Introduction to multilevel algorithms

III: Factorization of the quark determinant

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Schwarz alternating procedure (SAP)

Based on iterative improvement

$$D\psi = \eta, \qquad \psi = \psi_0 + \psi_1 + \ldots,$$

$$D\psi_0 \simeq \eta,$$

$$D\psi_1 \simeq \eta - D\psi_0,$$

$$D\psi_2 \simeq \eta - D(\psi_0 + \psi_1), \quad \ldots$$

Hermann Amandus
Schwarz
(1843–1921)

Here we shall use the

"Multiplicative overlapping Schwarz alternating procedure"

as preconditioner for D

Domain decomposition

QCD with Wilson quarks & open bc

Projector to Λ_k

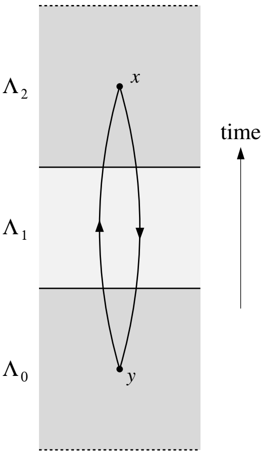
$$I_k\psi(x) = \begin{cases} \psi(x) & \text{if } x \in \Lambda_k \\ 0 & \text{otherwise} \end{cases}$$

Projector to the inner boundaries of Λ_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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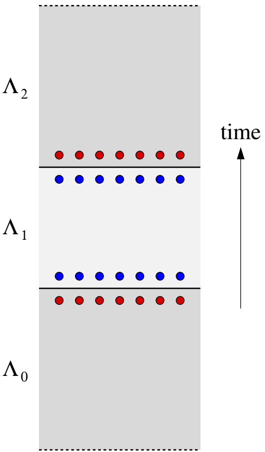


Overlapping Schwarz procedure

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

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

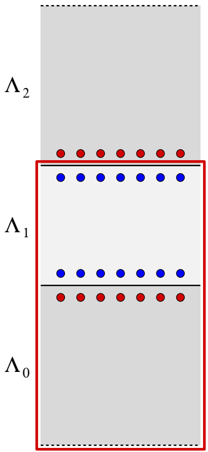
$$\psi_0 = D_0^{-1}(1 - I_2)\eta$$

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

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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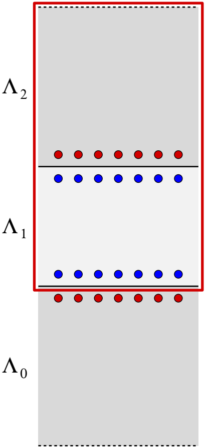


SAP preconditioner

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

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

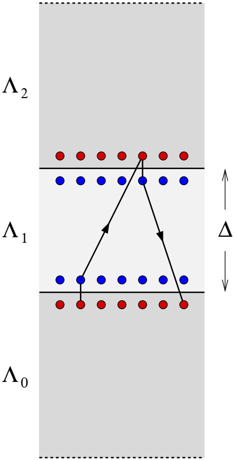
$$DM_{\mathrm{sap}} = 1 + \text{small}$$

More precisely

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

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

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

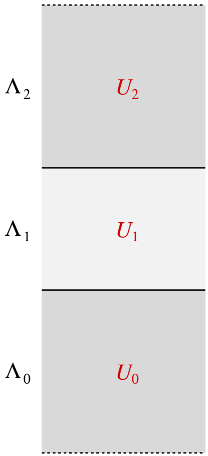


Factorization of $\det D$

After some algebra ...

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

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



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

Multiboson representation of $\det(1-w)$

For even N and using the γ_5-Hermiticity of D

$$\det(1-w) = R_N \prod_{k=1}^{N/2} \left|\det(z_k - w)\right|^{-2}, \qquad z_k = \exp\left\{2\pi i \frac{k}{N+1}\right\}$$

$$R_N \propto \det(1-w^{N+1}) = 1 + \mathrm{O}\left(\mathrm{e}^{-(N+1)M_\pi \Delta}\right)$$

The multiboson action

$$S_{\mathrm{mb}}(U,\phi) = \sum_{k=1}^{N/2} \|(z_k - w)\phi_k\|^2$$

however does not decouple U_0 from U_2!

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

Multiboson representation (cont.)

Consider doublets of pseudo-fermion fields

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

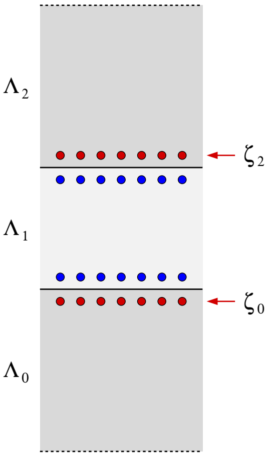
and, for any $v \in \mathbb{C}$, the operator

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

A correct multiboson action is then

$$S_{\rm mb}(U,\phi) = \sum_{k=1}^{N/2} \|W_{v_k}\phi_k\|^2, \quad v_k = \sqrt{z_k}$$

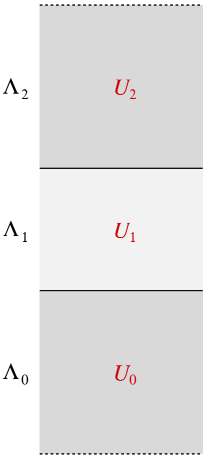
$\Rightarrow$ U_0 and U_2 are decoupled!



Summarizing . . .

Partition function with factorized $\det D$

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



Multilevel HMC simulations

- *May update all U or just U_0 or U_2*
- *Forces deriving from S_{mb} are small*
- *Established acceleration methods (Hasenbusch factorization, local deflation, etc.) apply*

Example: Vector-meson 2-point function

Assume exact isospin symmetry

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

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

The addition of the source term amounts to

$$D \to D + J_\mu^a i\tau^a\gamma_\mu$$

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

Before factorization

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

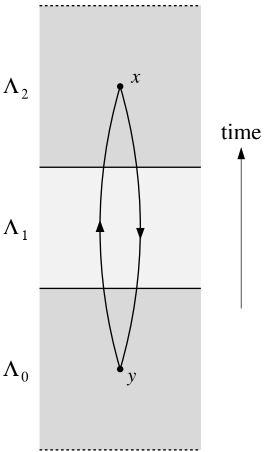
$$= \det D \operatorname{tr}\left\{\tau^a \gamma_\mu S(x,y) \tau^b \gamma_\nu S(y,x)\right\}$$

After factorization

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

$$= \left\langle \frac{\partial S_{\rm mb}}{\partial J^a_\mu(x)} \frac{\partial S_{\rm mb}}{\partial J^b_\nu(y)} \right\rangle_{J=0} + \mathrm{O}\left(\mathrm{e}^{-N M_\pi \Delta}\right)$$

$\Rightarrow$ factorized observable!



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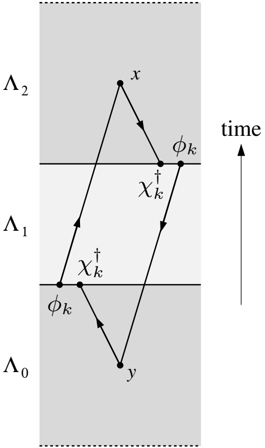

$$\chi_k = W_{v_k}\phi_k$$

Concluding remarks

Multilevel simulations of QCD work out $\rightarrow$ references

Will likely see some large-scale applications in the coming years (HVP, ...)

The factorization of the observables however deserves further study & development