Is the $\bar{\theta}$ Parameter of QCD Constant?

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(Received 29 April 2022; revised 22 June 2022; accepted 19 September 2022; published 11 October 2022)

Testing the cosmological variation of fundamental constants of nature can provide valuable insights into new physics scenarios. While many such constraints have been derived for standard model coupling constants and masses, the $\bar{\theta}$ parameter of QCD has not been as extensively examined. In this Letter, we discuss potentially promising paths to investigate the time dependence of the $\bar{\theta}$ parameter. While laboratory searches for CP-violating signals of $\bar{\theta}$ yield the most robust bounds on today's value of $\bar{\theta}$, we show that CP-conserving effects provide constraints on the variation of $\bar{\theta}$ over cosmological timescales. We find no evidence for a variation of $\bar{\theta}$ that could have implied an "iron-deficient" Universe at higher redshifts. By converting recent atomic clock constraints on a variation of constants, we infer $d(\bar{\theta}^2)/dt \leq 6 \times 10^{-15}\ \mathrm{yr}^{-1}$, at 1σ. Finally, we also sketch an axion model that results in a varying $\bar{\theta}$ and could lead to excess diffuse gamma ray background, from decays of axions produced in high redshift supernova explosions.

DOI: 10.1103/PhysRevLett.129.161802

Introduction.—The modern understanding of particle physics compels us to treat any fundamental "constant" of nature as a possible parameter that could vary over time and space. One of the earliest advocates of this view was Dirac [1], who attempted to explain why certain combinations of constants yield enormously large numbers. According to his proposal, these numbers could be rationalized if one assumes that they start out as having natural values and then evolve over long cosmological times.

Dirac's proposal is no longer the main motivation for considering variation of constants. Nonetheless, it remains a possibility that values of various parameters in the standard model (SM) were, at very early times, right after the big bang, different. Masses of fermions, for example, are set by the Higgs field, after electroweak symmetry breaking (EWSB). This also indicates that, if the Universe started out very hot and dense, as is generally assumed, even the symmetries of the vacuum could have evolved, as would be the case for EWSB.

At a more theoretical level, for example, in the context of string theory, various constants of nature are assumed to be set by the values of certain moduli, early on (see, e.g., Ref. [2]). However, one could imagine that these moduli may have continued to evolve over cosmological times leading to variations in the value of physical parameters, assumed to be constants (see Ref. [3] for a statistical interpretation; for early work in the context of extra-dimensional theories, see Ref. [4]). This is the point of view we will adopt here. In particular, we will focus on variation of one parameter, namely, the θ angle of QCD, which is associated with the level of CP violation in strong interactions.

In Ref. [5], it was argued that θ cannot depend on space-time. The gist of the argument is that θ parametrizes topological transformations corresponding to the winding number of QCD gauge configurations. This notion will become ill defined if θ is a space-time-dependent field. However, θ by itself is not a measurable quantity in QCD. Instead, a new quantity $\bar{\theta}_q \equiv \theta + \arg[\det(M_q)]$, where M_q is the quark mass matrix, is the effective parameter that would lead to CP-violating phenomena in QCD. The smallness of $\bar{\theta}_q \lesssim 10^{-10}$, as implied by the upper bound on neutron electric dipole moment (EDM) $d_n < 1.8 \times 10^{-26}\ e\,\mathrm{cm}$ (90% confidence level) [6–8], remains a conceptual puzzle and is often referred to as the "strong CP problem."

One of the most theoretically appealing resolutions of the above puzzle was proposed by Peccei and Quinn [9,10], by promoting $\bar{\theta}_q$ to a field that relaxes to zero in the early Universe. This is accomplished by introducing a global U(1) symmetry, anomalous under QCD. Once the U(1) is broken, a pseudo-Goldstone mode, called the axion [11,12] and denoted by a with decay constant f_a, would appear. This field gets a mass, from a potential generated by nonperturbative QCD interactions. The axion has a minimum at $\langle a\rangle = -(f_a/\xi)\bar{\theta}_q$, with ξ an $\mathcal{O}(1)$ parameter, such that CP is conserved in strong interactions. The quantity of interest is now $\bar{\theta}$,

$$\bar{\theta} \equiv \bar{\theta}_q - \xi(\langle a\rangle/f_a). \tag{1}$$

In the following, we will assume that $\bar{\theta}$ changes due to a change in the axion potential over time. For example, this change could come from the effects of other light scalars (see Supplemental Material, where this idea is explained in more detail [13]) such that $\bar{\theta}$ is not constant in time. Alternatively, one could consider a change in f_a; a model for this has been proposed in Ref. [34]. The $\bar{\theta}$ parameter also runs in the SM, but the running starts at seven loops [35]. This running allows us to introduce a space-time dependence of $\bar{\theta}$, through threshold corrections and new interactions with the background density (e.g., of dark matter), in analogy with the mechanisms discussed in [36–38].

In this Letter, we derive novel bounds on the cosmological time evolution of $\bar{\theta}$. Though there have been many past studies constraining the change of fundamental constants and examining the sensitivity of physical phenomena to the value of $\bar{\theta}$ [14,39–41], this is the first study of the $\bar{\theta}$ variation effects on proton-to-electron mass ratio over cosmological timescales, which allows us to set tighter bounds than previously obtained. We will focus on the effect of changing $\bar{\theta}$ on observables in atomic and nuclear physics. In models with an axion, additional constraints due to the presence of the axion field can also be derived, as discussed in the Supplemental Material [13], which further contains Refs. [15–33,42] (see also, for example, Ref. [39]).

Signatures of varying $\bar{\theta}$.—The phenomenological consequences of $\bar{\theta}$ are elusive, as they are typically not visible in perturbation theory. Nonetheless, the $\bar{\theta}$ parameter is physical [43–45] and the theory is CP conserving for $\bar{\theta}=0,\pi$. We therefore think of $\bar{\theta}$ as a continuous variable and distinguish between CP-conserving effects of varying $\bar{\theta}$ and CP-violating effects. The most prominent CP-conserving effect of varying $\bar{\theta}$ is the change in hadron masses. In fact, it can be shown that $\bar{\theta}=\pi$ corresponds to a negative determinant of the quark mass matrix [46]. We can construct a combination of the kaon and pion masses whose value is predicted by current algebra [47,48],

$$r = (m_{K^0}^2 - m_{K^\pm}^2 - m_{\pi^0}^2 + m_{\pi^\pm}^2)/m_\pi^2 = \frac{m_d \mp m_u}{m_d \pm m_u}, \quad (2)$$

where the upper (lower) sign corresponds to $\bar{\theta}=0$ ($\bar{\theta}=\pi$). Here, $m_u=2.16$ and $m_d=4.67$ MeV [49] are the up and the down quark masses, respectively. The quantity r is predicted to be less (greater) than 1 for $\bar{\theta}=0$ ($\bar{\theta}=\pi$). We will consider small variations around $\bar{\theta}=0$, since, in nature, the observed value of this ratio is less than 1, and consequently, $\bar{\theta}$ near zero is preferred today.

CP-violating effects—EDM, atomic effects: Before discussing the CP-conserving effects of nonzero $\bar{\theta}$, we will briefly summarize the most prominent phenomenological consequences of CP violation induced by $\bar{\theta}$. Nonzero $\bar{\theta}$ implies a nonvanishing EDM for hadrons. Intensive searches for neutron EDM so far have resulted in only an upper bound, which is the strongest experimental constraint: $\bar{\theta}\lesssim 10^{-10}$ [6,7]. In neutron EDM experiments, neutrons are placed in external electric and magnetic fields and one measures changes in their Larmor precession [6] (see Refs. [50–56] for future proposals to improve the experimental sensitivity on the neutron EDM and Ref. [57] for a proposal using a proton storage ring to improve future experimental sensitivity to the proton EDM).

For atomic systems, the EDM measurements are more challenging. Schiff's theorem forbids effects linear in electron and proton EDMs. The theorem is valid in the nonrelativistic pointlike approximation; thus observable effects of EDMs are restricted to higher order, relativistic effects, or effects related to the finite nucleus size.

Experiments looking for EDMs in complex systems apply external fields and search for tiny splittings of energy levels due to the nonzero EDM [58]. A classic example of such searches is the measurement of the ^{199}Hg EDM [59]. If no source of CP violation other than $\bar{\theta}$ is assumed, this measurement provides a strong bound $\bar{\theta}\lesssim 1.5\times 10^{-10}$, comparable to neutron EDM. However, theoretical interpolation of the experimental results is less clean due to numerous possible sources of CP violation in complex atomic systems and less precise computations of the relation between $\bar{\theta}$ and ^{199}Hg EDM [60,61].

We see that CP violation effects of $\bar{\theta}$ are nontrivial to observe and require precise control over external fields. While such conditions can be realized in terrestrial experiments, it is not feasible to search for EDMs over astronomical distances. We therefore turn to the CP-conserving effects of $\bar{\theta}$, which, though less sensitive, are much easier to observe over astronomical distances.

For a recent review about EDMs see Ref. [62]; for reviews about using atoms to constrain new physics, see Refs. [63,64].

CP-conserving effects—hadron masses, molecular effects: The value of $\bar{\theta}$ affects various hadronic properties like the proton and neutron masses but also binding energies of nuclei. Of particular interest to obtain constraints on $\bar{\theta}$ is the dependence of the pion mass on $\bar{\theta}$ as this affects the nucleon masses, the neutron-proton mass difference, and the neutron decay width, which play a role in big bang nucleosynthesis (BBN).

The leading order $\bar{\theta}$ dependence of the pion mass in the two-flavor approximation is [65,66]

$$m_\pi^2(\bar{\theta}) = m_\pi^2 \cos(\bar{\theta}/2)\sqrt{1+\epsilon^2\tan^2(\bar{\theta}/2)}, \quad (3)$$

where the pion mass $m_\pi = m_\pi(\bar{\theta}=0) = 139.57$ MeV and $\epsilon = (m_d - m_u)/(m_d + m_u) \approx 0.37$ quantifies the departure from the isospin symmetric limit $\epsilon = 0$. With this expression, the nucleon mass in the $\epsilon \to 0$ limit is given as [66]

$$m_N(\bar{\theta}) = m_0 - 4c_1 m_\pi^2(\bar{\theta}) - \frac{3g_A^2 m_\pi^3(\bar{\theta})}{32\pi f_\pi^2}, \qquad (4)$$

with the nucleon mass in the chiral limit $m_0 = 869.5$ MeV [67], $g_A = 1.27$ is the axial-vector coupling constant, $f_\pi = 92.2$ MeV is the pion decay constant, and $c_1 = -1.1\ \text{GeV}^{-1}$ [68] is a low-energy constant from the second-order chiral pion-nucleon Lagrangian (see Ref. [69] for a review on this topic). The neutron mass is well approximated by Eq. (4); for the proton mass, one needs to include the $\bar{\theta}$ dependence of the QCD contribution to the neutron-proton mass difference [40,70]

$$(m_n - m_p)^{\text{QCD}}(\bar{\theta}) \simeq 4c_5 B_0 \frac{m_\pi^2}{m_\pi(\bar{\theta})^2}(m_u - m_d), \qquad (5)$$

with $B_0 = m_\pi^2/(m_u + m_d)$ and $c_5 = (-0.074 \pm 0.006)\ \text{GeV}^{-1}$. The pion mass affects the strength of the nuclear force. However, the effects of $\bar{\theta}$ on a multinucleon system are difficult to quantify; we only have a qualitative notion that with increasing $\bar{\theta}$ the nuclear binding energy will increase and the relative importance of the Coulomb interaction will decrease [40]. An increase in the binding energy mimics a lighter nucleus, and so does a decrease in the nucleon mass. Therefore, to obtain a conservative lower bound on the effect of a variation of $\bar{\theta}$ in systems with many nucleons, we will focus on the effect due to the shift in the nucleon mass only. This allows us to make use of the very powerful data from spectroscopic measurements of molecular transitions at various redshifts. These observations have been used to constrain the ratio of proton-to-electron mass, $\mu \equiv m_p/m_e$, during the evolution of the Universe, as it affects atomic transitions [71,72]. Under the assumption that the effect of the nucleon mass change [73] is the dominant effect of $\bar{\theta}$, we can obtain a conservative bound on $\Delta\bar{\theta}$ from changes of μ. We constrain ourselves to using few-nucleon systems like H_2 and HD (hydrogen deuteride) in order to obtain the most reliable bounds. In the Supplemental Material [13], we provide details on our treatment of diatomic molecules. By using the ratio of the expression in Eq. (4) for free $\bar{\theta}$ over that evaluated at $\bar{\theta} = 0$, we arrive at the relation between μ and $\Delta(\bar{\theta}^2)$ as

$$\Delta(\bar{\theta}^2) \approx -1.4 \times 10^2 \frac{\Delta\mu}{\mu}. \qquad (6)$$

Notice that a change in $\bar{\theta}$ can only decrease the nucleon masses and therefore $\Delta\mu/\mu$. Even though the deuteron is a multinucleon system where, instead of the one-pion exchange, the exchange of the ω, ρ, σ mesons determines the binding energy [40], we find that the numerical dependence of a change in the deuteron mass on a variation in $\bar{\theta}$ is comparable and even slightly smaller than for a change in μ. Therefore, including HD data (which, in fact, represents a rather small fraction of the total dataset) leads to conservative bounds on $\Delta(\bar{\theta}^2)$. We show the constraints on $\Delta(\bar{\theta}^2)$ from H_2 and HD observations in Table I for various values of the redshift.

TABLE I. Constraints on the variation of $\bar{\theta}^2$ for various redshifts making use of different systems. We reinterpret the constraints on $\Delta\mu/\mu$ coming from methods involving H_2 and HD using Eq. (6). The errors indicate 1σ uncertainties.

z	$\Delta(\bar{\theta}^2)$ $(\times 10^3)$	Object	Reference
2.059	-1.06 ± 0.49	$J2123-005$	[71,74,75]
2.34	-2.66 ± 1.44	Q1232 + 082	[76]
2.402	1.06 ± 1.44	$HE0027-1836$	[77]
2.426	0.95 ± 3.89	$Q2348-011$	[78]
2.597	-1.05 ± 0.74	$Q0405-443$	[71,79–82]
2.659	-1.04 ± 0.93	$J0643-504$	[83]
2.66	-1.44 ± 0.64	$B0642-5038$	[71,83,84]
2.688	0.61 ± 0.88	J1237 + 0648	[85]
2.811	0.07 ± 0.38	$Q0528-250$	[71,81,86–88]
3.025	-0.71 ± 0.63	$Q0347-383$	[71,81,82,89,90]
4.224	1.33 ± 1.06	J1443 + 2724	[91]

Using the upper limit on $\bar{\theta}$ from neutron EDM experiments on Earth [6,7] we can constrain $\bar{\theta}$ during the evolution the Universe. In Fig. 1, we plot the best fit values of $\Delta(\bar{\theta}^2)$ and their 1σ errors. Since today's value of $\bar{\theta}$ is bounded to be smaller than $\sim 10^{-10}$, the corresponding bound on $\bar{\theta}$ in this figure can, to a very approximation, be obtained from $\sqrt{\Delta(\bar{\theta}^2)}$. Some of the results for $\Delta(\bar{\theta}^2)$ in Table I are negative, which leads to unphysical values of $\bar{\theta}$. These correspond to best fit values in the gray region of the figure. We deduce from Fig. 1 that the data used in our study, taken all together, offer no evidence for any time variation in $\bar{\theta}$ and strongly favor $\Delta(\bar{\theta}^2) = 0$.

Our results are compatible and even stronger than direct constraints on the value of $\bar{\theta}$ in the early Universe coming from the ^{4}He mass fraction at BBN [40], stellar dynamics [14,39–41], x-ray emissions from the surroundings of compact stellar objects [39], and the measured value of the proton and neutron mass today.

In fact, a change in $\bar{\theta}$ affects the abundance of ^{56}Fe and ^{56}Co in the Universe as ^{56}Co would be the most tightly bound nucleus instead of ^{56}Fe for large $\bar{\theta}$. The increase in the neutron-proton mass difference for large $\bar{\theta}$ [14] leads to ^{56}Fe being heavier than ^{56}Co by ~ 5 MeV [39], and ^{56}Fe produced in the stars would have decayed to ^{56}Co. Therefore, large $\bar{\theta}$ leads to an iron-deficient Universe. From this effect, one can also derive an upper limit of $\bar{\theta} \lesssim \mathcal{O}(1)$ [39] making use of the observation of the Fe Kα line around white dwarfs and neutron stars combined with the nonobservation of a ^{56}Co line. Variation of $\bar{\theta}$ could also affect the shape of the light curve of type Ia supernovae, through its effect on the mass of ^{56}Co whose radioactive

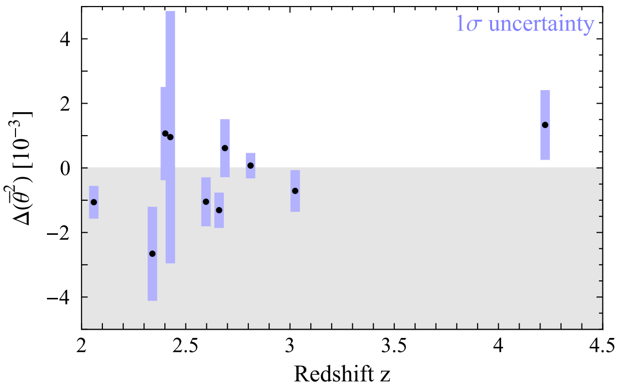

FIG. 1. Constraints on $\Delta(\bar{\theta}^2)$ derived from bounds on $\Delta\mu/\mu$ in Table I across a range of redshifts z. The two data points at $z = 2.659$ and 2.66 have been combined and averaged. The best fit points are shown as black circles and the 1σ uncertainties are shown in blue. Some data points from Table I lead to negative $\Delta(\bar{\theta}^2)$ and therefore to unphysical values of $\bar{\theta}$, which we show in the gray region.

decay is the dominant heating source for the supernova remnant [92].

Local time variation of physical constants is currently constrained very precisely by atomic clocks [64]. In particular, recent measurements have yielded $\dot{\mu}/\mu = -8 \pm 36 \times 10^{-18}$ yr^{-1} [93]. Using this result, and employing Eq. (6) as a conservative bound on the conversion factor between the $\dot{\mu}/\mu$ and the $d(\bar{\theta}^2)/dt$ for complex nuclei (such as $^{171}Yb^{+}$ used in Ref. [93]), we obtain the upper bound on the local time variation of $\bar{\theta}^2$,

$$\frac{d(\bar{\theta}^2)}{dt} \leq 6 \times 10^{-15}\ \mathrm{yr}^{-1}, \tag{7}$$

where the bound should be interpreted as corresponding to 1σ level. Without a specific model for the time dependence of $\bar{\theta}$, one cannot infer a bound on $\bar{\theta}$ at earlier epochs.

Summary and conclusions.—Testing the constancy of fundamental constants of the SM can provide valuable insights into physics beyond the SM. In this Letter, we established for the first time constraints on the variation of the $\bar{\theta}$ parameter of QCD over cosmological timescale from data on molecular transitions at different redshifts. As $\bar{\theta}$ affects hadronic properties, a change in $\bar{\theta}$ translates to a change in the proton-to-electron mass ratio that has been constrained with various observations. Making use of the observations involving H_2 and HD molecules, we find that generally $\bar{\theta} \lesssim 0.1$ for redshifts $z \sim 2$–4. By converting atomic clock constraints on the local variation of constants, we infer $d(\bar{\theta}^2)/dt \leq 6 \times 10^{-15}$ yr^{-1}.

Our results constrain models that predict a change in $\bar{\theta}$ at late times, while various direct limits on $\bar{\theta}$, including bounds from early Universe physics, lead to weaker constraints of $\bar{\theta} \lesssim 1$ [14,39–41]. To further constrain variations of $\bar{\theta}$ in the future, one could make use of the effects of $\bar{\theta}$ on nuclear properties. For example, for varying $\bar{\theta}$ we also expect long-lived isotopes to become short lived and hence rarer than observed, or as the phase space changes, some decays might become forbidden. These studies require complicated nuclear calculations, which is beyond the scope of this Letter.

Other effects of varying $\bar{\theta}$ are more model dependent, for example, signatures related to the change in the axion mass (see the Supplemental Material [13] for a discussion). If the change in $\bar{\theta}$ is due to a shift in the axion potential, larger $\bar{\theta}$ for high z corresponds to heavier axions in the early Universe. This could lead to the prediction of gamma rays from the decay of axions produced in supernovae or neutron stars.

Disentangling a change in $\bar{\theta}$ from a change in other quantities like α, μ, and α_s is challenging; however, a few avenues exist. Varying α leads to a change in the fine-structure doublets, whereas a change in μ can be measured by comparing molecular hydrogen vibrational and rotational modes [72]. Furthermore, the quantities α, μ, and α_s are not related to parity violation, whereas $\bar{\theta}$ is generally assumed to be a measure of parity violation in QCD. Therefore, if $\bar{\theta}$ was larger at high z, one could expect electric and magnetic multipole nuclear transitions to mix. This could affect the relative intensity of various spectral lines. Its observation could be used to distinguish $\bar{\theta}$ variation from a change in α_s or μ, which would have a homogeneous effect on the spectrum. This effect is solely due to the parity-violating effects of $\bar{\theta}$. However, the $\bar{\theta}$ induced parity nonconserving forces would be spin dependent and, consequently, subleading to the dominant parity-conserving binding effects.

In conclusion, any discovery that establishes time dependence of fundamental parameters would have revolutionary implications for our understanding of the Universe. In this context, searches for cosmological-scale space-time dependence of the $\bar{\theta}$ parameter are well motivated and it is essential to explore new avenues.

We thank Bob Scherrer for pointing out the relation between the lifetime of ^{56}Co and the light curve of supernovae type Ia. The authors acknowledge support by the United States Department of Energy under Grant Contract No. DE-SC0012704.

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