Currents, chemical potential and boundary conditions in lattice QCD

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A connection between the operator fermionic currents $\hat{J}$ and corresponding ‘Grassmannian’ currents $J$ in the functional integral formalism is studied. The QCD action with non–zero chemical potential $\mu$ is derived. A connection between the fermionic Fock space and boundary conditions along the forth direction is discussed.

1. Introduction

One needs transfer matrix (TM) formalism :\textsuperscript{a}) to define boundary conditions (b.c.’s) for $\psi, \psi_x$ and $U_{x\mu}$ in the functional integrals, in particular, along the forth (‘time’) direction ;\textsuperscript{b}) to establish connection between correlators of currents $\hat{J}$ and corresponding masses.

In Wilson approach the average of any functional $\langle O(U; \psi; \bar{\psi}) \rangle$ is \textsuperscript{[1]}

$$\langle O \rangle_W = \frac{1}{Z_W} \int [d\psi][d\bar{\psi}] \ O(U; \psi; \bar{\psi}) \ e^{-S_W} \tag{1}$$

where $S_W$ is the standard Wilson action and $Z_W$ is given by $\langle 1 \rangle_W = 1$. Given boundary conditions, the average $\langle O \rangle_W$ is (mathematically) well defined and can be calculated numerically.

In the TM approach the connection between the TM $\hat{V}$ and the Hamiltonian $\hat{H}$ is given by $\hat{V} = e^{-a\hat{H}}$. The average of any operator $\hat{O}$ is

$$\langle \hat{O} \rangle_H = \frac{1}{Z_H} \text{Tr} \left( \hat{V}^{N_4} \hat{O} P_0 \right) \tag{2}$$

where $P_0$ projects on colorless states and $N_4$ is a number of sites along the forth direction. The partition function $Z_H$ is given by $\langle 1 \rangle_H = 1$. The consistency between two approaches, i.e. $Z_W = Z_H \equiv Z$, defines the transfer matrix $\hat{V}$ \textsuperscript{[2] \textsuperscript{[3] \textsuperscript{[4]}}.

Here it will be shown that the connection between operators $\hat{O}$ and corresponding functionals $O(U; \psi; \bar{\psi})$ is more complicated than in the continuum.

It will be also shown a connection between b.c.’s and the choice of the fermionic Fock space (FFS). Another b.c.’s for $\psi, \bar{\psi}$ will be proposed.

2. Transfer matrix formalism

Let $c_i^\dagger(c_i)$ and $d_i^\dagger(d_i)$ be creation(annihilation) operators of quarks and antiquarks, respectively, $[c_i, c_j^\dagger]_+ = [d_i, d_j^\dagger]_+ = \delta_{ij}$ and $i,j = (\vec{x}; \alpha; s)$ where $\vec{x}$ is a 3d coordinate, $\alpha$ is a color index and $s$ is a spin index.

Let $\{U_{\vec{x},k}\}$ and $\{U_{\vec{x}';k}\}$ be two gauge field configurations defined on spacelike links. 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 \textsuperscript{[5]}:

$$V(U; U') = T_F(U) V_G(U; U') T_F(U') \ ; \tag{3}$$

$$\hat{T}_F(U) = C_0 \ e^{d^\dagger Q(U)e^{-c^\dagger R(U)e^{-d^\dagger R^*(U)}d}}$$

where $V_G(U; U')$ corresponds to a pure gauge part \textsuperscript{[6]} Matrix $Q$ is

$$Q_{\vec{x} \vec{y}} = \frac{i}{2} \sum_{k=1}^{3} \left[ \delta_{\vec{y}, \vec{x}+k} U_{x,k} - \delta_{\vec{y}, \vec{x}-k} U_{x,k}^\dagger \right] \sigma_k . \tag{4}$$

\textsuperscript{*}Talk given at \textit{LATTICE 2002} Int.Symp. (June 24–29, 2002, Cambridge, Massachusetts, USA)

\textsuperscript{†}Supported by the grant INTAS–00–00111 and RFBR grant 02–02–17308.
and $R$ is given by

$$ e^R = B^{1/2}/\sqrt{2}\kappa $$

with

$$ B_{\bar{x}\bar{y}} = \delta_{\bar{x}\bar{y}} - \kappa \sum_{k=1}^{3} \left[ \delta_{\bar{x},\bar{x}-k} U_{\bar{x}k} + \delta_{\bar{x},\bar{x}+k} U^\dagger_{\bar{x}k} \right] . \quad (5) $$

$C_0$ is a constant, $\kappa$ is a hopping parameter and $\sigma_k$ are Pauli matrices. One can prove the equality $Z_H = Z_W$ using the Grassmannian coherent state basis $|\eta\xi\rangle = e^{\xi^a\eta^d\xi^a\eta^d}|0\rangle$ and $\langle \eta\xi| = (0)e^{\bar{\xi}^d\bar{\eta}^a}$, where $\eta_{\bar{x}}(x_1), \ldots, \eta_{\bar{x}}(x_4)$ are Grassmannian variables and $\bar{\epsilon}^a = \sum_x c^a_{\bar{x}}\eta_{\bar{x}}$, etc.. The bispinors $\psi_{\bar{x}}(x_4), \bar{\psi}_{\bar{x}}(x_4)$ are given by

$$ \psi(x_4) = \bar{B} \left( \begin{array}{c} \bar{\eta} \\ \xi \end{array} \right) ; \quad \bar{\psi}(x_4) = \left( \begin{array}{c} \xi^T \\ \bar{\eta} \end{array} \right) \gamma_4 \bar{B} $$

(6)

where $\bar{B}_{\bar{x}\bar{y}} = \bar{B}^{-1/2}$. Note that on the lattice the connection between $\psi, \bar{\psi}$ and $\eta, \bar{\xi}$ is rather nontrivial.

Another important point is the choice of the fermionic Fock space. Assuming that the FFS spanned by all possible fermionic states

$$ \{|n_i\}; \{m_j\}\rangle \equiv \prod_{i=1}^N (c^a_i)^{n_i} \prod_{j=1}^N (d^\dagger_j)^{m_j} |0\rangle, $$

(7)

where $n_i, m_j = 0, 1$, one arrives at b.c.’s

$$ \psi_{\bar{x}}(L_4) = -\bar{\psi}_{\bar{x}}(0) ; \quad \bar{\psi}_{\bar{x}}(L_4) = -\bar{\psi}_{\bar{x}}(0) $$

(8)

and $U_{\bar{x}k}(L_4) = U_{\bar{x}k}(0)$ where $L_4 = N_4 a$.

3. Fermionic currents

3.1. Pseudoscalar current

Pseudoscalar current $\tilde{J}^P_{\bar{x}}$ is given by

$$ \tilde{J}^P_{\bar{x}} = :i\chi^\dagger_{\bar{x}}\gamma_4\gamma_5 \chi_{\bar{x}}: = ic^\dagger_{\bar{x}} d_{\bar{x}}^T - d_{\bar{x}}^T c^\dagger_{\bar{x}} , $$

(9)

where $\chi_{\bar{x}} = \left( \begin{array}{c} \xi \\ d_{\bar{x}}^T \end{array} \right)$, $\chi^\dagger_{\bar{x}} = \left( \begin{array}{c} c_{\bar{x}}^T \\ \bar{\xi} \end{array} \right)$ and $\gamma_\nu$ are euclidian $\gamma$-matrices. The average is

$$ \langle \tilde{J}^P \rangle_H = \frac{1}{Z} \text{Tr} \left( \hat{\psi}^N \hat{P}_0 \right) $$

(10)

where $\hat{J}^P = \sum_{\bar{x}} \tilde{J}^P_{\bar{x}}$. Following [3], let us choose the FFS as in eq. (3). One obtains [3]

$$ \langle \tilde{J}^P \rangle_H = \frac{1}{Z} \int [dU][d\bar{\psi}] J^P(\psi, \bar{\psi}, U) \cdot e^{-Sw} $$

(11)

where Grassmannian current $J^P(\psi, \bar{\psi}, U)$ is

$$ J^P = -i \sum_{\bar{x}y} \bar{\psi}_y(0) B_{\bar{x}y}(0) \gamma_5 \psi_{\bar{x}}(0) $$

(12)

and boundary conditions given in eq. (3). The zero–momentum pseudoscalar correlator is

$$ \Gamma^P(\tau) = \frac{1}{Z} \text{Tr} \left( \hat{V}^{N_4 - \tau} \hat{J}^P \hat{V}^\tau \hat{J}^P P_0 \right) $$

$$ = \frac{1}{Z} \int [dU][d\bar{\psi}\psi] J^P(\tau) J^P(0) \cdot e^{-Sw} . $$

(13)

Note that $J^P$ depends on fields $U_{x\mu}$ and does not coincide with the naive expression

$$ J^P_{\text{naive}} = (\bar{\psi}\gamma_5 \psi)(0) = \sum_{\bar{x}} \bar{\psi}_{\bar{x}}(0) \gamma_5 \psi_{\bar{x}}(0) . $$

(14)

3.2. Scalar current

Pseudoscalar current $\tilde{J}^S_{\bar{x}}$ is given by

$$ \tilde{J}^S_{\bar{x}} = :\chi^\dagger_{\bar{x}} \gamma_5 \chi_{\bar{x}}: = c^\dagger_{\bar{x}} c_{\bar{x}} + d_{\bar{x}}^T d_{\bar{x}} , $$

(15)

and $\tilde{J}^S = \sum_{\bar{x}} \tilde{J}^S_{\bar{x}}$. One obtains [3]

$$ \langle \tilde{J}^S \rangle_H = \frac{1}{Z} \text{Tr} \left( \hat{J}^S \hat{V}^{N_4} P_0 \right) $$

$$ = \frac{1}{Z} \int [dU][d\bar{\psi}\bar{\psi}] J^S(\psi, \bar{\psi}, U) \cdot e^{-Sw} $$

(16)

where Grassmannian current $J^S(\psi, \bar{\psi}, U)$ is

$$ J^S = 2\kappa \left[ \bar{\psi}(0) P_{\dagger}^{(1)} U_{\dagger}^0(0) \psi(0) + \bar{\psi}(0) P_{\dagger}^{(-)} U_{\dagger}^0(0) \psi(a) - 2\bar{\psi}(0) P_{\dagger}^{(-)} C(0) \psi(0) \right] . $$

(17)

$$ C_{\bar{x}y}(x_4) = \frac{1}{2} \sum_{k=1}^3 \left[ \delta_{\bar{x},\bar{x}+k} U_{\bar{x}k} - \delta_{\bar{x},\bar{x}-k} U^\dagger_{\bar{x}k} \right] \gamma_k $$

(18)

Evidently, $J^S$ does not coincide with

$$ J^S_{\text{naive}} = (\bar{\psi}\psi)(0) = \sum_{\bar{x}} \bar{\psi}_{\bar{x}}(0) \psi_{\bar{x}}(0) . $$

(19)
3.3. Non–zero chemical potential \( \mu \)

The partition function \( Z(\mu) \) with nonzero chemical potential \( \mu \) is given by

\[
Z(\mu) = \text{Tr} \left( \hat{V} N \epsilon \hat{N}/T P_0 \right)
\]

(20)

where \( \hat{N} = \sum_x (\epsilon^c_x c_x - \epsilon^d_x d_x) \). One obtains

\[
Z(\mu) = \int [dU][d\bar{\psi}] d\psi \exp \{-SW + \delta S_F\}
\]

(21)

where

\[
\delta S_F = 2\kappa \sum_x \left[ \left(e^{\mu/T} - 1\right) \bar{\psi}(a) P^{(+)}_4 U^+_4(0) \psi(0)
\right.

\[
\left. + \left(e^{-\mu/T} - 1\right) \bar{\psi}(0) P^{(-)}_4 U^0_4(0) \psi(0) \right]\right].
\]

(22)

Making the change of variables

\[
\psi(x_4) \rightarrow \begin{cases} 
  e^{-x_4 \mu} \psi(x_4) & x_4 \neq 0 \\
  e^{-L_4 \mu} \psi(x_4) & x_4 = 0
\end{cases}
\]

(23)

\[
\bar{\psi}(x_4) \rightarrow \begin{cases} 
  e^{x_4 \mu} \bar{\psi}(x_4) & x_4 \neq 0 \\
  e^{L_4 \mu} \bar{\psi}(x_4) & x_4 = 0
\end{cases}
\]

(24)

one obtains (see also [2]) the modified fermionic matrix \( \mathcal{M}(U; \mu) = 1 - 2\kappa D(U; \mu) \) where

\[
D_{x_4} = \sum_{k=1}^3 \left[ \delta_{y,x+k} \bar{P}^{(-)}_{4} U^{(+)}_{x+k} + \delta_{y,x-k} \bar{P}^{(+)}_{4} U^{(-)}_{x-k,k} \right]
\]

\[
+ \left[ e^{-\alpha \mu} \delta_{y,x+4} \bar{P}^{(-)}_{4} U^{(-)}_{x+4} + e^{\alpha \mu} \delta_{y,x-4} \bar{P}^{(+)}_{4} U^{(+)}_{x-4,4} \right].
\]

Evidently, \( \mathcal{M}(U; \mu) \) coincides with the fermionic matrix for the non–zero chemical potential proposed many years ago in [3].

4. Fermionic Fock space and boundary conditions

The important observation is that b.c.’s for Grassmannian variables \( \psi, \bar{\psi} \) along the forth direction depend on the choice of the FFS. This choice depends on the model (physical) assumptions.

For example, QCD vacuum is supposed to have an equal number of quarks and antiquarks, and in the zero temperature limit vacuum eigenstate is expected to give a main contribution. So, one can choose the fermionic Fock (sub)space as in eq. (8) but with additional condition

\[
\sum_i n_i = \sum_i m_i.
\]

(25)

In the infinite volume limit one obtains \( \bar{\psi} \)

\[
Z = \int 2\pi i d\varphi \int [dU] [d\bar{\psi} d\psi] e^{-S_W(U; \psi, \bar{\psi})}
\]

(26)

with fermionic boundary conditions

\[
\psi(x_4) = -e^{i \varphi} \psi(x_0); \quad \bar{\psi}(x_4) = -e^{-i \varphi} \bar{\psi}(x_0)
\]

(27)

One may expect that at \( N_c < \infty \) these b.c.’s could be a better choice for the zero temperature calculations, e.g., for the hadron spectroscopy study.

Another interesting case is a finite temperature transition in the (early) Universe with zero baryon asymmetry: \( \Delta B = 0 \). Note that in this case for Polyakov loop \( \mathcal{P} \) one obtains \( \langle \mathcal{P} \rangle_W = 0 \) and \( \langle [\mathcal{P}] \rangle_W \) is expected to be a good order parameter as in quenched QCD.

5. Summary

A connection between operator current \( \hat{J} \) and corresponding Grassmannian current \( J \) is shown to be more complicated than in continuum. In particular, \( J \)’s depend on fields \( U_{x \mu} \), i.e. \( J = J(\psi, \bar{\psi}, U) \) , and \( J \neq J_{\text{naive}} \).

The modified action with non–zero chemical potential \( \mu \neq 0 \) is derived.

A choice of the b.c.’s along the forth direction and their connection to FFS is discussed. Another b.c.’s for \( \psi, \bar{\psi} \) are proposed which could be a better choice for, e.g., the hadron spectroscopy study.

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