Neutron Electric Dipole Moment in Lattice QCD

Sinya Aoki[(a)] and Andreas Gocksch
Physics Department, Brookhaven National Laboratory, Upton, New York 11973
(Received 12 May 1989)

We present an exploratory computation of the electric dipole moment of the neutron induced by a CP-violating θ term in the QCD Lagrangian in the framework of quenched lattice QCD. We find $d_N \approx -4\times 10^{-14}\theta\, e\,\text{cm}$.

PACS numbers: 13.40.Fn, 11.30.Er, 12.38.Gc

Some time ago it was discovered[1] that a term of the form (we use a Euclidean metric throughout)

$$\mathcal{L}_\theta = \frac{+i\theta g^2}{32\pi^2} F F^* \qquad (1)$$

could be present in the QCD Lagrangian. Despite the fact that $\mathcal{L}_\theta$ can be written as a total divergence it can lead to observable effects due to the existence of the celebrated instanton solutions[2] in QCD. Certainly one of the more dramatic consequences of having such a term present would be the nonvanishing of the neutron electric dipole moment. This comes about because of the P- and T-violating nature of $\mathcal{L}_\theta$. The nonobservation of an electric dipole moment for the neutron[3] at a level of $2.6\times 10^{-25}\, e\,\text{cm}$ puts a severe bound on the magnitude of θ. Most theoretical analyses favor a value of $d_N \sim 10^{-16}\theta\, e\,\text{cm}$ leading to a vacuum angle θ smaller than $O(10^{-9})$. The smallness of θ is sometimes referred to as the strong CP problem. There are possible solutions of this problem, most notably the elegant mechanism of Peccei and Quinn.[4] Their proposal leads,[5] however, to the existence of a light weakly interacting pseudoscalar particle, the axion, which to date has not been observed.

In this Letter we report on a computation of the neutron electric dipole moment in lattice QCD. To put our calculation into a proper perspective let us quickly review a few important points about previous estimates of this quantity. The divergence of the axial current in QCD is nonvanishing and is in fact proportional to $\mathcal{L}_\theta$ in the limit of vanishing quark masses. This fact can be utilized to eliminate $\mathcal{L}_\theta$ in favor of a complex phase in the quark mass matrix by a chiral rotation. There are, in principle, infinitely many physically equivalent ways of including this phase due to the freedom of making further chiral rotations. However, one particular form of the effective CP-violating interaction at the *quark level* can be picked out on the basis of simple physical arguments. The answer[6] is $\delta\mathcal{L}_{CP} = \theta\bar{m}\bar{\psi}\gamma_5\psi$, where $\bar{m}$ is the reduced mass of the light quarks in the theory. $\delta\mathcal{L}_{CP}$ vanishes if any one-quark flavor is exactly massless. The quantity of interest is

$$\mathbf{d}_N = \langle N|\mathbf{d}_N|N\rangle = Q\int d^3x \langle N|\mathbf{x}\bar{\psi}\gamma_0\psi(\mathbf{x})|N\rangle\,, \qquad (2)$$

where Q is the quark charge matrix. Since θ is small, treating $\delta\mathcal{L}_{CP}$ as a perturbation is adequate and one is led to the computation of products of the type $\langle N|\mathbf{d}_N|X\rangle\langle X|\delta\mathcal{L}_{CP}|N\rangle$, where $|X\rangle$ is an intermediate state that can be reached from the nucleon via $\delta\mathcal{L}_{CP}$. These matrix elements are calculable in QCD—they are, however, strictly nonperturbative. Baluni[6] uses the bag model to compute these matrix elements. Crewther *et al.*[7] argue that in the limit $m_\pi \to 0$ the intermediate state $|N\pi\rangle$ dominates and then use an effective πN Lagrangian to estimate the matrix elements. Physically this means that with a light pion the neutron obtains a dipole moment by dissociating into a proton and a pion. The above approaches obviously have some shortcomings. The bag-model result is sensitive to the value of the bag radius ($d_N \sim \bar{m}R^2$ on dimensional grounds). As to the other calculation, it is not clear if the pion is light enough in the real world.

Lattice QCD offers the possibility of calculating the effect from first principles. We will discuss the uncertainties associated with this approach later on when we discuss our results. As can be seen from Eq. (1) simply including $\mathcal{L}_\theta$ in the gauge part of the action is impossible from a numerical point of view since it is imaginary. There are no efficient ways of dealing with complex actions at this time. We therefore use the following trick: We imagine having done a chiral rotation in the continuum in order to trade $\mathcal{L}_\theta$ for a phase in the mass term. We then use a lattice regularization of the resulting Dirac operator—in the present case we use Wilson fermions. Since Wilson fermions have the correct anomaly, this procedure can be shown to be valid on the lattice directly.[8] (More generally we can use the CP-violating Wilson term[8] as well as the CP-violating mass term. In this case the true θ is equal to the difference of complex phases between the two. By the chiral rotation we can set one of the phases to zero without loss of the generality.) Hence we use the following fermion action:

$$S_F = \sum_n \bar{\psi}(n)[1 - i(1-8\kappa)\tan(\theta)\gamma_5]\psi(n) - \kappa\sum_{n,\mu}\bar{\psi}(n)(1-\gamma_\mu)U_\mu(n)\psi(n+\hat{\mu}) + \bar{\psi}(n)(1+\gamma_\mu)U_\mu^\dagger(n-\hat{\mu})\psi(n-\hat{\mu})\,. \qquad (3)$$

Note that the θ-dependent term disappears for $\kappa = \frac{1}{8}$, i.e., for vanishing bare mass. (Because of the effect of the chiral-symmetry breaking by the Wilson term the pion is massive at nonzero gauge coupling even though the bare mass is set equal to zero. By setting one of the bare quark masses to zero we may solve the strong *CP* problem while producing a nonzero pion mass[9] in the continuum limit.) With this action we go on to use the quenched approximation; i.e., we compute propagators in background gauge fields that were generated using the Wilson action. Note that in the present case the meaning of "quenching" is not unique. One could also compute propagators without any θ dependence but instead include a factor of e^{iQ} in the average over the gauge configurations. Here Q is the topological charge. The two ways of quenching are obviously not equivalent. We shall return to this point later on.

To extract the electric dipole moment of hadrons we chose to use the techniques which had previously been successfully applied to the computation of baryon magnetic moments.[10] By modifying the links $U_3(n) \to e^{qEt}U_3(n)$ and $U_3(n)^\dagger \to e^{-qEt}U_3(n)^\dagger$, we introduce a constant-background electric field in the $+z$ direction. We will only be concerned with u and d quarks for which $q=\frac{2}{3}$ and $-\frac{1}{3}$, respectively. The above substitution violates the periodicity of the lattice—we keep this violation small by working with small fields. In this background electric field we measure the masses of the hadrons of interest. We measured proton, neutron, ρ, and pion propagators. From the difference between spin-up and spin-down masses in the case of the nucleon, or the difference in mass between longitudinally and transversely polarized ρ's, one can infer the value of the electric dipole moment at fixed θ. Only the former is phenomenologically interesting. If the strong interactions break *CP* the ρ will certainly have an electric dipole moment. It will, however, decay before it can ever be measured. We therefore simplified our life by computing the meson propagators only approximately. The relation $\gamma_5 M^{-1}\gamma_5 = M^{-1\dagger}$ which one uses in the computation of meson propagators is violated by terms or order $\tan(\theta)$. We dropped these terms and therefore do not quote any numbers for the ρ. (We can measure the meson propagators exactly if we perform one more inversion of the Dirac operator each time.)

One might be worried that in the presence of an electric field the usual technique of extracting masses from zero-momentum propagators might fail. A charged particle ("quark") accelerates, thereby leading to a t dependence of the "mass." However, by appealing to the analytic form of the propagator in an external electromagnetic field[11] one sees that to order linear in E only the mass is modified by the electric dipole moment interaction and thus is independent of t. As a matter of fact the other effects of E, which may produce a t dependence of the "mass," must enter through even powers of E since they respect P. Fortunately, it turns out that the effect of acceleration of individual quark to the hadrons is numerically small since the QCD force is stronger than the electric field we add. It is also noted that a term of the form $\bar\psi\gamma_5\psi$ in the action gives an elementary electric dipole moment to the quarks. This can also be seen in a nonrelativistic expansion of the Dirac Hamiltonian. As a check on our numerical methods we successfully computed the induced electric dipole moment for a free Wilson fermion. Both linearity in E of the shift in mass and the θ dependence of the dipole moment were very nicely satisfied.

Let us now discuss the QCD calculation. We used an $8^3\times 20$ lattice with periodic boundary conditions on both gauge fields and quarks. All results in this Letter were obtained by averaging over twelve gauge configurations separated by 400 pseudoheatbath sweeps. The numbers that we show below were obtained from simulations at an inverse gauge coupling of $\beta=6.0$. Since the dipole moment $\mathbf{d}$ has the dimension of a length, it is desirable to go to weak coupling so as to make the dimensionless quantity $\mathbf{d}/a$ big. This may lead to larger finite-size effects; as a matter of fact, the deconfining transition for $n_t=8$ is at $\beta=6.02\pm0.02$.[12] We have checked that on our lattices the spatial Wilson lines average to zero. The masses of the nucleons are determined by fitting the spin-up and spin-down propagators to the form $C_1e^{-mt}+C_2e^{-m(20-t)}$ with the *same* mass in the exponent. This is due to the mixing of the upper and lower spinor components in the presence of the *P*-violating term in the action. We use relativistic wave functions throughout. The electric dipole moment is computed from the formula

$$2d_zE=[m_\uparrow(E)-m_\uparrow(0)]-[m_\downarrow(E)-m_\downarrow(0)]\,. \quad (4)$$

The zero-field value of the mass shift *must* be subtracted on any finite sample of gauge configurations.[10]

On a single configuration we found, using $\kappa=0.14$, $\theta=0.4$, a linear behavior of the mass shift for E less than 0.02. For the rest of the calculation we fixed E to be 0.01. Our results are summarized in Table I. Errors were computed using the "jackknife" procedure.[13] Note that at $\theta=0$, $\kappa=0.14$ corresponds to a very heavy quark. The other value $\kappa=0.1565$ corresponds to κ_c ($\theta=0$) at $\beta=6.0$.[14] The fact that with a small *CP*-violating term in the propagator one can run at κ_c might come in handy

TABLE I. Results for electric dipole moments at $\beta=6.0$. R is the ratio of the proton-to-neutron electric dipole moment.

κ	θ	Nucleon	$2pE$	R
0.14	0.2	Neutron	−0.019 (0.018)	···
0.14	0.2	Proton	0.016 (0.020)	···
0.14	0.4	Neutron	−0.029 (0.018)	···
0.14	0.4	Proton	0.050 (0.020)	···
0.14	0.4	···	···	−1.7 (0.6)
0.1565	0.4	Neutron	−0.029 (0.010)	···
0.1565	0.4	Proton	0.028 (0.020)	···
0.1565	0.4	···	···	−1.0 (0.3)

also in ordinary spectroscopy on the lattice. An extrapolation in the CP-violating "magnetic field" might be easier than the usual extrapolations to κ_c. We are presently exploring this possibility.

To discuss our data let us concentrate on the $\theta=0.4$ data which have smaller errors. The value for the ratio of the neutron-to-proton electric dipole moment at the lower value of κ is close to what one would expect on the basis of a nonrelativistic SU(6) quark model which predicts $R=-\frac{3}{2}$. This is interesting. It suggests that the bulk of the electric dipole moment of the nucleon in our calculation is just the sum of the quark electric dipole moments. This is reasonable since we have seen before that the θ-dependent mass term induces a quark dipole moment. The sign of this contribution to the neutron electric dipole moment is *opposite* to what has been computed in Refs. 6 and 7. This is in agreement with what has been found in the cloudy bag model.[15] At the larger value of κ the ratio seems to be closer to unity.[16] Before we translate our results into physical units we must point out the following: The quenched approximation as we implement it underestimates the "pion" contribution to the dipole moment. This can easily be seen in the hopping parameter expansion. The other way of quenching that was mentioned before would leave out the quark component completely. Which contribution is more important? On the basis of previous experience with the quenched approximation we would claim that we have computed the dominant contribution. The part of the "pion" effect that we neglect is due to dynamical fermion loops and we feel that it should therefore be small. (Our quenched approximation includes some of the pion effect. This can be seen by the hopping parameter expansion. We would like to thank M. Creutz for pointing it out to us.) Apart from the quoted statistical errors there are systematic effects. We have mentioned finite-size effects before. At $\theta=0.4$ all masses (including the pion) are quite large so that the "squeezing" of the nucleons due to the finiteness of the box is probably not a big problem. We have tried to extract an electric dipole moment from twelve configurations at $\beta=5.7$ but did not succeed. This is presumably due to the fact that the lattice spacing is roughly a factor of 2 larger. The same effect can also be seen in Table I: A factor of 2 change in θ brings the signal down to the level of the error. The other source of systematic uncertainty, the quenched approximation, was discussed above. One potentially serious problem could be the oppositely directed electric field at the boundary of our lattice which exists due to the nonperiodicity of the electric potential. An indication that this field is not contaminating our results is the fact that in the nucleon propagator the "forward" and "backward" propagating contributions come in with the same mass. We have also repeated our calculation at $\kappa=0.1565$, $\theta=0.4$ on five configurations with fixed boundary conditions in the time direction. We find $2pE=-0.2$ $(+0.04)$ for the neutron (proton). Both the order of magnitude and the sign agree with the numbers quoted in the table.

Let us now estimate the neutron electric dipole moment in physical units. Since we are working at κ_c $(\theta=0)$ and we are interested in very small θ, we use the value of the lattice spacing at $\beta=6.0$ and $\kappa=\kappa_c$. From Ref. 14 we find $a\approx 0.58\ \mathrm{GeV}^{-1}$. Hence

$$d_N\sim -e\left(\frac{\theta}{0.4}\right)\frac{0.029}{2\times 0.01}a\approx -4\times 10^{-14}\theta\, e\,\mathrm{cm}.$$

with an error of $1.4\times 10^{-14}\theta\, e\,\mathrm{cm}$. Taken at face value this translates into a bound of θ smaller than $O(10^{-11})$. The magnitude of the dipole moment is about 100 times larger than most continuum estimates of this quantity. Before a serious disagreement can be claimed, the present computation, which to a large extent should be considered exploratory in character, must be repeated on larger lattices. In particular, one must go to smaller θ to check that nothing funny happens when the masses of the particles become smaller. Nevertheless, to conclude, let us speculate as to the possible origins of a disagreement. Wilson fermions give the correct axial anomaly in the continuum limit at the expense of chiral symmetry. Hence mass counterterms are generated leading to a difference between "bare" and "current" masses. The dipole moment that we compute is proportional to the bare mass which does *not* vanish in the chiral moment. The continuum calculations, on the other hand, always involve the current mass which is related to the square of the pion mass. This leads to an effective chiral suppression $\sim m_\pi^2$ relative to our calculation. All this may point to a rather subtle problem in QCD. If one wants to define the theory nonperturbatively, a regularization must be introduced. If this regularization is to treat the axial anomaly correctly, chiral symmetry must be broken (Pauli-Villars regularization is a good example).

We would like to thank W. Marciano for suggesting this calculation and for helpful discussions. We are also grateful to I-Hsiu Lee for help during the early stages of this work. Finally we recall helpful discussions with M. Creutz and G. Valencia. This manuscript has been authored under Contract No. DE-AC02-76-CH00016 with the U.S. Department of Energy. The computations reported here were performed on a CRAY-2 computer at the National Magnetic Fusion Energy Computer Center.

[a]Present address: Institute for Theoretical Physics, State University of New York at Stony Brook, Stony Brook, NY 11794.

[1]G. 't Hooft, Phys. Rev. Lett. **37**, 8 (1983).

[2]A. A. Belavin, A. M. Polyakov, A. S. Schwartz, and Yu. S. Tyupkin, Phys. Lett. **59B**, 85 (1975).

[3]N. F. Ramsey, Ann. Rev. Nucl. Part. Sci. **32**, 211 (1982).

[4]R. Peccei and H. Quinn, Phys. Rev. Lett. **38**, 1440 (1977).

[5]S. Weinberg, Phys. Rev. Lett. **40**, 223 (1978); F. Wilczek, Phys. Rev. Lett. **40**, 279 (1978).

[6]V. Baluni, Phys. Rev. D **19**, 2227 (1979).

[7]R. J. Crewther, P. Di Vecchia, G. Veneziano, and E. Witten, Phys. Lett. **88B**, 123 (1979).

[8]E. Seiler and I. O. Stamatescou, Phys. Rev. D **25**, 2177 (1982).

[9]D. Kaplan and V. Manohar, Phys. Rev. Lett. **56**, 2004 (1986); K. Choi, C. Kim, and W. Sze, Phys. Rev. Lett. **61**, 794 (1988).

[10]C. Bernard, T. Draper, K. Olynik, and M. Rushton, Phys. Rev. Lett. **49**, 1076 (1982); G. Martinelli, G. Parisi, R. Petronzio, and F. Rapuano, Phys. Lett. **116B**, 434 (1982).

[11]J. Schwinger, Phys. Rev. **82**, 664 (1951).

[12]S. Gottlieb *et al.*, Phys. Rev. Lett. **55**, 1958 (1985); N. Christ and H. Q. Deng, Phys. Rev. Lett. **60**, 1367 (1988).

[13]S. Gottlieb *et al.*, Nucl. Phys. **B263**, 704 (1986).

[14]R. D. Loft and T. DeGrand, University of Colorado Report No. COLO-HEP-178, 1988 (to be published).

[15]M. A. Morgan and G. A. Miller, Phys. Lett. B **179**, 379 (1986).

[16]S. M. Barr and W. J. Marciano, in *CP Violation,* edited by C. Jarlskog (World Scientific, Singapore, 1989).