Is there a third-order phase transition in quenched QCD?

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We discuss the connection between the contributions of large field configurations and the large order behavior of perturbation theory. For quenched QCD, the sensitivity of the average plaquette to a removal of large field configurations has a narrow peak near $\beta = 5.6$. Various analysis of the order 10 weak coupling series for the plaquette give robust indications for a singularity in the third derivative of the free energy (second derivative of the plaquette) with respect to $\beta$, near $\beta = 5.7$. We report results of numerical calculations. The peak in the third derivative of the free energy present on $4^4$ lattices disappears if the size of the lattice is increased isotropically up to a $10^4$ lattice. On the other hand, on $4 \times L^3$ lattices, it persists when $L$ increases. The location of the peak coincides with the onset of a non-zero average for the Polyakov loop and seems related to the finite temperature transition. We also discuss the discrepancy between the perturbative series and the numerical values of the plaquette.
1. Introduction

Perturbation theory can be a frustrating tool for field theorists. Sometimes, it provides extremely accurate answers, sometimes it is not even qualitatively correct. In recent years, our main goal has been to construct modified perturbative series which are converging and accurate. As briefly reviewed in Section 2, our approach consists in removing large field configurations in a way that preserves the closeness to the correct answer.

In the case of quenched QCD, there are several questions that are relevant for this approach and that have been addressed. How sensitive is the average plaquette $P$ to a large field cutoff [1]? How does $P$ behave when the coupling becomes negative [2]? How does $P$ differ from its weak coupling expansion [3, 4]? Are all the derivatives of $P$ with respect to $\beta$ continuous in the crossover region? The analysis [3, 5] of the weak series for $P$ up to order 10 [6] suggests an (unexpected) singularity in the second derivative of $P$, or in other words in the third derivative of the free energy.

In the following, we report our recent attempts to find this singularity. As all the technical details regarding this question have just appeared in a preprint [5], we will only summarize the main results leaving room for more discussion regarding the difference between series and the numerical values of $P$.

2. Large field configurations and perturbation theory

The reason why perturbation theory sometimes fail is well understood for scalar field theory. Large field configurations have little effect on commonly used observables but are important for the average of large powers of the field and dominate the large order behavior of perturbative series. A simple way to remove the large field configurations consists in restricting the range of integration for the scalar fields.

$$\prod_x \int_{-\phi_{\text{max}}}^{\phi_{\text{max}}} d\phi_x .$$

For a generic observable $\text{Obs.}$ in a $\lambda \phi^4$ theory, we have then

$$\text{Obs.}(\lambda) \simeq \sum_{k=0}^{K} a_k(\phi_{\text{max}}) \lambda^k$$

The method produces series which apparently converge in nontrivial cases such as the anharmonic oscillator and $D = 3$ Dyson hierarchical model [7, 8].

The modified theory with a field cutoff differs from the original theory. Fortunately, it seems possible, for a fixed order in perturbation theory, to adjust the field cutoff to an optimal value $\phi_{\text{max}}(\lambda, K)$ in order to minimize or eliminate the discrepancy with the (usually unknown) correct value of the observable in the original theory. In a simple example [5], the strong coupling can be used to calculate approximately this optimal $\phi_{\text{max}}(\lambda, K)$. This method provides an approximate treatment of the weak to strong coupling crossover and we hope it can be extended to gauge theory where this crossover [14] is a difficult problem. The calculation of the modified coefficients remains a challenge, however approximately universal features of the transition between the small and large field cutoff limits for the modified coefficients of the anharmonic oscillator [13], suggest...
the existence of simple analytical formulas to describe the field cutoff dependence of large order coefficients.

This method needs to be extended to the case of lattice gauge theories. Important differences with the scalar case need to be understood. For compact groups such as SU(N), the gauge fields are not arbitrarily large. Consequently, it is possible to define a sensible theory at negative $\beta = 2N/g^2$. However, the average plaquette tends to two different values in the two limits $g^2 \to \pm 0$ [3]. This precludes the existence of a regular perturbative series about $g^2 = 0$. A first order phase transition near $\beta = -\frac{22}{6}$, was also observed [2] for SU(3).

The impossibility of having a convergent perturbative series about $g^2 = 0$ is well understood [12] in the case of the partition function for a single plaquette which after gauge fixing to the identity on three links reads.

$$Z = \int dU e^{-\beta(1-4\text{ReTr}U)} ,$$

If we expand the group element $U = e^{igA}$ with $A = A^a T^a$ and the Haar measure in powers of $g$, we obtain a converging sum that allows us to calculate $Z$ accurately, however, the “coefficients” are $g$-dependent. This comes from the finite bounds of integration of the gauge fields that are proportional to $1/g$. If $g^2$ is small and positive, we can extend the range of integration to infinity with errors that seem controlled by $e^{-2\beta}$. By “decompactifying” the gauge fields, we have transformed a converging sum into a power series in $g$ with constant coefficients growing factorially with the order. The situation is now reminiscent to the scalar case and can be treated using this analogy.

We can introduce a gauge invariant field cutoff that is treated as a $g$-independent quantity. For a given order in $g$, one can use the strong coupling expansion to determine the optimal value of this cutoff. This provides a significant improvement in regions where neither weak or strong coupling is adequate [12].

This program can in principle be extended to LGT on $D$-dimensional lattices, however the calculation of the modified coefficients is difficult. An appropriately modified version of the stochastic method seems to be the most promising for this task. As the technology for completing this task is being developed, we will discuss several questions about the average plaquette and its perturbative expansion.

### 3. The average plaquette and its perturbative expansion in quenched QCD

We now consider a SU(3) lattice gauge theory in 4 dimensions without quarks (quenched QCD). We use the Wilson action without improvement. Our main object will be the average plaquette action denoted $P$ and can be expressed as $-\partial(\ln(Z)/6L^4)/\partial \beta$. The effect of a gauge invariant field cutoff is very small but of a different size below, near or above $\beta = 5.6$ (see Fig. 6 of Ref. [3]). This is in agreement with the idea that modifying the weight of the large field configurations affects the crossover behavior [13]. The weak coupling series for $P$ has been calculated up to order 10 in Ref. [3]:

$$P_W(1/\beta) = \sum_{m=1}^{10} b_m \beta^{-m} + \ldots .$$

The coefficients are given in table 1. The values corresponding to the series and the numerical data calculated on a $16^4$ lattice is shown in Fig. [3]. A discrepancy becomes visible below $\beta = 6$. The
situation can be improved by using Padé approximants, however, they do not show any change in curvature and often have poles near $\beta = 5.2$. For comparison, Padé approximant for the strong coupling expansion \[14\] depart visibly from the numerical values when $\beta$ becomes slightly larger than 5. In conclusion, it is not clear that by combining the two series we can get a complete information regarding the crossover behavior.

The difference between the weak coupling expansion $P_W$ and the numerical data $P$ can be further analyzed. From the example of the one-plaquette model \[12\], one could infer that by adding the tails of integration, we should make errors of order $e^{-C\beta}$, for some constant $C$. Consistently with this argument, the difference should scale as a power of the lattice spacing, namely

$$P_{\text{NonPert.}} = (P - P_W) \propto a^A \propto \left(e^{\frac{4\pi^2}{3\beta}}\right)^A. \tag{3.1}$$

A case for $A = 2$ has been made in Ref. \[3\] based on a series of order 8. Another analysis supports $A = 4$ (the canonical dimension of $F_{\mu\nu}F^{\mu\nu}$) \[4, 15\]. Fig. 3 shows fits at different orders and in different regions that support each of these possibilities. It would be interesting to study cases where long series are available and non-perturbative effects well understood in order to define a prescription to extract the power properly.

The series $P_W$ has another intriguing feature: $r_m = b_m/b_{m-1}$, the ratio of two successive coefficients seem to extraplates near 6 when $m \to \infty$ when $m$ becomes large \[4\]. This suggests a
behavior of the form

\[ P = (1/\beta_c - 1/\beta)^{-\gamma}(A_0 + A_1(\beta_c - \beta)^\lambda + \ldots), \]

as encountered in the study of the critical behavior of spin models. We have reanalyzed [5] the series using estimators [16] known as the extrapolated ratio (\( \hat{R}_m \)) and the extrapolated slope (\( \hat{S}_m \)) in order to estimate \( \beta_c \) and \( \gamma \). We found that the weak series suggests

\[ P \propto (1/5.74 - 1/\beta)^{1.08}. \tag{3.2} \]

These estimators are sensitive to small variations in the coefficients and show a remarkable stability when the volume is increased from \( 8^4 \) to \( 24^4 \). The numbers are in good agreement with the estimates of Ref. [4] with other methods. A finite radius of convergence is not expected and one does not expect any singularity between the limits where confinement and asymptotic freedom hold. It may simply be that the series is too short to draw conclusion about its asymptotic behavior. A simple example where this happens [5] is

\[ Q(\beta) = \int_0^\infty dt e^{-t[1 - t\beta_c/(\alpha\beta)]^{-\gamma}}, \tag{3.3} \]

with \( \alpha \) sufficiently large. If \( m \ll \alpha \), \( r_m \approx \beta_c(1 + (\gamma - 1)/m) \), For \( m \gg \alpha \) we have \( r_m \propto m \) and the coefficients grow factorially.

If we take Eq. (3.2) seriously, it implies that the second derivative of \( P \) diverges near \( \beta = 5.7 \). We have searched for such a singularity [5]. We have shown that the peak in the third derivative of the free energy present on \( 4^4 \) lattices disappears if the size of the lattice is increased isotropically up to a \( 10^4 \) lattice. On the other hand, on \( 4 \times L^3 \) lattices, a jump in the third derivative persists when \( L \) increases. Its location coincides with the onset of a non-zero average for the Polyakov loop and seems consequently related to the finite temperature transition. It should be noted that the possibility of a third-order phase transition has been discussed for effective theories of the Polyakov’s loop [17].

A few words about the tadpole improvement [18] for the weak series. If we consider the resummation

\[ P_W(1/\beta) = \sum_{m=1}^{K} e_m \beta_R^{-m} + O(\beta_R^{-K-1}) \tag{3.4} \]

with \( \beta_R = \beta(1 - \sum_{m=1} b_m \beta^{-m}) \), the ratios \( e_m/e_{m-1} \) stay close to -1.5 for \( m \) up to 7, but seem to start oscillating more for large \( m \).

| \( m \) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-------|---|---|---|---|---|---|---|---|---|----|
| \( b_m \) | 2 | 1.2208 | 2.9621 | 9.417 | 34.39 | 136.8 | 577.4 | 2545 | 11590 | 54160 |
| \( e_m \) | 2 | -2.779 | 3.637 | -3.961 | 4.766 | -3.881 | 6.822 | -1.771 | 17.50 | 48.08 |

**Table 1:** \( b_m \): regular coefficients; \( e_m \): tadpole improved coefficients

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