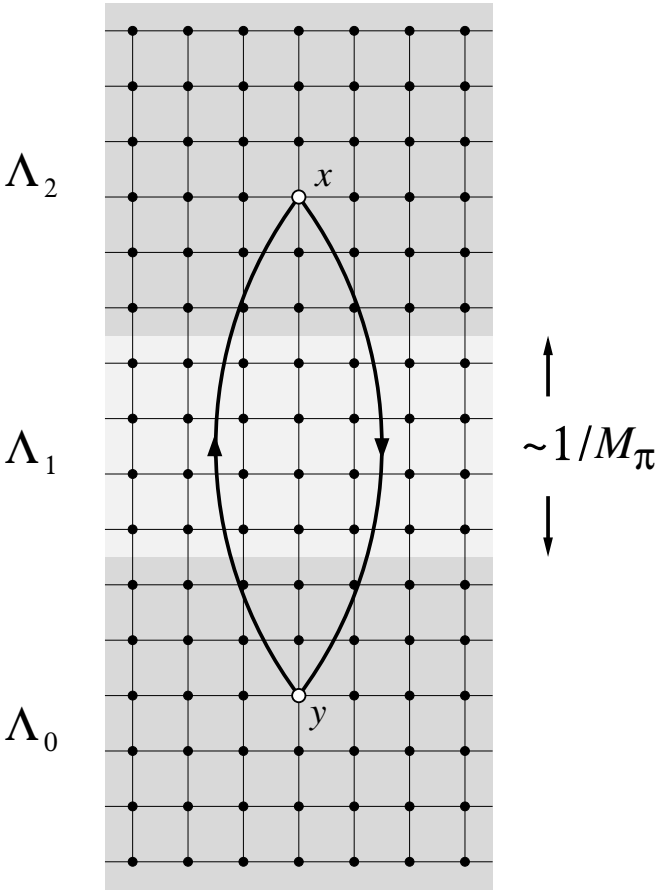
Cè, Giusti & Schaefer '16, '17

To decouple $\Lambda_0$ from $\Lambda_2$ use

- ⋆ *Overlapping SAP preconditioner*

$$\det D = \frac{\det DM_{\rm sap}}{\det M_{\rm sap}}$$

- ⋆ *Multiboson representation for the residual term* $\det DM_{\rm sap}$




open bc

## Domain decomposition of $D$

Wilson quarks & open bc

Projector to $\Lambda_k$

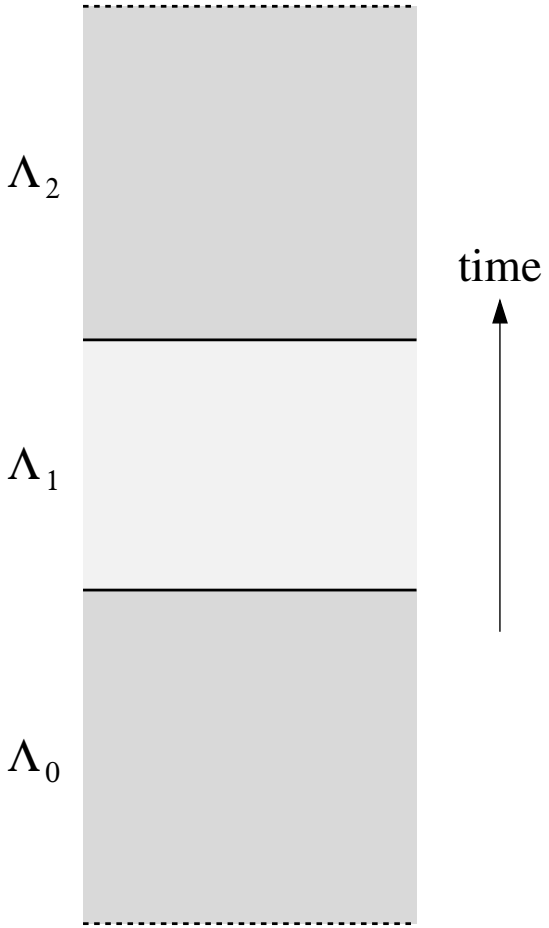
$$I_k\psi(x) = \begin{cases} \psi(x) & \text{if } x \in \Lambda_k \\ 0 & \text{otherwise} \end{cases}$$

Projector to the inner boundaries of $\Lambda_k$

$$P_k\psi(x) = \begin{cases} \psi(x) & \text{if } x \in \partial\Lambda_k^* \\ 0 & \text{otherwise} \end{cases}$$

Decomposition of $D$

$$D = D_{00} + D_{01} + D_{10} + \ldots, \qquad D_{kl} = I_k D I_l$$



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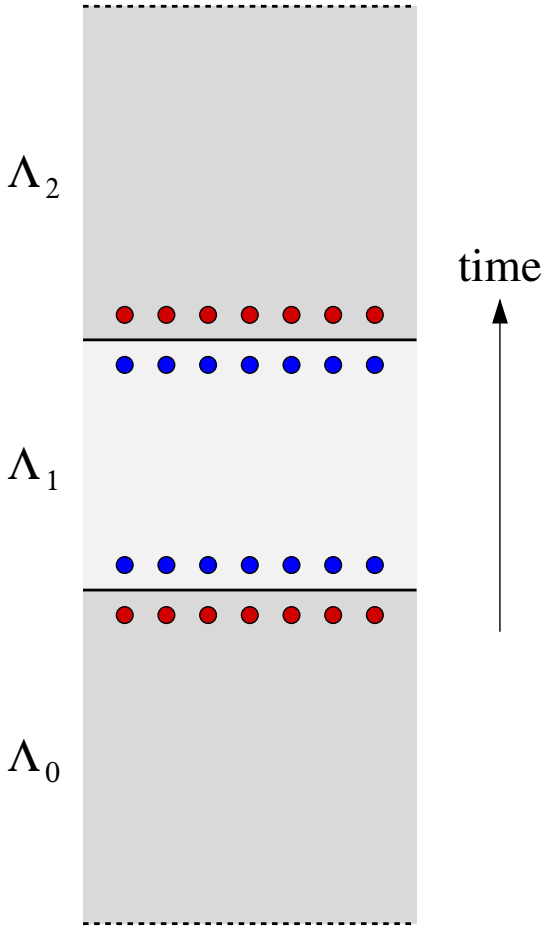


## Overlapping Schwarz procedure

Approximately solve $D\psi = \eta$ in two steps

**Step 1:** Solve equation in $\Lambda_0 \cup \Lambda_1$

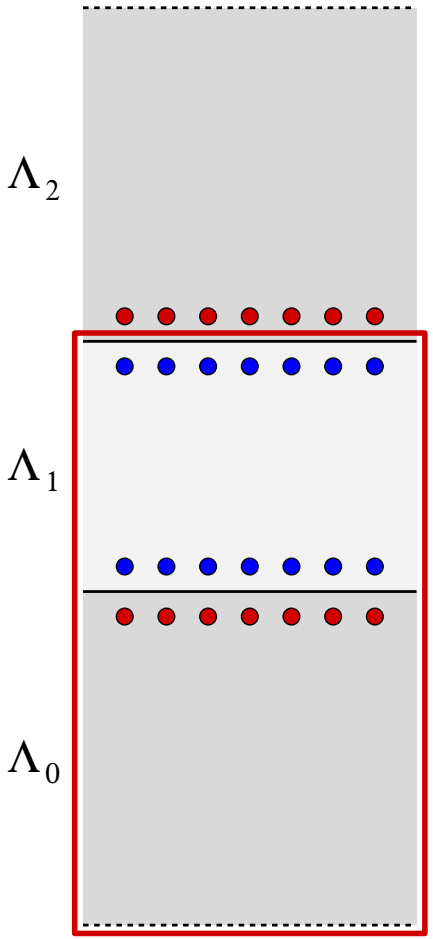
$$\psi_0 = D_0^{-1}(1 - I_2)\eta$$

$$\begin{aligned}\eta_0 &= \eta - D\psi_0 \\ &= I_2\eta - D_{21}D_0^{-1}(1 - I_2)\eta\end{aligned}$$

**Step 2:** Solve equation in $\Lambda_2 \cup \Lambda_1$

$$\psi_1 = D_2^{-1}(1 - I_0)\eta_0$$

$$\begin{aligned}\eta_1 &= \eta - D(\psi_0 + \psi_1) \\ &= -D_{01}D_2^{-1}(1 - I_0)\eta_0\end{aligned}$$



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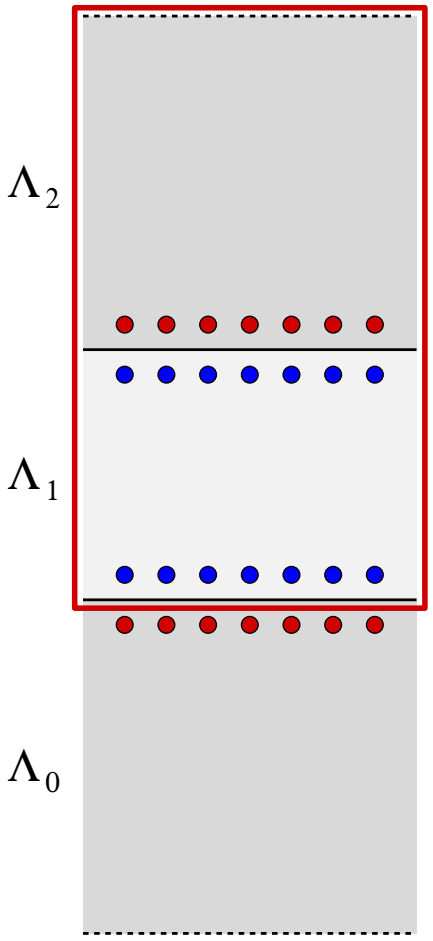


## SAP preconditioner

$$\psi_0 + \psi_1 = M_{\rm sap}\eta$$

$$M_{\rm sap} = D_2^{-1}(1 - I_0) + \ldots$$

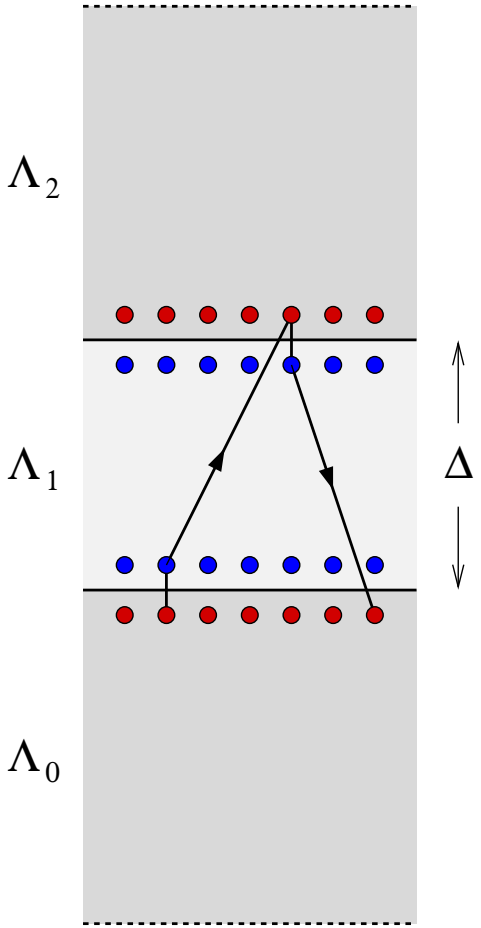
$$DM_{\rm sap} = 1 + \text{small}$$

More precisely

$$\det(DM_{\rm sap}) = \det(1 - w)$$

$$w = P_0 D_0^{-1} D_{12} D_2^{-1} D_{10} P_0$$

$$\Rightarrow \quad w = \mathrm{O}\left(\mathrm{e}^{-M_\pi \Delta}\right)$$

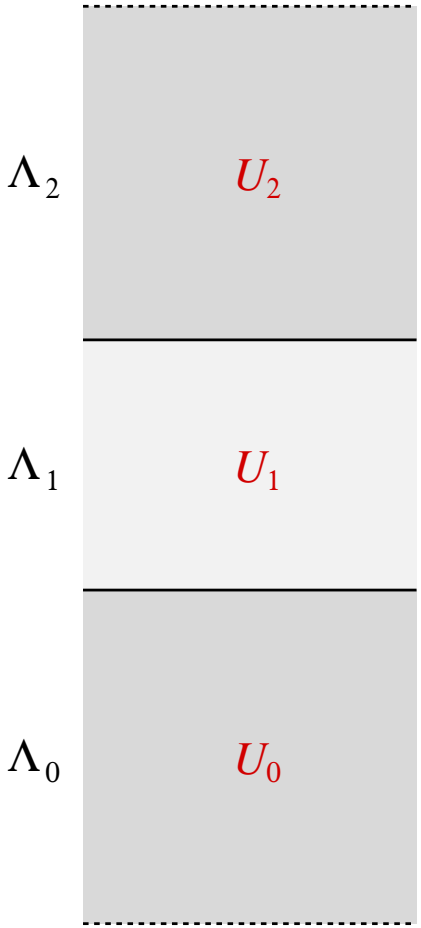


## Factorization of $\det D$

After some algebra ...

$$\det D = \frac{\det(DM_{\text{sap}})}{\det M_{\text{sap}}}$$

$$= \det D_0 \det D_2 \frac{\det(1-w)}{\det D_{11}}$$




- For fixed $U_1$, and if $\det(1-w)$ is neglected, the fields $U_0$ and $U_2$ are decoupled!
- Use multiboson representation for $\det(1-w)$
  $\Rightarrow$ decoupling up to terms $\propto \mathrm{tr}\{w^{N+1}\}$

## Multiboson representation

Consider doublets of pseudo-fermion fields

$$\phi = \begin{pmatrix} \zeta_0 \\ \zeta_2 \end{pmatrix}, \quad P_0\zeta_0 = \zeta_0, \ \ldots$$

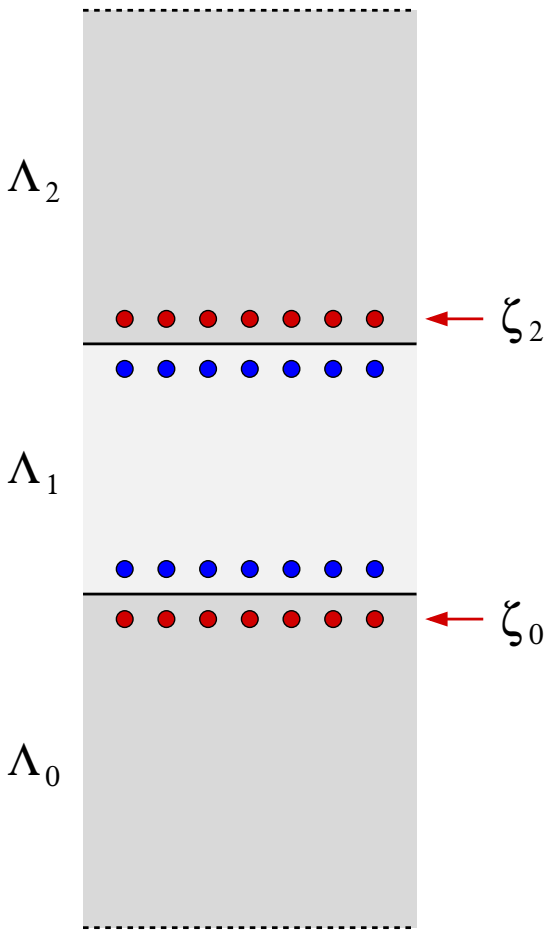
and, for any $v \in \mathbb{C}$, the operator

$$W_v = \begin{pmatrix} vP_0 & P_0 D_0^{-1} D_{12} \\ P_2 D_2^{-1} D_{10} & vP_2 \end{pmatrix}$$

A correct multiboson action is then

$$S_{\mathrm{mb}} = \sum_{k=1}^{N/2} \|W_{v_k}\phi_k\|^2, \quad v_k = \sqrt{z_k}$$

$\Rightarrow$ $U_0$ and $U_2$ are decoupled!



## Summarizing . . .

Factorized functional integral

$$\int \mathrm{D}[U]\,\mathrm{e}^{-S_{\mathrm{G}}} \prod_{u,d,s,\ldots} \mathrm{D}[\phi]\,\frac{\det D_0 \det D_2}{\det D_{11}}\,\mathrm{e}^{-S_{\mathrm{mb}}}$$

- ⋆ *2-level update cycle as before*
- ⋆ *Forces deriving from $S_{\mathrm{mb}}$ are small*
- ⋆ *Established acceleration methods apply:*
  *Local deflation, SAP, etc.*

## Factorization of the vector-meson propagator

Assume exact isospin symmetry

$$S \to S + \sum_x J^a_\mu(x)(\overline{\psi} i\tau^a \gamma_\mu \psi)(x)$$

$$\langle(\overline{\psi}\tau^a\gamma_\mu\psi)(x)\,(\overline{\psi}(y)\tau^b\gamma_\nu\psi)(y)\rangle = -\left.\frac{\partial^2 \ln \mathcal{Z}}{\partial J^a_\mu(x)\partial J^b_\nu(y)}\right|_{J=0}$$

The addition of the source term amounts to

$$D \to D + J^a_\mu i\tau^a\gamma_\mu$$

$\Rightarrow$ $\det D$ factorizes as before!

Before factorization of $\det D$

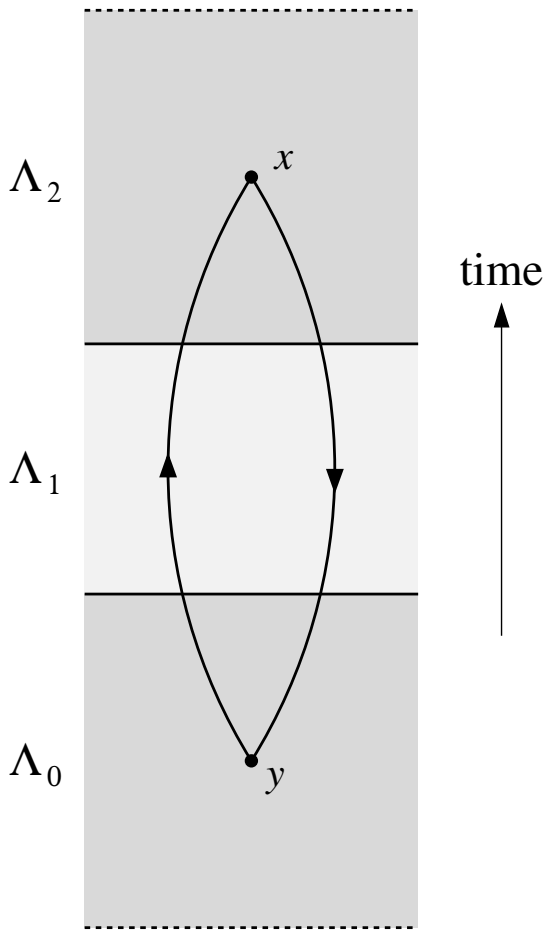
$$\left.\frac{\partial^2 \ln \mathcal{Z}}{\partial J^a_\mu(x)\partial J^b_\nu(y)}\right|_{J=0}$$

$$= \left\langle \mathrm{tr}\left\{\tau^a \gamma_\mu S(x,y)\tau^b \gamma_\nu S(y,x)\right\}\right\rangle$$

After factorization

$$= \left\langle \frac{\partial S_{\mathrm{mb}}}{\partial J^a_\mu(x)} \frac{\partial S_{\mathrm{mb}}}{\partial J^b_\nu(y)} \right\rangle + \mathrm{O}\left(\mathrm{e}^{-NM_\pi \Delta}\right)$$

$\Rightarrow$ Factorized observable!



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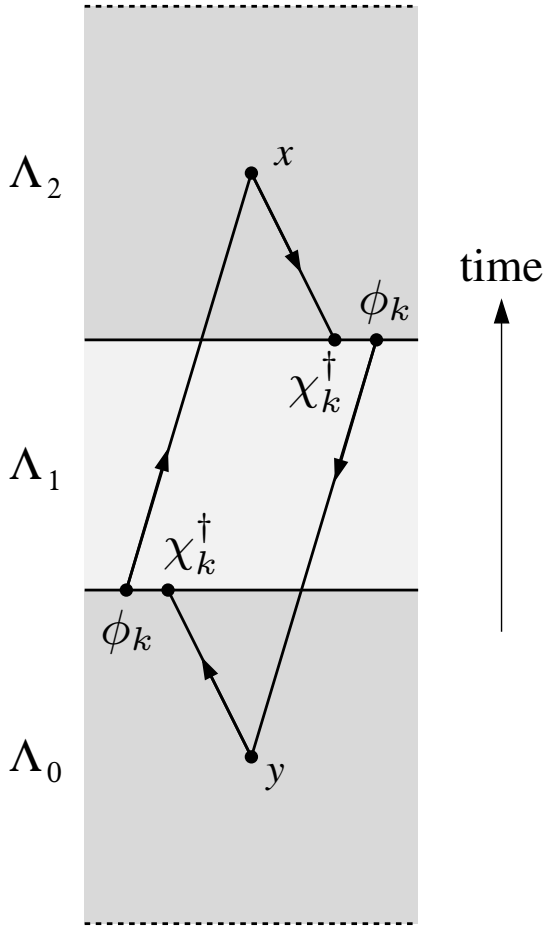


$$\chi_k = W_{v_k}\phi_k$$

## Concluding remarks

*Works out for*

* *Improved actions*
* *Disconnected diagrams and baryon propagators*

*DW and twisted-mass quarks?*

*Propagator factorizations using random fields*

Giusti, Harris, Nada & Schaefer '18, ...

*A version of* `openQCD` *supporting multilevel simulations is in preparation*

Giusti & ML '22f