Transfer matrix and nonperturbative renormalization of fermionic currents in lattice QCD

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Abstract

The functional integral representation for fermionic observables on the lattice is studied. In particular, Grassmannian representations of the scalar $\hat{J}^{(S)}$ and pseudoscalar $\hat{J}^{(P)}$ currents and pseudoscalar correlator are derived. It is also discussed the connection between the fermionic Fock space and boundary conditions along the time direction.

1 Introduction

The ‘functional’ integral approach to the quantization with lattice regularization in the euclidean space is very convenient for numerical calculations and gives a possibility for the non–perturbative study of the gauge theories [1]. However, a consistent quantization scheme needs a canonical Hamiltonian (or transfer matrix) approach to answer questions that do not obviously hold in the functional integral formulation.

The canonical quantization formalism is necessary to define boundary conditions for $U_{x\mu}$ and $\psi, \bar{\psi}$ in the integrals in eq.’s (1.5), (1.6), in particular along the forth (imaginary time) direction. It is the canonical quantization formalism which establishes the connection between correlators of currents (e.g., pseudoscalar current $\hat{J}^{(P)}$) and masses of corresponding particles.

The standard Wilson action $S_W$ with $SU(N_c)$ gauge group is [1]

$$S_W(U; \psi; \bar{\psi}) = S_G(U) + S_F(U; \psi; \bar{\psi})$$  

(1.1)

where pure gauge part $S_G$ and fermionic part $S_F$ are given by
\[ S_G = \beta \sum_{x, \mu > \nu} \left[ 1 - \frac{1}{N_c} \text{Re Tr} \left( U_{x\mu} U_{x+\mu,\nu} U_{x+\nu,\mu}^\dagger \right) \right] ; \quad \beta = \frac{2N_c}{g^2} ; \]

\[ S_F = \sum_{f=1}^{N_f} \sum_{x,y} \sum_{s,s'} \bar{\psi}_x^{f,s} \mathcal{M}_{xy}^{f,s,s'} \psi_y^{f,s'} \equiv \bar{\psi} \mathcal{M} \psi . \quad (1.2) \]

In equations above \( U_{x\mu} \in SU(N_c) \) are gauge fields, \( \psi_x, \bar{\psi}_x \) are fermionic Grassmann variables and \( g = g_0(a) \) is a bare coupling, \( a \) being a lattice spacing. Wilson’s fermionic matrix \( \mathcal{M}(U) \) (with \( N_f = 1 \)) is given by

\[ \mathcal{M}_{xy} = \delta_{xy} - 2\kappa \sum_{\mu} \left[ \delta_{y,x+\mu} P_{\mu}^{(-)} U_{x\mu} + \delta_{y,x-\mu} P_{\mu}^{(+)} U_{x-\mu,\mu}^\dagger \right] , \quad (1.3) \]

where \( \kappa \) is a hopping parameter and \( P_{\mu}^{(\pm)} = (1 \pm \gamma_{\mu})/2 \). The action \( S_W \) is invariant with respect to the local transformations

\[ U_{x\mu} \xrightarrow{\Omega} U_{x+\mu}^{\Omega} = \Omega_x U_{x\mu} \Omega_x^{\dagger} ; \quad \psi_x \xrightarrow{\Omega} \Omega_x \psi_x ; \quad \bar{\psi}_x \xrightarrow{\Omega} \bar{\psi}_x \Omega_x^{\dagger} , \quad (1.4) \]

with \( \Omega_x \in SU(N_c) \). The partition function \( Z_W \) is

\[ Z_W = \int [dU][d\psi d\bar{\psi}] \ e^{-S_W(U;\psi;\bar{\psi})} , \quad (1.5) \]

where \([dU]\) denote product \( \prod_{x\mu} dU_{x\mu} \), etc.. The average of any functional \( \mathcal{O}(U;\psi;\bar{\psi}) \) is chosen to be

\[ \langle \mathcal{O} \rangle = \frac{1}{Z_W} \int [dU][d\psi d\bar{\psi}] \ \mathcal{O}(U;\psi;\bar{\psi}) \cdot e^{-S_W(U;\psi;\bar{\psi})} . \quad (1.6) \]

Given some boundary conditions, the average \( \langle \mathcal{O} \rangle \) is (mathematically) well defined and can be calculated numerically.

In the canonical quantization approach, the connection between the transfer matrix \( \hat{V} \) and the Hamiltonian \( \hat{H} \) is given by

\[ \hat{V} = e^{-a \hat{H}} , \quad (1.7) \]

The corresponding partition function \( Z_H \) is

\[ Z_H = \text{Tr} \left( e^{-\frac{1}{T} \hat{H}} \right)_{\text{colorless}} = \text{Tr} \left( \hat{V}^{N_4} \right)_{\text{colorless}} , \quad (1.8) \]

where \( N_4 \) is the lattice size along the forth direction, \( T = 1/aN_4 = 1/L_4 \) and the trace is defined on some colorless space of states. The consistency between two definitions of the partition function given in eq. (1.3) and eq. (1.8), i.e. \( Z_W = Z_H \equiv Z \), defines the transfer matrix \( \hat{V} \) \[ \hat{V} \] \[ \hat{V} \] \[ \hat{V} \] \[ \hat{V} \]. The average of any field operator \( \hat{O} \) is

\[ \langle \hat{O} \rangle = \frac{1}{Z} \text{Tr} \left( \hat{O} \hat{V}^{N_4} \right)_{\text{colorless}} . \quad (1.9) \]
Let $|\Psi_k\rangle$ be eigenstates of the transfer matrix $\hat{V}$ with eigenvalues $\lambda_k$

$$\hat{V}|\Psi_k\rangle = \lambda_k |\Psi_k\rangle ; \quad \lambda_k = e^{-aE_k} ,$$

and $E_k$ are eigenvalues of the Hamiltonian. Then

$$\langle \hat{O} \rangle \sim \sum_{k \geq 0} e^{-\frac{1}{2}E_k} \cdot \langle \Psi_k | \hat{O} | \Psi_k \rangle .$$

Similar expressions can be written for the correlators of currents, e.g. pseudoscalar current $\hat{J}^{(P)}$, etc..

The question of interest is the connection between operators $\hat{O}$ defined as normal products of creation and annihilation operators and corresponding functionals $O(U; \psi; \overline{\psi})$ in the functional integral approach. Another problem of interest is the choice of the boundary conditions along the imaginary time direction.

This paper is dedicated to the connection between the operator (canonical quantization) formalism and functional integral approach. The transfer matrix formalism is briefly reviewed in the second section. In the third section the statistical averages of the scalar $\hat{J}^{(S)}$ and pseudoscalar $\hat{J}^{(P)}$ currents are calculated as well as pseudoscalar correlator. Boundary conditions are discussed in the forth section. The last section is reserved for conclusions.

## 2 Transfer matrix formalism

Let us give an outline of the transfer matrix formalism following the paper. The main modification is connected with the introduction of the projection operator $P_0$ (see below) which is necessary to take into account the Gauss law.

Let $c_i^\dagger (c_i)$ and $d_i^\dagger (d_i)$ be creation(annihilation) operators of fermions and antifermions, respectively, that satisfy canonical anticommutation relations:

$$[c_i, c_j^\dagger]_+ = [d_i, d_j^\dagger]_+ = \delta_{ij} ,$$

and other anticommutation relations are equal to zero. Indices $i, j$ are composite: $i = (\vec{x}; \alpha; s)$ where $\vec{x}$ is a three dimensional coordinate, $\alpha = 1, \ldots, N_c$ is a color index and $s = 1, 2$ is a spin index. Therefore, $i, j = 1, \ldots, N$ where $N = 2N_cV_3$ and $V_3$ is a three-dimensional volume.

Let $\{U_{\vec{x};k}\}$ and $\{U'_{\vec{x};k}\}$ be two configurations of the gauge fields defined on the spacelike links $l_s = (\vec{x}; k)$. The transfer matrix $\hat{V}$ is an integral operator with respect to the gauge fields. Its kernal $V(U; U')$ is an operator in the fermion Hilbert space and has the following form

$$V(U; U') = \hat{T}_F(U)V_G(U; U')\hat{T}_F(U') ;$$

In paper the gauge $U_{\vec{x};4} = 1$ has been chosen which is not possible on the finite torus.
\[
\hat{T}_F(U) = C_0 \cdot \exp\left\{d^T Q(U)c\right\} \exp\{-c^\dagger R(U)c - d^\dagger R^T(U)d\};
\]
\[
\hat{T}_F^\dagger(U) = C_0 \cdot \exp\{-c^\dagger R(U)c - d^\dagger R^T(U)d\} \exp\{c^\dagger Q(U)d^\dagger\},
\]
where \(V_G(U;U') \equiv \langle U|\hat{V}_G|U'\rangle\) corresponds to a pure gauge part [2]. Hermitian matrices \(Q, R\) are given by
\[
e^R = \frac{1}{\sqrt{2\kappa}} B^{1/2};
\]
\[
B_{\bar{x}\bar{y}} = \delta_{\bar{x}\bar{y}} - \kappa \sum_{k=1}^3 \left[ \delta_{\bar{y},\bar{x}+k} U_{xk} + \delta_{\bar{y},\bar{x}-k} U_{x-k,k}^\dagger \right],
\]
and
\[
Q_{\bar{x}\bar{y}} = \frac{i}{2} \sum_{k=1}^3 \left[ \delta_{\bar{y},\bar{x}+k} U_{xk} - \delta_{\bar{y},\bar{x}-k} U_{x-k,k}^\dagger \right] \cdot \sigma_k.
\]
\(C_0 = C_0(U;U')\) is a constant to be defined later and \(\sigma_k\) are Pauli matrices.

It is convenient to define Grassmannian coherent states
\[
|\eta\zeta\rangle = \exp\left\{ \sum_{\bar{x}} (c_{\bar{x}}^\dagger \eta_{\bar{x}} + d_{\bar{x}}^\dagger \zeta_{\bar{x}}) \right\} |0\rangle; \quad \langle\eta\zeta| = \langle0| \exp\left\{ \sum_{\bar{x}} (\eta_{\bar{x}} c_{\bar{x}} + \zeta_{\bar{x}} d_{\bar{x}}) \right\},
\]
where \(\eta_{\bar{x}}, \ldots, \zeta_{\bar{x}}\) are some Grassmannian variables (spin and color indices suppressed). It is easy to see that
\[
c_{\bar{x}}|\eta\zeta\rangle = \eta_{\bar{x}}|\eta\zeta\rangle; \quad \langle\eta\zeta|c_{\bar{x}}^\dagger = \langle\eta\zeta|\eta_{\bar{x}}\rangle,
\]
and
\[
\langle\eta\zeta|\eta'\zeta'\rangle = e^{\eta\eta' + \zeta\zeta'}, \quad \hat{1} = \int [d\eta][d\zeta][d\zeta'] e^{-\eta\eta' - \zeta\zeta'} |\eta\zeta\rangle\langle\eta\zeta|.
\]
To prove the equivalence between the transfer matrix and functional integral approaches one can start with
\[
Z_H = \text{Tr} \left( \hat{V}^{N_s}_{\text{colorless}} \right) = \text{Tr} \left( \hat{V}^{N_s}_{\text{colorless}} P_0 \right),
\]
where \(P_0\) is the projection operator on the colorless state
\[
P_0 = \int [d\Lambda] R(\Lambda); \quad [d\Lambda] = \prod_{\bar{x}} d\Lambda(\bar{x}),
\]
and \(R(\Lambda)\) is the gauge transformation operator. In particular,
\[
R(\Lambda) \chi_{\bar{x}} R^\dagger(\Lambda) = \Lambda_{\bar{x}} \chi_{\bar{x}}; \quad R(\Lambda) \chi_{\bar{x}}^\dagger R^\dagger(\Lambda) = \chi_{\bar{x}}^\dagger \Lambda_{\bar{x}},
\]
\[4\]
where
\[
\chi_{\vec{x}} = \begin{pmatrix} c_{\vec{x}} \\ d_{\vec{x}}^T \end{pmatrix} ; \quad \chi_{\vec{x}}^\dagger = \begin{pmatrix} c_{\vec{x}}^\dagger \\ d_{\vec{x}} \end{pmatrix} .
\] (2.11)

To obtain the functional integral representation of \( Z_H \) one needs to represent \( \hat{V}^{N_4} \) as a product: \( \hat{V}^{N_4} = \hat{V} \cdot \hat{V} \cdot \ldots \cdot \hat{V} \) and insert unit operators \( U \) defined in eq. (2.7). For every time slice \( x_4 \) one can introduce new Grassmannian variables \( \psi_{\vec{x}}(x_4), \bar{\psi}_{\vec{x}}(x_4) \):

\[
\psi_{\vec{x}}(x_4) = \sum_\vec{y} B_{\vec{x}\vec{y}}^{1/2} \left( \eta_\vec{y} \right) ; \quad \bar{\psi}_{\vec{x}}(x_4) = \sum_\vec{y} \left( \eta_\vec{y} - \zeta_\vec{y}^T \right) B_{\vec{y}\vec{x}}^{-1/2} .
\] (2.12)

Therefore, \( [d\eta d\eta][d\zeta d\zeta] = J^2 \cdot [d\bar{\psi} d\psi] \). The constant \( C_0 \) is chosen to cancel the Jacobian \( J \) of this transformation. Assuming that the fermionic Fock space spanned by all possible fermionic states, one obtains

\[
Z_H = \int \prod_\vec{x} d\Lambda_{\vec{x}} \prod_\vec{x} \prod_{k=1}^3 dU_{\vec{x}k}(x_4) \prod_\vec{x} d\bar{\psi}_{\vec{x}} \psi_{\vec{x}} \exp \left\{ -S_W(U; \psi; \bar{\psi}) \right\},
\] (2.13)

where \( S_W \) is the Wilson action with \( U_{\vec{x}1}(x_4) = 1 \) and boundary conditions

\[
\psi_{\vec{x}}(x_4 = N_4a) = -\psi_{\vec{x}}^\Lambda(x_4 = 0) ; \quad \bar{\psi}_{\vec{x}}(x_4 = N_4a) = -\bar{\psi}_{\vec{x}}^\Lambda(x_4 = 0) ;
\]

\[
U_{\vec{x}k}(x_4 = N_4a) = U_{\vec{x}k}^\Lambda(x_4 = 0) .
\] (2.14)

The final step is a change of variables

\[
\psi_{\vec{x}}(x_4 = N_4a) \longrightarrow \Lambda_{\vec{x}} \psi_{\vec{x}}(x_4 = N_4a) ; \quad \bar{\psi}_{\vec{x}}(x_4 = N_4a) \longrightarrow \bar{\psi}_{\vec{x}}(x_4 = N_4a) \Lambda_{\vec{x}}^\dagger ,
\] (2.15)

and similar for the gauge fields \( U \). One obtains

\[
Z_H = \int \prod_\vec{x} dU_{\vec{x}4}(x_4 = N_4a-a) \prod_\vec{x} \prod_{k=1}^3 dU_{\vec{x}k}(x_4) [d\bar{\psi} d\psi] \exp \left\{ -S_W(U; \psi; \bar{\psi}) \right\},
\] (2.16)

where

\[
U_{x4} = 1 \quad \text{at} \quad 0 \leq x_4 \leq N_4a-2a ; \quad U_{\vec{x}4}(x_4 = N_4a-a) = \Lambda_{\vec{x}} ,
\] (2.17)

and boundary conditions

\[
\psi_{\vec{x}}(x_4 = N_4a) = -\psi_{\vec{x}}(x_4 = 0) ; \quad \bar{\psi}_{\vec{x}}(x_4 = N_4a) = -\bar{\psi}_{\vec{x}}(x_4 = 0) ;
\]

\[
U_{\vec{x}k}(x_4 = N_4a) = U_{\vec{x}k}(x_4 = 0) .
\] (2.18)
Evidently, $Z_H$ coincides with $Z_W$ in the temporal gauge defined in eq. (2.17). This proves the equivalence of two approaches.

Two comments are in order.

i) In the functional integral formalism Grassmannian variables $\eta, \bar{\eta}, \zeta, \bar{\zeta}$ correspond to the operators $c, c^\dagger, d, d^\dagger$. However, new Grassmannian variables $\psi, \bar{\psi}$ are connected with $\eta, \bar{\eta}, \zeta, \bar{\zeta}$ in a rather nontrivial way given in eq. (2.12). This observation will appear to be important for the calculation of fermionic matrix elements.

ii) Antiperiodic boundary conditions in eq. (2.18) stem from the choice of the fermionic Fock space which is, in fact, a physical assumption. Another choice of the fermionic Fock space gives another boundary conditions for fermionic variables $\psi, \bar{\psi}$ along the time direction. In details this question will be discussed later.

3 Fermionic currents

3.1 Pseudoscalar current

Pseudoscalar current $\hat{J}_\xi^{(P)}$ is given by

$$\hat{J}_\xi^{(P)} = :i\gamma_4\gamma_5\chi_\xi: = i(c_\xi^\dagger d_\xi^T - d_\xi^T c_\xi) ,$$

(3.1)

where $\gamma_4, \gamma_5$ are euclidian $\gamma$-matrices

$$\gamma_k = \begin{pmatrix} 0 & i\sigma_k \\ -i\sigma_k & 0 \end{pmatrix}; \quad \gamma_4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4 .$$

(3.2)

Evidently, $\hat{J}_\xi^{P^\dagger} = \hat{J}_\xi^{P}$.

Let us derive the functional integral representation of the statistical average

$$\langle \hat{J}^{(P)} \rangle \equiv \frac{1}{Z} \text{Tr} \left( \hat{J}^{(P)} \hat{V} N_4 P_0 \right) ,$$

(3.3)

where

$$\hat{J}^{(P)} = \sum_\xi \hat{J}_\xi^{(P)} .$$

(3.4)

As well as in the previous section, we assume that the fermionic Fock space spanned by all possible fermionic states. To derive the desired expression one should proceed in a same way as outlined in the second section and use the properties of the Grassmannian coherent states in eq. (2.6). Taking into account

$$\left( \bar{\eta}_\xi T \xi - \bar{\zeta}_\xi T \bar{\eta}_\xi \right)(x_4) = \sum_{\bar{\xi}} \bar{\psi}_{\bar{\xi}}(x_4) B^{1/2}(x_4) \gamma_5 B^{1/2}(x_4) \psi_{\bar{\xi}}(x_4) ,$$

(3.5)

one obtains
\[ \langle \hat{J}^{(P)} \rangle = -\frac{i}{Z} \int [dU][d\bar{\psi}\psi] \left( \bar{\psi}B\gamma_5\psi \right)(0) \cdot \exp\{ -S_W(U; \bar{\psi}; \psi) \} , \quad (3.6) \]

where

\[ \left( \bar{\psi}B\gamma_5\psi \right)(0) = \sum_{\vec{x}y} \bar{\psi}_{\vec{x}}(x_4)B_{\vec{x}y}(x_4)\gamma_5\psi_{\vec{y}}(x_4) \bigg|_{x_4=0} , \quad (3.7) \]

and boundary conditions given in eq. (2.18).

For the zero–momentum pseudoscalar correlator

\[ \Gamma^{(P)}(\tau) = \frac{1}{Z} \Tr \left( \tilde{V}^{N_4} \hat{J}^{(P)} \tilde{V}^\tau \hat{J}^{(P)} P_0 \right) , \quad (3.8) \]

one arrives at

\[ \Gamma^{(P)}(\tau) = -\frac{1}{Z} \int [dU][d\bar{\psi}\psi] \left( \bar{\psi}B\gamma_5\psi \right)(\tau)\left( \bar{\psi}B\gamma_5\psi \right)(0) \cdot \exp\{ -S_W(U; \bar{\psi}; \psi) \} . \quad (3.9) \]

One can see that Grassmannian current \( J^{(P)} \) has no naive expression \( J_{\text{naive}}^{(P)} = \sum_{\vec{x}} \bar{\psi}_{\vec{x}}\gamma_5\psi_{\vec{x}} \). Instead, it has rather complicated expressions and depends on the gauge field \( U_{\vec{x}\mu} \). However, in the continuum limit \( a \to 0 \)

\[ J^{(P)} = \sum_{\vec{x}} \left[ \bar{\psi}_{\vec{x}}\gamma_5\psi_{\vec{x}} - \kappa \sum_{k=1}^3 \left( \bar{\psi}_{\vec{x}} U_{\vec{x}k} \gamma_5 \psi_{\vec{x}+k} + \bar{\psi}_{\vec{x}} U^\dagger_{\vec{x}-k,k} \gamma_5 \psi_{\vec{x}-k} \right) \right] (x_4) \]

\[ \to (1 - 6\kappa) \sum_{\vec{x}} \left( \bar{\psi}_{\vec{x}}\gamma_5\psi_{\vec{x}} \right)(x_4) \sim J_{\text{naive}}^{(P)} . \quad (3.10) \]

Therefore, at nonzero spacing \( a \) there is a nonperturbative renormalization of the matrix element and correlator.

### 3.2 Generalized partition function and chemical potential

Let us derive the functional integral representation for the generalized partition function \( Z(\lambda_\tau, \lambda_\bar{\tau}) \) defined as

\[ Z(\lambda_\tau, \lambda_\bar{\tau}) = \Tr \left( \tilde{V}^{N_4} \cdot \exp\{ \lambda_\tau \hat{N}_\tau + \lambda_\bar{\tau} \hat{N}_{\bar{\tau}} \} P_0 \right) , \quad (3.11) \]

where

\[ \hat{N}_\tau = \sum_{\vec{x}} c^\dagger_{\vec{x}} c_{\vec{x}} ; \quad \hat{N}_{\bar{\tau}} = \sum_{\vec{x}} d^\dagger_{\vec{x}} d_{\vec{x}} . \quad (3.12) \]

Choosing the standard fermionic Fock space and repeating calculations outlined in the second section one obtains

\[ Z(\lambda_\tau, \lambda_\bar{\tau}) = \int [dU][d\bar{\psi}\psi] \exp \{ -S_W + \delta S_\tau \} \quad (3.13) \]
with
\[
\delta S_F = 2\kappa \sum_{\vec{x}} \left[ (e^{\lambda q} - 1) \overline{\psi}_{\vec{x}}(a) P_4^{(+)} U_{\vec{x}4}^\dagger(0) \psi_{\vec{x}}(0) + (e^{\lambda q} - 1) \overline{\psi}_{\vec{x}}(0) P_4^{(-)} U_{\vec{x}4}(0) \psi_{\vec{x}}(a) \right] 
- (e^{\lambda q} + \lambda q - 1) \sum_{\vec{y}} \overline{\psi}_{\vec{y}}(0) P_4^{(-)} C_{\vec{x}\vec{y}}(0) \psi_{\vec{x}}(0),
\]
(3.14)
and
\[
C_{\vec{x}\vec{y}} = \frac{1}{2} \sum_{k=1}^3 \left[ \delta_{\vec{y},\vec{x}+k} U_{xk} - \delta_{\vec{y},\vec{x}-k} U_{x-k,k}^\dagger \right] \gamma_k.
\]
(3.15)

The partition function \( Z(\mu) \) with nonzero chemical potential \( \mu \) is given by
\[
Z(\mu) = \text{Tr} \left( \exp \left\{ -\frac{1}{T} (\hat{H} - \mu \hat{N}) \right\} P_0 \right) = \text{Tr} \left( \hat{V} \cdot \exp \left\{ \frac{\mu}{T} \hat{N} \right\} P_0 \right),
\]
(3.16)
where \( \hat{N} = \hat{N}_q - \hat{N} \). Choosing
\[
\lambda_q = -\lambda q = \frac{\mu}{T}.
\]
(3.17)
one obtains
\[
\delta S_F = 2\kappa \sum_{\vec{x}} \left[ (e^{\mu/T} - 1) \overline{\psi}_{\vec{x}}(a) P_4^{(+)} U_{\vec{x}4}^\dagger(0) \psi_{\vec{x}}(0) + (e^{-\mu/T} - 1) \overline{\psi}_{\vec{x}}(0) P_4^{(-)} U_{\vec{x}4}(0) \psi_{\vec{x}}(a) \right].
\]
(3.18)

Making the change of variables
\[
\psi_{\vec{x}}(x_4) \rightarrow \begin{cases} 
  e^{-x_4\mu} \psi_{\vec{x}}(x_4) & x_4 \neq 0 \\
  e^{-L_4\mu} \psi_{\vec{x}}(x_4) & x_4 = 0
\end{cases}
\text{ and } \quad \overline{\psi}_{\vec{x}}(x_4) \rightarrow \begin{cases} 
  e^{x_4\mu} \overline{\psi}_{\vec{x}}(x_4) & x_4 \neq 0 \\
  e^{L_4\mu} \overline{\psi}_{\vec{x}}(x_4) & x_4 = 0
\end{cases},
\]
(3.19)
one obtains the modified fermionic matrix \( \mathcal{M}(U; \mu) \)
\[
\mathcal{M}_{xy}(U; \mu) = \delta_{xy} - 2\kappa \sum_{k=1}^3 \left[ \delta_{y,x+k} P_k^{(-)} U_{x+k} + \delta_{y,x-k} P_k^{(+)} U_{x-k,k}^\dagger \right] 
- 2\kappa \left[ e^{-a\mu} \cdot \delta_{y,x+4} P_4^{(-)} U_{x} + e^{a\mu} \cdot \delta_{y,x-4} P_4^{(+)} U_{x-4}^\dagger \right].
\]
(3.20)

Evidently, \( \mathcal{M}(U; \mu) \) coincides with the fermionic matrix for the nonzero chemical potential proposed in [5].
3.3 Scalar ‘condensate’

Let us obtain the functional integral representation of the statistical average \( \langle \hat{J}^{(S)} \rangle \) of the scalar current

\[
\hat{J}^{(S)} = \sum_{\vec{x}} : \chi^\dagger_{\vec{x}}(a)\chi_{\vec{x}} : = \hat{N}_q + \hat{N}_\bar{q} .
\]  

In what follows this average will be referred to as scalar condensate. Evidently,

\[
\langle \hat{J}^{(S)} \rangle = \frac{1}{Z} \text{Tr} \left( \hat{J}^{(S)} \hat{V}^N P_0 \right) = \frac{1}{Z} \frac{d}{d\lambda} Z(\lambda) \bigg|_{\lambda = 0} ,
\]

where

\[
Z(\lambda) = \text{Tr} \left( \hat{V}^N \cdot \exp\{\lambda(\hat{N}_q + \hat{N}_\bar{q})\} P_0 \right) .
\]

From eq.’s (3.13), (3.14) one derives at

\[
\lambda_q = \lambda_{\bar{q}} \equiv \lambda
\]

\[
Z(\lambda) = \int [dU][d\psi d\bar{\psi}] \exp \{-S_W + \delta S_F\} ;
\]

\[
\delta S_F = 2\kappa \left[ \langle e^\lambda - 1 \bar{\psi}(a)P_4^{(+)}U_4^\dagger(0)\psi(0) + \langle e^\lambda - 1 \bar{\psi}(0)P_4^{(-)}U_4(0)\psi(a) \right.
\]

\[
- \left. \langle e^{2\lambda} - 1 \bar{\psi}(0)P_4^{(-)}C(0)\psi(0) \right] ,
\]

where the notations are used

\[
\bar{\psi}(a)P_4^{(+)}U_4^\dagger(0)\psi(0) = \sum_{\vec{x}} \bar{\psi}_{\vec{x}}(x_4 = a)P_4^{(+)}U_{\vec{x},4}^\dagger(x_4 = 0)\psi_{\vec{x}}(x_4 = 0) ,
\]

eetc. Finally, one obtains

\[
\langle \hat{J}^{(S)} \rangle = \frac{1}{Z} \int [dU][d\psi d\bar{\psi}] e^{-S_W(U,\psi,\bar{\psi})} \]

\[
\cdot 2\kappa \left[ \bar{\psi}(a)P_4^{(+)}U_4^\dagger(0)\psi(0) + \bar{\psi}(0)P_4^{(-)}U_4(0)\psi(a) \right. \]

\[
- \left. 2\bar{\psi}(0)P_4^{(-)}C(0)\psi(0) \right] ,
\]

Evidently, the Grassmannian current

\[
J^{(S)} = 2\kappa \left[ \bar{\psi}(a)P_4^{(+)}U_4^\dagger(0)\psi(0) + \bar{\psi}(0)P_4^{(-)}U_4(0)\psi(a) \right. \]

\[
- \left. 2\bar{\psi}(0)P_4^{(-)}C(0)\psi(0) \right] ,
\]

does not coincide with

\[
J_{\text{naive}}^{(S)} = \left( \bar{\psi}\psi \right)(0) = \sum_{\vec{x}} \bar{\psi}_{\vec{x}}(x_4 = 0)\psi_{\vec{x}}(x_4 = 0) .
\]
In the continuum limit $a \rightarrow 0$ one obtains

$$J^{(S)} \rightarrow 2\kappa \langle \bar{\psi} \psi \rangle (0) \sim J_{\text{naive}}^{(S)} .$$

As well as in the case of the pseudoscalar current, there is a nonperturbative renormalization of the scalar condensate at nonzero spacing $a$.

## 4 Fermionic Fock space and boundary conditions

One or another choice of the fermionic Fock space depends on the model (physical) assumptions. For example, QCD vacuum is expected to have an equal number of quarks and antiquarks and it puts a restriction on the choice of the states. The important observation is that boundary conditions for Grassmannian variables $\psi, \bar{\psi}$ along the imaginary time direction depend on this choice.

Till now it has been assumed that the fermionic Fock space is spanned by all possible fermionic states, i.e. states

$$|\{n_i\}; \{m_j\} \rangle = \prod_{i=1}^{N} (c_i^\dagger)^{n_i} \prod_{j=1}^{N} (d_j^\dagger)^{m_j} |0 \rangle ,$$

where $n_i, m_j = 0, 1$ and $N = 2N_c V_3$ is a maximal value of parameters $i, j$. This choice of the Fock space results in the antiperiodic boundary conditions for fermionic Grassmannian variables in eq. (2.18). Indeed, the trace of any fermionic operator $\hat{O}$ can be written as

$$\text{Tr} \chi \hat{O} = \int [d\eta d\eta'] [d\zeta d\zeta'] \exp \left\{ -\eta \eta' - \zeta \zeta' - \eta' \eta - \zeta' \zeta \right\} \cdot \langle \eta \zeta | \hat{O} | \eta' \zeta' \rangle \cdot \text{Tr} \left( |\eta \zeta \rangle \langle \eta' \zeta' | \right) .$$

Choosing Fock space as in eq. (4.1) one obtains

$$\text{Tr} \left( |\eta \zeta \rangle \langle \eta' \zeta' | \right) = \exp \left\{ -\sum_{i=1}^{N} \left( \bar{\eta}_i \eta_i + \bar{\zeta}_i \zeta_i \right) \right\} ,$$

and

$$\text{Tr} \chi \hat{O} = \int [d\eta d\eta'] [d\zeta d\zeta'] \exp \left\{ -\eta \eta' - \zeta \zeta' \right\} \cdot \langle \eta \zeta | \hat{O} | -\eta; -\zeta \rangle .$$

Minuses in $| -\eta; -\zeta \rangle$ presume antiperiodic boundary conditions for $\psi, \bar{\psi}$ along the imaginary time direction.

However, the choice of the fermionic Fock space made in eq. (4.1) is not a unique one. As an example, let us consider the zero temperatures limit $T \rightarrow 0$. In this case the main contribution to the partition function $Z$ is expected to come from the vacuum eigenstate $|\text{vac} \rangle$.
\[ Z = \langle \text{vac} | \hat{\psi}^N | \text{vac} \rangle ; \quad T \to 0 . \]  

The corresponding Fock space is supposed to have the equal number of quarks and antiquarks. Therefore, it looks reasonable to choose the fermionic Fock space spanned by the vectors

\[ | \{ n_i \}; \{ m_j \} \rangle = \prod_{i=1}^{N} (c_i^\dagger)^{n_i} \prod_{j=1}^{N} (d_j^\dagger)^{m_j} | 0 \rangle \text{ with } \sum_i n_i = \sum_i m_i . \]  

Using the following representation for the delta–symbol

\[ \delta \sum_j n_j ; \sum_j m_j = \frac{1}{N} \sum_{k=0}^{N-1} \exp \left\{ \frac{i2\pi}{N} k \sum_j (n_j - m_j) \right\} , \]  

one obtains

\[ \text{Tr} \left( | \eta \zeta \rangle \langle \eta' \zeta' | \right) = \frac{1}{N} \sum_{k=0}^{N-1} \exp \left\{ -q_k \eta \eta' - q_k^* \zeta \zeta' \right\} , \]  

where

\[ q_k = \exp \left\{ \frac{2\pi ik}{N} \right\} ; \quad k = 0; 1; \ldots; N - 1 . \]  

Therefore,

\[ \text{Tr} \hat{O} = \frac{1}{N} \sum_{k=0}^{N-1} \int [d \eta d \eta'] [d \zeta d \zeta'] \exp \{-\eta \eta - \zeta \zeta \} \cdot \langle \eta \zeta | \hat{O} | - e^{i\varphi} \eta ; -e^{-i\varphi} \zeta \rangle . \]  

In the infinite volume limit \( V_3 \to \infty \) one arrives at

\[ \text{Tr} \hat{O} = \frac{1}{2\pi} \int_0^{2\pi} d \varphi \int [d \eta d \eta'] [d \zeta d \zeta'] \exp \{-\eta \eta - \zeta \zeta \} \cdot \langle \eta \zeta | \hat{O} | - e^{i\varphi} \eta ; -e^{-i\varphi} \zeta \rangle . \]  

Finally, fermionic boundary conditions for \( \psi, \bar{\psi} \) are

\[ \psi_x(x_4 = N_4 a) = -e^{i\varphi} \psi_x(x_4 = 0) ; \quad \bar{\psi}_x(x_4 = N_4 a) = -e^{-i\varphi} \bar{\psi}_x(x_4 = 0) \]  

with integration over \( \varphi \) between 0 and \( 2\pi \). On the finite lattice the temperature is nonzero and higher excitation states can give the (artifact) contributions. Therefore, one may expect that at \( N_4 < \infty \) the boundary conditions given in eq. (4.12) could be a better choice for the zero temperature calculations (e.g., for the hadron spectroscopy study) as compared to the choice of antiperiodic boundary conditions.

Another interesting case is the finite temperature transition(s) in the Universe. The baryon asymmetry \( \Delta B \) of the Universe is small and it is expected to be zero in QCD.
Therefore, also in this case the choice of the boundary conditions given in eq. (4.12) looks preferable. It is worthwhile to note that for Polyakov loop $P$ one obtains

$$\langle P \rangle = 0,$$

(4.13)

and $\langle |P| \rangle$ is expected to be a good order parameter as in quenched QCD.

Of course, different physical problems need different assumptions about the structure of the fermionic Fock space. For example, finite temperature phase transition with nonzero baryon density ($\Delta B \neq 0$) presume another choice of the fermionic Fock space. One can expect that the phase transition temperature $T_c$ depends on the choice of this Fock space and, therefore, on the choice of the boundary conditions along the forth direction.

5 Conclusions

The first goal of this work is the study of the connection between the fermionic currents $\hat{J}$ in the canonical quantization approach and corresponding currents $J$ in the functional integral (Wilson’s) scheme. In the canonical quantization approach the fermionic currents $\hat{J}$ (e.g. pseudoscalar current, etc.) are defined as normal products of operators $\chi_{\vec{x}}, \chi_{\vec{x}}^\dagger$, while in the functional integral formalism the fermionic currents $J$ are constructed out of Grassmannian variables $\psi_{\vec{x}}, \overline{\psi}_{\vec{x}}$.

As an example, two operator currents $\hat{J}^{(S)} = :\chi_{\vec{x}}^\dagger \gamma_4 \chi_{\vec{x}}:$ and $\hat{J}^{(P)} = :\chi_{\vec{x}}^\dagger \gamma_4 \gamma_5 \chi_{\vec{x}}:$ have been considered. It appears that corresponding Grassmannian currents $J$ have no naive expressions $J_{naive}^{(S)} = \overline{\psi}_{\vec{x}} \psi_{\vec{x}}$ and $J_{naive}^{(P)} = \overline{\psi}_{\vec{x}} \gamma_5 \psi_{\vec{x}}$. Instead, Grassmannian currents have rather complicated expressions and depend on the gauge field $U_{x\mu}$. However, Grassmannian currents $J^{(S,P)}$ become $\sim J_{naive}^{(S,P)}$ in the continuum limit $a \rightarrow 0$. Therefore, at nonzero spacing there is a nonperturbative renormalization of the matrix elements and correlators.

Another scope of this paper is the study of the boundary conditions along the imaginary time direction. The important observation is that boundary conditions for $\psi, \overline{\psi}$ along the imaginary time direction depend on the choice of the fermionic Fock space, and the choice of the fermionic Fock space depends on the model (physical) assumptions. For example, in the zero temperatures limit the main contribution to the partition function $Z$ is expected to come from the vacuum eigenstate $|\text{vac}\rangle$ which is supposed to have an equal number of quarks and antiquarks (if any). In this case it is reasonable to choose the fermionic Fock space as shown in eq. (4.12) which results in the boundary conditions for $\psi, \overline{\psi}$ given in eq. (4.12). One may expect that on the finite lattice with $N_4 < \infty$ the choice in eq. (4.12) can be better one for the zero temperature calculations as compared to the case of antiperiodic boundary conditions. These boundary conditions look also reasonable for the study of the finite temperature transition on the cosmological scale with zero baryon density.

In this paper the derivation of Grassmannian currents has been performed in the theory with Wilson fermions. It could be interesting to make a comparison with another versions of lattice QCD, e.g., with staggered fermions [6, 7].
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