Instanton Distribution in Quenched and Full QCD

R.C. Brower, T.L. Ivanenko, J.W. Negele, K.N. Orginos

Department of Physics, Boston University, Boston, MA 02215, USA
Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA
Department of Physics, Brown University, Providence, RI 02912, USA

In order to optimize cooling as a technique to study the instanton content of the QCD vacuum, we have studied the effects of alternative algorithms, improved actions and boundary conditions on the evolution of single instantons and instanton anti-instanton pairs. Using these results, we have extracted and compared the instanton content of quenched and full QCD.

1. Introduction

Because of the significant role that instantons play in light hadron structure and the intrinsic importance of understanding topological excitations in QCD, it is of fundamental interest to understand the instanton content of the QCD vacuum and, in particular the effect of dynamical quarks on it. Although cooling is a powerful technique to preferentially filter out non-topological excitations relative to instantons, it is limited by the removal of instantons due to lattice artifacts and instanton anti-instanton annihilation. We address this problem and compare quenched and unquenched results.

2. Relaxation Algorithm

In order to extract the instanton content of the lattice configurations efficiently on a parallel computer, we used a variant of the cooling method by discretizing the relaxation equation,

\[ U^\dagger \frac{dU}{d\tau} = -\frac{\delta S}{\delta U}, \]

introducing a small step size parameter \( \epsilon \) in the “relaxation time” \( \tau \) and updating simultaneously all links on the lattice. For large values of \( \epsilon \) this algorithm is unstable but in the limit \( \epsilon \to 0 \) it converges to the solution of the relaxation equation. We have found that for SU(3) gauge field the value \( \epsilon = 0.025 \) gives fast and stable relaxation and we have used this value in our measurements. Comparing the evolution of the action for our relaxation method with \( \epsilon = 0.025 \) and the “standard” Cabbibo-Marinari cooling, we found that one cooling step is approximately equivalent to 4 relaxation steps and that the cooling histories are very similar.

3. Identifying Instantons

We used the following procedure to identify instantons in our configurations. We consider all peaks in the action and topological charge density as candidates for the instantons. With an initial value of the instanton position \( x_0 \) (peak position) and instanton size \( \rho_0 = (48/S_0)^{1/4} \) (with the normalization \( S(x) \to a^4\tilde{F}^2 \) in the continuum), we perform a least squares fit to the action and topological charge densities of a classical continuum instanton,

\[ S_0(x, x_0) = \frac{48\rho^4}{((x-x_0)^2 + \rho^2)^4}. \]

as a function of \( x_0, \rho \). If the fitting process converges and the final values for the instanton position \( x_0 \) and size \( \rho \) are within a pre-defined range close to the initial values, we record the identified instanton. If one of the conditions above is not satisfied, the candidate peak in the action or
topological charge is discarded. Full details of the algorithm will be published elsewhere. Although there is some degree of arbitrariness in selecting the parameters in the algorithm, we were able to identify around 50% of the peaks in the action distribution as instantons with the remaining peaks corresponding to small instantons or other excitations.

4. Isolated Instantons

Several effects can distort the instanton distribution during the relaxation process. The smallest instantons may disappear by falling through the mesh. The larger instantons may shrink because of interaction with periodic images or may disappear by instanton anti-instanton pairs annihilate. We separated these effects by studying the evolution of discretized semiclassical instanton configurations.

First, we have investigated the shrinking of a single isolated instanton for a variety of instanton sizes and two lattice sizes, $16^4$ and $24^4$. We studied two actions, the Wilson action and a first order improved action:

$$S_{\text{imp}} = \frac{4}{3} \text{Tr}(1 - W_1 x_1) - \frac{1}{48} \text{Tr}(1 - W_2 x_2).$$

The first order term in the Wilson action expansion in $a^2/\rho^2$ is negative and the relaxation process forces instantons to shrink. The coefficients in the improved action were chosen so that the first order term is zero and the second order term is positive. In Fig. 1, we show the evolution of a single isolated instantons with sizes $\rho = 3.0$ and $\rho = 7.0$. Notice that during relaxation the trajectories terminate for the smaller instantons as they “fall through the lattice” and that the small instantons are much more stable with the improved action. Adding more terms to the action could further stabilize instantons but the first-order improved action was simple and already sufficient for our studies. For large instantons the evolution does not depend appreciably on the choice of the action but the boundary effects are substantial. Since we are ultimately interested on the order of 100 relaxation steps at most, we conclude that with the improved action and significantly larger lattices, the artificial loss of single instantons in cooling is negligible.

![Figure 1. Evolution of isolated instantons size $\rho = 3.0$ and $\rho = 7.0$ under relaxation for Wilson and improved actions on lattice sizes $16^4$ and $24^4$.](image-url)

Next, we studied the evolution of an instanton anti-instanton (I-A) pair. Figure 2 shows the history in a typical case: instantons of initial sizes $\rho_I = \rho_A = 6.0a$ with the separation between centers $s = 12.0a$. On the small lattice $16^4$, the boundary effects are much stronger than the interaction between objects and they shrink in place before they have a chance to interact. On the larger lattices the instanton and anti-instanton attract each other and annihilate. The finite volume effects have stabilized on the largest lattices. We have also checked that the discretization effects are negligible by comparing the evolution of the two appropriately rescaled configurations. (In Fig 2, the “data” for the $36^4$ lattice are actually obtained by a re-scaling from a $24^4$ lattice.)

The “interaction” time during which the instanton move toward each other is much less then the “shrinking” time and the individual instantons in a pair do not shrink significantly. In the case of a real dynamical configurations, we expect the instantons to interact more strongly and hence we believe the conventional use of periodic boundary conditions will not introduce serious finite volume distortions.
5. QCD Results

We have studied 21 full QCD configurations for $\beta = 5.5$, 2 flavors of Wilson fermions and $\kappa = 0.160$. As measured by LANL group [3], this choice of parameters corresponds to the lattice spacing $a(f_\pi) = 0.11$fm and pion mass $m_\pi = 360$MeV. Configurations were separated by 50 HMC trajectories with average length 50 steps of size $\epsilon = 0.01$. Those configurations have the same value of $\kappa_c = 0.16145$ as quenched QCD for $\beta = 5.898$ (See Ref. [3]). To compare quenched and full QCD in roughly the same physical region, we have generated 23 quenched configurations for $\beta = 5.85$ separated by 500 heat-bath iterations. We checked also that the Creutz ratios in both cases are comparable in the range of 3-5 lattice units.

Figure 3 shows the distribution of instantons in sizes after 20, 30 and 50 relaxation steps. Since our method for identifying instantons is not reliable before 20 steps, we can not determine the early evolutions of the distribution, but after 20 the distribution certainly changes dramatically with relaxation. Given that the number of instantons are $O(200)$ or larger in a $16^4$ box, the average distance between instantons is about 4 lattice units, comparable to the average instanton size. Under these conditions the interaction between instantons is very strong and consequently the effects of I-A pair annihilation are much stronger than boundary effects.

Since the erosion of the instantons distribution with cooling should be the same for the quenched and unquenched samples, we believe the fact that the distributions shown in Fig. 3 are essentially identical within errors provides strong evidence that the physical instanton distributions are very similar in quenched and full QCD, at least at this sea quark mass, which is of the order of $m_s$.

Figure 3. The instanton distribution in quenched and full QCD. The smooth curve is the measured distribution convoluted with a Gaussian curve of width 0.01fm. Error bars are estimated by the jackknife method.

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