

Opening up a Window on the Postinflationary QCD Axion

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The QCD axion cosmology depends crucially on whether the QCD axion is present during inflation or not. We point out that contrary to the standard criterion, the Peccei-Quinn (PQ) symmetry could remain unbroken during inflation, even when the axion decay constant, f_a , is (much) above the inflationary Hubble scale, H_I . This is achieved through the heavy lifting of the PQ scalar field due to its leading nonrenormalizable interaction with the inflaton, encoded in a high-dimensional operator which respects the approximate shift symmetry of the inflaton. The mechanism opens up a new window for the post-inflationary QCD axion and significantly enlarges the parameter space, in which the QCD axion dark matter with $f_a > H_I$ could be compatible with high-scale inflation and free from constraints on axion isocurvature perturbations. There also exist nonderivative couplings, which still keep the inflaton shift symmetry breaking under control, to achieve the heavy lifting of the PQ field during inflation. Additionally, by introducing an early matter domination era, more parameter space of high f_a could yield the observed DM abundance.

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Introduction.—The QCD axion is of great interest in solving the strong CP problem of the standard model [1–4], and serving as a classical cold dark matter (DM) candidate [5–7]. It is a naturally light pseudo-Nambu-Goldstone boson from spontaneous breaking of a global symmetry—the $U(1)$ Peccei-Quinn (PQ) symmetry—at a high energy scale f_a , which is often referred to as the axion decay constant. It is one of the best motivated feebly coupled particles beyond the standard model and has attracted continuously growing theoretical and experimental studies even four decades after the original proposal (e.g., discussions of future plans and open questions in some recent Snowmass studies [8–10]).

The QCD axion has a close intriguing interplay with cosmic inflation, a leading paradigm to understand the origin of our universe [11–13]. Depending on when the PQ symmetry is broken, the QCD axion cosmologies fall into two classes: the inflationary axion with the PQ symmetry breaking during inflation and the post-inflationary axion (PIA) with the PQ breaking happening afterward. To determine which class the QCD axion is in, we need to compare f_a with the temperature of the universe during inflation, which is given by the Gibbons-Hawking

temperature [14], $T_{\text{GH}} = H_I/(2\pi)$ with H_I the inflationary Hubble scale. More details could be found in recent reviews [15–17].

When $f_a > H_I/(2\pi)$, the QCD axion is in the first category and is present during inflation [18]. In this case, the exponential expansion stretches each patch of the initial misalignment angle θ_i , and our current Hubble patch owns a single uniform central value of θ_i at the end of inflation. The massless axion during inflation undergoes random quantum fluctuations set by T_{GH} , resulting in an axion isocurvature perturbation $\langle \delta\theta_i^2 \rangle = H_I^2/(2\pi f_a)^2$ [21–25]. This leads to the serious axion isocurvature problem: inflationary QCD axion DM could be incompatible with high-scale inflation (e.g., $f_a \sim 10^{11}$ GeV requires $H_I \lesssim 10^7$ GeV), due to the observation bound on the isocurvature perturbations [26]. (Solutions to the axion isocurvature problem have been proposed. For example, the isocurvature perturbation is suppressed if during inflation, the PQ breaking scale is temporarily enhanced [25,27–33] or QCD is much stronger [34]).

When $f_a < H_I/(2\pi)$, the QCD axion is in the post-inflation regime, with a quite different cosmic evolution. Because of the absence of axion during inflation, there is no axion isocurvature problem. Each Hubble patch has a θ_i drawn randomly from a uniform distribution between $-\pi$ and π , with $\langle \theta_i^2 \rangle = \pi^2/3$. In addition to the misalignment component, topological defects such as axion strings and domain walls (If the axion domain wall number is larger than one, the domain walls could be long-lived and incompatible with the observations [35]). We will assume

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the domain wall number to be one and thus the walls decay during the early universe [36–38].) are generated, and their decays contribute to the axion abundance [39–48]. The latest simulation indicates that the decays of the topological defects could be the dominant contribution and $f_a \sim 10^{10-11}$ GeV for the QCD axion to be the major component of DM in the minimal scenario [47,48]. For this case, ultradense compact minihalos might be formed as proposed in [49–52], giving rise to a plethora of interesting phenomenology and detection opportunities [53–61].

In this Letter, we will point out that the inclusion of the leading high-dimensional operator between the inflaton and the PQ scalar field (the phase becomes the QCD axion after symmetry breaking) could change the standard story briefly reviewed above significantly. In particular, it will modify the conventional boundary between inflationary and post-inflationary axion drastically. We require the operator to respect the (approximate) shift symmetry of the inflaton. (References [25,62–66] discuss renormalizable interactions between the inflaton and the PQ scalar field, which could lead to large quantum corrections to the inflaton potential and works only in the specific hybrid inflation scenario.) The nonrenormalizable operator, though suppressed by a high cutoff scale, could open up a new window for the PIA. More specifically, we will show that even when $f_a \gg H_I/(2\pi)$, the PQ symmetry could remain unbroken during inflation thanks to “heavy lifting” of the high-dimensional operator. As a result, part of the region in the (H_I, f_a) plane used to be labeled as an inflationary axion and suffers from the axion isocurvature problem that could belong to the PIA. The cosmological evolutions and consequences will be modified correspondingly. We will also comment on other types of operators that could achieve the same goal.

Our mechanism also enlarges the parameter space in which high-scale inflation scenarios and the QCD axion DM could be compatible with each other. QCD axion DM with $f_a > H_I/(2\pi)$ will not lead to unacceptable isocurvature perturbations since it is not present during inflation in our model. Large f_a may lead to too much QCD axion DM relic abundance through the standard production, which could be diluted subsequently to the observed value by the early matter domination (EMD) mechanism [21,67–76].

We present our inflationary heavy-lifting mechanism in Sec. II and map out the new window for PIA in Sec. III. We conclude in Sec. IV. Details of the relic abundance computations in the EMD epoch are collected in Appendix A.

Inflationary heavy-lifting mechanism.—During inflation, we have the following effective field theory (EFT) for the inflaton, denoted by a real scalar ϕ , and the complex PQ scalar field χ in the $(+---)$ convention:

$$\begin{aligned} \mathcal{L} &= (\partial_\mu \phi)^2/2 + |\partial_\mu \chi|^2 - V(\phi, \chi), \\ V(\phi, \chi) &= V(\phi) + \frac{\lambda}{2} \left(|\chi|^2 - \frac{f_a^2}{2} \right)^2 + \frac{c(\partial\phi)^2}{\Lambda^2} |\chi|^2, \end{aligned} \quad (1)$$

where Λ denotes the UV cutoff of the EFT, c and λ are positive dimensionless Wilson coefficients, and $V(\phi)$ stands for the inflaton potential that drives inflation. Here χ is the spectator field during inflation, and our discussions below are insensitive to different forms of $V(\phi)$. Our key new ingredient is the dimension-six operator [77] in Eq. (1), which is the leading operator coupling ϕ and χ while respecting the (approximate) shift symmetry of ϕ . This type of operator has been discussed in completely different contexts, such as cosmological collider [78,79]. (An operator of this form coupling inflaton to the Higgs field could also lead to imprints on the inflaton spectrum from oscillating electroweak symmetry breaking during inflation [80].) Following [78], we name our mechanism inflationary heavy lifting of the PQ field.

During inflation, the homogeneous background $\langle \partial_\mu \phi \rangle = \dot{\phi}_0 \delta_{\mu 0}$ then generates the effective quadratic term of the PQ scalar:

$$V(\phi, \chi) \supset \left(\frac{c\dot{\phi}_0^2}{\Lambda^2} - \frac{\lambda}{2} f_a^2 \right) |\chi|^2. \quad (2)$$

Note that the first term $\propto c$ has the opposite sign of the second term. When it is large enough, it can protect the PQ field from breaking during inflation. After the inflation ends, the expectation of $\partial\phi$ becomes smaller, allowing the PQ symmetry to be spontaneously broken by the tachyonic mass term. In addition, to reproduce the conventional post-inflationary behavior, the PQ scalar needs to be heavier than the Hubble scale during inflation to settle at the minimum, with its large-scale fluctuations exponentially suppressed. This translates to

$$m_{\text{PQ,eff}}^2 \approx \frac{c\dot{\phi}_0^2}{\Lambda^2} - \frac{\lambda}{2} f_a^2 \gtrsim (1.5H_I)^2, \quad (3)$$

where $1.5H_I$ is the boundary value for a field to be heavy enough in the inflationary background [81].

We then turn to determine the range of parameters in Eq. (3). First, the validity of the EFT requires Λ to be sufficiently larger than the scale of infrared degrees of freedom. Without referring to a specific UV completion, the heavy-field-induced corrections to inflaton self-interactions generically scale as $\mathcal{O}(\dot{\phi}_0^2/\Lambda^4)(\partial\phi)^2$. Requiring that the power expansion in series of $\dot{\phi}_0^2/\Lambda^4$ does not spoil the EFT during inflation imposes the condition that $\Lambda \gtrsim \dot{\phi}_0^{1/2}$ [78,82]. Second, there is a lower limit of coupling λ when the c term is present. Considering the theory to be natural, the radiative correction to λ , $\delta\lambda$, induced by the inflaton loop shall be subdominant. Integrating out the loop momenta to the cutoff scale Λ , we have

$$\delta\lambda \sim \frac{c^2}{16\pi^2} \lesssim \lambda \Rightarrow c \lesssim 4\pi\sqrt{\lambda}. \quad (4)$$

Similarly, we require the radiative correction to the quadratic mass term of χ from the inflaton loop, δm_{PQ}^2 , to satisfy

$$\delta m_{\text{PQ}}^2 \sim \frac{c}{16\pi^2} \Lambda^2 \lesssim \lambda f_a^2. \quad (5)$$

Lastly, after inflation, the PQ field will acquire a vacuum expectation value (VEV) and the heavy-lifting operator contributes to the inflaton's kinetic term. To avoid a wrong-sign kinetic term,

$$c f_a^2 \ll \Lambda^2. \quad (6)$$

As a benchmark, we choose $\Lambda = 3\sqrt{\dot{\phi}_0}$ and $c = \pi\sqrt{\lambda}$. Then Eq. (3) turns into a quadratic relation for $\sqrt{\lambda}$. Requiring that λ satisfying this relation is real, we find that

$$f_a \lesssim \frac{\sqrt{2\pi} \dot{\phi}_0}{27 H_I}, \quad (7)$$

which is saturated when $\sqrt{\lambda} = 81H_I^2/(2\pi\dot{\phi}_0)$. One could check that all the requirements listed above are satisfied. It is also worth mentioning that our benchmark is chosen so that the EFT stays away from the boundaries of all the theoretical constraints but not to maximize the f_a/H_I ratio [i.e., a smaller Λ and larger c can lead to a larger upper bound on f_a than Eq. (7)]. Generically, as $\sqrt{\dot{\phi}_0} \gg H_I$ during inflation, PQ symmetry is not broken even for f_a exceeding the conventional upper limit on the PIA, $H_I/(2\pi)$, significantly. Note that $\lambda < c < 1$ at the upper bound of f_a , which implies that the PQ field has a shallow potential. This could be realized similarly to the supersymmetric saxion scenario in [83,84].

The size of $\dot{\phi}_0$ can be estimated by the CMB observations. For single-field slow-roll inflation (case 1), $\dot{\phi}_0$ is constrained by the observed primordial scalar power spectrum $A_s \approx H_I^4/(4\pi^2\dot{\phi}_0^2)$. From the Planck measurement that $A_s \approx 2.1 \times 10^{-9}$ at large scales [26], we have $\sqrt{\dot{\phi}_0} \approx 60H_I$. From Eq. (7), the viable range for the post-inflationary axion becomes

$$\text{case 1: } f_a \lesssim 600H_I. \quad (8)$$

There is an interesting alternative with $\dot{\phi}_0$ determined differently. In this scenario, A_s is generated by another spectator field σ with a mass $m_\sigma \ll H_I$ instead of the inflaton. Such a light field σ is often referred to as the curvaton [85–87] (case 2). During inflation, the expected value of σ is frozen due to the Hubble friction, while its quantum fluctuations generate A_s . (We do not consider the intermediate scenario with both the curvaton and inflaton contributing to A_s significantly as it is even more constrained [88].) It only dominates the universe much later after the inflation ends and eventually decays back to radiation. The constraint on $\dot{\phi}_0$, in this case, is given by the slow-roll parameter $\epsilon \approx \dot{\phi}_0^2/(2H_I^2 M_{\text{pl}}^2)$ with the reduced Planck scale $M_{\text{pl}} \approx 2.4 \times 10^{18}$ GeV instead. The upper bound f_a in Eq. (7) then relaxes to

$$\text{case 2: } f_a \lesssim 8 \times 10^{16} \text{ GeV} \sqrt{\frac{\epsilon}{0.02}}. \quad (9)$$

The benchmark of ϵ is the observational upper bound, determined by the relation that $n_s - 1 \approx -2\epsilon$ [89–91], with $n_s \approx 0.96$ the scalar spectral index [26]. [Notice that the other constraint $\epsilon \lesssim 0.004$ reported in [26] does not apply to the curvaton case since the relation $r = 16\epsilon$ (from single field inflation) it relies on no longer holds].

While we focus on the inflaton derivative coupling, it is also possible to consider nonderivative coupling which still keeps the inflaton shift symmetry breaking under control. As an example, we could consider an operator

$$\frac{c' V(\phi)}{\Lambda'^2} |\chi|^2, \quad (10)$$

where we treat $V(\phi)$ as the inflaton shift symmetry breaking spurion and do not introduce additional symmetry-breaking sources. In general, we could consider a different expansion series of inflaton coupling to the PQ field in powers of $V(\phi)/\Lambda'^4$. For this series to hold, $\Lambda' \gtrsim V(\phi)^{1/4}$. (When $\Lambda' \sim M_{\text{pl}}$, this term is reduced to the Hubble-induced mass term [92,93]. In addition, the Hubble-induced mass term in the Einstein frame could be transformed into the nonminimal coupling of the PQ field to gravity, $\mathcal{R}|\chi|^2$, with the Ricci scalar $\mathcal{R} = 12H^2$ during inflation.) The computation for the f_a range is similar to the derivative coupling, with $\dot{\phi}_0$ replaced by $\sqrt{V(\phi)}$. Since $\sqrt{V(\phi)} \sim \dot{\phi}_0/\sqrt{\epsilon}$, the upper bound on f_a in Eq. (7) could be raised by a factor $1/\sqrt{\epsilon}$ [$\sim O(10)$ for current upper bounds on ϵ].

New window of post-inflationary axion.—We illustrate how the heavy-lifting mechanism changes the classification of QCD axion cosmologies in Fig. 1. One could see that in the two panels representing case 1 (single-field slow-roll inflation) and case 2 (curvaton scenario), respectively, the upper bounds of f_a based on Eq. (8) and Eq. (9) extend the conventional PIA region (blue) substantially. In case 2, the entire space in the (H_I, f_a) plane could belong to PIA.

However, with a high f_a , the post-inflationary scenario often overproduces axion DM via the radiation and decay of the axion string network. For the case that the universe is purely radiation dominated between inflaton reheating and matter-radiation equality, only when $f_a \sim 10^{10-11}$ GeV the axion string network can produce the observed DM relic abundance $\Omega_{\text{DM}} h^2 \approx 0.12$ [47,48]. Here we take the numerical benchmark of $f_a \in [3.1, 14] \times 10^{10}$ GeV [48], represented as the meshed horizontal bands in Fig. 1. PIA is still allowed when f_a is lower, but additional sources of DM are needed (shown as orange regions in Fig. 1). More parameter space with a higher f_a is accessible if the DM abundance can be modified in a nonstandard cosmology. In this Letter, we focus on the EMD scenario, where the universe's energy density is dominated by some nonrelativistic particles after

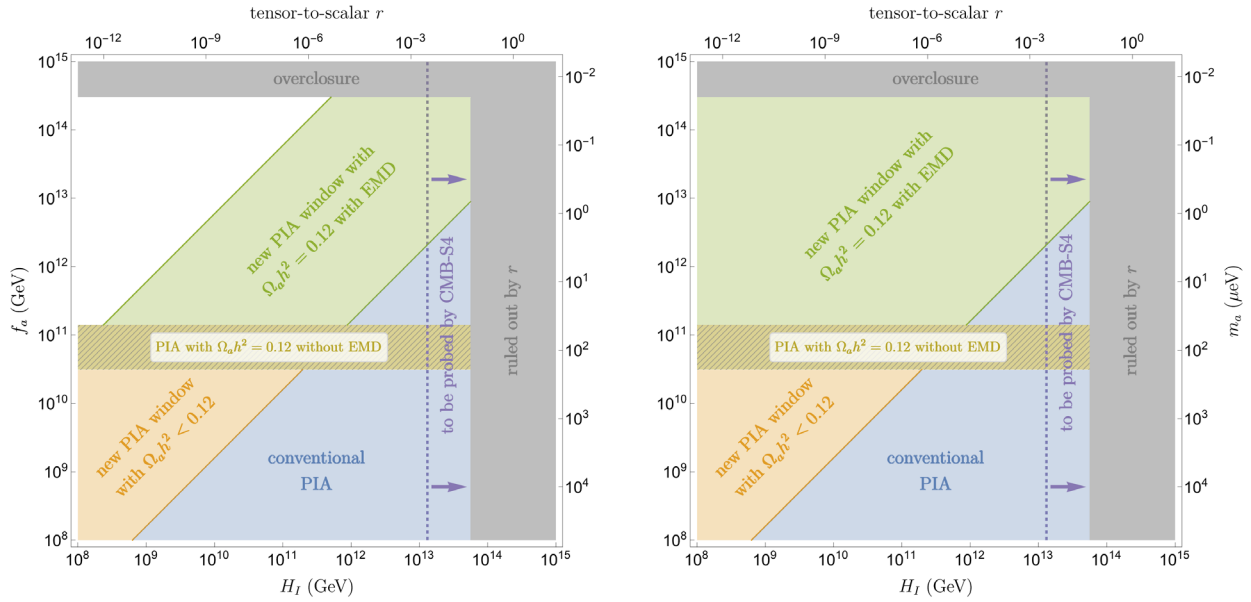


FIG. 1. New post-inflationary QCD axion window in the (H_I, f_a) plane. Left: case 1 single-field slow-roll inflation. Right: case 2 the curvaton scenario. Blue: the conventional PIA region with $f_a < H_I/(2\pi)$; orange: new PIA window with axion relic abundance $\Omega_a h^2 < 0.12$; meshed horizontal band: PIA with $\Omega_a h^2 = 0.12$ without EMD; green: new PIA window in which $\Omega_a h^2 = 0.12$ with EMD. Region right to the purple dashed line could be probed by CMB-S4 [99]. The gray regions are either ruled out by the upper bound on the tensor-to-scalar ratio r [26] (right vertical) or axion DM relic abundance overclosing the universe even with EMD (upper horizontal).

inflation reheating [67–71]. (Though nonminimal, EMD is highly motivated theoretically, e.g., it could be sourced by the moduli arising ubiquitously from string theory constructions [94,95] or dark glueballs [96].) In this case, the axion first oscillates during the EMD at a time t^* , which satisfies $3H(t^*) \approx m_a(t^*)$ [68,97]. (In this case, t^* could be very different from the one when the QCD axion starts to oscillate during the radiation domination epoch.) After that, the massive particles causing the EMD decay at the time scale of their lifetime $\sim \Gamma_{\text{EMD}}^{-1}$. The universe undergoes a secondary reheating as the energy density of the massive particles is converted into radiation, which dominates afterward. The entropy created by massive particles greatly dilutes the axion number density per comoving entropy density. The axion relic abundance $\Omega_a h^2$ is thus suppressed. Because of tight constraints, the EMD has to end before the big bang nucleosynthesis (BBN) era: Γ_{EMD}^{-1} must be shorter than the onset of BBN around $\mathcal{O}(1)$ second [98]. Equivalently, the radiation temperature right after the EMD ends, T_R , must be larger than $\mathcal{O}(1)$ MeV. When $T_R > 1$ MeV, $\Omega_a h^2 = 0.12$ can be satisfied when $f_a \lesssim 2.7 \times 10^{14}$ GeV. For a conservative range of $T_R > 10$ MeV, a large f_a of $\mathcal{O}(10^{13} - 10^{14})$ GeV is still allowed. More detailed computations can be found in Appendix A. The new parameter regime satisfying $\Omega_a h^2 = 0.12$ after introducing the EMD dilution mechanism with $T_R > 1$ MeV for the inflaton (curvaton) case is shown in green in Fig. 1.

One potential concern is that the EMD-inducing particles may have its own independent fluctuations as curvatons, resulting in additional isocurvature constraints. This is not

always true, at least in case 1. They could be generated by the thermal bath created from the inflaton reheating (see [100,101] for examples) so inheriting the inflaton’s perturbations; or they could have time-dependent potentials with much larger masses during inflation and thus have much suppressed quantum fluctuations [102,103]. Then in case 1, the density perturbations originate from a single source, the inflaton perturbations. Then there is no isocurvature constraint on the PIA in the new window.

In case 2, the curvaton scenario, the situation is more subtle. Now the curvaton σ induces the EMD. As a spectator field during inflation, the curvaton’s quantum fluctuation $\delta\sigma$ is not correlated with the inflaton’s fluctuation. Such differences can again introduce isocurvature perturbations between radiation, baryon, neutrino, and DM. Consequently, the isocurvature bounds could still be stringent if the PIA DM from the string networks obtains its perturbations from early radiation before the EMD [88]. While the axion string network is created much before EMD, it does not behave as the regular cold DM with a fixed comoving density. In contrast, it is well known that the comoving string density follows the attractive solution of the scaling law, which is insensitive to the initial conditions [104–109]. In other words, the large-scale correlation carried by the axion string network in the early universe could be washed out during the long EMD era. More discussions on axion dynamics with an EMD era can be found in the Appendix.

For other observational constraints, several cavity searches have already probed the QCD axion within

$m_a \in (1.9, 24.0) \mu\text{eV}$, or, correspondingly, $f_a \in (2.5 - 32) \times 10^{11} \text{ GeV}$ (not the full range; only discrete subsets) through the axion-photon coupling, assuming QCD axion is the entire DM [110–121]. More parameter space in Fig. 1 is still open to be explored.

Conclusions.—In this Letter, we propose an inflationary heavy-lifting mechanism to make the PQ field heavy during inflation, and thus the PQ symmetry remains unbroken even when $f_a \gg H_I$. This could be achieved by including the leading high-dimensional operator coupling the inflaton to the PQ field, which is inflaton shift symmetric. This simple inclusion drastically modifies the landscape of the QCD axion cosmologies. The post-inflationary QCD axion parameter space expands significantly in the (H_I, f_a) plane. The region subject to the axion isocurvature constraint shrinks in a correlated way, alleviating the tension between the QCD axion DM and high-scale inflation. Other types of operators, which keep the inflaton shift symmetry breaking under control, also exist to achieve the same goal. We also apply EMD to make more parameter space of high f_a consistent with the observed DM abundance.

We will outline several interesting consequences and possible future directions: (i) We describe our mechanism using an EFT. It could be useful to construct the UV completions and examine whether there could be other cosmological observables beyond r , such as primordial non-Gaussianities; (ii) our proposal demonstrates that the intriguing late-universe phenomenologies of PIA, such as the formation of miniclusters, could happen in a much larger territory of the inflation-axion parameter space than considered before, and thus calls for more studies; (iii) while we focus on the QCD axion, the mechanism could also be applied to axionlike particles in general and expand their post-inflationary regimes as well; (iv) beyond the well-motivated EMD, one could consider other mechanisms (e.g., [122]) to open up more parameter space for PIA DM of high f_a without overclosing the universe, and their associated model-dependent signals.

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Appendix: Axion relic abundance in early matter domination.—In this appendix, we first review the calculation of $\Omega_a h^2$ from misalignment mechanism without EMD [5–7]. During the radiation domination, the cosmic evolution of the homogeneous axion background is governed by the equation of motion:

$$\ddot{a} + 3H(T)\dot{a} + m_a(T)^2 a = 0, \quad (\text{A1})$$

in which $H(T)$ denotes the Hubble scale at the temperature T . In the early universe, we have $H \gg m_a$ so that the axion field value is frozen due to the Hubble

friction. However, as the radiation temperature drops, $m_a(T)$ increases while $H(T)$ decreases. Eventually, at the axion oscillating temperature T_* around $3H(T_*) \approx m_a(T_*)$, the axion potential becomes important, and the axion starts to oscillate about its minimum. The axion energy density at T_* can be approximated by

$$\rho_a(T_*) \approx \frac{1}{2} m_a(T_*)^2 a_i^2 = \frac{1}{2} m_a(T_*)^2 f_a^2 \theta_i^2, \quad (\text{A2})$$

in which the dimensionless angle $\theta \equiv a/f_a$ and the subscripts i denote the initial values of the quantities. In the discussions above, we assume that the axion potential is harmonic, which is not exact. However, as long as θ_i is not very close to π , the harmonic potential is still a good numerical approximation with only mild corrections [123–125]. With the approximate harmonic potential, the comoving axion number density is an adiabatic invariant when $T < T_*$:

$$R(T)^3 n_a(T) \approx R(T)^3 \frac{\rho_a(T)}{m_a(T)} \approx \frac{R(T_*)^3}{2} m_a(T_*) f_a^2 \theta_i^2, \quad (\text{A3})$$

where $R(T)$ is the scale factor at temperature T and $n_a(T)$ is the axion number density. It is then easy to estimate Ω_a since $\Omega_a \equiv \rho_a(T_0)/\rho_{\text{crit}} = m_a(T_0) n_a(T_0)/\rho_{\text{crit}}$, where T_0 is today's radiation temperature and ρ_{crit} is the current critical energy density of the universe.

The result above changes after a phase of EMD is induced by a massive particle ψ . In particular, if the axion starts to oscillate before the EMD ends, Ω_a will be diluted by the entropy generated during the reheating. We first estimate the new oscillation temperature T_* given the reheating temperature T_R . Here T_R is defined by the radiation temperature immediately after the massive particle decays. It is well known that during the EMD, the temperature of the radiation bath scales like $T \propto t^{-1} \propto \rho_\psi^{1/8}$ [21]. Then, using the approximation that $H(T_*) \approx m_a(T_*)/3$ and the Friedmann equation, we have [68]

$$\begin{aligned} 3H(T_*)^2 M_{\text{Pl}}^2 &\approx \rho_\psi(T_R) \frac{T_*^8}{T_R^8} \\ \Rightarrow m_a(T_*) M_{\text{Pl}} T_R^2 &\approx \sqrt{\frac{\pi^2 g_*(T_R)}{10}} T_*^4, \end{aligned} \quad (\text{A4})$$

where $g_*(T)$ is the effective degrees of freedom at T and we use $\rho_\psi(T_R) = \pi^2 g_*(T_R) T_R^4/30$.

After the reheating of EMD, Ω_a can be estimated via

$$\Omega_a \approx \frac{1}{\rho_{\text{crit}}} m_a(T_0) \frac{\rho_a(T_R) s(T_0)}{m_a(T_R) s(T_R)}, \quad (\text{A5})$$

where $s(T)$ is the entropy density at T . The relation above uses the fact that after EMD ends, n_a/s is conserved. The axion energy density at T_R is estimated by

$$\rho_a(T_R) = \rho_a(T_*) \frac{m_a(T_R) \rho_\psi(T_R)}{m_a(T_*) \rho_\psi(T_*)}. \quad (\text{A6})$$

In Eq. (A6) we used the fact that $n_a(T)/n_\psi(T) = \text{const}$ during EMD. Combining Eqs. (A2), (A5), and (A6), one finds that the axion relic density generated by the misalignment mechanism during EMD is

$$\Omega_a^{\text{mis}} h^2 = \frac{h^2}{2\rho_{\text{crit}}} m_a(T_*) m_a(T_0) f_a^2 \theta_i^2 \frac{h_*(T_0) T_0^3 T_R^5}{h_*(T_R) T_*^8}, \quad (\text{A7})$$

where $h_*(T)$ is the effective degrees of freedom that contributes to the entropy at T and $h \approx 0.7$.

To estimate the temperature dependence of $m_a(T_*)$, we use the result extrapolated from lattice simulations [126]

$$m_a(T) = \begin{cases} \frac{\sqrt{\chi(0)}}{f_a}, & T < T_2, \\ \frac{\sqrt{\chi(T_0)}}{f_a} \left(\frac{T_0}{T}\right)^{n/2}, & T_2 < T < T_0, \\ \frac{\sqrt{\chi(T_0)}}{f_a} \left(\frac{T_0}{T}\right)^4, & T > T_0, \end{cases} \quad (\text{A8})$$

in which the zero-temperature QCD susceptibility $\chi(0) = 3.6 \times 10^{-5} \text{ GeV}^4$, the demarcating temperature for the high-temperature regime $T_0 = 1.5 \text{ GeV}$, the high-temperature susceptibility $\chi(T_0) = 3.7 \times 10^{-14} \text{ GeV}^4$, and the intermediate-temperature benchmark $T_2 = [\chi(T_0)/\chi(0)]^{1/n} T_0$ which makes $\chi(T)$ continuous. The intermediate power dependence n is a number ranging from 7 to 20. Combining Eqs. (A5), (A6), (A7), and (A8), one can obtain the relic density of the QCD axion DM from misalignment mechanism as a function of f_a and T_R . For PIA, the effective θ_i^2 takes the average value $\langle \theta_i^2 \rangle = \pi^2/3$.

However, the dominant contribution to Ω_a in the PIA case is the radiation and decay of the axion string network, which could be much larger than Ω_a^{mis} . The numerical simulation of the axion relic density contributed from the string network Ω_a^{str} is known to be difficult. Here we take the simplified approach that the ratio between Ω_a^{str} and Ω_a^{mis} is a fixed constant $\alpha > 1$ [97]. Recent simulation [48] estimates that $\alpha \sim 6$ to 8. Using $\alpha \sim 8$, we find that for $T_R = 1 \text{ MeV}$, the constraint that $\Omega_a^{\text{mis}} + \Omega_a^{\text{str}} = \Omega_{\text{DM}}$ provides an upper bound on $f_a \lesssim 2.7 \times 10^{14} \text{ GeV}$, which is insensitive to the choice of n in Eq. (A8). On the other hand, when $T_R = 10 \text{ MeV}$, the parameter n could be a dominant source of uncertainty. Nonetheless, one still find that the upper bound for the PQ scale lands on $\sim \mathcal{O}(10^{13} - 10^{14}) \text{ GeV}$ for $T_R = 10 \text{ MeV}$.

For the complicated axion string dynamics, multiple uncertainties may be present in our calculation. For example, the axion string density may scale with time differently from the one extrapolated in lattice simulations as the physical time span greatly exceeds the capability of simulations [127]. It is also possible that dimensionless parameters describing the string network evolution differ

from our reference values by $\mathcal{O}(1)$ factors [128], as most lattice simulations assume a radiation-dominated background cosmology. Therefore, the upper bound on f_a derived when $T_R \approx 1 \text{ MeV}$ is a suggestive value, while a dedicated lattice simulation during EMD is needed for more precise predictions. However, most newly opened-up parameter space pointed out by this Letter is still valid aside from the part very close to the overclosure line.

Finally, we would like to comment briefly on other possible sources of isocurvature in the curvaton scenario with PIA DM. In Sec. III, we focus on the isocurvature from axion string decays. We argue that the attractor solution of the string network washes out the initial-condition dependence of the PIA profile. The fluctuation of PIA relic density is mainly due to that of the curvaton. Other components of PIA DM either come from axion string radiation before the string decays or the misalignment mechanism. However, PIA DM from string radiation is relativistic and redshift as radiation; thus, this contribution is expected to be minor and dominated by late-time contributions during the EMD without significant isocurvature [109]. On the other hand, for the misalignment mechanism contribution to the PIA DM abundance, the misalignment angle is randomized over $[-\pi, \pi]$. Hence, no large-scale isocurvature is generated like the standard PIA in a radiation domination epoch. Only small-scale fluctuations, such as axion minihalos, can be produced and observed. A dedicated numerical study of this scenario is needed in the future to validate the arguments above fully.

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