Transfer matrices and temporal factorization of the Wilson fermion determinant

Urs Wenger

Albert Einstein Center for Fundamental Physics
University of Bern

b
UNIVERSITÄT
BERN

in collaboration with Patrick Bühlmann

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Introduction and motivation

- Consider the grand-canonical partition function at finite μ,

$$Z_{\mathrm{GC}}(\mu) = \int \mathcal{D}\mathcal{U}\, e^{-S_b[\mathcal{U}]} \int \mathcal{D}\psi^\dagger \mathcal{D}\psi\, e^{-\psi^\dagger M[\mathcal{U};\mu]\psi}$$
$$= \int \mathcal{D}\mathcal{U}\, e^{-S_b[\mathcal{U}]} \det M[\mathcal{U};\mu]$$

where $\det M[\mathcal{U};\mu]$ is highly non-local in $\mathcal{U}$, difficult to calculate...

- In the Hamiltonian formulation one has

$$Z_{\mathrm{GC}}(\mu) = \mathrm{Tr}\left[e^{-\mathcal{H}(\mu)/T}\right] = \mathrm{Tr}\prod_t \mathcal{T}_t(\mu)$$
$$= \sum_N e^{-N\mu/T} \cdot Z_C(N)$$

where $Z_C(N) = \mathrm{Tr}\prod_t \mathcal{T}_t^{(N)}$.

Fermion matrix and dimensional reduction

- The fermion matrix $M[\mathcal{U};\mu]$ has generic (temporal) structure

$$M = \begin{pmatrix} B_0 & e^{+\mu} C'_0 & 0 & \dots & \pm e^{-\mu} C_{L_t-1} \\ e^{-\mu} C_0 & B_1 & e^{+\mu} C'_1 & & 0 \\ 0 & e^{-\mu} C_1 & B_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & & \\ & & & B_{L_t-2} & e^{+\mu} C'_{L_t-2} \\ \pm e^{+\mu} C'_{L_t-1} & 0 & & e^{-\mu} C_{L_t-2} & B_{L_t-1} \end{pmatrix}$$

  for which the determinant can be reduced to

$$\det M[\mathcal{U};\mu] = \prod_t \det \tilde{B}_t \cdot \det\left(1 \mp e^{\mu L_t} \cdot \mathcal{T}\right)$$

  where $\mathcal{T} = \mathcal{T}_0 \cdot \ldots \cdot \mathcal{T}_{L_t-1}$ and $\mathcal{T}_t = \mathcal{T}_t[B_t, C_t, C'_t]$.

- $M[\mathcal{U};\mu]$ is $(L \cdot L_t) \times (L \cdot L_t)$, while $\mathcal{T}$ is $L \times L$.

Fugacity expansion and canonical determinants

- Fugacity expansion

$$\det M[\mathcal{U};\mu] = \sum_N e^{-N\cdot\mu/T} \cdot \det{}_N M[\mathcal{U}]$$

yields the canonical determinants

$$\det{}_N M[\mathcal{U}] = \sum_J \det \mathcal{T}^{JJ}[\mathcal{U}] = \mathrm{Tr}\left[\prod_t \mathcal{T}_t^{(N)}\right],$$

where $\det \mathcal{T}^{JJ}$ is the principal minor of order N.

- States are labeled by index sets $J \subset \{1,\ldots,L\}, |J| = N$
  - number of states grows exponentially with L at half-filling

$$N_{\text{states}} = \binom{L}{N} = N_{\text{principal minors}}$$

  - sum can be evaluated stochastically with MC

Transfer matrices and factorization

- Use Cauchy-Binet formula

$$\det(A \cdot B)^{\not I \not K} = \sum_J \det A^{\not I \not J} \cdot \det B^{\not J \not K}$$

to factorize into product of transfer matrices

- Transfer matrices in sector N are hence given by

$$\det \mathcal{T}^{\not J \not J} = \sum_J \det(\mathcal{T}_0 \cdot \ldots \cdot \mathcal{T}_{L_t - 1})^{\not J \not J} = (\mathcal{T}_0)_{JI} \cdot (\mathcal{T}_1)_{IK} \cdot \ldots \cdot (\mathcal{T}_{L_t-1})_{LJ}$$

with $(\mathcal{T}_t)_{IK} = \det \tilde{B}_t \cdot \det \mathcal{T}_t^{\not I \not K}$.

- Finally, we have

$$\det{}_N M[\mathcal{U}] = \prod_t \det \tilde{B}_t \cdot \sum_{\{J_t\}} \prod_t \det \mathcal{T}_t^{\not J_{t-1} \not J_t}$$

where $|J_t| = N$ and $J_{L_t} = J_0$.

Dimensional reduction of QCD

- Consider the Wilson fermion matrix for a single quark with chemical potential μ:

$$M_\pm(\mu) = \begin{pmatrix} B_0 & P_+A_0^+ & & & \pm P_-A_{L_t-1}^- \\ P_-A_0^- & B_1 & P_+A_1^+ & & \\ & P_-A_1^- & B_2 & \ddots & \\ & & \ddots & \ddots & \\ & & & & P_+A_{L_t-2}^+ \\ \pm P_+A_{L_t-1}^+ & & & P_- & B_{L_t-1} \end{pmatrix}$$

  - temporal hoppings are

$$A_t^+ = e^{+\mu} \cdot \mathbb{I}_{4\times 4} \otimes \mathcal{U}_t = \left(A_t^-\right)^{-1}$$

  - Dirac projectors $P_\pm = \frac{1}{2}(\mathbb{I} \mp \Gamma_4)$
  - B_t are (spatial) Wilson Dirac operators on time-slice t
  - all blocks are $(4 \cdot N_c \cdot L_s^3 \times 4 \cdot N_c \cdot L_s^3)$-matrices

Dimensional reduction of QCD

- Reduced Wilson fermion determinant is given by

$$\det M_{p,a}(\mu) \propto \prod_t \det Q_t^+ \cdot \det\left[\mathbb{I} \pm e^{+\mu L_t}\mathcal{T}\right]$$

where $\mathcal{T}$ is the product of spatial matrices given by

$$\mathcal{T} = \prod_t Q_t^+ \cdot \mathcal{U}_t \cdot (Q_{t+1}^-)^{-1} \equiv \prod_t \mathcal{T}_t$$

$$Q_t^{\pm} = B_t P_{\mp} + P_{\pm}, \qquad B_t = \begin{pmatrix} D_t & C_t \\ -C_t & D_t \end{pmatrix}$$

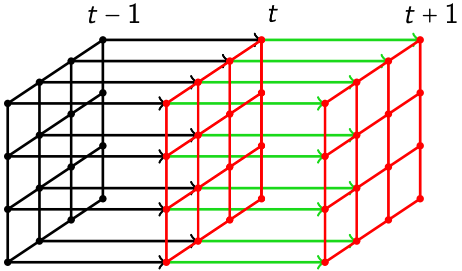
and

$$Q_t^+ = \begin{pmatrix} 1 & C_t \\ 0 & D_t \end{pmatrix}, \quad (Q_t^-)^{-1} = \begin{pmatrix} D_t^{-1} & 0 \\ C_t \cdot D_t^{-1} & 1 \end{pmatrix}.$$

Structure of building blocks

- Product of spatial matrices:

$$\mathcal{T} = \prod_t Q_t^+ \cdot \mathcal{U}_t \cdot (Q_{t+1}^-)^{-1} \qquad \text{or} \qquad \mathcal{T} = \prod_t \mathcal{U}_{t-1}^- \cdot (Q_t^-)^{-1} \cdot Q_t^+ \cdot U_t^+$$



$$Q_t^+ \cdot \mathcal{U}_t \cdot (Q_{t+1}^-)^{-1}$$

Structure of building blocks

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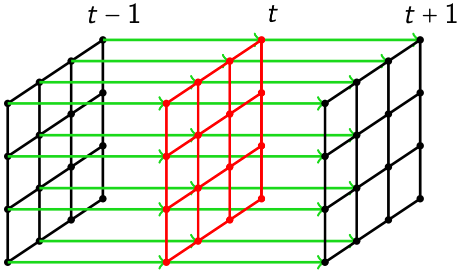


$$\mathcal{U}_{t-1}^- \cdot (Q_t^-)^{-1} \cdot Q_t^+ \cdot \mathcal{U}_t^+$$

Canonical projection and factorization

Canonical projection of QCD

$$\det M_{N_q} = \prod_t \det Q_t^+ \cdot \sum_A \det \mathcal{T}^{\not{A}\not{A}}$$

- sum is over all index sets $A \in \{1, 2, \ldots, 2N_q^{\max}\}$ of size

$$|A| = N_q^{\max} + N_q, \qquad N_q^{\max} = 2 \cdot N_c \cdot L_s^3$$

- i.e., the trace over the minor matrix of rank N_q of $\mathcal{T}$

Factorization of QCD determinant

$$\det M_{N_q} = \prod_t \det Q_t^+ \cdot \prod_t M\left((Q_t^-)^{-1}\right)_{\not{A}_t \not{B}_t} M(Q_t^+)_{\not{B}_t \not{C}_t} M(\mathcal{U}_t)_{\not{C}_t \not{A}_{t+1}}$$

Relation between quark and baryon number in QCD

- Consider $\mathbb{Z}(N_c)$-transformation by $z_k = e^{2\pi i \cdot k/N_c} \in \mathbb{Z}(N_c)$:

$$\mathcal{U}_t \to \mathcal{U}'_t = z_k \cdot \mathcal{U}_t \qquad \text{at one fixed } t.$$

- As a consequence we have

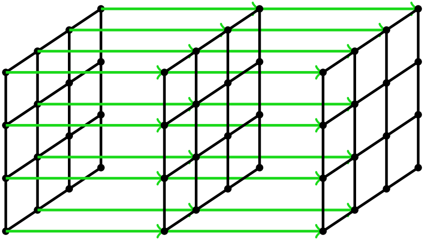
$$\begin{aligned} \det M_{N_q} \to \det M'_{N_q} &= \prod_t \det Q_t^+ \cdot \sum_A \det(z_k \cdot \mathcal{T})^{\bcancel{A}\bcancel{A}} \\ &= z_k^{-N_q} \cdot \det M_{N_q} \end{aligned}$$

and summing over z_k therefore yields

$$\det M_{N_q} = 0 \qquad \text{for } N_q \neq 0 \bmod N_c$$

Multi-level integration schemes

- Temporal gauge links in $\mathcal{U}_t$ are completely decoupled:



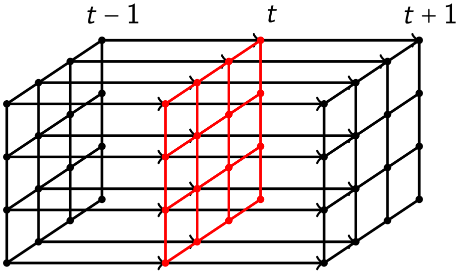
$$M(\mathcal{U}_{t-1})_{\cancel{C_{t-1}}\cancel{A_t}} \cdot M\left((Q_t^-)^{-1}\right)_{\cancel{A_t}\cancel{B_t}} \cdot M(Q_t^+)_{\cancel{B_t}\cancel{C_t}} \cdot M(\mathcal{U}_t)_{\cancel{C_t}\cancel{A_{t+1}}}$$

  - spatial matrix $\mathcal{U}_t$ is block diagonal:

$\Rightarrow M(\mathcal{U}_t)$ trivial to calculate!

Multi-level integration schemes

- Spatial gauge links in $\color{red}{Q_t^{\pm}}$ coupled through temporal plaquettes only:



$$M(\mathcal{U}_{t-1})_{\not{C}_{t-1}\not{A}_t} \cdot M\left(\color{red}{(Q_t^-)^{-1}}\right)_{\not{A}_t\not{B}_t} \cdot M(\color{red}{Q_t^+})_{\not{B}_t\not{C}_t} \cdot M(\mathcal{U}_t)_{\not{C}_t\not{A}_{t+1}}$$

  - spatial matrices $\color{red}{Q_t^{\pm}}$ can be treated together:

$$M\left(\color{red}{(Q_t^-)^{-1}}\right)_{\not{A}_t\not{B}_t} \cdot M(\color{red}{Q_t^+})_{\not{B}_t\not{C}_t} = M\left(\color{red}{(Q_t^-)^{-1} \cdot Q_t^+}\right)_{\not{A}_t\not{C}_t}$$

Correlation functions

- Source and sink operators $\mathcal{S}$ and $\overline{\mathcal{S}}$:
  - remove or re-add indices from/to the available index set,
  - potentially change quark number N_q, e.g.,

$$\ldots \cdot \mathcal{T}_{t-1}^{(N_q)} \cdot \mathcal{S}_{N_q \to N_q+3} \cdot \mathcal{T}_t^{(N_q+3)} \cdot \ldots \cdot \mathcal{T}_{t'}^{(N_q+3)} \cdot \overline{\mathcal{S}}_{N_q+3 \to N_q} \cdot \mathcal{T}_{t'+1}^{(N_q)} \cdot \ldots$$

  - vacuum sector corresponds to $N_q = 0$

- Natural to contruct improved estimators:
  - simulate directly the correlation function at $C(t'-t)$,
  - measure $C(t'+1-t)$ relative to $C(t'-t)$

$$\langle C(t'+1-t) \rangle_{C(t'-t)} \sim e^{-aE}$$

from additional insertion $\mathcal{T}_{t'+1}^{(N_q)} \to \mathcal{T}_{t'+1}^{(N_q+3)}$

- All spectral information is contained in $\langle \mathcal{T}_t^{(N_q)} \rangle$.

Summary and outlook

- Complete temporal factorization of the Wilson fermion determinant:

$$\det M_{N_q} = \prod_t \det Q_t^+ \cdot \prod_t M\left((Q_t^-)^{-1}\right)_{\not{A}_t \not{B}_t} M(Q_t^+)_{\not{B}_t \not{C}_t} M(\mathcal{U}_t)_{\not{C}_t \not{A}_{t+1}}$$

  - works for fixed quark numbers N_q
  - allows for very flexible multi-level integration schemes
  - cf. [Gattringer et al, Giusti et al, Chandrasekharan et al]

Caveats: positivity? potential sign problem?

$Q^\pm$ are strictly positive, $(\mathcal{T}_t)_{\not{B}\not{C}}$ not necessarily. . .