Series expansion of the quark determinant in the number of quark-antiquark pairs

Fabrizio Palumbo *

INFN – Laboratori Nazionali di Frascati
P. O. Box 13, I-00044 Frascati, ITALIA
Internet: palumbo@lnf.infn.it

November 30, 2021

April 15, 1997

Abstract

We propose a formulation of the QCD partition function which leads to a series expansion for the quark determinant in any given baryonic sector. The $r$-th term gives the gauge-invariant contribution of the valence quarks plus $r$ quark-antiquark pairs. This expansion can be used to investigate any baryonic sector, starting from the nucleon up to high baryonic densities.

*Work supported in part by the European Community’s Human Potential Programme under contract HPRN-CT-2000-00131 Quantum Spacetime
1 Introduction

A clearcut separation of the valence and sea quark contributions to the QCD partition function might help in the study of a number of issues, starting with the spin content of the nucleon [1] up to QCD at finite baryonic density [2]. The identification of the different contributions can be achieved by means of an expansion of the partition function with respect to the number of quark-antiquark pairs, which is the goal of the present paper. But the practical usefulness of such an expansion depends on the number of terms necessary to get the desired accuracy.

In the case of the nucleon, for instance, only a few quarks of the sea are expected to contribute significantly. If the partition function is split in the corresponding terms only a few will be important.

At first sight the case of QCD at nonzero baryon density appears quite different, because in principle one is interested in the thermodynamic limit. To investigate this limit an infinite number of terms would obviously be necessary, making our expansion of little use. In actual numerical simulations, however, the physical volumes accessible are of the order of a few $fm^3$. If we consider that normal nuclear density is about $3$ quarks/$6 fm^3$, with 6 valence quarks we are already at about twice the ordinary nuclear density, and it is reasonable to expect that the number of important quark-antiquark pairs be comparable to the number of valence quarks at least at moderate density and temperature.

To our knowledge there exists no clearcut separation of the contributions we are discussing. To tackle this problem we need, to start with, a formulation of the partition function in a given baryonic sector. One such formulation has been constructed by introducing an imaginary chemical potential in the grand canonical partition function and by projecting in a given baryonic sector by a Fourier transformation [3], [4]. But the result is not very transparent with respect to the distinction of the different contributions we are interested in.

We consider here a different form of projection, which leads to a series expansion for the quark determinant. The terms of this expansion have the desired physical meaning: The $r$-th term gives the gauge-invariant contribution of the valence quarks plus $r$ quark-antiquark pairs. In view of the above considerations, we hope that our expansion will have a reasonable convergence in present numerical simulations.

The technique we employ is fairly general, requiring only the knowledge
of the transfer matrix in the Fock space of the quarks. But in this paper we restrict ourselves to the case of Wilson fermions. We hope to be able to treat the Kogut-Susskind fermions in a future work.

We outline the derivation of the series expansion in Sec.2 focussing on the strategy, leaving out many details of the calculations for Sec.3. In Sec.4 we give our conclusions.

2 The series expansion of the quark determinant in a given baryonic sector

In this Section we outline the steps leading to a series expansion of the quark determinant in a given baryonic sector. As already said the presentation will be somewhat schematic.

The quark determinant in the absence of any condition on the baryon number is

\[ \det Q = \int [d\bar{\psi}\psi] \exp S_F. \]  

(1)

\(S_F\) is the quark action and \(Q\) the standard quark matrix which will be spelled out later. Our strategy is to write \(\det Q\) as the trace of the transfer matrix acting in the quark Fock space, impose the restriction to a given baryonic sector, and then rewrite the trace as the determinant of a modified quark matrix. The round trip is done by mapping the Grassmann algebra generated by the quark fields into the Fock space following the construction of Lüscher. But while his paper is based on the mere existence of the map, for us it is essential a concrete realization by means of coherent states.

In the transfer matrix formalism the (euclidean) time is treated differently from the spatial coordinates. So we must also treat it differently, and we assume a convention of summation over intrinsic quantum numbers and spatial sites only. These have coordinates \(n\), while the time will be denoted by \(n_0\). The link variables \(U_\mu\) are matrices in color and have spatial matrix elements

\[
(U_0(n_0))_{m,n} = U_0(m,m_0)\delta_{m,n} \\
(U_j(m_0))_{m,n} = U_j(m,m_0)\delta_{m+j,n}.
\]  

(2)

The quark field \(\psi\) carries Dirac, color and flavor indices, denoted altogether by \(\alpha\), and space-time label \(n\). We will use with the same convention Grassmann variables \(x\)'s and \(y\)'s and quark creation and annihilation operators
\[ \hat{x}^+, \hat{x}, \hat{y}^+, \hat{y}. \] But unlike Grassmann variables, the creation and annihilation operators do not carry a temporal index. Thus according to our convention

\[ \overline{\psi}(n_0)\psi(n_0) = \sum_{n,\alpha} \overline{\psi}_{n,\alpha}(n_0)\psi_{n,\alpha}(n_0) \]
\[ \hat{x}^+\hat{x} = \sum_{n,\alpha} \hat{x}_{n,\alpha}^+\hat{x}_{n,\alpha}, \]
\[ \hat{x}^+x(n_0) = \sum_{n,\alpha} \hat{x}_{n,\alpha}^+x_{n,\alpha}(n_0) \]  

(3)

and the quark action is

\[ S_F = \sum_{m_0,n_0} \overline{\psi}(m_0)Q(m_0,n_0)\psi(n_0) \]
\[ = \sum_{m,\alpha,n,\beta} \overline{\psi}_{m,\alpha}(m_0)Q_{m\alpha,n,\beta}(m_0,n_0)\psi_{n,\beta}(n_0). \]  

(4)

Let us come back to the evaluation of the quark determinant in a given baryonic sector.

The first step is to write the unconstrained determinant as a trace in Fock space

\[ det\ Q = Tr\ \hat{T}. \]  

(5)

\( \hat{T} \) is the transfer matrix whose definition will be given in the next Section. The second step is to impose the restriction to a sector with baryon number \( n_B \) by inserting in the trace the appropriate projection operator \( P_{n_B} \)

\[ det\ Q|_{n_B} = Tr\left( \hat{T}P_{n_B} \right). \]  

(6)

To rewrite the above expression as a determinant we choose coherent states \[ \text{coherent states} \]

as a basis

\[ |x> = |\exp(-x\hat{x}^+)>, \quad |y> = |\exp(-y\hat{y}^+)>. \]  

(7)

In such a basis the trace takes again the form of a Berezin integral

\[ det\ Q|_{n_B} = \int [dx^+dx\ dy^+dy] \exp(-x^+x - y^+y) <x, y|\hat{T}P_{n_B}|-x, -y > \]  

(8)

which will be expressed in terms of the determinant of a modified quark matrix.
So far for the strategy. Now we show how we get a series expansion, what is its the physical interpretation and what is the final result.

The kernel $\langle x, y | \hat{T} P_{nB} | x, -y \rangle$ has the integral form
\[
\langle x, y | \hat{T} P_{nB} | x, -y \rangle = \int [dz^+ dz dw^+ dw] \exp \left( -z^+ z - w^+ w \right) \cdot \langle x, y | \hat{T} | z, w > < z, w | P_{nB} | x, -y \rangle.
\]
(9)

The kernel $\langle x, y | \hat{T} | z, w >$ will be given in the next Section, while that of $P_{nB}$ is immediately calculated
\[
\langle z, w | P_{nB} | x, -y \rangle = \sum_{r=0}^{\infty} \left( \begin{array}{c} -1 \\ n_B \end{array} \right)^{n_B} \frac{1}{(n_B + r)!r!} \cdot \langle \hat{y}w^+ \rangle^r (\hat{x}z^+)^{n_B+r} \langle x^+ \rangle^{n_B+r} \langle y^+ \rangle^r.
\]
(10)

Since $\hat{x}^+, \hat{y}^+$ are creation operators of quarks and antiquarks respectively, we see that the r-th term of this series gives the gauge-invariant contribution of $n_B$ valence quarks plus $r$ quark-antiquark pairs.

Needless to say, for $n_B = 0$, $det Q |_{nB}$ does not reduce to the unconstrained determinant: Indeed also baryonic states are present in the unconstrained determinant, while they are not in $det Q |_{nB=0}$. In QCD at nonvanishing temperature it makes a difference whether we impose or not the condition $n_B = 0$. In view of the relatively low value of the critical temperature with respect to the nucleon mass, however, we do not expect significant effects from this restriction unless we go to exceedingly high temperatures.

Let us now proceed to derive our final result. By evaluating the vacuum expectation values appearing in the last equation we express the kernel of the projection operator in terms of Grassmann variables only
\[
\langle z, w | P_{nB} | x, -y \rangle = \sum_{r=0}^{\infty} \left( \begin{array}{c} -1 \\ n_B \end{array} \right)^{n_B} \frac{1}{(n_B + r)!r!} (z^+)^{n_B+r} (w^+)^r.
\]
(11)

To evaluate the integral of Eq.(9) we rewrite the above equation in exponential form
\[
\langle z, w | P_{nB} | x, y \rangle = \sum_{r=0}^{\infty} \left( \begin{array}{c} -1 \\ n_B \end{array} \right)^{n_B} \frac{1}{(n_B + r)!r!} \frac{\delta^{n_B+r}}{\delta j_1^{n_B+r}} \frac{\delta^r}{\delta j_2^r} \exp(-j_1 z^+ x - j_2 w^+ y) |_{j_1=j_2=0}.
\]
(12)

The integrals of Eqs.(9),(11) are gaussian and we get the constrained determinant in terms of the determinant of a modified quark matrix
\[
det Q |_{nB} = \sum_{r=0}^{\infty} \left( \begin{array}{c} -1 \\ n_B \end{array} \right)^{n_B} \frac{1}{(n_B + r)!r!} \frac{\delta^{n_B+r}}{\delta j_1^{n_B+r}} \frac{\delta^r}{\delta j_2^r} (Q + \delta Q) |_{j_1=j_2=0}.
\]
(13)
The variation of the quark matrix is

\[
\delta Q = K \left[ (j_1 - 1) (1 + \gamma_0) d(N_0 - 1) U_0 (N_0 - 1) T_0^{(+)} + \\
(j_2 - 1) (1 - \gamma_0) d(N_0) T_0^{(-)} U_0^+ (N_0 - 1) \\
+ (j_1 j_2 - 1) d(N_0) C(N_0) (1 + \gamma_0) \right],
\]

(14)

where

\[
(T(\pm))_{m,n} = \delta_{m,0\pm 1,n_0} \delta_{m,n},
\]

(15)

\[
(d(N_0))_{m,n} = \delta_{m_0,N_0} \delta_{m_0,n_0} \delta_{m,n}.
\]

\(K\) is the hopping parameter and the matrix \(C\) is given in the next Section. The particular time \(N_0\) appearing depends on the fact that we inserted the projection operator at the latest time, but the value of \(\det Q|_{n_B}\) does not depend on this arbitrary choice, as it will be clear from the derivation.

3 Evaluation of the quark matrix in a given baryonic sector

In the first part of this Section we report the definition of the transfer matrix \(\hat{T}\) and the proof of Eq. (5). These results have been derived by Lüscher, and we will follow his paper even in the notation with minor changes. Then we will evaluate the integral (9) getting the quark matrix in a given baryonic sector.

To start with we report the explicit expression of the quark matrix

\[
Q = K \left[ (1 + \gamma_0) U_0 T^{(+)} + (1 - \gamma_0) T^{(-)} U_0^+ + 2C \right] - B
\]

(16)

where

\[
C = \frac{1}{2} \sum_{j=1}^{3} \left( U_j - U_j^+ \right) \gamma_j,
\]

\[
B = \mathbb{1} - K \sum_{j=1}^{3} \left( U_j + U_j^+ \right)
\]

(17)

and the lattice spacing has been set equal to 1. The modifications necessary at nonzero temperature are obvious. The transfer matrix is defined in terms
of the operator
\[
\hat{T}_F(n_0) = \exp \left( 2K \hat{x}^+ B(n_0)^{-\frac{1}{2}} c(n_0) B(n_0)^{-\frac{1}{2}} \hat{y}^+ \right) \\
\quad \cdot \exp \left( -\hat{x}^+ M(n_0) \hat{x} - \hat{y}^+ M(n_0) \hat{y} \right)
\]
according to the ordered product
\[
\hat{T} = \mathcal{J} \prod_{n_0=-N_0}^{N_0-1} (\hat{T}_F(n_0))^+ \hat{T}_F(n_0 + 1).
\]
\(\mathcal{J}\) is the jacobian of a transformation which will be defined later, and two new matrices have made their appearance
\[
M = -\ln \left( (2K)^{\frac{1}{2}} U_0^+ B^{-\frac{1}{4}} \right) \\
c = \frac{1}{2} \sum_{j=1}^{3} \left( U_j - U_j^+ \right) i\sigma_j.
\]
The \(\sigma_j\) are the Pauli matrices and the operator \(\hat{T}_F(n_0)\) depends on the time \(n_0\) only through the dependence on it of the gauge fields.

We then use the following equations. Firstly, for arbitrary matrices \(M\) and \(N\)
\[
<x| \exp \hat{x}^+ M \hat{x} |x'> = \exp \left( x^+ \exp M x' \right),
\]
\[
<x| \exp(\hat{x}^+ M \hat{x}) \exp(\hat{x}^+ N \hat{x}) |x'> = \exp \left( x^+ e^M e^N x' \right).
\]
Secondly, if \(B = B(\hat{x}^+)\) and \(C = C(\hat{x})\) are operators which depend on \(\hat{x}^+, \hat{x}\) only, for any operator \(A\)
\[
<x|B \cdot A \cdot C |x'> = B(x^+) A(x^+, x') C(x').
\]
We thus get the kernel
\[
<x(n_0), y(n_0)|\hat{T}_F^+(n_0) \hat{T}_F(n_0 + 1)|x(n_0 + 1), y(n_0 + 1) >= \\
\quad \exp \left( 2K x(n_0) B(n_0)^{-\frac{1}{2}} c(n_0) B(n_0)^{-\frac{1}{2}} y(n_0) \right) \\
\quad \cdot \exp \left( x^+(n_0) e^{M(n_0)} e^{M(n_0+1)} x(n_0 + 1) - y^+(n_0) e^{M(n_0)} e^{M(n_0+1)} y(n_0 + 1) \right) \\
\quad \cdot \exp \left( 2Ky(n_0 + 1) B(n_0 + 1)^{-\frac{1}{2}} c(n_0 + 1) B(n_0 + 1)^{-\frac{1}{2}} x(n_0 + 1) \right).
\]
\(^1\)Lüscher assumes the gauge \(U_0 = 1\) to prove reflection positivity. We are not concerned here with this most important issue and do not fix the gauge.
Now to go back from the Grassmann variables $x'$ and $y'$ to the quark field $\psi$ we only need the relations

$$
\psi = B^{-\frac{1}{2}} \begin{pmatrix} x \\ y^+ \end{pmatrix},
$$

$$
\bar{\psi}' = (x^+ \ y) \gamma_0 B^{-\frac{1}{2}}.
$$

(25)

This transformation cancels out the jacobian $J$. Inserting the identity between the factors in Eq.(19), using the equality

$$
\bar{\psi}_n (B\psi)_n = x^+_n x_n + y^+_n y_n,
$$

(26)

and collecting all the exponents we get Eq. (5). At this point two observations are in order. The first is that the interpretation of $\hat{x}, \hat{y}$ as annihilation operators of quarks and antiquarks follows from the action of the charge conjugation on the quark field

$$
\psi' = C^{-1} \bar{\psi}
$$

$$
\bar{\psi}' = -\tilde{C} \bar{\psi},
$$

(27)

where, with Lüscher’s convention for the $\gamma$-matrices,

$$
C = \gamma_0 \gamma_2.
$$

(28)

In fact these transformations imply

$$
x' = -i \sigma_2 y
$$

$$
y' = i \sigma_2 x.
$$

(29)

The second observation is that all the above construction requires the Wilson parameter $r$ to be equal to 1.

There remains the evaluation of Eq. (4). We notice that

$$
<x, y | \tilde{T} | z, w> = \tau \exp \left( x^+ (N_0 - 1) D z + y^+ (N_0 - 1) D^* w + w E z \right),
$$

(30)

where $\tau$ does not depend on $z, w$, the star means complex conjugation and

$$
D = B^{-\frac{1}{2}} (N_0 - 1) U_0 (N_0 - 1) B^{-\frac{1}{2}} (N_0)
$$

$$
E = B^{-\frac{1}{2}} (N_0) c(N_0) B^{-\frac{1}{2}} (N_0).
$$

(31)
We must therefore perform the gaussian integral

\[
< x, y | \mathcal{T} P_{n_B} | - x, - y > = \int [dz^+ dw^+] \tau \exp \left( -z^+ z - w^+ w \right) \cdot \\
\exp \left( - j_1 z^+ x - j_2 w^+ y + x^+(N_0 - 1)Dz + y^+(N_0 - 1)D^* w + w E z \right) \\
= \tau \exp \left( - j_1 x^+(N_0 - 1)D x - j_2 y^+(N_0 - 1)D^* y + j_1 j_2 y E x \right). \quad (32)
\]

Comparing the kernel of the unconstrained transfer matrix with the above and taking into account the antiperiodic boundary conditions of the quark field in euclidean time we get the expression of Eq. (14) for \( \delta Q \).

4 Conclusion

In principle by the present approach one can perform investigations of QCD in any definite baryonic sector at any temperature, starting from baryon number zero up to high baryonic densities. In practice, apart from the lowest baryonic numbers, we are confined to small physical volumes. With the volumes actually accessible in numerical simulations, perhaps this is not a too severe limitation, and we can hope to get reasonable results with the first few terms at least for not too high density and temperature.

One could think of different applications of our expansion by further specifying or changing the projection operator. In the case of baryonic number 1, for instance, by evaluating the expectation value of the total angular momentum \( \mathcal{J} \) one can disentangle the valence and cloud contributions to the spin of the nucleon. Remaining to the lowest baryonic numbers, one might try to attack the study of the deuteron.

Another obvious field where our approach is potentially relevant is the QCD phase diagram. In particular one could investigate the various superconductive phases with spontaneous breaking of the color symmetry (see for instance \( \mathcal{E} \)) by replacing the projection operator by the trial state of the BCS theory.

Acknowledgements

It is a pleasure to thank dr. G. DiCarlo for many conversations about QCD at finite baryonic density.
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