Four-dimensional domain decomposition for the factorization of the fermion determinant

Matteo Saccardi Leonardo Giusti

UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

INFN Istituto Nazionale di Fisica Nucleare

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Based on: *L. Giusti, M. Saccardi, Physics Letters B 829 (2022) 137103*

Overview

Introduction and Motivations

- The analytical integration of fermionic degrees of freedom

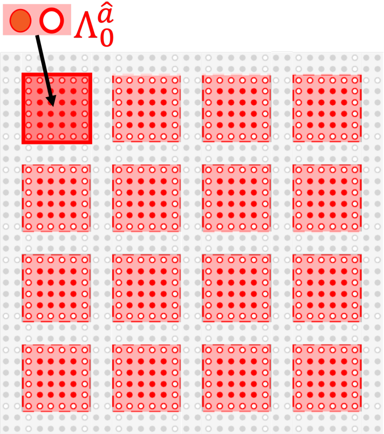
$$\int \mathcal{D}U e^{-S_G[U]} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-\bar{\psi}D[U]\psi} = \int \mathcal{D}U e^{-S_G[U]} \det D[U]$$

leads to an effective bosonic theory with action

$$S^{eff}[U] = \underbrace{S_G[U]}_{\text{local}} + \underbrace{S_F^{eff}[U]}_{\text{global}}, \qquad S_F^{eff}[U] = -\ln\det D[U]$$

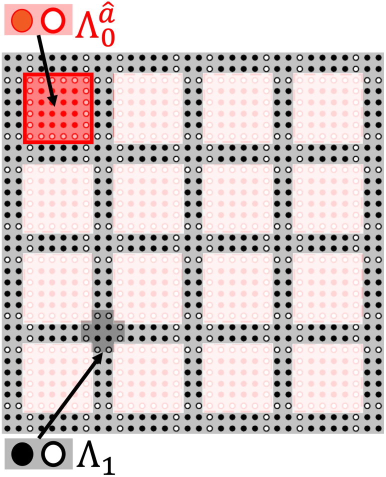
- Aim: factorize $\det D[U]$
- Here: factorization via an overlapping $4d$ domain decomposition

Domain decomposition: bulk



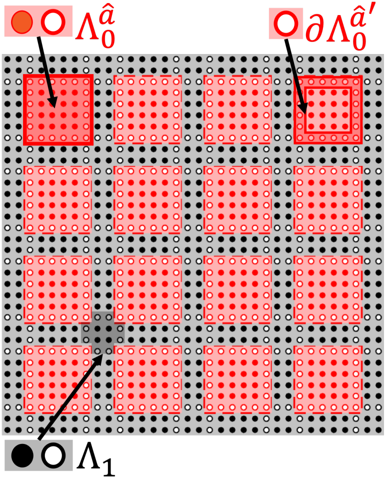
- Aim: factorize dependence on local hypercubic blocks $\Lambda_0^{\hat{a}}$ (red)
- *Active* disconnected $\Lambda_0 \equiv \bigcup_{\hat{a}} \Lambda_0^{\hat{a}}$

Domain decomposition: bulk



- Aim: factorize dependence on local hypercubic blocks $\Lambda_0^{\hat{a}}$ (red)
- *Active* disconnected $\Lambda_0 \equiv \bigcup_{\hat{a}} \Lambda_0^{\hat{a}}$
- *Inactive* connected Λ_1 (grey)

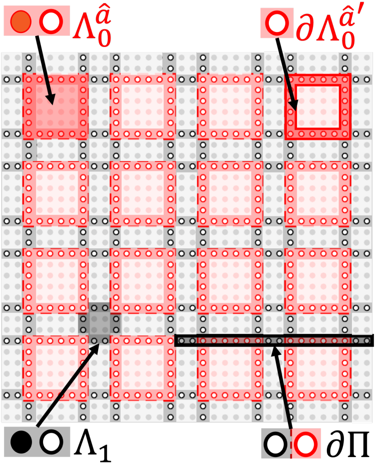
Domain decomposition: boundaries



- Internal boundaries of each $\Lambda_0^{\hat{a}}$ (empty circles in the red region)

$$\partial\Lambda_0^{\hat{a}}, \quad \partial\Lambda_0 \equiv \bigcup_{\hat{a}} \partial\Lambda_0^{\hat{a}}$$

Domain decomposition: boundaries



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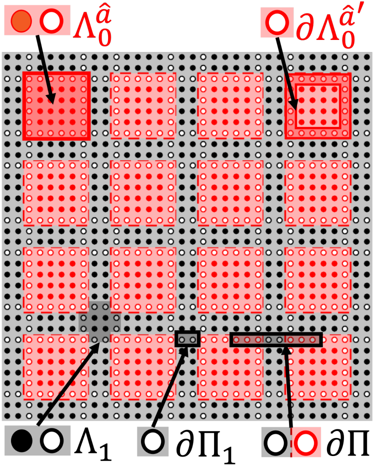
$$\partial\Lambda_0^{\hat{a}}, \quad \partial\Lambda_0 \equiv \bigcup_{\hat{a}} \partial\Lambda_0^{\hat{a}}$$

- $\partial\Pi$ union of hyperplanes passing by $\partial\Lambda_0$ (all empty circles)

Domain decomposition: boundaries



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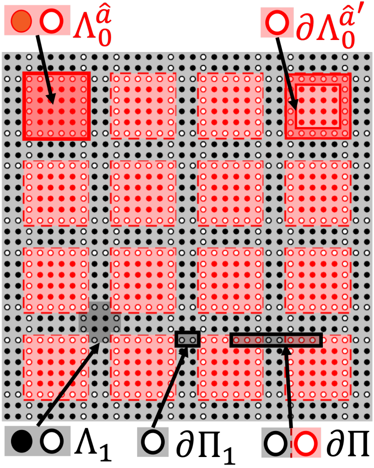
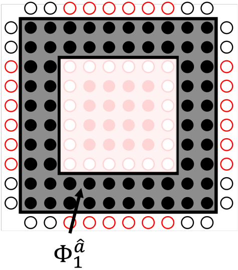
$$\partial\Lambda_0^{\hat{a}}, \quad \partial\Lambda_0 \equiv \bigcup_{\hat{a}} \partial\Lambda_0^{\hat{a}}$$

- $\partial\Pi$ union of hyperplanes passing by $\partial\Lambda_0$ (all empty circles)

- $\partial\Pi_1 = \partial\Pi \backslash \partial\Lambda_0$ (empty circles in the grey region)

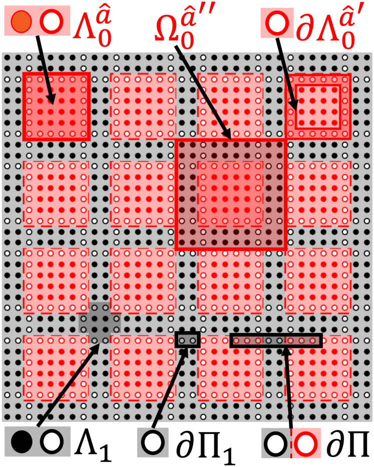
Domain decomposition: framed domains

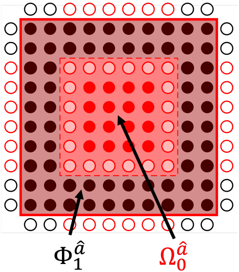




- Frame $\Phi_1^{\hat{a}} \in \Lambda_1$ for each $\Lambda_0^{\hat{a}}$

Domain decomposition: framed domains

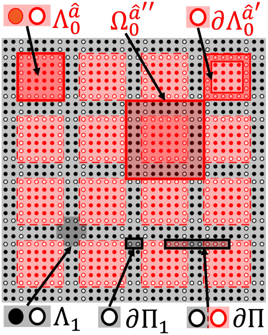




- Frame $\Phi_1^{\hat{a}} \in \Lambda_1$ for each $\Lambda_0^{\hat{a}}$
- Framed domain $\Omega_0^{\hat{a}} \equiv \Lambda_0^{\hat{a}} \cup \Phi_1^{\hat{a}}$

Block decomposition of det D

From this domain decomposition we obtain



$$\det D = \frac{\det W_1}{\det D_{\Lambda_1}^{-1} \prod_{\hat{a}} \left[\det D_{\Phi_1^{\hat{a}}} \det D_{\Omega_0^{\hat{a}}}^{-1}\right]}$$

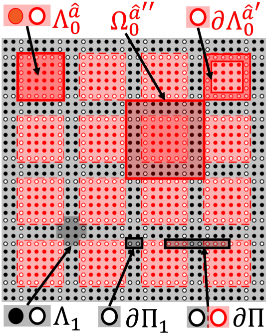
$$\det W_1 = 1 + \ldots$$

$$S_F^{eff}[U] = -\sum_{\hat{a}} \underbrace{\ln \det D_{\Omega_0^{\hat{a}}}}_{\text{block–local}} + \sum_{\hat{a}} \ln \det D_{\Phi_1^{\hat{a}}} - \ln \det D_{\Lambda_1} - \underbrace{\ln \det W_1}_{\text{still global}}$$

$\Rightarrow$ To accomplish our aim: factorize $\ln \det W_1$

Recovering the one-dimensional case

Direct generalization of the 1d case [Giusti et al. 16-18, Dalla Brida et al. 21]



$$\det D = \frac{\det W_1}{\det D_{\Lambda_1}^{-1} \prod_{\hat{a}} \left[\det D_{\Phi_1^{\hat{a}}} \det D_{\Omega_0^{\hat{a}}}^{-1}\right]}$$

$$W_z = \left(\begin{array}{c|c} zP_{\partial\Lambda_0} + [\hat{D}^{\mathrm{d}}_{\partial\Lambda_0}]^{-1}\hat{D}^{\mathrm{h}}_{\partial\Lambda_0} & W_{\partial\Lambda_0,\partial\Pi_1} \\ \hline W_{\partial\Pi_1,\partial\Lambda_0} & zP_{\partial\Pi_1} \end{array}\right)$$

$$\hat{D}^{\mathrm{d}}_{\partial\Lambda_0} = \sum_{\hat{a}} \hat{D}_{\partial\Lambda_0^{\hat{a}}}, \quad \hat{D}^{\mathrm{h}}_{\partial\Lambda_0} = \sum_{\hat{a}\neq\hat{a}'} \hat{D}_{\partial\Lambda_0^{\hat{a}},\partial\Lambda_0^{\hat{a}'}}$$

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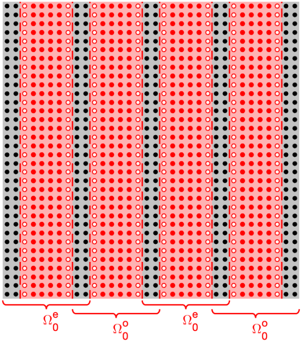


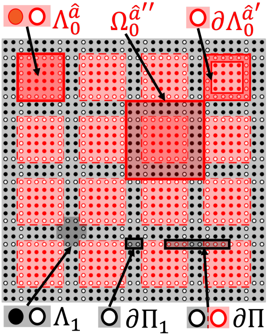
$$\det D = \frac{\det W_1}{\det D_{\Lambda_1}^{-1} \prod_{\hat{a}} \left[\det D_{\Phi_1^{\hat{a}}} \det D^{-1}_{\Omega_0^{\hat{a}}}\right]}$$

$$W_z = \left(\begin{array}{c|c} zP_{\partial\Lambda_0} + [\hat{D}^{\mathrm{d}}_{\partial\Lambda_0}]^{-1}\hat{D}^{\mathrm{h}}_{\partial\Lambda_0} & \cancel{W_{\partial\Lambda_0,\partial\Pi_1}} \\ \hline \cancel{W_{\partial\Pi_1,\partial\Lambda_0}} & \cancel{zP_{\partial\Pi_1}} \end{array}\right)$$

- $\partial\Pi_1$ absent, $\Phi_1^{\hat{a}} = \Lambda_1$ disconnected
- Even-odd decomposition $\hat{a} \in \{e, o\}$ to recover the 1d result

$$\det D = \frac{\det W_1}{\det D_{\Lambda_1} \det D^{-1}_{\Omega_0^e} \det D^{-1}_{\Omega_0^o}}$$

Block decomposition of det D



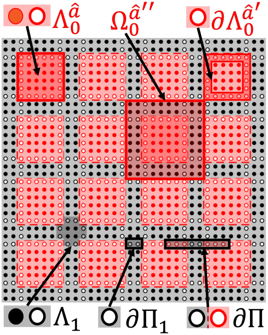
$$W_z = \left(\begin{array}{c|c} zP_{\partial\Lambda_0} + [\hat{D}^{\mathrm{d}}_{\partial\Lambda_0}]^{-1}\hat{D}^{\mathrm{h}}_{\partial\Lambda_0} & W_{\partial\Lambda_0,\partial\Pi_1} \\ \hline W_{\partial\Pi_1,\partial\Lambda_0} & zP_{\partial\Pi_1} \end{array} \right)$$

$$\hat{D}^{\mathrm{d}}_{\partial\Lambda_0} = \sum_{\hat{a}} \hat{D}_{\partial\Lambda_0^{\hat{a}}}, \quad \hat{D}^{\mathrm{h}}_{\partial\Lambda_0} = \sum_{\hat{a}\neq\hat{a}'} D_{\partial\Lambda_0^{\hat{a}},\partial\Lambda_0^{\hat{a}'}}$$

The generalization is not straightforward due to

- existence of corners in $4d$, i.e. $\partial\Pi_1$ and off-diagonal terms of W_1
- Λ_1 connected in $4d$

Block decomposition of det D



$$W_z = \left(\begin{array}{c|c} zP_{\partial\Lambda_0} + [\hat{D}^{\mathrm{d}}_{\partial\Lambda_0}]^{-1}\hat{D}^{\mathrm{h}}_{\partial\Lambda_0} & W_{\partial\Lambda_0,\partial\Pi_1} \\ \hline W_{\partial\Pi_1,\partial\Lambda_0} & zP_{\partial\Pi_1} \end{array} \right)$$

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- $W_1 = \mathbb{1}+$ off-diagonal terms suppressed with the thickness of Λ_1 (~ 0.5 fm or so) $\Rightarrow$ Multi-boson representation
- Only dependence on U_{Λ_0} in the red terms in the first line $\Rightarrow$ Multi-boson factorization [Lüscher 94, 04, 05; Borici Forcrand 95, 96]

Multi-boson factorization of det W_1

$$\det W_1 = \frac{1}{\det W_1^{-1}} = \frac{\mathcal{W}_N}{\prod_{k=1}^{N/2} \det \left[W_{u_k}^\dagger W_{u_k}\right]}, \; N \sim O(10)$$

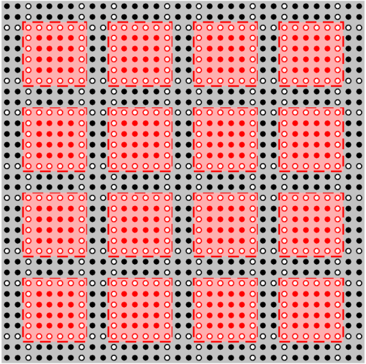
$$\frac{1}{\det \left[W_{u_k}^\dagger \, W_{u_k}\right]} \propto \int d\chi_k d\chi_k^\dagger \, e^{-|W_{u_k}\chi_k|^2},$$

$$|W_z\chi|^2 = \sum_{\hat{a}} \left| P_{\partial\Lambda_0^{\hat{a}}}\left[z\,\chi_{\partial\Lambda_0} + \hat{D}^{-1}_{\partial\Lambda_0^{\hat{a}}}\hat{D}^{\mathrm{h}}_{\partial\Lambda_0}\chi_{\partial\Lambda_0} + W_{\partial\Lambda_0^{\hat{a}},\partial\Pi_1}\chi_{\partial\Pi_1}\right]\right|^2$$

$$+\left|z\,\chi_{\partial\Pi_1} + W_{\partial\Pi_1,\partial\Lambda_0}\chi_{\partial\Lambda_0}\right|^2$$

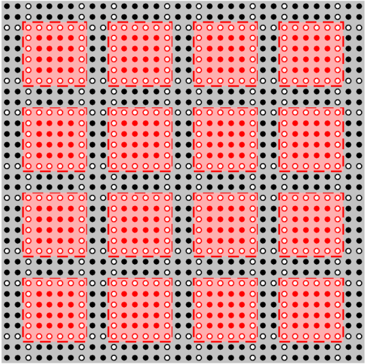
- $N/2$ multi-boson fields χ_k living on $\partial\Pi = \partial\Lambda_0 \cup \partial\Pi_1$
- Only first line of W_z depends on U_{Λ_0} $\Rightarrow$ factorized multi-boson action
- $\mathcal{W}_N$ = reweighting factor

Conclusions



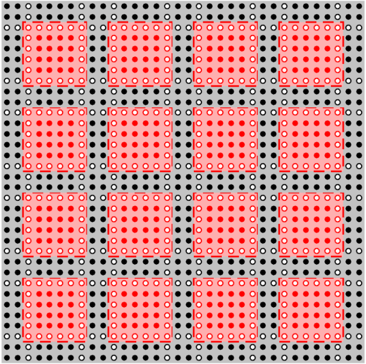
- Four-dimensional overlapping domain decomposition
- Block factorization of $\det D[U]$
- Multi-boson factorization and reweighting
- Factorized gauge field dependence of $S_F^{eff}[U]$

Outlook



- **Multi-level**: local updates and averages
- **Master-field**: fully factorized molecular-dynamics evolution
- **Parallelization** on heterogeneous architectures

Outlook



- **Multi-level**: local updates and averages
- **Master-field**: fully factorized molecular-dynamics evolution
- **Parallelization** on heterogeneous architectures

Thank you for your attention!

Backup slides

LU decomposition of a 2×2 block matrix

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I & BD^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} S_A & 0 \\ C & D \end{pmatrix}, S_A = A - BD^{-1}C$$

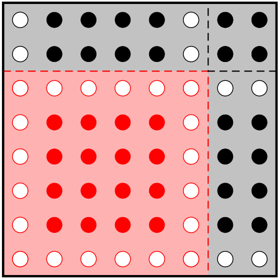
$$\det M = \det D \det S_A$$

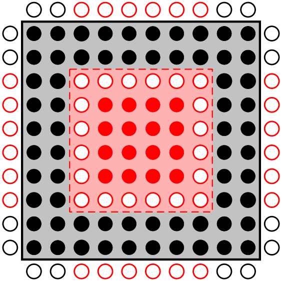
$$M^{-1} = \begin{pmatrix} S_A^{-1} & -S_A^{-1}BD^{-1} \\ -D^{-1}CS_A^{-1} & D^{-1} + D^{-1}CS_A^{-1}BD^{-1} \end{pmatrix}$$

$$\det \begin{pmatrix} A & \mathcal{B} \\ \mathcal{C} & D \end{pmatrix} = \det A \det D \det \begin{pmatrix} 1 & \mathcal{A}^{-1}\mathcal{B} \\ \mathcal{D}^{-1}\mathcal{C} & 1 \end{pmatrix}$$

$$\mathcal{A}^{-1} = P_1 A^{-1} P_1, \mathcal{B} = P_1 B P_2, \mathcal{C} = P_2 C P_1, \mathcal{D}^{-1} = P_2 D^{-1} P_2$$

Definition of the domains





$$L = \bigcup_{\hat{a}} \Gamma^{\hat{a}}, \qquad \hat{a} = \{a_0, a_1, a_2, a_3\}$$

$$a_\mu = 0, \ldots, \frac{L_\mu}{G_\mu} - 1, \qquad \mu = 0, \ldots, 3$$

$$G_\mu = B_\mu + b_\mu, \qquad x_\mu = G_\mu \cdot a_\mu$$

$$\Gamma^{\hat{a}} = \Lambda_0^{\hat{a}} \bigcup_{\hat{d} \neq \hat{0}, d_\mu = 0,1} \Lambda_1^{(\hat{a},\hat{d})}$$

$$x_\mu = G_\mu \cdot a_\mu + B_\mu \cdot d_\mu$$

$$\Phi_1^{\hat{a}} = \bigcup_{\substack{(\hat{c},\hat{d}) \neq (\hat{0},\hat{0}), \\ c_\mu, d_\mu = 0,1 | (d-c)_\mu = 0,1}} \Lambda_1^{(\hat{a}-\hat{c},\hat{d})}$$

$$\Omega_0^{\hat{a}} = \Lambda_0^{\hat{a}} \cup \Phi_1^{\hat{a}}$$

Derivation of block decomposition

- First decomposition: $L = \partial\Lambda_0 \cup \left(\bar{\Lambda}_0 \cup \Lambda_1\right)$ so that

$$\det D = \det D_{\bar{\Lambda}_0} \det D_{\Lambda_1} \det \tilde{D}_{\partial\Lambda_0},$$

$$\tilde{D}_{\partial\Lambda_0} = D_{\partial\Lambda_0} - D_{\partial\Lambda_0,\bar{\Lambda}_0} D^{-1}_{\bar{\Lambda}_0} D_{\bar{\Lambda}_0,\partial\Lambda_0} - D_{\partial\Lambda_0,\Lambda_1} D^{-1}_{\Lambda_1} D_{\Lambda_1,\partial\Lambda_0}$$

- Second decomposition: $\Lambda_1 = \Phi_1^{\hat{a}} \cup (\Lambda_1 \backslash \Phi_1^{\hat{a}})$ so that

$$\tilde{D}_{\partial\Lambda_0} = \hat{D}_{\partial\Lambda_0} - \hat{D}_{\partial\Lambda_0,\partial\Pi_1} \hat{D}^{-1}_{\partial\Pi_1} \hat{D}_{\partial\Pi_1,\partial\Lambda_0},$$

$$\hat{D}_{\partial\Lambda_0} = \hat{D}^d_{\partial\Lambda_0} + \hat{D}^h_{\partial\Lambda_0}, \quad \hat{D}^d_{\partial\Lambda_0} = \sum_{\hat{a}} \hat{D}_{\partial\Lambda_0^{\hat{a}}}, \quad \hat{D}^h_{\partial\Lambda_0} = \sum_{\hat{a}\neq\hat{a}'} \hat{D}_{\partial\Lambda_0^{\hat{a}},\partial\Lambda_0^{\hat{a}'}},$$

$$\hat{D}_{\partial\Lambda_0^{\hat{a}}} = D_{\partial\Lambda_0^{\hat{a}}} - D_{\partial\Lambda_0^{\hat{a}},\bar{\Lambda}_0^{\hat{a}}} D^{-1}_{\bar{\Lambda}_0^{\hat{a}}} D_{\bar{\Lambda}_0^{\hat{a}},\partial\Lambda_0^{\hat{a}}} - D_{\partial\Lambda_0^{\hat{a}},\Phi_1^{\hat{a}}} D^{-1}_{\Phi_1^{\hat{a}}} D_{\Phi_1^{\hat{a}},\partial\Lambda_0^{\hat{a}}},$$

$$\hat{D}_{\partial\Lambda_0^{\hat{a}},\partial\Lambda_0^{\hat{a}'}} = -\frac{1}{2} D_{\partial\Lambda_0^{\hat{a}},\Phi_1^{\hat{a}}} \left[D^{-1}_{\Phi_1^{\hat{a}}} - D^{-1}_{\Phi_1^{\hat{a}}} D_{\Phi_1^{\hat{a}},\partial\bar{\Omega}_0^{\hat{a}*}} D^{-1}_{\Phi_1^{\hat{a}'}} \right.$$

$$\left. + D^{-1}_{\Phi_1^{\hat{a}'}} - D^{-1}_{\Phi_1^{\hat{a}}} D_{\partial\bar{\Omega}_0^{\hat{a}'*},\Phi_1^{\hat{a}'}} D^{-1}_{\Phi_1^{\hat{a}'}} \right] D_{\Phi_1^{\hat{a}'},\partial\Lambda_0^{\hat{a}'}}$$

$$\hat{D}_{\partial\Pi_1} = D_{\partial\Pi_1} - D_{\partial\Pi_1,\bar{\Lambda}_1} D^{-1}_{\Lambda_1} D_{\bar{\Lambda}_1,\partial\Pi_1}$$

Derivation of block decomposition

$$\det D = \frac{\det W_1}{\det D_{\Lambda_1}^{-1} \prod_{\hat{a}} \left[\det D_{\Phi_1^{\hat{a}}} \det D_{\Omega_0^{\hat{a}}}^{-1} \right]}$$

$$W_z = \left(\begin{array}{c|c} z\mathbb{P}_{\partial\Lambda_0} + [\hat{D}^{\mathrm{d}}_{\partial\Lambda_0}]^{-1} \hat{D}^{\mathrm{h}}_{\partial\Lambda_0} & W_{\partial\Lambda_0,\partial\Pi_1} \\ \hline W_{\partial\Pi_1,\partial\Lambda_0} & z\mathbb{P}_{\partial\Pi_1} \end{array} \right)$$

$$W_{\partial\Lambda_0,\partial\Pi_1} = \sum_{\hat{a}} \mathbb{P}_{\partial\Lambda_0^{\hat{a}}} D_{\Omega_0^{\hat{a}}}^{-1} D_{\Phi_1^{\hat{a}},\partial\bar{\Omega}_0^{\hat{a}*}} = W_{\partial\Lambda_0,\partial\Pi_1} P_{\partial\Pi_1}$$

$$W_{\partial\Pi_1,\partial\Lambda_0} = \hat{D}_{\partial\Pi_1}^{-1} \hat{D}_{\partial\Pi_1,\partial\Lambda_0} = W_{\partial\Pi_1,\partial\Lambda_0} P_{\partial\Lambda_0}$$

$$P_{\partial\Lambda_0^{\hat{a}}} \psi(x) = \begin{cases} 0 & \text{if } x \notin \partial\Lambda_0^{\hat{a}}\,, \\ \dfrac{1-\gamma_\mu}{2}\psi(x) & \text{if } x \in \partial\Lambda_0^{\hat{a}} \text{ and } \exists!\ \mu \,\big|\, (x-\hat{\mu}) \in \partial\Lambda_0^{\hat{a}*}\,, \\ \dfrac{1+\gamma_\mu}{2}\psi(x) & \text{if } x \in \partial\Lambda_0^{\hat{a}} \text{ and } \exists!\ \mu \,\big|\, (x+\hat{\mu}) \in \partial\Lambda_0^{\hat{a}*}\,, \\ \psi(x) & \text{otherwise}\,, \end{cases}$$

Derivation of multi-boson factorization

$$\det D = \frac{\det W_1}{\det D_{\Lambda_1}^{-1} \prod_{\hat{a}} \left[\det D_{\Phi_1^{\hat{a}}} \det D_{\Omega_0^{\hat{a}}}^{-1} \right]}$$

- First, we define the approximating polynomial

$$P_N(z) = \frac{1 - R_{N+1}(z)}{z} = c_N \prod_{k=1}^{N} (z - z_k)$$

- With this definition, we can rewrite $\det D$ by noticing that

$$\frac{1}{\det P_N(W_1)} = C \prod_{k=1}^{N/2} \det^{-1} \{ (z_k - W_1)^\dagger (z_k - W_1) \} = C \prod_{k=1}^{N/2} \det^{-1} (W_{u_k}^\dagger W_{u_k}),$$

$$u_k = 1 - z_k = \cos\left(\frac{2\pi k}{N+1}\right) + i\sqrt{1 - c^2} \sin\left(\frac{2\pi k}{N+1}\right), \; k = 1, \ldots, N$$

Derivation of multi-boson factorization

- The multi-boson action comes from the term

$$\frac{1}{\det(W_{u_k}^{\dagger} W_{u_k})} \propto \int d\chi_k d\chi_k^{\dagger} e^{-|W_{u_k}\chi_k|^2},$$

$$|W_z\chi|^2 = \sum_{\hat{a}} \left| P_{\partial\Lambda_0^{\hat{a}}} \left[z\,\chi_{\partial\Lambda_0} + \hat{D}^{-1}_{\partial\Lambda_0^{\hat{a}}} \hat{D}^{\mathrm{h}}_{\partial\Lambda_0} \chi_{\partial\Lambda_0} + D^{-1}_{\Omega_0^{\hat{a}}}\, D_{\Phi_1^{\hat{a}},\partial\bar{\Omega}_0^{\hat{a}*}} \chi_{\partial\Pi_1} \right] \right|^2$$

$$+ \left| z\,\chi_{\partial\Pi_1} + W_{\partial\Pi_1,\partial\Lambda_0} \chi_{\partial\Lambda_0} \right|^2$$

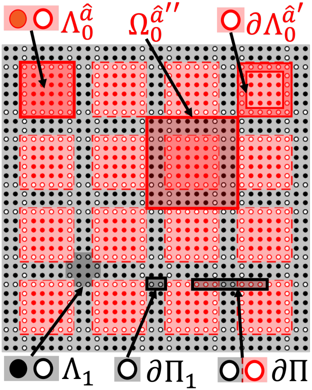
where $U[\Lambda_0]$ appears only in the first line $\Rightarrow$ factorized dependence of the multi-boson action on the gauge field in the blocks $\Lambda_0^{\hat{a}}$

- We can define the reweighting term $\mathcal{W}_N = \det\{1 - R_{N+1}(W_1)\}$ so that

$$\langle O \rangle = \frac{\langle O \mathcal{W}_N \rangle_N}{\langle \mathcal{W}_N \rangle_N}$$

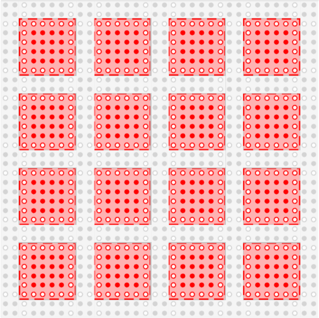
$$\frac{\det D}{\mathcal{W}_N} \propto \frac{1}{\det D_{\Lambda_1} \prod_{\hat{a}} \left[\det D_{\Phi_1^{\hat{a}}} \det D_{\Omega_0^{\hat{a}}} \right] \prod_{k=1}^{N/2} \det(W_{u_k}^{\dagger} W_{u_k})}$$

Block-local updates



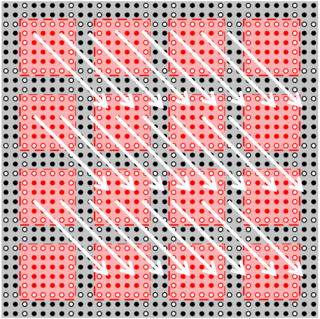
- ➢ Single level-0 global update
- ➢ Generation of new pseudo-fermion and multi-boson fields

Block-local updates



- Single level-0 global update
- Generation of new pseudo-fermion and multi-boson fields
- n_1 level-1 local updates: molecular-dynamics evolution restricted to local, active links in Λ_0, which are decoupled in n_b blocks $\Lambda_0^{\hat{a}}$ (multi-bosons and inactive links in Λ_1 fixed)
- Level-1 local accept-reject step *independent* on different blocks

Block-local updates



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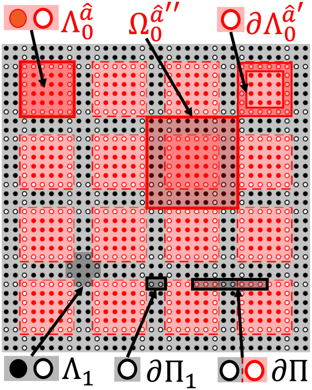
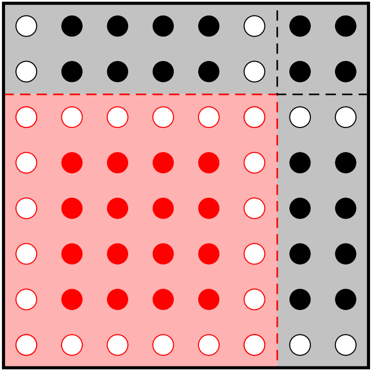
- n_1 level-1 local updates: molecular-dynamics evolution restricted to local, active links in Λ_0, which are decoupled in n_b blocks $\Lambda_0^{\hat{a}}$ (multi-bosons and inactive links in Λ_1 fixed)
- Level-1 local accept-reject step *independent* on different blocks
- Translation of the gauge field by a random vector v, i.e. $U_\mu(x) \to U_\mu(x+v)$

Block-local updates



- Single level-0 global update
- Generation of new pseudo-fermion and multi-boson fields
- n_1 level-1 local updates: molecular-dynamics evolution restricted to local, active links in Λ_0, which are decoupled in n_b blocks $\Lambda_0^{\hat{a}}$ (multi-bosons and inactive links in Λ_1 fixed)
- Level-1 local accept-reject step *independent* on different blocks
- Translation of the gauge field by a random vector v, i.e. $U_\mu(x) \to U_\mu(x+v)$
- Repeat n_0 times
- Averages over $n_0 \cdot n_1^{n_b}$ configurations, generated at a cost proportional to $n_0 \cdot n_1$

Size of the blocks



We need to ensure that a good fraction of the link variables can be updated in each step. If, for instance, we consider blocks with an extension of 2.5 fm and a frame of 0.5 fm in all directions, the fraction of the active links is

$$\frac{V_{\Lambda_0}}{V_{cell}} = \frac{(3-0.5)^4\,\mathrm{fm}^4}{(3\,\mathrm{fm})^4} \simeq 50\%$$