

Transfer matrices and temporal factorization of the Wilson fermion determinant

Urs Wenger^{a,*}

^a*Albert Einstein Center for Fundamental Physics, Institute for Theoretical Physics, University of Bern, Sidlerstrasse 5, CH-3012 Bern, Switzerland*

E-mail: wenger@itp.unibe.ch

When lattice QCD is formulated in sectors of fixed quark numbers, the canonical fermion determinants can be expressed explicitly in terms of transfer matrices. This in turn provides a complete factorization of the fermion determinants in temporal direction. Here we present a generic overview of this factorization, apply it to Wilson-type fermions and provide explicit constructions of the transfer matrices. Possible applications of the factorization include multi-level integration schemes and the construction of improved estimators for generic n -point correlation functions.

*The 39th International Symposium on Lattice Field Theory (Lattice2022),
8-13 August, 2022
Bonn, Germany*

*Speaker

1. Introduction and motivation

The temporal factorization of fermion determinants is a generic feature of fermionic quantum field theories on the lattice. The key steps for achieving the factorization are 1) the dimensional reduction of the fermion determinant, 2) the projection to canonical sectors with fixed fermion numbers, and 3) the factorization of the canonical determinants in terms of transfer matrices. In these proceedings we summarize these three steps first for a generic fermionic gauge field theory and then exemplify the steps by applying them to QCD with Wilson fermions.

The dimensional reduction of the fermion determinant has been known since a long time [1–3] and has been used in different contexts [4–12] since then. Canonical ensembles and determinants have found their use in various applications [13, 14]. In some cases they lead to a solution of the fermion sign problem [15]. For the factorization it is important use the canonical projection of the fermion determinant as first proposed [16] and applied [17, 18] in the context of supersymmetric Yang-Mills quantum mechanics. Moreover, the factorization of the fermion determinant has also been demonstrated for the Hubbard model [19].

The dimensional reduction and temporal factorization of the fermion determinant is most interesting from an algorithmic point of view. First, the dimensional reduction offers the possibility to reduce the complexity of calculating the fermion determinant. Second, the factorization allows the construction and application of multi-level integration schemes following [20]. Since the factorization in terms of the transfer matrices presented here is the most atomic one, it may serve as the basis for more flexible and efficient factorization schemes [21, 22]. The factorization also enables the construction of improved estimators for generic n -point correlation functions [19]. Moreover, the transfer matrices naturally accommodate open boundary conditions in time.

To set the stage we consider a generic fermionic gauge field theory with gauge fields \mathcal{U} and fermion fields ψ^\dagger, ψ . Its grand-canonical partition function at finite chemical potential μ is

$$Z_{\text{GC}}(\mu) = \int \mathcal{D}\mathcal{U} e^{-S_b[\mathcal{U}]} \int \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-\bar{\psi} M[\mathcal{U}; \mu] \psi} \quad (1)$$

$$= \int \mathcal{D}\mathcal{U} e^{-S_b[\mathcal{U}]} \det M[\mathcal{U}; \mu], \quad (2)$$

where $S_b[\mathcal{U}]$ is the bosonic gauge field action and $M[\mathcal{U}; \mu]$ the fermion matrix. After integrating out the fermion fields one obtains the fermion determinant $\det M[\mathcal{U}; \mu]$ as indicated in Eq. (2). In general, this determinant is very difficult to calculate, due to its highly non-local dependence on the gauge field. In the Hamiltonian formulation one can formally write the partition function as a trace of the Hamiltonian Boltzman weight over all the states of the system,

$$Z_{\text{GC}}(\mu) = \text{Tr} \left[e^{-\mathcal{H}(\mu)/T} \right] = \text{Tr} \prod_t \mathcal{T}_t(\mu), \quad (3)$$

where the last equation indicates that on a space-time lattice the temporal evolution can be written in terms of grand-canonical transfer matrices \mathcal{T}_t defined at fixed (Euclidean) times t . Finally, one can use a fugacity expansion to relate the grand-canonical partition function to the canonical one, $Z_C(N)$, for which the fermion number N is fixed,

$$Z_{\text{GC}}(\mu) = \sum_N e^{-N\mu/T} \cdot Z_C(N) = \sum_N e^{-N\mu/T} \cdot \text{Tr} \prod_t \mathcal{T}_t^{(N)}. \quad (4)$$

Here, $\mathcal{T}_t^{(N)}$ are the corresponding canonical transfer matrices at fixed fermion number N . They can be obtained, at least formally, by restricting \mathcal{T}_t to states with fixed N . In the following we show that these relations are not just formal, but can be made explicit.

2. Step 1: Dimensional reduction of the fermion determinant

For generic gauge field theories discretized on a space-time lattice with $L_s \times L_t$ lattice sites and a total of L fermionic degrees of freedom per time slice, the fermion matrix $M[\mathcal{U}; \mu]$ has the (temporal) structure

$$M[\mathcal{U}; \mu] = \begin{pmatrix} B_0 & e^{+\mu} C'_0 & 0 & \dots & \pm e^{-\mu} C_{L_t-1} \\ e^{-\mu} C_0 & B_1 & e^{+\mu} C'_1 & & 0 \\ 0 & e^{-\mu} C_1 & B_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & & \vdots \\ \pm e^{+\mu} C'_{L_t-1} & 0 & & B_{L_t-2} & e^{+\mu} C'_{L_t-2} \\ & & & e^{-\mu} C_{L_t-2} & B_{L_t-1} \end{pmatrix}. \quad (5)$$

Here, the matrices B_t describe the spatial fermion hoppings and only depend on the spatial gauge fields at fixed time t , while the matrices C'_t and C_t describe the temporal fermion hoppings forward and backward in time, respectively. They only contain temporal gauge fields. The \pm signs in the upper right and lower left block of the matrix indicate periodic or antiperiodic boundary conditions for the fermions in the temporal direction.

Given this structure, the determinant of M can be reduced by iterative Schur decompositions yielding

$$\det M[\mathcal{U}; \mu] = \prod_{t=0}^{L_t-1} \det \tilde{B}_t \cdot \det \left(1 \mp e^{\mu L_t} \cdot \mathcal{T} \right), \quad (6)$$

where $\mathcal{T} = \mathcal{T}_0 \cdot \dots \cdot \mathcal{T}_{L_t-1}$ with $\mathcal{T}_t = \mathcal{T}_t[B_t, C_t, C'_t]$, i.e., the matrices \mathcal{T}_t only depend on the spatial blocks associated with the time slice at time t . The matrices \tilde{B}_t are equal to B_t up to constant factors of the fugacity $e^{\pm\mu}$. Since the prefactor $\prod_t \det \tilde{B}_t$ is already factorized and hence not relevant in the remaining derivation of the factorization, we neglect it for simplicity and only reintroduce it at the very end.

The key object from step 1 is the matrix $\mathcal{T}[\mathcal{U}]$ given as the product of spatial matrices,

$$\mathcal{T}[\mathcal{U}] \equiv \prod_{t=0}^{L_t-1} \mathcal{T}_t. \quad (7)$$

The matrices \mathcal{T}_t are of size $L \times L$ only, while in contrast $M[\mathcal{U}; \mu]$ is of size $(L \cdot L_t) \times (L \cdot L_t)$.

3. Step 2: Projection of the fermion determinant to canonical sectors

The projection of the fermion determinant to canonical sectors starts from the expansion of the fermion determinant in terms of the fugacity $e^{-\mu/T}$,

$$\det M[\mathcal{U}; \mu] = \sum_{N=-L/2}^{L/2} e^{-N \cdot \mu/T} \cdot \det_N M[\mathcal{U}], \quad (8)$$

where $\det_N M[\mathcal{U}]$ denote the canonical determinants at fixed fermion number N . Up to a constant multiplicative factor they are simply given by the coefficients in the fugacity expansion of the characteristic polynomial of the reduced matrix in Eq. (6),

$$\sum_{N=-L/2}^{L/2} e^{-N \cdot \mu/T} \cdot \det_N M[\mathcal{U}] \propto \det \left(e^{-\mu/T} + \mathcal{T}[\mathcal{U}] \right), \quad (9)$$

where for simplicity we now restrict ourselves to antiperiodic temporal boundary conditions for the fermions. The coefficients can be calculated through the elementary symmetric functions S_k of order k of the eigenvalues $\{\tau_i\}$ of \mathcal{T} ,

$$\det_N M[\mathcal{U}] \propto S_{L/2+N}(\mathcal{T}),$$

where

$$S_k(\mathcal{T}) \equiv S_k(\{\tau_i\}) = \sum_{1 \leq i_1 < \dots < i_k \leq L} \prod_{j=1}^k \tau_{i_j} = \sum_{|J|=k} \det \mathcal{T}^{\mathcal{J}\mathcal{J}}. \quad (10)$$

In the last equality we have made use of the fact that the symmetric functions S_k can be expressed in terms of the principal minors of order k denoted by $\det \mathcal{T}^{\mathcal{J}\mathcal{J}}$. We recall that the principal minors are obtained by computing the determinant of the matrix $\mathcal{T}^{\mathcal{J}\mathcal{J}}$ from which the columns and rows labeled by the index set J of size k are removed.

Summarizing the derivation above we have

$$\det_N M[\mathcal{U}] \propto \sum_J \det \mathcal{T}^{\mathcal{J}\mathcal{J}}[\mathcal{U}] \propto \text{Tr} \left[\prod_t \mathcal{T}_t^{(N)} \right]. \quad (11)$$

The last proportionality exposes the connection with the trace over the fermionic states with fixed fermion number N of the product of transfer matrices in Eq. (4), except that here the trace is taken for a fixed gauge field \mathcal{U} .

We note that the fermionic states are labeled by index sets $J \subset \{1, \dots, L\}$, $|J| = L/2 + N$, hence the number of states is given by

$$N_{\text{states}} = \binom{L}{L/2 + N} = N_{\text{principal minors}}, \quad (12)$$

i.e., at half-filling ($N = 0$) the number of states grows exponentially with L . For relativistic gauge field theories, half-filling corresponds to the vacuum sector where all states have equal numbers of fermions and antifermions, hence $N = 0$. At first sight, the exponential growth of states looks like an obstacle for numerical Monte-Carlo simulations, however, one can treat the index set J as a (discrete) dynamical degree of freedom which can be evaluated stochastically [14, 16–19].

4. Step 3: Temporal factorization of the fermion determinant

Having the canonical fermion determinant at hand, we are now in the position to derive its temporal factorization. To do so, we use the Cauchy-Binet formula

$$\det(A \cdot B)^{\mathcal{K}\mathcal{K}} = \sum_J \det A^{\mathcal{K}J} \cdot \det B^{J\mathcal{K}} \quad (13)$$

to factorize the minor matrix of a product of matrices $A \cdot B$ into the product of the corresponding minor matrices of A and B . Applying the Cauchy-Binet formula to the principal minors in Eq. (11) achieves the factorization. Reintroducing the prefactors $\det \tilde{B}_t$ and defining $(\mathcal{T}_t)_{IK} = \det \tilde{B}_t \cdot \det \mathcal{T}_t^{\mathbb{K}\mathbb{K}}$ for simplicity we eventually obtain the expression in terms of the transfer matrices,

$$\det \mathcal{T}^{\mathcal{Y}\mathcal{Y}} = \det(\mathcal{T}_0 \cdots \mathcal{T}_{L_t-1})^{\mathcal{Y}\mathcal{Y}} = (\mathcal{T}_0)_{JI} \cdot (\mathcal{T}_1)_{IK} \cdots (\mathcal{T}_{L_t-1})_{LJ}, \quad (14)$$

where implicit sums over the index sets $\{J, I, K, \dots\}$ are assumed. Collecting everything we finally have

$$\det {}_N M[\mathcal{U}] = \prod_{t=0}^{L_t-1} \det \tilde{B}_t \cdot \sum_{\{J_t\}} \prod_{t=0}^{L_t-1} \det \mathcal{T}_t^{\mathcal{Y}_t \mathcal{Y}_{t+1}}, \quad (15)$$

where $|J_t| = L/2 + N$ and $J_{L_t} \equiv J_0$.

5. Application to QCD with Wilson fermions

We can now apply the three steps sketched in the previous sections to QCD with Wilson fermions. For this purpose we consider the Wilson fermion matrix $M[\mathcal{U}; \mu]$ for a single quark flavour with chemical potential μ ,

$$M_{\pm}[\mathcal{U}; \mu] = \begin{pmatrix} B_0 & P_+ A_0^+ & & & \pm P_- A_{L_t-1}^- \\ P_- A_0^- & B_1 & P_+ A_1^+ & & \\ & P_- A_1^- & B_2 & \ddots & \\ & & \ddots & \ddots & \\ \pm P_+ A_{L_t-1}^+ & & & & P_+ A_{L_t-2}^+ \\ & & & P_- A_{L_t-2}^- & B_{L_t-1} \end{pmatrix}$$

with the Dirac projectors $P_{\pm} = \frac{1}{2}(\mathbb{I} \mp \Gamma_4)$. Here, the temporal hoppings are

$$A_t^{\pm} = e^{\pm\mu} \cdot \mathcal{U}_t = (A_t^{\mp})^{-1} \quad \text{with} \quad \mathcal{U}_t = \{\mathbb{I}_{4 \times 4} \otimes U_4(\bar{x}, t), \bar{x} \in \{0, \dots, L_s^3 - 1\}\}$$

collecting the temporal gauge links at fixed time t , while the spatial fermion hoppings are collected in the spatial Wilson Dirac operators B_t containing only the spatial gauge links at time slice t . All block matrices appearing in $M[\mathcal{U}; \mu]$ are $(4 \cdot N_c \cdot L_s^3 \times 4 \cdot N_c \cdot L_s^3)$ matrices. The reduced Wilson fermion determinant is then given by

$$\det M_{p,a}(\mu) \propto \prod_{t=0}^{L_t-1} \det Q_t^+ \cdot \det [\mathbb{I} \pm e^{\pm\mu L_t} \mathcal{T}], \quad (16)$$

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

$$\mathcal{T} = \prod_{t=0}^{L_t-1} Q_t^+ \cdot \mathcal{U}_t \cdot (Q_{t+1}^-)^{-1} \equiv \prod_{t=0}^{L_t-1} \mathcal{T}_t \quad (17)$$

with

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

and hence

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

We refer to Ref. [11] for further details on the derivation of the dimensional reduction for Wilson fermions.

The product of the spatial matrices Q_t^\pm and temporal gauge links \mathcal{U}_t can be written in different ways. The form

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

emphasises the connection to the usual definition of transfer matrices between time slice at t and $t + 1$, while the form

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

with $\mathcal{U}_t^\pm = \mathcal{U}_t P_\mp + P_\pm$ points out the separation of the spatial gauge links within a fixed time slice t contained in Q_t^\pm from those within neighbouring time slices at $t \pm 1$. There are also several ways to express the spatial matrices. The form

$$\tilde{\mathcal{T}}_t \equiv (Q_t^-)^{-1} \cdot Q_t^+ = \begin{pmatrix} 1 & 0 \\ C_t & 1 \end{pmatrix} \begin{pmatrix} D_t^{-1} & 0 \\ 0 & D_t \end{pmatrix} \begin{pmatrix} 1 & C_t \\ 0 & 1 \end{pmatrix}$$

exposes the relation $\det \tilde{\mathcal{T}}_t = 1$ and hence the spectral property $\lambda \leftrightarrow 1/\lambda^*$ of the eigenvalues λ of $\tilde{\mathcal{T}}_t$. In contrast, the form

$$\tilde{\mathcal{T}}_t = \begin{pmatrix} D_t^{-1} & D_t^{-1} \cdot C_t \\ C_t \cdot D_t^{-1} & D_t + C_t \cdot D_t^{-1} \cdot C_t \end{pmatrix} \Leftrightarrow \tilde{\mathcal{S}}_t = \begin{pmatrix} C_t & D_t \\ D_t & -C_t \end{pmatrix}$$

expresses the relation between the matrix $\tilde{\mathcal{T}}_t$ and the three-dimensional scattering matrix $\tilde{\mathcal{S}}_t$.

Given the reduced determinant in Eq. (16) and the explicit form of \mathcal{T} in Eq. (17) it is now straightforward to apply step 2 for the case of Wilson fermions and project to the canonical determinants with N_q quarks,

$$\det M_{N_q} = \prod_t \det Q_t^+ \cdot \sum_A \det \mathcal{T}^{AA}. \quad (18)$$

Here, the sum is over all index sets $A \subset \{1, 2, \dots, 2N_q^{\max}\}$ of size $|A| = N_q^{\max} + N_q$ where $N_q^{\max} = 2 \cdot N_c \cdot L_s^3$ for gauge group $SU(N_c)$ and $N_q \in \{-N_c \cdot L_s^3, \dots, +N_c \cdot L_s^3\}$. Finally, the temporal factorization of the QCD determinant is achieved by applying step 3 to Eq. (18) yielding

$$\det M_{N_q} = \prod_t \det Q_t^+ \cdot \prod_t M \left((Q_t^-)^{-1} \right)_{A_t \setminus B_t} M (Q_t^+)_{B_t \setminus C_t} M (\mathcal{U}_t)_{C_t \setminus A_{t+1}} \quad (19)$$

where for notational simplicity we have introduced the notation $M(A)$ for the minor matrix of a generic matrix A .

We end this section by pointing out three interesting properties of the minor matrices appearing in Eq. (19). First, we note that transforming all temporal gauge links at one fixed time slice t with an element $z_k = e^{2\pi i \cdot k/N_c} \in \mathbb{Z}(N_c)$ of the center of the gauge group, i.e.,

$$\mathcal{U}_t \rightarrow \mathcal{U}'_t = z_k \cdot \mathcal{U}_t$$

we find

$$\det M_{N_q} \rightarrow \det M'_{N_q} = \prod_t \det Q_t^+ \cdot \sum_A \det(z_k \cdot \mathcal{T})^{\lambda\lambda} = z_k^{-N_q} \cdot \det M_{N_q}.$$

As a consequence, summing over $z_k, k = 1, \dots, N_c$ yields

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

i.e., only sectors with integer baryon numbers yield nonvanishing canonical partition functions. This nontrivial physical relation between the quark and baryon numbers in QCD becomes trivial in the factorized canonical formulation. Second, we note that with the relations

$$M(Q^{-1})_{\mathcal{A}\mathcal{B}} = (-1)^{p(A,B)} \frac{\tilde{M}(Q)_{BA}}{\det Q}, \quad \det Q_t^+ = \det Q_t^-,$$

where $\tilde{M}(Q)$ is the complementary minor matrix of Q and $p(A, B)$ the total parity of the index sets A and B , the inversion of Q_t^- can be avoided. Third, we note that \mathcal{U}_t is trivial in Dirac space and has a simple block structure in terms of the collection of temporal gauge links $W_t = \mathbb{I}_{4 \times 4} \otimes U_4(\bar{x}, t)$ at fixed spatial site \bar{x} . As a consequence, the corresponding minor matrix element $M(\mathcal{U}_t)_{\mathcal{C}_t \mathcal{A}_{t+1}}$ in Eq. (19) is nonzero only if $M(W_t)_{\mathcal{C}_t \mathcal{A}_{t+1}} \neq 0, \forall \bar{x}$, where $c_t(\bar{x}) \in \mathcal{C}_t$ and $a_{t+1}(\bar{x}) \in \mathcal{A}_{t+1}$ are the sub-index sets restricted to \bar{x} . Hence, $M(\mathcal{U}_t)_{\mathcal{C}_t \mathcal{A}_{t+1}} = 0$ if $|c_t(\bar{x})| \neq |a_{t+1}(\bar{x})|$ at any of the sites \bar{x} . This imposes a considerable restriction on the allowed index sets.

6. Multi-level integration schemes and improved estimators

The factorization provided by Eq. (19) allows for simple multi-level integration schemes, since the gauge fields on different time slices are no longer coupled through the fermion determinant. For example, the temporal gauge links \mathcal{U}_t at different times t are completely decoupled from each other. Since the spatial matrix \mathcal{U}_t is block-diagonal (see remark above), $M(\mathcal{U}_t)$ is trivial to calculate. Assuming Wilson's plaquette gauge action the only interaction between the temporal gauge links at fixed t is through the temporal plaquettes only.

The spatial gauge fields at fixed time t on the other hand interact with each other only through $M((Q_t^-)^{-1})$ and $M(Q_t^+)$. Of course the spatial gauge links at two neighbouring time slices are still coupled through the gauge action, however, assuming again Wilson's plaquette gauge action, the coupling is through the temporal plaquettes only.

The caveat for practical implementations of such multi-level integration schemes lies in the fact that a priori the factors in Eq. (19) are not necessarily positive. How severe the corresponding sign problem is and whether it can be ameliorated by multi-level integration schemes remains to be seen.

For the construction of fermionic observables, such as n -point correlation functions, we follow Ref. [19] where the construction is described using the Hubbard model as an example. Source and sink operators \mathcal{S} and $\bar{\mathcal{S}}$, respectively, inserted at time t simply remove or add indices from/to the index sets at time t . The operators \mathcal{S} and $\bar{\mathcal{S}}$ potentially change the quark number N_q and hence the canonical sector, e.g.,

$$\dots \cdot \mathcal{T}_{t-1}^{(N_q)} \cdot \mathcal{S}_{N_q \rightarrow N_q+3} \cdot \mathcal{T}_t^{(N_q+3)} \cdot \dots \cdot \mathcal{T}_{t'}^{(N_q+3)} \cdot \bar{\mathcal{S}}_{N_q+3 \rightarrow N_q} \cdot \mathcal{T}_{t'+1}^{(N_q)} \cdot \dots \quad (20)$$

Starting from, e.g., the vacuum sector with $N_q = 0$ the example in Eq. (20) corresponds to a baryon-antibaryon correlation function $C_{\text{B-}\bar{\text{B}}}(t' - t)$.

In the factorized formulation, it is natural to construct improved estimators as follows. Barring potential sign problems one can directly simulate a correlation function $C(t' - t)$, e.g., as given in Eq. (20), at large $t' - t$ and determine $C(t' + 1 - t)$ relative to $C(t' - t)$ through the expectation value

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

That is, the ground-state energy E of the correlator is essentially determined by measuring the effect of shifting $\bar{\mathcal{S}}_{N_q+3 \rightarrow N_q}$ from t' to $t' + 1$ and changing $\mathcal{T}_{t'+1}^{(N_q)} \rightarrow \mathcal{T}_{t'+1}^{(N_q+3)}$ on top of the correlation function $C(t' - t)$. If this can be implemented in practice, it would open the way to tackle signal-to-noise problems on top of using multi-level integration schemes.

The construction of improved estimators for correlation functions is closely related to the expectation value of the transfer matrix $\langle \mathcal{T}_t^{(N_q)} \rangle_{N_q}$. In principle, this object contains all the spectral information of the system in the canonical sector with N_q quarks, but in practice it is difficult to calculate since the size of the transfer matrix grows exponentially with the spatial lattice size L_s . Nevertheless, since the theory is local, one can expect that only a limited number of matrix elements are necessary to approximate the low-lying spectrum of the transfer matrix.

7. Summary and outlook

In these proceedings we have summarized the generic steps leading to a complete temporal factorization of the fermion determinant for generic fermionic gauge field theories. The steps involve 1) the dimensional reduction of the fermion determinant, 2) the projection to canonical sectors with fixed fermion numbers, and 3) the temporal factorization in terms of transfer matrices. Applying these three steps to QCD with Wilson fermions leads to the most atomic temporal factorization of the Wilson fermion determinant as given in Eq. (19). The factorization opens the way for more flexible and potentially more efficient multi-level integration schemes for QCD. The main caveat for making further progress in this direction lies in the fact that the factors in Eq. (19) are a priori not necessarily positive and hence may induce a potential sign problem. However, it is worthwhile to point out that the matrices Q^\pm are strictly positive, and hence also all their principal minors.

The generic canonical projection and subsequent factorization outlined here has already been applied successfully to a range of fermionic (gauge) field theories in various computational setups. In [16–18] the principal minors of the canonical projection have been simulated in one-dimensional supersymmetric $\text{SU}(N_c)$ Yang-Mills gauge theories. In [19] it was demonstrated in the Hubbard model that the Hubbard-Stratanovich field can be analytically integrated out from the factorized determinant such that the model can be simulated with the discrete index sets (representing the fermion occupation numbers) as the only remaining degrees of freedom. In low dimensions, the positivity of the fermion weights can then be proven for any arbitrary spin- and mass-imbalanced system. In [15] the dimensional reduction and determinant factorization has been used to derive the exact three-dimensional effective Polyakov-loop action for QCD in the heavy-dense limit. Similar to the Hubbard model, the temporal gauge fields can be integrated out analytically leading to a system which is free of the fermion sign problem at finite baryon density. In [14] we reported on the canonical projection of the Wilson fermion determinant for the case of the two-flavour Schwinger

model. The canonical fermion determinants can then be used, e.g., to calculate meson-scattering phase shifts from finite-volume effects. A summary of the results of some of these applications is currently in preparation.

The temporal factorization presented here is loosely related to other approaches to determinant factorizations. For example, it is probably straightforward to derive the factorization based on winding number expansion techniques [23] starting from the transfer matrices derived here. Furthermore, fermion bags similar to the ones introduced in [24] can be identified straightforwardly using the index sets. In our approach, the bags are confined to time slices at fixed t (with weights given by the minor matrices $M(Q_t^\pm)$), however, the bags can be naturally extended in time by connecting the index sets in time. Following this line of thought a little further immediately leads to the interpretation of the index sets as fermion occupation numbers and fermion loops as suggested in [16]. Finally, we note that the factorization of the Wilson fermion determinant presented in Sec. 5 is closely related to the construction of the transfer matrices in [25]. However, we have so far not established the exact relation between the two constructions.

Acknowledgements: I would like to thank Patrick Bühlmann for useful discussions.

References

- [1] R. Blankenbecler, D. J. Scalapino and R. L. Sugar, *Monte Carlo Calculations of Coupled Boson - Fermion Systems. I.*, *Phys. Rev. D* **24** (1981) 2278.
- [2] J. E. Hirsch, D. J. Scalapino, R. L. Sugar and R. Blankenbecler, *An Efficient Monte Carlo Procedure for Systems With Fermions*, *Phys. Rev. Lett.* **47** (1981) 1628–1631.
- [3] U. Wolff, *A REDUCTION OF THE KOGUT-SUSSKIND FERMION DETERMINANT*, *Phys. Rev. D* **30** (1984) 2236.
- [4] A. Hasenfratz and D. Toussaint, *Canonical ensembles and nonzero density quantum chromodynamics*, *Nucl. Phys. B* **371** (1992) 539–549.
- [5] D. H. Adams, *A Dimensionally reduced expression for the QCD fermion determinant at finite temperature and chemical potential*, *Phys. Rev. D* **70** (2004) 045002, [hep-th/0401132].
- [6] P. de Forcrand and U. Wenger, *New baryon matter in the lattice Gross-Neveu model*, *PoS LAT2006* (2006) 152, [hep-lat/0610117].
- [7] P. de Forcrand, M. A. Stephanov and U. Wenger, *On the phase diagram of QCD at finite isospin density*, *PoS LATTICE2007* (2007) 237, [0711.0023].
- [8] Z. Fodor, K. K. Szabo and B. C. Toth, *Hadron spectroscopy from canonical partition functions*, *JHEP* **08** (2007) 092, [0704.2382].
- [9] E. Bilgici, J. Danzer, C. Gattringer, C. B. Lang and L. Liptak, *Canonical fermion determinants in lattice QCD: Numerical evaluation and properties*, *Phys. Lett. B* **697** (2011) 85–89, [0906.1088].

- [10] K. Nagata and A. Nakamura, *Wilson Fermion Determinant in Lattice QCD*, *Phys. Rev. D* **82** (2010) 094027, [1009.2149].
- [11] A. Alexandru and U. Wenger, *QCD at non-zero density and canonical partition functions with Wilson fermions*, *Phys. Rev. D* **83** (2011) 034502, [1009.2197].
- [12] M. Giordano, K. Kapas, S. D. Katz, D. Nogradi and A. Pasztor, *New approach to lattice QCD at finite density; results for the critical end point on coarse lattices*, *JHEP* **05** (2020) 088, [2004.10800].
- [13] S. Kratochvila and P. de Forcrand, *The Canonical approach to finite density QCD*, *PoS LAT2005* (2006) 167, [hep-lat/0509143].
- [14] P. Bühlmann and U. Wenger, *Finite-volume effects and meson scattering in the 2-flavour Schwinger model*, *PoS LATTICE2021* (2022) 463, [2112.15228].
- [15] U. Wenger and P. Bühlmann, *Heavy-dense QCD at fixed baryon number without a sign problem*, *PoS LATTICE2021* (2022) 584, [2110.15021].
- [16] K. Steinhauer and U. Wenger, *Loop formulation of supersymmetric Yang-Mills quantum mechanics*, *JHEP* **12** (2014) 044, [1410.0235].
- [17] G. Bergner, H. Liu and U. Wenger, *Canonical simulations of supersymmetric SU(N) Yang-Mills quantum mechanics*, *PoS LATTICE2015* (2016) 241, [1509.01446].
- [18] G. Bergner, H. Liu and U. Wenger, *A local update algorithm for supersymmetric Yang-Mills quantum mechanics*, *PoS LATTICE2016* (2016) 395, [1612.04291].
- [19] S. Burri and U. Wenger, *The Hubbard model in the canonical formulation*, *PoS LATTICE2019* (2019) 249, [1912.09361].
- [20] M. Cè, L. Giusti and S. Schaefer, *Domain decomposition, multi-level integration and exponential noise reduction in lattice QCD*, *Phys. Rev. D* **93** (2016) 094507, [1601.04587].
- [21] M. Cè, L. Giusti and S. Schaefer, *A local factorization of the fermion determinant in lattice QCD*, *Phys. Rev. D* **95** (2017) 034503, [1609.02419].
- [22] L. Giusti and M. Saccardi, *Four-dimensional factorization of the fermion determinant in lattice QCD*, *Phys. Lett. B* **829** (2022) 137103, [2203.02247].
- [23] J. Danzer and C. Gattringer, *Winding expansion techniques for lattice QCD with chemical potential*, *Phys. Rev. D* **78** (2008) 114506, [0809.2736].
- [24] S. Chandrasekharan, *The Fermion bag approach to lattice field theories*, *Phys. Rev. D* **82** (2010) 025007, [0910.5736].
- [25] M. Luscher, *Construction of a Selfadjoint, Strictly Positive Transfer Matrix for Euclidean Lattice Gauge Theories*, *Commun. Math. Phys.* **54** (1977) 283.