# Temporal factorization of the Wilson fermion determinant and multi-level integration 

Urs Wenger<br>Albert Einstein Center for Fundamental Physics<br>\section*{$\boldsymbol{u}^{b}$}<br> BERN

in collaboration with Sebastian Burri and Patrick Bühlmann

Numerical Challenges in QCD 15 August 2022, Meinerzhagen, Germany

## Overview

- Temporal factorization of fermion determinants in LQFTs:

Step 1: dimensional reduction

Step 2: projection to canonical sectors

Step 3: temporal factorization

- Application to QCD


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Step 1: dimensional reduction

Step 2: projection to canonical sectors

Step 3: temporal factorization

- Application to QCD
- Application to the Hubbard model


## Introduction and motivation

- Consider the grand-canonical partition function at finite $\mu$,

$$
\begin{aligned}
Z_{\mathbf{G C}}(\mu) & =\int \mathcal{D} \mathcal{U} e^{-S_{b}[\mathcal{U}]} \int \mathcal{D} \bar{\psi} \mathcal{D} \psi e^{-\bar{\psi} M[\mathcal{U} ; \mu] \psi} \\
& =\int \mathcal{D} \mathcal{U} e^{-S_{b}[\mathcal{U}]} \operatorname{det} M[\mathcal{U} ; \mu]
\end{aligned}
$$

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

- In the Hamiltonian formulation one has

$$
\begin{aligned}
Z_{\mathrm{GC}}(\mu) & =\operatorname{Tr}\left[e^{-\mathcal{H}(\mu) / T}\right]=\operatorname{Tr} \prod_{t} \mathcal{T}_{t}(\mu) \\
& =\sum_{N} e^{-N \mu / T} \cdot Z_{C}(N)
\end{aligned}
$$

where $Z_{C}(N)=\operatorname{Tr} \Pi_{t} \mathcal{T}_{t}^{(N)}$.

## Step 1: dimensional reduction

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

$$
M=\left(\begin{array}{ccccc}
B_{0} & e^{+\mu} C_{0}^{\prime} & 0 & \cdots & \pm e^{-\mu} C_{L_{t}-1} \\
e^{-\mu} C_{0} & B_{1} & e^{+\mu} C_{1}^{\prime} & & 0 \\
0 & e^{-\mu} C_{1} & B_{2} & \ddots & \vdots \\
\vdots & \ddots & \ddots & & \\
\pm e^{+\mu} C_{L_{t}-1}^{\prime} & 0 & & B_{L_{L^{-}}-2} & e^{+\mu} C_{L_{t}-2}^{\prime} \\
{ }^{-\mu} C_{L_{t}-2} & B_{L_{t}-1}^{\prime}
\end{array}\right)
$$

for which the determinant can be reduced to

$$
\operatorname{det} M[\mathcal{U} ; \mu]=\prod_{t} \operatorname{det} \tilde{B}_{t} \cdot \operatorname{det}\left(1 \mp e^{\mu L_{t}} \cdot \mathcal{T}\right)
$$

where $\mathcal{T}=\mathcal{T}_{0} \ldots \cdot \mathcal{T}_{L_{t}-1}$ and $\mathcal{T}_{t}=\mathcal{T}_{t}\left[B_{t}, C_{t}, C_{t}^{\prime}\right]$.

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


## Fugacity expansion and canonical determinants

- Fugacity expansion

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

yields the canonical determinants

$$
\operatorname{det}_{N} M[\mathcal{U}]=\sum_{J} \operatorname{det} \mathcal{T}^{Y Y}[\mathcal{U}]=\operatorname{Tr}\left[\prod_{t} \mathcal{T}_{t}^{(N)}\right]
$$

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

## Fugacity expansion and canonical determinants

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$$

where $\operatorname{det} \mathcal{T} \nmid X$ is the principal minor of order $N$.

Key object from step 1:

$$
\mathcal{T}[\mathcal{U}] \equiv \prod_{t=0}^{L_{t}-1} \mathcal{T}_{t} \quad \Leftrightarrow \quad \text { product of spatial matrices }
$$

## Fugacity expansion and canonical determinants

## Key step 2:

$$
\mathcal{T}[\mathcal{U}] \equiv \prod_{t=0}^{L_{t}-1} \mathcal{T}_{t} \quad \Rightarrow \quad \operatorname{det}{ }_{N} M[\mathcal{U}]=\sum_{J} \operatorname{det} \mathcal{T}^{X Y}[\mathcal{U}]
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$$

- Fugacity expansion:

$$
\operatorname{det} M[\mathcal{U} ; \mu] \propto \operatorname{det}\left(e^{-\mu / T}+\mathcal{T}[\mathcal{U}]\right)=\sum_{N} e^{-N \cdot \mu / T} \cdot \operatorname{det}{ }_{N} M[\mathcal{U}]
$$

## Fugacity expansion and canonical determinants

Key step 2:

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\mathcal{T}[\mathcal{U}] \equiv \prod_{t=0}^{L_{t}-1} \mathcal{T}_{t} \quad \Rightarrow \quad \operatorname{det}_{N} M[\mathcal{U}]=\sum_{J} \operatorname{det} \mathcal{T}^{X X}[\mathcal{U}]
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$$

- Coefficients given by the elementary symmetric functions $S_{k}$ of order $k$ of $\left\{\tau_{i}\right\}$ :

$$
\operatorname{det}_{N} M[\mathcal{U}]=S_{L-N}(\mathcal{T})
$$

where

$$
S_{k}(\mathcal{T}) \equiv S_{k}\left(\left\{\tau_{i}\right\}\right)=\sum_{1 \leq i_{1}<\cdots<i_{k} \leq L} \prod_{j=1}^{k} \tau_{i_{j}}=\sum_{|J|=k} \operatorname{det} \mathcal{T}^{\not X X} .
$$

## Canonical determinants

$$
\sum_{J} \operatorname{det} \mathcal{T}^{Y Y}[\mathcal{U}]=\operatorname{Tr}\left[\prod_{t} \mathcal{T}_{t}^{(N)}\right]
$$

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

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

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- treat index set $J$ as dynamical degree of freedom


## Canonical determinants

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$$

- Efficient stochastic evaluation of $\sum_{J}$ :
- treat index set $J$ as dynamical degree of freedom
- update $J \rightarrow J^{\prime}$ using Fisher-Yates reshuffling and

$$
p_{J \rightarrow J^{\prime}}=\min \left[1, A_{J \rightarrow J^{\prime}}\right] \quad \text { with } \quad A_{J \rightarrow J^{\prime}}=\left|\frac{\operatorname{det} \mathcal{T} \chi^{\prime} \nmid \chi^{\prime}}{\operatorname{det} \mathcal{T} \nmid X}\right| \text {. }
$$

## Transfer matrices and factorization

- Use Cauchy-Binet formula

$$
\operatorname{det}(A \cdot B)^{\wedge K}=\sum_{J} \operatorname{det} A^{\wedge \chi} \cdot \operatorname{det} B^{Y K}
$$

to factorize into product of transfer matrices

- Transfer matrices in sector $N$ are hence given by

$$
\operatorname{det} \mathcal{T}^{\text {XX }}=\operatorname{det}\left(\mathcal{T}_{0} \cdot \ldots \cdot \mathcal{T}_{L_{t}-1}\right)^{\text {KY }}=\left(\mathcal{T}_{0}\right)_{J /} \cdot\left(\mathcal{T}_{1}\right)_{I K} \cdot \ldots \cdot\left(\mathcal{T}_{L_{t}-1}\right)_{L J}
$$

with $\left(\mathcal{T}_{t}\right)_{I K}=\operatorname{det} \tilde{B}_{t} \cdot \operatorname{det} \mathcal{T}_{t}{ }^{\text {KK }}$ and implicit sums $\{J, I, K, \ldots\}$.

- Finally, we have

$$
\operatorname{det}{ }_{N} M[\mathcal{U}]=\prod_{t} \operatorname{det} \tilde{B}_{t} \cdot \sum_{\left\{J_{t}\right\}} \prod_{t} \operatorname{det} \mathcal{T}_{t}^{X_{t-1} X_{t}}
$$

where $\left|J_{t}\right|=N$ and $J_{L_{t}}=J_{0}$.

## Factorization and fermion bags

Key step 3:

$$
\sum_{J} \operatorname{det} \mathcal{T}^{\not Y Y}=\sum_{J} \operatorname{det}\left(\mathcal{T}_{0} \cdot \ldots \cdot \mathcal{T}_{L_{t}-1}\right)^{\not Y X}=\left(\mathcal{T}_{0}\right)_{J l} \cdot\left(\mathcal{T}_{1}\right)_{I K} \cdot \ldots \cdot\left(\mathcal{T}_{L_{t}-1}\right)_{L J}
$$



## Factorization and fermion bags

Key step 3:

$$
\sum_{J} \operatorname{det} \mathcal{T}^{\not Y X}=\sum_{J} \operatorname{det}\left(\mathcal{T}_{0} \cdot \ldots \cdot \mathcal{T}_{L_{t}-1}\right)^{\not X X}=\left(\mathcal{T}_{0}\right)_{J l} \cdot\left(\mathcal{T}_{1}\right)_{I K} \cdot \ldots \cdot\left(\mathcal{T}_{L_{t}-1}\right)_{L J}
$$



$$
\ldots \quad N=L
$$



## Factorization and fermion bags

Key step 3:

$$
\sum_{J} \operatorname{det} \mathcal{T}^{\not Y X}=\sum_{J} \operatorname{det}\left(\mathcal{T}_{0} \cdot \ldots \cdot \mathcal{T}_{L_{t}-1}\right)^{\not Y X}=\left(\mathcal{T}_{0}\right)_{J I} \cdot\left(\mathcal{T}_{1}\right)_{I K} \cdot \ldots \cdot\left(\mathcal{T}_{L_{t}-1}\right)_{L J}
$$


... $\quad N=L$


## Dimensional reduction of QCD - Step 1

- Consider the Wilson fermion matrix for a single quark with chemical potential $\mu$ :

$$
M_{ \pm}(\mu)=\left(\begin{array}{ccccc}
B_{0} & P_{+} A_{0}^{+} & & & \pm P_{-} A_{L_{t}-1}^{-} \\
P_{-} A_{0}^{-} & B_{1} & P_{+} A_{1}^{+} & & \\
& P_{-} A_{1}^{-} & B_{2} & \ddots & \\
& & \ddots & \ddots & \\
& & & & P_{+} A_{L_{t}-2}^{+} \\
\pm P_{+} A_{L_{t}-1}^{+} & & & P_{-} & B_{L_{t}-1}
\end{array}\right)
$$

- temporal hoppings are

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

- Dirac projectors $P_{ \pm}=\frac{1}{2}\left(\mathbb{I} \mp \Gamma_{4}\right)$
- $B_{t}$ 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 - Step 1

- Reduced Wilson fermion determinant is given by

$$
\operatorname{det} M_{p, a}(\mu) \propto \prod_{t} \operatorname{det} Q_{t}^{+} \cdot \operatorname{det}\left[\mathbb{I} \pm e^{+\mu L_{t}} \mathcal{T}\right]
$$

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

$$
\begin{gathered}
\mathcal{T}=\prod_{t} Q_{t}^{+} \cdot \mathcal{U}_{t} \cdot\left(Q_{t+1}^{-}\right)^{-1} \equiv \prod_{t} \mathcal{T}_{t} \\
Q_{t}^{ \pm}=B_{t} P_{\mp}+P_{ \pm}, \quad B_{t}=\left(\begin{array}{cc}
D_{t} & C_{t} \\
-C_{t} & D_{t}
\end{array}\right)
\end{gathered}
$$

and

$$
Q_{t}^{+}=\left(\begin{array}{cc}
1 & C_{t} \\
0 & D_{t}
\end{array}\right), \quad\left(Q_{t}^{-}\right)^{-1}=\left(\begin{array}{cc}
D_{t}^{-1} & 0 \\
C_{t} \cdot D_{t}^{-1} & 1
\end{array}\right) .
$$

## Structure of building blocks

- Product of spatial matrices:

$$
\mathcal{T}=\prod_{t} Q_{t}^{+} \cdot \mathcal{U}_{t} \cdot\left(Q_{t+1}^{-}\right)^{-1} \quad \text { or } \quad \mathcal{T}=\prod_{t} \mathcal{U}_{t-1}^{-} \cdot\left(Q_{t}^{-}\right)^{-1} \cdot Q_{t}^{+} \cdot U_{t}^{+}
$$



$$
Q_{t}^{+} \cdot \mathcal{U}_{t} \cdot\left(Q_{t+1}^{-}\right)^{-1}
$$

## Structure of building blocks

- Product of spatial matrices:

$$
\mathcal{T}=\prod_{t} Q_{t}^{+} \cdot \mathcal{U}_{t} \cdot\left(Q_{t+1}^{-}\right)^{-1} \quad \text { or } \quad \mathcal{T}=\prod_{t} \mathcal{U}_{t-1}^{-} \cdot\left(Q_{t}^{-}\right)^{-1} \cdot Q_{t}^{+} \cdot \mathcal{U}_{t}^{+}
$$



$$
\mathcal{U}_{t-1}^{-} \cdot\left(Q_{t}^{-}\right)^{-1} \cdot Q_{t}^{+} \cdot \mathcal{U}_{t}^{+}
$$

## Structure of building blocks

- Several ways to rewrite spatial matrices:

$$
\widetilde{\mathcal{T}}_{t} \equiv\left(Q_{t}^{-}\right)^{-1} \cdot Q_{t}^{+}=\left(\begin{array}{cc}
1 & 0 \\
C_{t} & 1
\end{array}\right)\left(\begin{array}{cc}
D_{t}^{-1} & 0 \\
0 & D_{t}
\end{array}\right)\left(\begin{array}{cc}
1 & C_{t} \\
0 & 1
\end{array}\right)
$$

- spectral property and determinant:

$$
\lambda \leftrightarrow \frac{1}{\lambda^{*}}, \quad \operatorname{det}\left(Q_{t}^{-}\right)^{-1} \cdot Q_{t}^{+}=1
$$

- Relation to 1 d scattering matrix $\widetilde{\mathcal{S}}_{t}$ :

$$
\widetilde{\mathcal{T}}_{t}=\left(\begin{array}{cc}
D_{t}^{-1} & D_{t}^{-1} \cdot C_{t} \\
C_{t} \cdot D_{t}^{-1} & D_{t}+C_{t} \cdot D_{t}^{-1} \cdot C_{t}
\end{array}\right) \quad \Leftrightarrow \quad \widetilde{\mathcal{S}}_{t}=\left(\begin{array}{cc}
C_{t} & D_{t} \\
D_{t} & -C_{t}
\end{array}\right) .
$$

## Canonical projection and factorization - Step $2+3$

## Step 2: Canonical projection of QCD

$$
\operatorname{det} M_{N_{q}}=\prod_{t} \operatorname{det} Q_{t}^{+} \cdot \sum_{A} \operatorname{det} \mathcal{T}^{A \lambda A}
$$

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

$$
|A|=N_{q}^{\max }+N_{q}, \quad N_{q}^{\max }=2 \cdot N_{c} \cdot L_{s}^{3}
$$

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

Step 3: Factorization of QCD determinant

$$
\operatorname{det} M_{N_{q}}=\prod_{t} \operatorname{det} Q_{t}^{+} \cdot \prod_{t} M\left(\left(Q_{t}^{-}\right)^{-1}\right)_{A_{t} B_{t}} M\left(Q_{t}^{+}\right)_{B_{t} C_{t}} M\left(\mathcal{U}_{t}\right)_{C_{t} A_{t+1}}
$$

## Relation between quark and baryon number in QCD

## Step 3: Factorization of QCD determinant

$$
\operatorname{det} M_{N_{q}}=\prod_{t} \operatorname{det} Q_{t}^{+} \cdot \prod_{t} M\left(\left(Q_{t}^{-}\right)^{-1}\right)_{A_{t} B_{t}} M\left(Q_{t}^{+}\right)_{B_{t} C_{t}} M\left(\mathcal{U}_{t}\right)_{C_{t} A_{t+1}}
$$

- Consider $\mathbb{Z}\left(N_{c}\right)$-transformation by $z_{k}=e^{2 \pi i \cdot k / N_{c}} \in \mathbb{Z}\left(N_{c}\right)$ :

$$
\mathcal{U}_{t} \rightarrow \mathcal{U}_{t}^{\prime}=z_{k} \cdot \mathcal{U}_{t} \quad \text { at one fixed } t
$$

- As a consequence we have

$$
\operatorname{det} M_{N_{q}} \rightarrow \operatorname{det} M_{N_{q}}^{\prime}=\prod_{t} \operatorname{det} Q_{t}^{+} \cdot \sum_{A} \operatorname{det}\left(z_{k} \cdot \mathcal{T}\right)^{\langle\lambda|}=z_{k}^{-N_{q}} \cdot \operatorname{det} M_{N_{q}}
$$

and summing over $z_{k}$ therefore yields

$$
\operatorname{det} M_{N_{q}}=0 \quad \text { for } N_{q} \neq 0 \bmod N_{c}
$$

## Properties of minor matrices

## Step 3: Factorization of QCD determinant

$$
\operatorname{det} M_{N_{q}}=\prod_{t} \operatorname{det} Q_{t}^{+} \cdot \prod_{t} M\left(\left(Q_{t}^{-}\right)^{-1}\right)_{\mathcal{A}_{t} B_{t}} M\left(Q_{t}^{+}\right)_{B_{t} \mathcal{C}_{t}} M\left(\mathcal{U}_{t}\right)_{G_{t} X_{t+1}}
$$

- Note that

$$
M\left(Q^{-1}\right)_{A B}=(-1)^{p(A, B)} \frac{\widetilde{M}(Q)_{B A}}{\operatorname{det} Q}, \quad \operatorname{det} Q_{t}^{+}=\operatorname{det} Q_{t}^{-}
$$

avoids inverting $Q_{t}^{-}$.

- Consider temporal gauge link $W_{t}=\mathbb{I}_{4 \times 4} \otimes U_{4}(\bar{x}, t)$ at $\bar{x}$ :

$$
M\left(W_{t}\right)_{\gamma_{t} \phi_{t+1}}=0 \text { if }\left|c_{t}\right| \neq\left|a_{t}\right|
$$

for $c_{t} \in C_{t}$ and $a_{t+1} \in A_{t+1}$.

## Multi-level integration schemes

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

$M\left(\mathcal{U}_{t-1}\right)_{\mathcal{C}_{t-1} \mathcal{A}_{t}} \cdot M\left(\left(Q_{t}^{-}\right)^{-1}\right)_{\mathcal{A}_{t} Q_{t}} \cdot M\left(Q_{t}^{+}\right)_{\mathcal{B}_{t}{C_{t}}} \cdot M\left(\mathcal{U}_{t}\right)_{\mathcal{C}_{t} A_{k+1}}$
- spatial matrix $\mathcal{U}_{t}$ is block diagonal:
$\Rightarrow M\left(\mathcal{U}_{t}\right)$ trivial to calculate!


## Multi-level integration schemes

- Spatial gauge links in $Q_{t}^{ \pm}$coupled through temporal plaquettes only:

$M\left(\mathcal{U}_{t-1}\right)_{C_{t-1} A_{t}} \cdot M\left(\left(Q_{t}^{-}\right)^{-1}\right)_{A_{t} B_{t}} \cdot M\left(Q_{t}^{+}\right)_{B_{t} C_{t}} \cdot M\left(\mathcal{U}_{t}\right)_{C_{t} A_{k+1}}$
- spatial matrices $Q_{t}^{ \pm}$can be treated together:

$$
M\left(\left(Q_{t}^{-}\right)^{-1}\right)_{\chi_{t} \dot{\beta}_{t}} \cdot M\left(Q_{t}^{+}\right)_{\mathcal{k}_{t} \chi_{t}}=M\left(\left(Q_{t}^{-}\right)^{-1} \cdot Q_{t}^{+}\right)_{\chi_{t} \chi_{t}}
$$

## Correlation functions

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

$$
\ldots \cdot \mathcal{T}_{t-1}^{\left(N_{q}\right)} \cdot \mathcal{S}_{N_{q} \rightarrow N_{q}+3} \cdot \mathcal{T}_{t}^{\left(N_{q}+3\right)} \cdot \ldots \cdot \mathcal{T}_{t^{\prime}}^{\left(N_{q}+3\right)} \cdot \overline{\mathcal{S}}_{N_{q}+3 \rightarrow N_{q}} \cdot \mathcal{T}_{t^{\prime}+1}^{\left(N_{q}\right)} \cdot \ldots
$$

- vacuum sector corresponds to $N_{q}=0$
- Natural to construct improved estimators:
- simulate directly the correlation function at $C\left(t^{\prime}-t\right)$,
- measure $C\left(t^{\prime}+1-t\right)$ relative to $C\left(t^{\prime}-t\right)$

$$
\left\langle C\left(t^{\prime}+1-t\right)\right\rangle_{C\left(t^{\prime}-t\right)} \sim e^{-a E}
$$

from additional insertion $\mathcal{T}_{t^{\prime}+1}^{\left(N_{q}\right)} \rightarrow \mathcal{T}_{t^{\prime}+1}^{\left(N_{q}+3\right)}$

- All spectral information is contained in $\left\langle\mathcal{T}_{t}^{\left(N_{q}\right)}\right\rangle$.


## Summary and outlook

- Complete temporal factorization of the Wilson fermion determinant:
- 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, $\left(\mathcal{T}_{t}\right)_{B C}$ not necessarily...

## Hubbard model

- Consider the Hamiltonian for the Hubbard model

$$
\mathcal{H}(\mu)=-\sum_{\langle x, y\rangle, \sigma} t_{\sigma} \hat{c}_{x, \sigma}^{\dagger} \hat{c}_{y, \sigma}+\sum_{x, \sigma} \mu_{\sigma} N_{x, \sigma}+U \sum_{x} N_{x, \uparrow} N_{x, \downarrow}
$$

with particle number $N_{x, \sigma}=\hat{c}_{x, \sigma}^{\dagger} \hat{c}_{x, \sigma}$.

## Hubbard model with Trotter

- Consider the Hamiltonian for the Hubbard model

$$
\mathcal{H}(\mu)=-\sum_{\langle x, y\rangle, \sigma} t_{\sigma} \hat{c}_{x, \sigma}^{\dagger} \hat{c}_{y, \sigma}+\sum_{x, \sigma} \mu_{\sigma} N_{x, \sigma}+U \sum_{x} N_{x, \uparrow} N_{x, \downarrow}
$$

with particle number $N_{x, \sigma}=\hat{c}_{x, \sigma}^{\dagger} \hat{c}_{x, \sigma}$.

- Trotter decomposition and coherent state representation yields

$$
Z_{\mathrm{GC}}(\mu)=\int \mathcal{D} \psi^{\dagger} \mathcal{D} \psi e^{-S\left[\psi^{\dagger}, \psi ; \mu\right]}
$$

with Euclidean action

$$
S\left[\psi^{\dagger}, \psi ; \mu\right]=\sum_{\sigma} \psi_{\sigma}^{\dagger} \nabla_{t} \psi_{\sigma}+H\left[\psi^{\dagger}, \psi ; \mu\right]
$$

## Hubbard model with Trotter and Stratonovic

- Consider the Hamiltonian for the Hubbard model

$$
\mathcal{H}(\mu)=-\sum_{\langle x, y\rangle, \sigma} t_{\sigma} \hat{c}_{x, \sigma}^{\dagger} \hat{c}_{y, \sigma}+\sum_{x, \sigma} \mu_{\sigma} N_{x, \sigma}+U \sum_{x} N_{x, \uparrow} N_{x, \downarrow}
$$

with particle number $N_{x, \sigma}=\hat{c}_{x, \sigma}^{\dagger} \hat{c}_{x, \sigma}$.

- After a Hubbard-Stratonovich transformation we have

$$
Z_{\mathrm{GC}}(\mu)=\int \mathcal{D} \psi^{\dagger} \mathcal{D} \psi \mathcal{D} \phi \rho[\phi] e^{-\sum_{\sigma} S\left[\psi_{\sigma}^{\dagger}, \psi_{\sigma}, \phi ; \mu_{\sigma}\right]}
$$

with $S\left[\psi_{\sigma}^{\dagger}, \psi_{\sigma}, \phi ; \mu_{\sigma}\right]=\psi_{\sigma}^{\dagger} M\left[\phi ; \mu_{\sigma}\right] \psi_{\sigma}$, and hence

$$
=\int \mathcal{D} \phi \rho[\phi] \prod_{\sigma} \operatorname{det} M\left[\phi ; \mu_{\sigma}\right] .
$$

## Fermion matrix and dimensional reduction

- The fermion matrix has the structure

$$
M\left[\phi ; \mu_{\sigma}\right]=\left(\begin{array}{cclc}
B & 0 & \cdots & \pm e^{\mu_{\sigma}} C\left(\phi_{N_{t}-1}\right) \\
-e^{\mu_{\sigma}} C\left(\phi_{0}\right) & B & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & -e^{\mu_{\sigma}} C\left(\phi_{N_{t}-2}\right) & B
\end{array}\right)
$$

for which the determinant can be reduced to

$$
\operatorname{det} M\left[\phi ; \mu_{\sigma}\right]=\operatorname{det} B^{N_{t}} \cdot \operatorname{det}\left(1 \mp e^{N_{t} \mu_{\sigma}} \mathcal{T}[\phi]\right)
$$

where $\mathcal{T}[\phi]=B^{-1} C\left(\phi_{N_{t}-1}\right) \cdot \ldots \cdot B^{-1} C\left(\phi_{0}\right)$.

## Fermion matrix and dimensional reduction

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-e^{\mu_{\sigma}} C\left(\phi_{0}\right) & B & \ldots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \ldots & -e^{\mu_{\sigma}} C\left(\phi_{N_{t}-2}\right) & B
\end{array}\right)
$$

for which the determinant can be reduced to

$$
\operatorname{det} M\left[\phi ; \mu_{\sigma}\right]=\operatorname{det} B^{N_{t}} \cdot \operatorname{det}\left(1 \mp e^{N_{t} \mu_{\sigma}} \mathcal{T}[\phi]\right)
$$

where $\mathcal{T}[\phi]=B^{-1} C\left(\phi_{N_{t}-1}\right) \cdot \ldots \cdot B^{-1} C\left(\phi_{0}\right)$.

- Transfer matrices are hence given by

$$
\begin{aligned}
\left(\mathcal{T}_{t}\right)_{I K} & =\operatorname{det} B \cdot \operatorname{det}\left[B^{-1} \cdot C\left(\phi_{t}\right)\right]^{\text {IK }} \\
& =\operatorname{det} B \cdot \operatorname{det}\left(B^{-1}\right)^{\wedge \mathcal{A}} \cdot \operatorname{det} C\left(\phi_{t}\right)^{Y K} \\
& =(-1)^{p(I, J)} \operatorname{det} B^{J I} \cdot \operatorname{det} C\left(\phi_{t}\right)^{Y K} .
\end{aligned}
$$

## Transfer matrices

- Since $C\left(\phi_{t}\right)$ can be chosen diagonal, we have

$$
\operatorname{det} C\left(\phi_{t}\right)^{Y K}=\delta_{J K} \prod_{x \notin J} \phi_{x, t}
$$

and the HS field can be integrated out site by site:

$$
\int d \phi_{x, t} \rho\left(\phi_{x, t}\right) \phi_{x, t}^{\Sigma_{\sigma}} \delta_{x \neq J \sigma} \equiv w_{x, t}= \begin{cases}w_{2} & \text { if } x \notin J^{\uparrow}, x \notin J \downarrow \\ w_{1} & \text { else } \\ w_{0} & \text { if } x \in J^{\uparrow}, x \in J^{\downarrow}\end{cases}
$$

- Finally, with $\Pi_{x} w_{x, t} \equiv W\left(\left\{J_{t}^{\sigma}\right\}\right)$ we have

$$
Z_{C}\left(\left\{N_{\sigma}\right\}\right)=\sum_{\left\{J_{t}^{\sigma}\right\}} \prod_{t}\left(\prod_{\sigma} \operatorname{det} B^{J_{t-1}^{\sigma} J_{t}^{\sigma}}\right) W\left(\left\{J_{t}^{\sigma}\right\}\right), \quad\left|J_{t}^{\sigma}\right|=N_{\sigma}
$$

## Relation to fermion loop formulation

$$
Z_{C}\left(\left\{N_{\sigma}\right\}\right)=\sum_{\left\{J_{t}^{\sigma}\right\}} \prod_{t}\left(\prod_{\sigma} \operatorname{det} B^{J_{t-1}^{\sigma} J_{t}^{\sigma}}\right) W\left(\left\{J_{t}^{\sigma}\right\}\right)
$$

index sets $J_{t}$ :

$\{3,6\}$
$\{4,5\}$
$\{4,5\}$
$\{2,7\}$
$\{2,7\}$
$\{3,7\}$

## Relation to fermion bag formulation

- In $d=1$ dimension the 'fermion bags' $\operatorname{det} B^{I J}$ can be calculated analytically:

and one can prove that

$$
\begin{aligned}
& \quad \operatorname{det} B^{I J} \geq 0 \text { for open b.c. } \\
& \Rightarrow \text { there is no sign problem }
\end{aligned}
$$

- For periodic b.c. there is no sign problem either, because

$$
Z_{C}^{\mathrm{pbc}}\left(L_{s} \rightarrow \infty\right)=Z_{C}^{\mathrm{obc}}\left(L_{s} \rightarrow \infty\right)
$$

