

# The QCD axion beyond the classical level: A lattice study

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## Abstract

The axion is a hypothetical elementary particle postulated by the Peccei-Quinn theory to resolve the strong CP problem in QCD. If axions exist and have low mass, they are a candidate for dark matter as well. So far our knowledge of the properties of the QCD axion rests on semi-classical arguments and effective theory. In this Letter we perform a fully dynamical investigation of the Peccei-Quinn theory, focussing on the impact of QCD on key axion parameters, by simulating the Peccei-Quinn-Weinberg-Wilczek action on the lattice. The results of the simulation, including the axion mass and effective potential, are found to be in contradiction with current axion phenomenology and question the validity and use of the Peccei-Quinn theory.

# 1 The strong CP problem and axion

Quantum chromodynamics (QCD) describes the strong interactions remarkably well down to the smallest scales probed so far. Yet it faces a problem. The theory allows for a CP-violating term  $S_\theta$  in the action,

$$S = S_{\text{QCD}} + S_\theta, \quad (1)$$

the so-called  $\theta$  term. In Euclidean space-time  $S_\theta$  reads

$$S_\theta = i\theta Q, \quad Q = \int d^4x q(x) \in \mathbb{Z}, \quad (2)$$

where  $Q$  is the topological charge with charge density

$$q(x) = -\frac{1}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x). \quad (3)$$

In this formulation  $\theta$  enters as an arbitrary phase with values  $\theta \in [0, 2\pi)$ . The problem is that no CP violation has been observed in the strong interactions. A nonvanishing value of  $\theta$  would result in an electric dipole moment  $d_n$  of the neutron. Current experimental limits on  $|d_n|$  [1], paired with lattice calculations [2], lead to the upper bound  $|\theta| \lesssim 7.4 \times 10^{-7}$ . This anomalously small number is referred to as the strong CP problem, which is one of the most intriguing problems in particle physics.

In the Peccei-Quinn theory [3] the CP violating action  $S_\theta$  is augmented by the axion interaction

$$S_\theta \rightarrow S_\theta + S_{\text{Axion}} = \int d^4x \left[ \frac{1}{2} (\partial_\mu \phi_a(x))^2 + i \left( \theta + \frac{\phi_a(x)}{f_a} \right) q(x) \right], \quad (4)$$

where  $\phi_a(x)$  is the axion field, and  $f_a$  is the axion decay constant setting the scale at which the  $U_{\text{PQ}}(1)$  Peccei-Quinn symmetry is broken. The action is invariant under

$$\phi_a(x) \rightarrow \phi_a(x) + \delta f_a, \quad (5)$$

called shift symmetry. Replacing  $\phi_a(x)$  by  $\phi_a(x) - \theta f_a$  cancels the CP violating term in the action. A necessary condition though is that QCD allows all values of  $\phi_a/f_a$  to exist. This leaves us with the action

$$S = S_{\text{QCD}} + S_{\text{Axion}}, \quad S_{\text{Axion}} = \int d^4x \left[ \frac{1}{2} (\partial_\mu \phi_a(x))^2 + i \frac{\phi_a(x)}{f_a} q(x) \right]. \quad (6)$$

It is expected that QCD induces an effective potential for  $\phi_a$ ,  $U_{\text{eff}}(\phi_a)$ , whose minimum is at  $\phi_a = 0$ , thus restoring CP symmetry. In the following we will treat the axion field as a dynamical degree of freedom with the purpose to solve the strong CP problem, whether it arises from the spontaneously broken  $U_{\text{PQ}}(1)$  Peccei-Quinn symmetry or from a more fundamental theory, and focus on QCD interactions.

The key observable is the mass  $m_a$  of the axion. No such particle has been observed to date. In phenomenological applications of the Peccei-Quinn theory so far the axion is treated as an external source,  $\phi_a(x) \rightarrow \bar{\phi}_a = \frac{1}{V} \int d^4x \phi_a(x)$ , where  $V$  is the space-time volume. The

generating functional  $Z(\bar{\phi}_a)$  is read off from the  $\theta$  dependence of the vacuum energy density. In semi-classical approximation [4]  $Z(\bar{\phi}_a)$  may be written

$$Z(\bar{\phi}_a) = e^{-V U_{\text{eff}}(\bar{\phi}_a)}, \quad U_{\text{eff}}(\bar{\phi}_a) = \chi_t \left[ 1 - \cos\left(\frac{\bar{\phi}_a}{f_a}\right) \right] \approx \frac{1}{2} \frac{\chi_t}{f_a^2} \bar{\phi}_a^2, \quad (7)$$

where  $\chi_t$  is the topological susceptibility,  $\chi_t = \frac{\langle Q^2 \rangle}{V}$ . Expanding  $U_{\text{eff}}(\bar{\phi}_a)$  at the minimum gives the axion a mass [5],

$$m_a^2 = \frac{\partial^2}{\partial \bar{\phi}_a^2} U_{\text{eff}}(\bar{\phi}_a) \Big|_{\bar{\phi}_a=0} = \frac{\chi_t}{f_a^2}. \quad (8)$$

If correct, the axion can be made practically invisible by appropriate choice of  $f_a$ . Interactions at the quantum level between the axion and quarks and gluons are neglected in this approach. It needs to be seen whether (6) averages successfully over the physics at shorter length scales to be used as an effective action.

In Euclidean quantum field theory the mass  $m_a$  is given by the large time  $t$  decay of the axion correlation function,

$$\int d^3 \vec{x} \langle \phi_a(\vec{x}, t) \pi(0) \rangle \simeq A e^{-m_a t}, \quad (9)$$

where  $\pi$  is a pseudoscalar source. The value of the underlying path integral does not change under the shift of integration variables  $\phi_a(x) \rightarrow \phi_a(x) + \epsilon_a(x)$ , nor does the shift alter the integration measure. Expanding the path integral to first order in  $\epsilon_a(x)$ , we obtain the equation of motion

$$\frac{\partial^2}{\partial t^2} \int d^3 \vec{x} \langle \phi_a(\vec{x}, t) \pi(0) \rangle = \frac{i}{f_a} \int d^3 \vec{x} \langle q(\vec{x}, t) \pi(0) \rangle, \quad t > 0. \quad (10)$$

A special feature of the action  $S_{\text{Axion}}$  is that the coupling  $1/f_a$  can be factored out by the change of variable  $\phi_a(x) \rightarrow \tilde{\phi}_a(x)/f_a$ ,

$$S_{\text{Axion}} \equiv \frac{1}{f_a^2} \tilde{S}_{\text{Axion}}, \quad \tilde{S}_{\text{Axion}} = \int d^4 x \left[ \frac{1}{2} (\partial_\mu \tilde{\phi}_a(x))^2 + i \tilde{\phi}_a(x) q(x) \right], \quad (11)$$

similar to the gauge coupling  $\beta = 6/g^2$  in the pure Yang-Mills theory. In terms of the new variable  $\tilde{\phi}_a(x)$  the equation of motion (10) reads

$$\frac{\partial^2}{\partial t^2} \int d^3 \vec{x} \langle \tilde{\phi}_a(\vec{x}, t) \pi(0) \rangle = i \int d^3 \vec{x} \langle q(\vec{x}, t) \pi(0) \rangle, \quad t > 0. \quad (12)$$

The axion mass  $m_a$  thus depends on  $1/f_a$  only through the topological charge density  $q(x)$ . This suggests that  $m_a$  stays finite at small couplings  $1/f_a$ , with values in between the pion and the  $\eta'$  mass, in contrast to common lore (8).

The interaction between the axion and QCD is mediated by a dimension-five operator. As a result, fluctuations of both axion and gluons are expected to lead to significant renormalization effects, which demands a nonperturbative, ‘bottom-up’ [6] evaluation of the theory. In this Letter we shall subject the Peccei-Quinn theory to a first quantitative test on the lattice.

## 2 The QCD axion on the lattice

At finite lattice spacing  $a$  the topological charge gets multiplicatively and additively renormalized [7]. As a result, the periodicity of the action  $S_\theta$  in  $\theta$  is lost. To circumvent this problem, we may chirally rotate the  $\theta$  term into the fermionic part of the action, making use of the axial anomaly [8]. Assuming three quark flavors, substituting  $\phi_a/f_a$  for  $\theta$  in the chirally rotated action [2] and replacing the integral by a sum over  $x$ , we arrive at

$$S_{\text{Axion}} = a^4 \sum_x \left[ \frac{1}{2} (\partial_\mu \phi_a(x))^2 - i \hat{m} \sin\left(\frac{\phi_a(x)}{3f_a}\right) (\bar{u}(x)\gamma_5 u(x) + \bar{d}(x)\gamma_5 d(x) + \bar{s}(x)\gamma_5 s(x)) \right], \quad (13)$$

where  $\hat{m}^{-1} = (m_u^{-1} + m_d^{-1} + m_s^{-1})/3$ , plus a factor  $\cos(\phi_a(x)/3f_a)$  in the mass term of  $S_{\text{QCD}}$ . It makes a difference whether  $\theta$  is replaced before or after the chiral rotation. The difference is a term involving the derivative of  $\phi_a(x)$ , which is not expected to change the static properties of the theory. Our choice (13) corresponds to the Peccei-Quinn-Weinberg-Wilczek parameterization of the action [9].

The action (13) is complex and still does not lend itself to numerical simulation on the Euclidean lattice. It has been shown that the finite volume partition function of the action (1) is analytic in  $\theta$  for  $|\theta| < \pi$  [10]. Assuming that this holds for the action (6) and parameter  $1/f_a$  as well, and that  $\phi_a/f_a$  remains small, we may resort to simulations at imaginary values of  $f_a$ ,

$$f_a^* = i f_a, \quad (14)$$

being followed by analytic continuation to physical numbers. The range of  $\phi_a$  values can be estimated from the effective theory with Gaussian distributed topological charge  $Q$  [11], described by the partition function

$$Z = \int dQ d\bar{\phi}_a e^{-[Q^2/2\langle Q^2 \rangle + i(\bar{\phi}_a/f_a)Q + (m_a^2/2)\bar{\phi}_a^2 V]}, \quad (15)$$

including a hypothetical mass term. This predicts

$$\langle \bar{\phi}_a^2 \rangle \propto \frac{1}{(\chi_t/f_a^2 + m_a^2)V}, \quad (16)$$

stating that  $\phi_a$  can be kept small for sufficiently large volumes. On that assumption contributions of higher order in  $\phi_a$  can be neglected in (13), and in  $S_{\text{QCD}}$  as well. This leaves us with the action

$$S_{\text{Axion}} = a^4 \sum_x \left[ \frac{1}{2} (\partial_\mu \phi_a(x))^2 + \frac{\hat{m} \phi_a(x)}{3 f_a^*} (\bar{u}(x)\gamma_5 u(x) + \bar{d}(x)\gamma_5 d(x) + \bar{s}(x)\gamma_5 s(x)) \right]. \quad (17)$$

The action satisfies the shift symmetry (5) with  $f_a \rightarrow f_a + O(\phi_a) = f_a + O(1/\sqrt{V})$ .

We use the SLiNC action with Symanzik improved glue for QCD [12]. The kinetic part of the axion action is discretized as

$$\frac{1}{2} a^4 \sum_{x,\mu} \left( \frac{\phi_a(x + a\hat{\mu}) - \phi_a(x)}{a} \right)^2 = a^2 \sum_{x,\mu} (\phi_a(x) - \phi_a(x + a\hat{\mu}))^2. \quad (18)$$

#	$a^{-4}V$	$\kappa_0$	$1/af_a^*$
1	$12^3 \times 24$	0.12090	0.01825
2	$12^3 \times 24$	0.12090	0.1825
3	$12^3 \times 24$	0.12090	1.825
4	$24^3 \times 48$	0.12090	0.01825
5	$24^3 \times 48$	0.12090	0.1825
6	$24^3 \times 48$	0.12090	1.825

Table 1: The parameters of our present QCD + axion ensembles, generated at the SU(3) flavor symmetric point, for a wide range of bare axion decay constants,  $2\kappa_0\bar{m}/3af_a^* = 0.00001$ ,  $0.0001$  and  $0.001$ , respectively. The parameters match previous pure QCD runs [14].

We assume periodic boundary conditions for axion and gauge fields. The gauge fields are updated using BQCD [13]. As a first step, we focus on the SU(3) flavor symmetric point, defined by  $m_u = m_d = m_s \equiv \bar{m}$  and  $m_\pi^2 = m_K^2 = (m_\pi^{2\text{phys}} + 2m_K^{2\text{phys}})/3 \approx [420 \text{ MeV}]^2$ , where we can hope for a strong signal, and which is a good starting point for simulations at smaller pion masses [14]. The simulations are done at  $\beta = 10/g^2 = 5.50$  and restricted to  $12^3 \times 24$  and  $24^3 \times 48$  lattices, owing to the high computational cost. The quark mass  $\bar{m}$  is given by  $a\bar{m} = 1/2\kappa_0 - 1/2\kappa_{0,c}$ , where the hopping parameter  $\kappa_0$  marks the symmetric point, and  $\kappa_{0,c}$  is the critical hopping parameter at which  $\bar{m}$  vanishes on the SU(3) symmetric line. To a good approximation  $\kappa_0 = 0.12090$ , while  $\kappa_{0,c} = 0.12110$ . We use the center of mass of the nucleon octet to set the scale. This results in the lattice spacing  $a = 0.074(2) \text{ fm}$  [15]. The simulation parameters are listed in Table 1. Each ensemble consist of  $O(10,000)$  configurations on the  $12^3 \times 24$  lattice and  $O(1,500)$  configurations on the  $24^3 \times 48$  lattice.

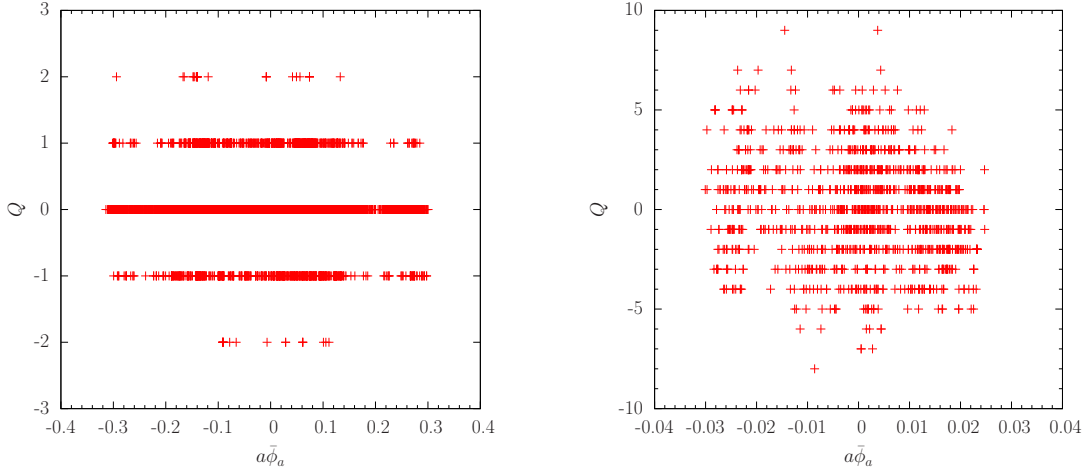


Figure 1: The topological charge  $Q$  plotted against the average axion field  $\bar{\phi}_a = \frac{a^4}{V} \sum_x \phi_a(x)$ , configuration by configuration, for  $1/af_a^* = 0.01825$  on the  $12^3 \times 24$  (left) and  $24^3 \times 48$  lattice (right).

A unique feature of SLiNC fermions is that the sum of Wilson term, mass ( $am_B = 1/2\kappa_{0,c} - 4$ ) and nonperturbative clover term are invariant under chiral rotations [16], thus preserving all chiral symmetries.

We monitor the topological charge  $Q$  and average axion field  $\bar{\phi}_a$ . In Fig. 1 we show  $Q$  as a function of  $\bar{\phi}_a$  on the  $12^3 \times 24$  and the  $24^3 \times 48$  lattice for  $1/af_a^* = 0.01825$ . The most striking feature is that the range of  $\bar{\phi}_a$  values shrinks drastically with increasing volume. We find  $\langle a^2 \bar{\phi}_a^2 \rangle \approx 0.14 \times 10^{-1}$  on the  $12^3 \times 24$  lattice and  $\langle a^2 \bar{\phi}_a^2 \rangle \approx 0.18 \times 10^{-3}$  on the  $24^3 \times 48$  lattice. No significant dependence of  $\langle \bar{\phi}_a^2 \rangle$  on  $f_a$  was observed. Equation (16) proves roughly correct if the difference in axion masses (Table 2) is taken into account. To solve the strong CP problem, the axion field would have to cover the full range  $0 < |\phi_a/f_a| < \pi$ . Beyond that, we do not see any correlation between the global charge  $Q$  and axion field  $\bar{\phi}_a$ . A measure for linear relationship is Pearson's correlation coefficient

$$r = \frac{\sum_1^N \bar{\phi}_a Q - \sum_1^N \bar{\phi}_a \sum_1^N Q/N}{\sqrt{\left(\sum_1^N \bar{\phi}_a^2 - \left(\sum_1^N \bar{\phi}_a\right)^2/N\right)\left(\sum_1^N Q^2 - \left(\sum_1^N Q\right)^2/N\right)}}, \quad (19)$$

where  $\sum_1^N$  is the ensemble sum. On the  $24^3 \times 48$  lattice we obtain  $r = 0.016(113)$ ,  $0.016(113)$  and  $-0.108(80)$  for  $1/af_a = 1.825$ ,  $0.1825$  and  $0.01825$ , respectively, which is compatible with zero. Cross correlations with  $-5 \leq \Delta at \leq 5$  give similar results. In contrast, the effective theory (15) predicts  $r = -1$ . The topological susceptibility  $\chi_t$  will be given later (Table 2) together with the axion masses. From the probability distribution of  $\bar{\phi}_a$ ,  $P(\bar{\phi}_a)$ , we obtain the effective potential [17, 18]

$$V U_{\text{eff}}(\bar{\phi}_a) = -\log P(\bar{\phi}_a) + c. \quad (20)$$

Both  $P(\bar{\phi}_a)$  and  $U_{\text{eff}}(\bar{\phi}_a)$  are shown in Fig. 2. From the potential we can read off the axion mass,  $m_a^2 = \partial^2 U_{\text{eff}}(\bar{\phi}_a)/\partial \bar{\phi}_a^2|_{\bar{\phi}_a=0}$ . A first estimate gives  $m_a = 190 - 250$  MeV on the  $24^3 \times 48$  lattice for  $1/af_a^* = 0.01825$ .

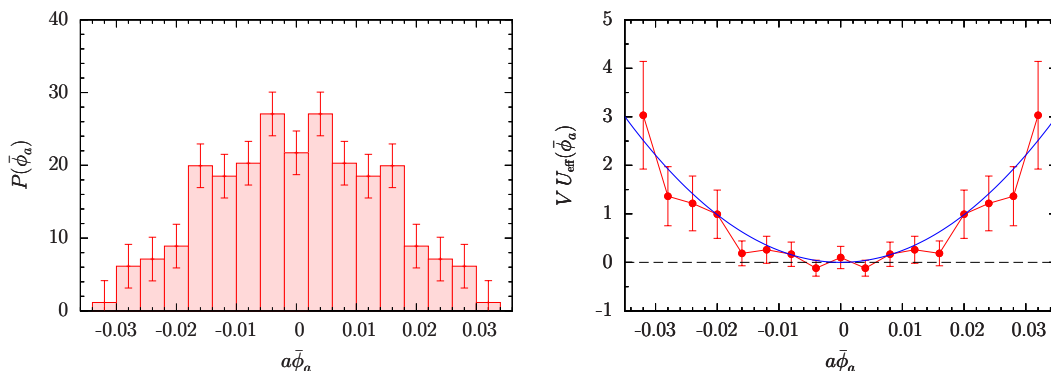


Figure 2: The probability distribution  $P(\bar{\phi}_a)$  (left) and the effective potential  $U_{\text{eff}}(\bar{\phi}_a)$  (right) on the  $24^3 \times 48$  lattice for  $1/af_a^* = 0.01825$ . The potential is normalized to zero at  $\bar{\phi}_a = 0$ . The solid curve represents the effective potential (22) suggested by the lattice,  $U_{\text{eff}}(\bar{\phi}_a) = (m_a^2/2) \bar{\phi}_a^2$ , with  $m_a = 230$  MeV.

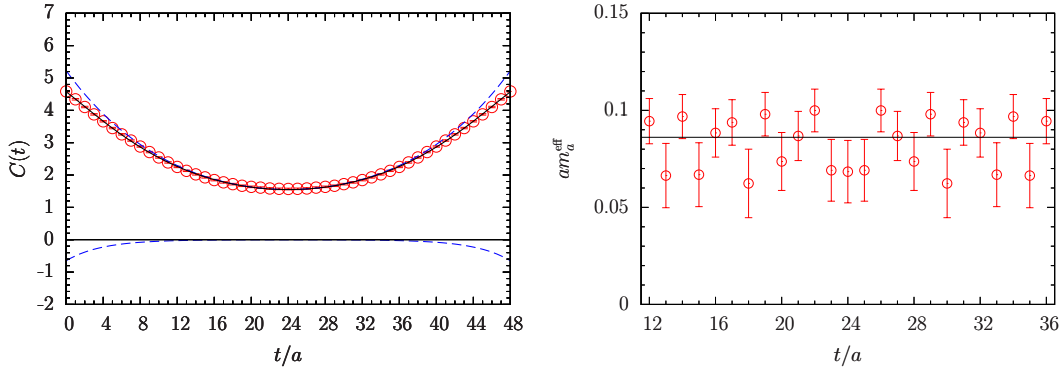


Figure 3: The correlation function  $C(t)$  (left) and the effective axion mass  $m_a^{\text{eff}}$  (right) on the  $24^3 \times 48$  lattice for  $1/f_a^* = 0.01825$ . The upper dashed curve shows the contribution of the axion,  $A \cosh(-m_a \tau)$ , while the lower dashed curve shows the contribution of the  $\eta'$ ,  $B \cosh(-m_{\eta'} \tau)$ .

### 3 The axion mass

To obtain the axion mass  $m_a$  we compute the correlation function  $C(t) = a^2 \sum_{\vec{x}} \langle \phi_a(\vec{x}, t) \phi_a(0) \rangle$ , which we parameterize as

$$C(t) = A \cosh(-m_a \tau) + B \cosh(-m_{\eta'} \tau), \quad \tau = t - T/2, \quad (21)$$

where  $T$  is the temporal extent of the lattice. We expect the operator  $\phi_a$  to couple to the axion and a flavor singlet quark-antiquark bound state, which we call the  $\eta'$  meson. In Fig. 3 we show the correlation function  $C(t)$  on the  $24^3 \times 48$  lattice together with a two-exponential fit, eq. (21), to the data. The individual contributions of the axion and the  $\eta'$  are shown by the dashed curves. As expected, the contribution of the  $\eta'$  is negative. Also shown is the effective mass of the axion,  $am_a^{\text{eff}} = \text{arcosh}[(C(t-a) + C(t+a))/2C(t)]$ , which dominates the correlation function at times  $8 \ll t/a \ll 40$ . In Table 2 we collect our results for the axion and  $\eta'$  masses. The  $12^3 \times 24$  lattice was too small to determine the  $\eta'$  mass reliably. The axion mass shows significant finite size corrections. We expect the corrections to be dominated by discretization effects of the axion propagator [19]. This suggests  $m_a(L) = m_a(1 - c/L^2)$ , where  $L$  is the spatial extent of the lattice.

#	$a^{-4}V$	$1/f_a^* [\text{GeV}^{-1}]$	$\chi_t^{1/4} [\text{MeV}]$	$m_a [\text{MeV}]$	$m_{\eta'} [\text{MeV}]$
1	$12^3 \times 24$	0.0068	$119 \pm 4$	$62 \pm 2$	
2	$12^3 \times 24$	0.068	$121 \pm 6$	$73 \pm 8$	
3	$12^3 \times 24$	0.68	$108 \pm 8$	$66 \pm 4$	
4	$24^3 \times 48$	0.0068	$153 \pm 11$	$230 \pm 13$	$700 \pm 110$
5	$24^3 \times 48$	0.068	$148 \pm 9$	$221 \pm 13$	$660^{+50}_{-350}$
6	$24^3 \times 48$	0.68	$151 \pm 8$	$238 \pm 11$	$670 \pm 120$

Table 2: The axion and  $\eta'$  masses, as well as the topological susceptibility, according to volume and bare axion decay constant  $f_a^*$ , in physical units using  $a = 0.074(2)$  fm.

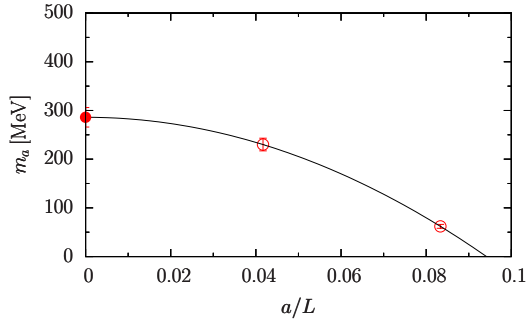


Figure 4: The axion mass  $m_a$  for  $1/f_a^* = 0.0068 \text{ GeV}^{-1}$  extrapolated to the infinite volume.

In Fig. 4 we attempt an extrapolation to the infinite volume, which lifts the axion masses to approximately 300 MeV. The  $\eta'$  masses lie within the expected range [20]. We expect the axion to mix with the  $\pi^0$ ,  $\eta$  and  $\eta'$  mesons. The topological susceptibility  $\chi_t$  turns out to be in agreement with pure QCD at the given mass, but shows no dependence on  $1/f_a^*$ .

The most remarkable result is that the axion mass is independent of  $1/f_a^2$  over a wide range of decay constants  $f_a$ , covering two orders of magnitude. In Fig. 5 we contrast the lattice result with the semi-classical prediction (8). While the lattice axion mass stays constant in the limit  $1/f_a^2 \rightarrow 0$ , the semi-classical result (8) rapidly drops to zero in that limit. Our results come not completely unexpected. They are consistent with the conclusion drawn from the equation of motion (12), assuming that the topological charge density  $q(x)$  receives no or little feedback from the axion, which seems to be the case. Further support comes from the path integral. As a consequence of (16), the action will be dominated by the term linear in  $\phi_a$  at sufficiently large volumes. The result is that the axion decay constant can be absorbed into the integration

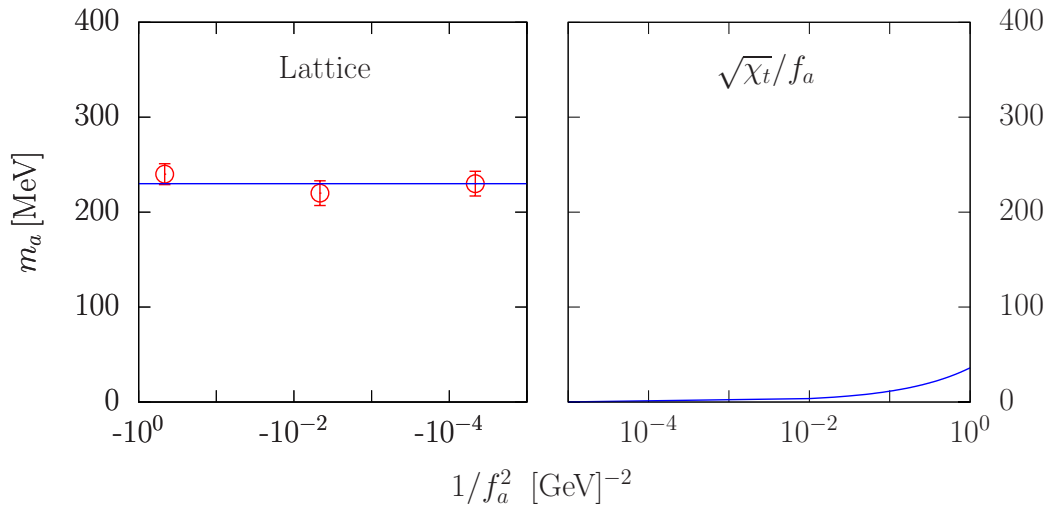


Figure 5: The axion mass  $m_a$  as a function of  $1/f_a^2$  on the  $24^3 \times 48$  lattice (left), compared with the prediction (8) of the semi-classical approximation (right).



variable, which makes the path integral independent of  $f_a$ . This suggests that the axion mass in Fig. 5 continues linearly across  $1/f_a^2 = 0$  to positive values of  $1/f_a^2$ .

A key element in phenomenological applications of the Peccei-Quinn theory, notably the estimate of the dark matter axion mass, has been the effective potential (7) and resulting mass formula (8). Our simulations suggest however

$$U_{\text{eff}}(\bar{\phi}_a) = \frac{m_a^2}{2} \bar{\phi}_a^2 \quad (22)$$

with  $m_a \approx 230$  MeV, up to finite size corrections. For (22) to be true, it must match the constrained effective potential (20) derived earlier. This is indeed the case. In Fig. 2 (right figure) we compare (22) with (20) on one of our  $24^3 \times 48$  lattices. Both (20) and (22) produce consistent results. Possible contributions of higher order to (22) appear to be small. Similar matches are found for the other lattices.

## 4 Conclusion and outlook

In this Letter we have performed a fully dynamical simulation of the Peccei-Quinn theory on the lattice for three flavors of quarks. Our results, above all the axion mass, are found to be in conflict with current axion phenomenology and experiment. In particular, we can exclude a very light axion which would qualify as dark matter candidate. To account for the quantum fluctuations consistently in the framework of effective field theory, a mass term for the axion will have to be added to the action,

$$S_{\text{Axion}} = \int d^4x \left[ \frac{1}{2} (\partial_\mu \phi_a(x))^2 + i \frac{\phi_a(x)}{f_a} q(x) + \frac{1}{2} m_a^2 \phi_a^2(x) \right], \quad (23)$$

and possibly operators of higher powers of  $\phi_a$  as well. The axion mass term does not affect the transformation properties of the action under  $U_{\text{PQ}}(1)$ . It appears though that QCD allows only small values of  $\phi_a/f_a$  to exist, which thwarts the Peccei-Quinn solution of the strong CP problem.

So far the calculations have been done at a single value of the lattice spacing,  $a = 0.074$  fm. It is an open question what happens at larger momentum cut-offs and whether the QCD axion can be a self-consistent, fundamental quantum field theory with a well defined continuum limit. Simulations at varying lattice spacings, together with analytical investigations [21], will have to show.

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