On the loop formula for the fermionic determinant

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Introduction and a simple example

1. Introduction

We discuss here a formula which represents the lattice fermionic determinant (a large order polynomial) as an infinite product of determinants of a smaller, fixed dimension. The formula is based on the loop expansion [1] and has been used for HD-QCD [2]. It provides a systematic approximation to QCD, can however lead to missinterpretations. We rederive here this formula explcitly and discuss its features in detail.

2. A simple example

We consider

$$\det(1-k(X+Y)) = \mathrm{e}^{\mathrm{tr}\ln(1-\mathrm{k}(\mathrm{X}+\mathrm{Y}))} \quad (1)$$

The traces distinguish between the strings $XXYY$ and $XYXY$, say, but identify cyclic permutation, such as $XXYY$ and $XYYX$.
Expanding the exponent in (1) we obtain:

$$\begin{aligned}
&-\ k\mathrm{tr}(X+Y) - \frac{1}{2}k^2\mathrm{tr}(X^2+2XY+Y^2) - \ldots \\
&-\ \frac{1}{4}k^4\mathrm{tr}(X^4+4X^3Y+2(XY)^2+4X^2Y^2+\ldots) \\
&=\ -k\mathrm{tr}X - \frac{1}{2}k^2\mathrm{tr}X^2 - \frac{1}{3}k^3\mathrm{tr}X^3\ldots \\
&-\ k^2\mathrm{tr}XY - \frac{1}{2}k^4\mathrm{tr}(XY)^2\ldots \quad (2)
\end{aligned}$$

with further regrouping of the terms observing the order in which the monomials are formed in the products $(X+Y)(X+Y)(X+Y)$....
We immediately see that resumming the terms which are powers of a lowest order monomial (what we call "s-resummation") we get the ln series.

After exponentiation we thus obtain

$$\begin{aligned}
&\det(1-k(X+Y)) \quad (3)\\
&= \det(1-kX)\det(1-kY)\det(1-k^2XY)\\
&\det(1-k^3X^2Y)\det(1-k^3XY^2)\ldots
\end{aligned}$$

To simplify the further discussion we shall consider $X = x$ and $Y = y$ just complex numbers. The formula holds just as well:

$$\begin{aligned}
&\ln(1-k(x+y)) \quad (4)\\
&= \ln(1-kx)+\ln(1-ky)+\ln(1-k^2xy)\ldots\\
&1-k(x+y) = (1-kx)(1-ky)(1-k^2xy)\\
&(1-k^3x^2y)(1-k^3xy^2)\ldots \quad (5)
\end{aligned}$$

On the LHS we have a polynomial in k while on the RHS we have an infinite product. Since the derivation is formally correct it is clear that the validity of Eqs. (3),(5) implies cancelations between infinite series which calls for convergence arguments.
The LHS in Eq. (5) has just one zero at $k = \frac{1}{x+y}$ while the RHS appears to have an infinite series of zeroes at $k = 1/x, 1/y, 1/\sqrt{xy}, \ldots$. For $k < \frac{1}{|x|+|y|}$ convergence is ensured. The formula provides a series of approximations of the LHS, so, e.g. cutting after the 3-d order factor and expanding the product gives $1-kx-ky+O(k^4)$, correct to this order.
What we did was to apparently replace the one log cut on LHS in (4) by a superposition of log cuts on the RHS, correspondingly the one zero of the LHS in (5) by a superposition of zeroes on the RHS.
The RHS zeroes (cuts) are not approximations of the LHS ones, but truncations of the product give approximations to the LHS which may be very good in the convergence domain (see also sect. 8).

The loop formula

3. Definitions

Wilson's fermionic matrix in $d = 2,\ 4,\ \ \mu > 0$ is

$$\begin{aligned}
W &= \mathbb{1} - \kappa Q \quad (6)\\
&= \mathbb{1}\ -\kappa\sum_{i=1}^{d-1}\left(\Gamma_{+i}U_iT_i + \Gamma_{-i}T_i^{-1}U_i^{-1}\right)\\
&-\ \kappa\ \left(\mathrm{e}^{\mu}\Gamma_{+\mathrm{d}}\mathrm{U_d}\mathrm{T_d} + \mathrm{e}^{-\mu}\Gamma_{-\mathrm{d}}\mathrm{T_d^{-1}}\mathrm{U_d^{-1}}\right)\\
\Gamma_{\pm\nu} &= \mathbb{1}\pm\gamma_\nu,\ \gamma_\nu = \gamma_\nu^*,\ \gamma_\nu^2 = \mathbb{1},\ \mathrm{tr}\Gamma_{\pm\nu} = d \quad (7)
\end{aligned}$$

(T: lattice translations, $U_\nu \in SL(3,C)$: links).

4. The loop formula

The loop expansion and formula for Det$W$ are

$$\begin{aligned}
\mathrm{Det}\ W &= \mathrm{Det}(\mathbb{1}-\kappa Q) = \mathrm{e}^{\mathrm{Tr}\ln(\mathbb{1}-\kappa\mathrm{Q})} \quad (8)\\
&= \exp\left[-\sum_{l=1}^{\infty}\sum_{\{\mathcal{C}_l\}}\sum_{s=1}^{\infty}\frac{{g_{\mathcal{C}_l}}^s}{s}\mathrm{tr}_{\mathrm{D,C}}\left[\mathcal{L}_{\mathcal{C}_l}^s\right]\right] \quad (9)\\
&= \prod_{l=1}^{\infty}\prod_{\{\mathcal{C}_l\}}\det_{\mathrm{D,C}}\left(\mathbb{1}\ -\ g_{\mathcal{C}_l}\mathcal{L}_{\mathcal{C}_l}\right)\ , \quad (10)\\
g_{\mathcal{C}_l} &= \kappa^l\left(\epsilon\,\mathrm{e}^{\mathrm{N_d}\mu}\right)^r,\ \mathcal{L}_{\mathcal{C}_l} = \prod_{\lambda\in\mathcal{C}_l}\Gamma_\lambda U_\lambda. \quad (11)
\end{aligned}$$

Here $\mathcal{C}_l$ are *distinguishable, non-exactly-self-repeating lattice closed paths of length* l: *primary paths*. r is the net winding number of the path in the time direction (d), with p.b.c. or a.p.b.c. and $\epsilon = +1(-1)$ correspondingly (p.b.c. in the 'spatial' directions). Det, Tr imply Lattice, Dirac, and colour d.o.f., $\mathcal{L}_{\mathcal{C}_l}$ is the chain of links and Γ factors along a *primary path* (a *primary loop*), closing under the trace after s repeted coverings of the path $\mathcal{C}_l$. From Eq. (9) to (10) we use "s-resummation".

Q implies unit steps on the lattice and Q^n generates a (closed) path of length n, with the weight $\frac{1}{n}$. This can be the s repetion of a closed path of length l, called a *primary path*. The primary path can start cyclically at each of its points, has therefore multiplicity l, its repetitions do not bring different paths. (NB: Pauli's principle was used to obtain the determinant, after that it's matrix algebra.)
The colour and Dirac traces close over the whole chain of length ls, the s power of the *primary loop* $\mathcal{L}_{\mathcal{C}_l}$ Eq. (11) and do not depend on the starting point of the latter. Their contribution comes therefore with the weight $\frac{l}{ls} = \frac{1}{s}$ and the factor $g_{\mathcal{C}_l}$ coming from the links - see Eq. (9). We recognize here the logarithm series, and partial summations over s and exponentiation lead to Eq. (10).
The loops in Eq. (11) can be rewritten as

$$\begin{aligned}
\mathcal{L}_{\mathcal{C}_l} &= \Gamma_{\mathcal{C}_l}U_{\mathcal{C}_l},\ \Gamma_{\mathcal{C}_l} = \prod_{\lambda\in\mathcal{C}_l}\Gamma_\lambda,\ U_{\mathcal{C}_l} = \prod_{\lambda\in\mathcal{C}_l}U_\lambda \quad (12)\\
\mathrm{tr}_{D,C}\mathcal{L}_{\mathcal{C}_l}^s &= \mathrm{tr}_D\Gamma_{\mathcal{C}_l}^s\,\mathrm{tr}_C U_{\mathcal{C}_l}^s \equiv \mathrm{tr}\Gamma_{\mathcal{C}_l}^s\,\mathrm{tr}U_{\mathcal{C}_l}^s
\end{aligned}$$

since the Dirac and colour traces factorise. The Dirac factors $\mathrm{tr}_D\Gamma_{\mathcal{C}_l}$ can be calculated for each $\mathcal{C}_l$ geometrically [1] or numerically.
For linear and planar loops we have moreover [1]

$$\frac{2}{d}\mathrm{tr}\left[\Gamma_{\mathcal{C}_l}^s\right] = \left[\frac{2}{d}\mathrm{tr}\Gamma_{\mathcal{C}_l}\right]^s = h_{\mathcal{C}_l}^s \quad (13)$$

which simplifies the contributions of these loops to

$$\begin{aligned}
&\det_C(1-g_{\mathcal{C}_l}h_{\mathcal{C}_l}U_{\mathcal{C}_l}) \quad (14)\\
&= (1+C_{\mathcal{C}_l}^3)(1+a\mathrm{tr}U_{\mathcal{C}_l}+b\mathrm{tr}U_{\mathcal{C}_l}^{-1}), \quad (15)\\
&C_{\mathcal{C}_l} = g_{\mathcal{C}_l}h_{\mathcal{C}_l},\ a = \frac{C_{\mathcal{C}_l}}{(1+C_{\mathcal{C}_l}^3)},\ b = aC_{\mathcal{C}_l} \quad (16)
\end{aligned}$$

Applications

5. HD-QCD

For QCD at chemical potential $\mu > 0$ the coefficients of primary loops of length l with positive net winding number $r > 0$ in the time direction are

$$g_{\mathcal{C}_l} = \kappa^{l_\sigma}\epsilon^r\zeta^{rN_\tau},\ \ l_\sigma = l - r\,N_\tau \geq 0, \quad (17)$$

$d = 2, 4$, $\epsilon = \mp 1$ for (a.)p.b.c.. Since ζ and κ play different roles we order the contributions after l_σ.
HD-QCD in leading order ensues in the limit [3]

$$\kappa\to 0,\ \mu\to\infty,\ \zeta = \kappa\mathrm{e}^{\mu}:\mathrm{fixed} \quad (18)$$

(LO, $l_\sigma = 0$). It describes gluon dynamics with static quarks. Only the straight Polyakov loops P in Eq. (10) survive. With $l_\sigma = 2$ we retrieve Polyakov loops with one decoration, $\tilde{P}$, and the quarks have some mobility - [2]. The corresponding contributions are of the form Eq. (14), with

$$C_P \equiv C = \epsilon(\frac{d}{2}\zeta)^{N_\tau},\ C_{\tilde{P}} \equiv C_r = \kappa^2C^r, \quad (19)$$

respectively. The decoration can be inserted anywhere along the Polyakov loop and have any length. There are therefore $2(d-1)N_\tau(N_\tau-1)$ primary decorated loops of length $l = N_\tau + 2$. However, we can attach to each of them any number $r > 1$ of straight Polyakov loops while still at order κ^2.
We obtain to this order (up to a constant factor)

$$\begin{aligned}
\det W^{[2]} &= \prod_{\vec{x}}(1+a\mathrm{Tr}P_{\vec{x}}+b\mathrm{Tr}P_{\vec{x}}^{-1}) \quad (20)\\
&\times\prod_q\prod_{r\geq 1}(1+a_r\mathrm{Tr}\tilde{P}_{q,r,\vec{x}}+b_r\mathrm{Tr}\tilde{P}_{q,r,\vec{x}}^{-1}), \quad (21)\\
a &= C(1+C^3)^{-1},\ b = aC, \quad (22)\\
a_r &= C_r(1+C_r^3)^{-1},\ b_r = a_rC_r \quad (23)
\end{aligned}$$

Here q identifies the $2(d-1)N_\tau(N_\tau-1)$ shortest decorated Polyakov loops. The second factor in Eq. (21), however, is an infinite product. For κ small enough to ensure convergence we can cut the product, e.g. at $r = 1$, this was done in [2] for a reweighting simulation to produce the phase diagram of QCD with 3 flavours of heavy quarks.

6. Complex Langevin Simulation

The CL process associated to a partition function Z with complex measure proceeds in the manifold of a complex variable z and involves a drift force K as the logarithmic derivative of the measure

$$\begin{aligned}
dz(t) &= K(z)dt + \omega(z,t), \quad (24)\\
K(z) &= \frac{\rho'(z)}{\rho(z)},\ Z = \int dz\,\rho(z), \quad (25)
\end{aligned}$$

with ω an appropriately normalized random noise.
A CL process to simulate QCD at nonzero μ takes place in the complexified space of the link variables $U \in SL(3,C)$ [4], [5]. The drift incorporates the logarithmic derivative of the determinant and needs the evaluation of the inverse of W, Eq. (6) which is a large matrix of rang $N_\sigma^{d-1}N_\tau N_c d$.
Using the loop formula Eq. (10) we have

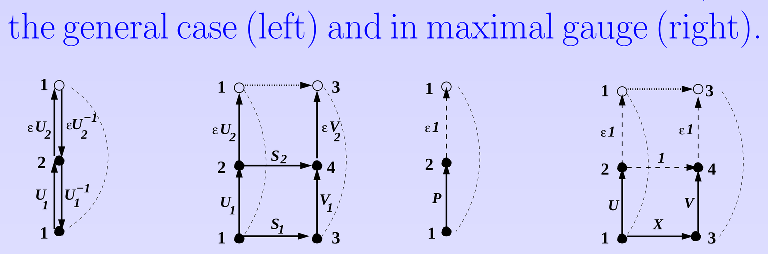
$$K(U_\lambda) = \sum_{\{\mathcal{C}_\lambda\}}\frac{\partial_{U_\lambda}\det_{\mathrm{D,C}}\left(\mathbb{1}\ -\ g_{\mathcal{C}_\lambda}\mathcal{L}_{\mathcal{C}_\lambda}\right)}{\det_{\mathrm{D,C}}\left(\mathbb{1}\ -\ g_{\mathcal{C}_\lambda}\mathcal{L}_{\mathcal{C}_\lambda}\right)} \quad (26)$$

where the sum involves all loops $\mathcal{L}_\lambda$ which contain the link U_λ and the terms are easily calculable. There are of course infinitely many such loops and they may also contain powers of U_λ, a simulation on these lines can only be achieved if we can meaningfully limit the number of terms in Eq. (26).

Examples and discussion

7. Two more simple examples

For illustration we present here 2 simple examples: a 1-d a.p.b.c. chain and a 2×2 lattice with a.p.b.c. in the one and free b.c. in the other direction, for the general case (left) and in maximal gauge (right).



The chain has only one primary loop $P = U_1U_2$ and the loop formula reproduces the exact $\det W$

$$\det W = 1 + 4\zeta^2P + 4\kappa^4\zeta^{-2}P^{-1} + 16\kappa^4 \quad (27)$$

In the second example there are 12 primary loops of length $l \leq 6$, listed here with their weights: $L_{1,2}$: U_1U_2, $V_1V_2(4\epsilon\zeta^2)$, $L_{3,4}$: $S_1V_1S_2^{-1}U_1^{-1}$, $S_2V_2S_1^{-1}U_2^{-1}(-4\kappa^4)$, $L_{5,6}$: $S_1V_1S_2^{-1}U_2$, $S_2V_2S_1^{-1}U_1(4\epsilon\zeta^2\kappa^2)$, L_{7-12} : $S_1V_1V_2V_1S_2^{-1}U_2$, $S_2V_2S_1^{-1}U_1U_2U_1$, $S_1V_1V_2V_1S_2^{-1}U_2$, $S_2V_2V_1V_2S_1^{-1}U_1$, $S_1V_1V_2S_1^{-1}U_1U_2$, $S_2V_2V_1S_2^{-1}U_2U_1(-16\zeta^4\kappa^2)$.
The loop formula keeping only the loops of length up to 6 gives to 2-nd order in κ (in maximal gauge)

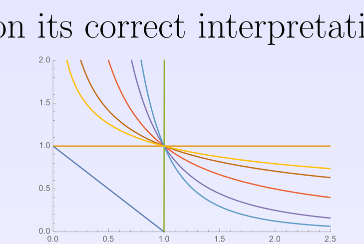
$$\begin{aligned}
&D^{[0]}(1,2) = 1 - 4\epsilon\zeta^2(U+V) + 16\zeta^4U\,V \quad (28)\\
&D^{[2]}(3-6) = -4\epsilon\kappa^2\zeta^2(V\,X+U\,X^{-1}) \quad (29)\\
&D^{[2]}(7-12) = 1 - 16\kappa^2\zeta^4(2\,U\,V + X\,V\,U\\
&+X^{-1}U\,V + X^{-1}U^2 + X\,V^2)) \quad (30)
\end{aligned}$$

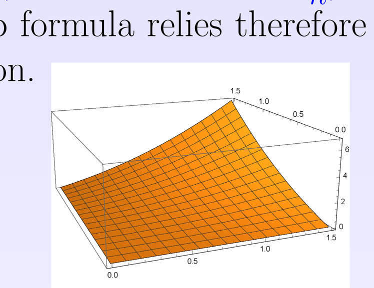
and we obtain the determinant to order κ^2 including all loops up to length 6, in complete agreement with the exact determinant to this order

$$\begin{aligned}
&\det W^{[2,6]} = 1 - 4\epsilon\zeta^2(U+V) + 16\zeta^4U\,V\\
&-4\epsilon\zeta^2\kappa^2(V\,X+U\,X^{-1}) - 32\zeta^4\kappa^2U\,V \quad (31)
\end{aligned}$$

8. Discussion

As appealing as the loop formula appears its use is involved. The formula does not allow an interpretation in terms of "linear factors" decomposition, but provides a systematic approximation in κ approaching the true determinant in the convergence domain.
Fixing the parameters we may enquire which is the variable's manifold on which the determinant vanishes. For the example in sect. 2 we find the zeroes of the factors always lying above the exact one (the diagonal of the square) with the lowest order ones (the straight lines) nearest to it. The first 3 factors give $1-\kappa(x+y)+\kappa^3xy(x+y)$, a 3-d order approximation whose error increases drastically beyond the true zero at $x+y = 1/\kappa$ (unit in the figure is $\frac{1}{\kappa}$).
The usefulness of the loop formula relies therefore on its correct interpretation.





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