

Collider fingerprints of freeze-in dark matter produced during the fast expansion phase of Universe

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We examine a simple dark sector extension where the observed dark matter (DM) abundance arises from a freeze-in process through the decay of heavy vectorlike quarks into a scalar dark matter candidate. The detection prospects of such DM are challenging due to the feeble nature of the interactions, but these vectorlike quarks can be produced copiously at the LHC, where they decay to standard model quarks along with DM. Depending on the decay rate, this scenario is typically probed through long-lived particle or displaced vertex signatures, assuming a radiation-dominated cosmological background. An alternative hypothesis suggests that the Universe may have experienced a rapid expansion phase instead of the standard radiation-dominated one during freeze-in. This would significantly alter the dark matter phenomenology, requiring a substantial increase in the interaction rate to match the observed relic density, resulting in the rapid decay of the parent particle. As a result, much of the parameter space for this scenario is beyond the reach of traditional long-lived particle and displaced vertex searches. Due to this nonstandard cosmic evolution, existing constraints do not cover the expanded dark matter parameter space. We propose a complementary search strategy to explore this scenario, offering additional limits alongside searches for long-lived particles and displaced vertices. In our search, we investigate the feebly interacting massive particle (FIMP) dark matter model at the LHC using boosted fatjets and significant missing transverse momentum. To improve precision, we include one-loop QCD corrections for LHC production processes and employ a boosted decision tree multivariate analysis, leveraging jet substructure variables to explore a vast parameter space for this minimally extended FIMP dark matter model at the 14 TeV LHC.

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I. INTRODUCTION

Extensive studies with astrophysical and cosmological observations [1–4] have jointly established the existence of a yet unidentified nonluminous form of matter (also known as dark matter) as a dominant matter component of the Universe that exerts its presence over a vast range of scales, from galaxies to the cosmological length. In particular, the observation of cosmic microwave background (CMB) has provided a crucial input for studying the properties and evolution of dark matter by quantifying its contribution around 27% of the total energy budget of the Universe, featuring the relic density, $\Omega h^2 = 0.12$ [4,5]. Among

numerous proposals on particle candidates of dark matter, weakly interacting dark matter particle (WIMP) [6–40] snatches most of the attention due to its rich phenomenology and search prospects at various frontiers owing to its simple production mechanism and miraculous weak scale interactions with the standard model (SM) particles. Unfortunately, after decades of rigorous searches using direct [41–44] and indirect [45] detection experiments, as well as collider experiments [46–48], the elusive nature of dark matter persists. Despite their apparent ubiquity, the fundamental properties and evolution mechanism of dark matter (DM) particles still remain obscure. However, such null results significantly constrained different DM models, including a favorable range of electro-weak mass scale and the coupling of the dark matter. That resulted in vigorous scientific efforts to look for possible dark matter signatures outside the electro-weak mass scale and investigate different unconventional dark matter scenarios where the production mechanism supports a minuscule SM interaction, unlike the WIMP paradigm.

One such exciting alternative dark matter candidate is a feebly interacting massive particle (FIMP) [49–78], which

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naturally answers the nonobservation of any signature at experimental grounds owing to its tiny interaction with the visible particles. Due to its feeble interaction, the FIMP has never been in thermal contact with the SM particles, and the scattering and decay of some particles at the thermal bath populates the FIMP gradually via the so-called freeze-in mechanism. Early cosmological history is crucial since such dark matter production occurs in the early Universe. Typically, studies of such dark matter computation assume a radiation-dominated background, although there is no direct evidence of the energy budget prior to the big bang nucleosynthesis (BBN). It is worth investigating the scenario without such particular prejudice that radiation dominated the early Universe. It is even more critical since such an assumption not only changes the evolution of dark matter at early times but also modifies its imprint on our present experiments and how one would scrutinize and constrain such DM models.

Recently, studies of dark matter phenomenology in the presence of nontrivial evolution of cosmological background have become the domain of growing interest [26,27,32,38–40,55,61,79]. One such exciting nonstandard cosmological picture is a fast expansion [80,81], where the energy budget is dominated via a species ϕ with $\rho_\phi \propto a^{-(4+n)}$ provided $n > 0$ and with $a(t)$ being the scale factor, redshifting faster than the radiation. Although ϕ drives the early Universe's expansion, the subsequent radiation-dominated background can be realized naturally since the energy density of ϕ dilutes faster than radiation. Several works have investigated the effect of fast expansion on freeze-in production of dark matter, see, for example, Refs. [55,79,81].

One of the main difficulties of freeze-in dark matter is its detection prospects due to the feeble nature of the interaction with the SM. However, it is possible to probe freeze-in dark matter at a collider if the DM is directly produced from the decay of a heavy dark sector mediator that can substantially interact with the SM. This Yukawa-type interaction involves a heavy particle beyond the standard model (BSM), a SM particle, and a DM. Such dark matter particles can be as light as keV, but one must remember that it cannot be lower than 12 keV, and this strong lower bound comes from the Lyman- α constraint [82–84]. Here, the heavy mediator can be produced abundantly at the collider and then decays further to SM particles and DM through a feeble interaction.

Interestingly, the same decay process also enters the freeze-in dark matter production mechanism and helps to realize the desired relic density of DM. Hence, this picture has an exciting natural connection between the collider signature and the cosmological background. For a heavy mediator mass of around a few hundred GeV, signatures with long-lived particle (LLP) searches or displaced vertex (DV) provide us with an excellent avenue to probe this picture. At least, that was the setup in almost all of the previous works while considering DM evolution in a

radiation-dominated background. As mentioned earlier, this picture is bound to change if the freeze-in occurs in a fast-expanding Universe. In that case, such modified cosmology demands a larger interaction strength than a conventional radiation-dominated case, resulting in the prompt decay of heavy mediators and poor performance by LLP or DV searches at the LHC.

In this work, we study the impact of nonstandard cosmology on dark matter production and demonstrate how to probe such DM at colliders in the context of the simplified hadrophilic model. Here, dark matter generation occurs via the vectorlike heavy quark, where alternative cosmology mandates a more considerable interaction strength than usual to satisfy the relic density constraints. Naturally, the probing methodology at the collider also changes since prompt decay occurs instead of offering a DV signature. The hadrophilic model is the minimal extension of the SM and contains a single vectorlike quark (VLQ) that mediates the interaction between the FIMP dark matter and the SM quarks. The VLQ is an isospin singlet, but depending on its hypercharge, it can have either $2/3e$ or $-1/3e$ electromagnetic charge. The present study offered a collider analysis of this model for a $2/3e$ charge VLQ, a pair of which can be copiously produced at the LHC. Interestingly, this study probes the model entirely independent of the BSM couplings¹ and solely depends on the QCD coupling constant (α_s) and the mass of the VLQ. After pair production, each VLQ promptly decays into a top quark along with the dark matter. The resulting products from top quarks in the final state can form toplike boosted fatjets because of the significant mass difference between the VLQ and DM. We utilize jet substructure variables to exploit the internal structure within the fatjets that help to segregate three-pronged top fatjets from the vast SM backgrounds, generating two boosted fatjets with a significant missing transverse momentum (MET). Furthermore, our investigations incorporate one-loop QCD corrections of the VLQ pair production processes for an accurate event rate and differential distributions. We leverage an advanced multivariate analysis, employing a boosted decision tree to optimize our event selection, further enhancing signal and background discrimination.

This article is designed as follows. In Sec. II, we discuss the simplified dark matter model. Section III describes a brief sketch of the nonstandard cosmological picture. Dark matter phenomenology and the impact of modified

¹Model independence is ensured since the decay of the VLQ is prompt owing to the impact of nonstandard cosmology, as considered in this work. Hence, the projected constraint from this analysis is expected to be insensitive to the BSM coupling, as can be followed in the final result. This is contrary to the complementary searches through LLP or DV, which are most effective when the BSM coupling between the VLQ with the SM quark and dark matter is minuscule, producing displaced decay VLQs at a specific range of detectors.

cosmology are further demonstrated in Sec. IV. Sections V and VI are devoted to the proposed collider analysis and the current and expected reach of the LHC based on our analysis. Finally, we conclude in Sec. VII.

II. THE MODEL

We extend the SM by a real singlet scalar dark matter candidate S of mass m_S , neutral under SM symmetry group $SU(3)_c \times SU(2)_L \times U(1)_Y$, along with a vectorlike up-type quark Ψ with mass m_Ψ , an $SU(2)$ singlet. The dark sector particles transform odd under the discrete $\mathcal{Z}_2$ symmetry, while the SM particles transform trivially under it. The unbroken $\mathcal{Z}_2$ symmetry not only forbids the mixing between heavy VLQ with SM quarks or S with the SM Higgs doublet (H), but also it ensures the stability of DM provided $m_S < m_\Psi$. Charge assignments for the fields relevant to our study under different symmetry groups are displayed in Table I. In this minimal freeze-in dark matter scenario, DM interacts with the SM particles through the Yukawa-type interaction involving a left-handed component of the vectorlike quark and a right-handed up-type quark. The Lagrangian of the scalar can be written as

$$\mathcal{L} = |D^\mu H|^2 + \frac{1}{2}(\partial^\mu S)^2 - V(H, S) \quad (2.1)$$

with

$$D^\mu = \partial^\mu - ig \frac{\sigma^a}{2} W^{a\mu} - ig' Y B^\mu, \quad (2.2)$$

where g and g' refer to the $SU(2)_L$ and $U(1)_Y$ gauge couplings, respectively. The general form of the scalar potential can be given as

$$V(H, S) = -\mu_H^2(H^\dagger H) + \lambda_H(H^\dagger H)^2 + \frac{\mu_S^2}{2}S^2 + \frac{\lambda_S}{4}S^4 + \lambda_{SH}S^2(H^\dagger H). \quad (2.3)$$

In the limit, $\mu_H^2, \mu_S^2 > 0$, the vacuum expectation value of both the scalars can be obtained by minimizing the scalar potential as

$$\langle H \rangle = v, \quad \langle S \rangle = 0. \quad (2.4)$$

TABLE I. Charge assignments for some relevant fields under different symmetry groups.

	H	S	Ψ
$SU(3)_c$	1	1	3
$SU(2)_L$	2	1	1
$U(1)_Y$	1/2	0	2/3
$\mathcal{Z}_2$	Even	Odd	Odd

Note that the parameter μ_S is related to the DM mass, as followed from Eq. (2.3),

$$m_S^2 = \mu_S^2 + \lambda_{SH}v^2. \quad (2.5)$$

The Lagrangian for the BSM fermion is given by

$$\mathcal{L}_f = i\bar{\Psi}\gamma_\mu D^\mu \Psi - m_\Psi \bar{\Psi}\Psi - \sum_f \tilde{y}_f (S\bar{\Psi}P_R f + \text{H.c.}), \quad (2.6)$$

where $f = \{u, c, t\}$, $P_R (= \frac{1+\gamma_5}{2})$ is the right-handed projection operator, and $\tilde{y}_f$ represents the Yukawa coupling. Similar simplified models were considered in the Refs. [21,79,85].

In this work, we are interested in dark matter production through freeze-in processes via the BSM-Yukawa interaction. To simplify our demonstration, we set the Higgs portal interaction strength $\lambda_{SH} = 0$ that prohibits the additional channels. The self-coupling, λ_S , is also irrelevant to our study. We only consider the top quark interaction in the rest of our analysis.² In this case, the model is termed as a top-philic model. So, the relevant parameters for the dark matter phenomenology are $\{m_S, m_\Psi, \tilde{y}_t\}$.

III. FAST EXPANDING UNIVERSE

The most favored concept of the origin and evolution of our Universe is encapsulated in the form of the standard model of cosmology that assumes the radiation component dominated the energy budget of the early Universe. However, cosmological observations have yet to rule out the possibility that some other species have dominated the energy density of the early Universe instead of radiation before the onset of BBN. The new energy component can redshift faster (or slower) than the radiation energy density ρ_R , which evolves with $\rho_R \propto a(t)^{-4}$, with $a(t)$ being the scale factor. Several prior works have demonstrated the impact of such alternative cosmology on DM phenomenology [55,79,81].

Here, we consider a scenario where a new species, ϕ , dominantly contributes to the total energy density along with the radiation component of the Universe. It is important to mention that we assume that ϕ starts dominating the energy budgets of the early Universe once the inflationary reheating is over.³ The energy density of the

²Such a setup naturally leads to minimal flavor violation, and these effects are subdued as a result of the smallness of the freeze-in coupling.

³We have assumed that the reheating temperature is much larger than all the mass scales involved in our theory. It is essential to mention that in the case of early matter domination, the matter field has to decay to start radiation domination. However, in the case of fast expansion, radiation domination comes naturally. As a result, entropy injection occurs in an early matter domination scenario, which is absent in the expanding universe case.

field ϕ redshifts faster than radiation as $\rho_\phi \propto a(t)^{-(4+n)}$ with the equation of state $\omega = \frac{1}{3}(n+1)$ provided $n > 0$. Note that $\omega = \frac{1}{3}$ for $n = 0$ recreates the behavior like a radiation. In the presence of ϕ , the expansion in the early Universe is driven jointly by both the energy components, so the modified Hubble rate can be expressed by using the Friedmann equation as

$$H^2 = \frac{\rho_R + \rho_\phi}{3M_P^2}, \quad (3.1)$$

where $M_P (= 2.4 \times 10^{18} \text{ GeV})$ refers to the reduced Planck mass. Now, the total energy density of the Universe as a function of temperature can be described as [80]

$$\begin{aligned} \rho(T) &= \rho_R(T) + \rho_\phi(T) \\ &= \rho_R(T) \left[1 + \frac{g_*(T_r)}{g_*(T)} \left(\frac{g_{*S}(T)}{g_{*S}(T_r)} \right)^{(4+n)/3} \left(\frac{T}{T_r} \right)^n \right], \end{aligned} \quad (3.2)$$

where $\rho_R(T) = \frac{\pi^2}{30} g_*(T) T^4$, where T_r represents the temperature at which the fast expansion phase ends, after which the Universe enters to the radiation-dominated era. $g_*(T)$ and $g_{*S}(T)$ refer to the relativistic degrees of freedom of energy and entropy, respectively. In this case, the modified Hubble rate can be approximated as [80]

$$H(T) \simeq \frac{\pi\sqrt{g_*}}{3\sqrt{10}M_P} \left(\frac{T}{T_r} \right)^{n/2}, \quad (T \gg T_r). \quad (3.3)$$

It is clear from the expression that the Hubble rate at any point of the fast expansion stage is always larger than the same for the radiation-dominated background. Interestingly, the impact of nonstandard cosmology can be understood by the simple parametrization of two parameters, n and T_r . Increasing n (or decreasing T_r) points toward an even faster expansion of the Universe. Parametrizing the effect of the extra species ϕ by the effective number of relativistic degrees of freedom and then considering the observational bound on the same, one can obtain a bound on the reference temperature as $T_r \geq (15.4)^{1/n} \text{ MeV}$. In addition, the temperature smaller than the BBN temperature ($T_{\text{BBN}} \simeq 4 \text{ MeV}$) is in tension with the cosmological observation, and it also puts a stringent lower bound on T_r .

The scenario with $0 < n \leq 2$ can be reached by introducing a positive scalar potential, whereas a negative potential is associated with $n > 2$. The $n = 2$ case is particularly interesting, referring to the well-motivated quintessence fluid [80]. This regime is also known as the kination era, as kinetic energy dominates over potential energy, where the energy density falls as $\rho_\phi \propto a(t)^{-6}$. Throughout our present analysis, we primarily focus on the dark matter production during the kination phase

(i.e., $\omega = 1$) to showcase the DM evolution and collider signature exploring the dark sector.

IV. DARK MATTER PHENOMENOLOGY

In our present setup, the vectorlike quark (Ψ) remains part of the primordial thermal bath in addition to the SM particles owing to its gauge interaction with them. However, the dark matter particle S always remains out of thermal equilibrium due to the tiny Yukawa interaction ($\tilde{y}_t \ll 1$), which connects it with the SM quarks via the vectorlike fermion Ψ . Hence, starting from zero or a negligibly small initial number density of DM in the early Universe, it gradually populates from the decay and scattering of the bath particles. The freeze-in process attains the final DM number density. However, that essentially depends on the background of cosmology in the early Universe. In particular, it depends on the parameters n and T_r in the case of an expanding early Universe.

DM production can occur via the scatterings ($t\bar{t} \rightarrow SS, \Psi\Psi \rightarrow SS$) and⁴ the decay $\Psi \rightarrow tS$. Note that the scattering cross sections and decay rate are proportional to $\tilde{y}_t^4$ and $\tilde{y}_t^2$, respectively. For $\tilde{y}_t \ll 1$, the scattering remains subdominant compared to the decay, so the DM production mainly proceeds via the decay of Ψ . The following Boltzmann equation governs the freeze-in production of DM through the decay process:

$$\frac{dn}{dt} + 3Hn = \frac{g_\Psi m_\Psi^2 \Gamma_\Psi}{2\pi^2} T K_1 \left(\frac{m_\Psi}{T} \right). \quad (4.1)$$

The decay width of the vectorlike fermion is

$$\Gamma_\Psi = \frac{\tilde{y}_t^2}{32\pi} \frac{(m_\Psi^2 + m_t^2)(m_\Psi^2 - m_t^2)}{m_\Psi^3}, \quad (4.2)$$

and $n(t)$ represents the number density of DM, g_Ψ is the internal degrees of freedom of Ψ , and $K_1(\cdot)$ refers to the modified Bessel function of first kind. Rewriting the DM abundance in terms of $Y = n/s$, with s being the entropy density, and the dimensionless variable $x = m/T$, one can recast the Eq. (4.1) in the following form:

$$\frac{dY}{dx} = \frac{\langle \Gamma_\Psi \rangle}{Hx} Y_\Psi^{\text{eq}}(x), \quad (4.3)$$

where $Y_\Psi^{\text{eq}}(x)$ denotes equilibrium abundance of the vectorlike fermion. $\langle \Gamma_\Psi \rangle$ is the thermally averaged decay rate, expressed as $\Gamma_\Psi \frac{K_1(x)}{K_2(x)}$, with $K_2(x)$ being the modified Bessel function of second kind. Now, one can obtain the relic density after evaluating the final freeze-in DM abundance

⁴The scattering via Higgs mediation can also contribute, but for simplicity we do not consider this contribution by setting the Higgs portal coupling (λ_{SH}) to zero.

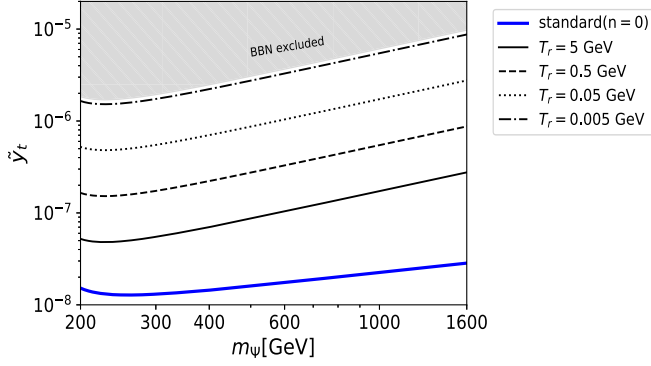


FIG. 1. In different early Universe cosmological evolution scenarios, contours that satisfy the dark matter relic density constraint $\Omega h^2 = 0.12$ are shown in the Yukawa coupling ($\tilde{y}_t$) and vectorlike quark mass m_ψ plane for the freeze-in dark matter model. The thick blue solid line refers to the standard radiation-dominated (or $n = 0$) background picture. In contrast, the thin (solid, dashed, dotted, and dash-dotted) lines correspond to different values of the nonstandard cosmological parameter $T_r (= 5, 0.5, 0.05, 0.005 \text{ GeV}$, respectively) for a fixed $n (= 2)$. The dark matter mass is set at $m_S = 12 \text{ keV}$.

by solving Eq. (4.3) numerically and plugging it in the following equation:

$$\Omega h^2 = 2.755 \times 10^8 \times m_S \times Y(x \rightarrow \infty). \quad (4.4)$$

In addition, one can also calculate the relic density of DM by using the following expression, deduced by solving Eq. (4.3) analytically:

$$\Omega h^2 \simeq \frac{2.755 \times 10^8 \times 45}{4\pi^4 \times 1.66} \times \frac{M_P g_\psi \Gamma_\psi T_r^{\frac{n}{2}}}{\sqrt{g_* g_{*s}}} \times \frac{m_S * 2^{2+\frac{n}{2}}}{m_\psi^{2+\frac{n}{2}}} \Gamma\left(\frac{6+n}{4}\right) \Gamma\left(\frac{10+n}{4}\right). \quad (4.5)$$

Here, g_* and g_{*s} are the effective number of relativistic degrees of freedom contributed to the energy and entropy density, respectively, and $\Gamma(\dots)$ denotes the standard notation for the gamma function. In Fig. 1, we show that the

relic density satisfied contours for the radiation-dominated (standard, $n = 0$) and modified cosmology with different values of T_r for a fixed $n = 2$. Here, the thick blue solid line represents a radiation-dominated scenario and $T_r = 5, 0.5, 0.05, 0.005 \text{ GeV}$ contours are denoted by the thin solid, dashed, dotted, and dot-dashed lines, respectively. The gray-shaded region is ruled out since the temperature T_r , if lower than the BBN temperature ($\simeq 4 \text{ MeV}$), conflicts with the cosmological observation. These contours clearly demonstrate the requirement for a larger coupling for a fixed mass as one decreases the value of T_r . Lowering T_r means that expansion will be faster, necessitating a larger interaction, i.e., larger coupling to compensate for this effect and satisfy the relic density. It is imperative to know whether the DM is still out of equilibrium for such a large coupling. One can check that the coupling required to reach thermal equilibrium with the thermal bath is almost 2 orders of magnitude larger than the same to satisfy correct order relic density, and it is further discussed in detail in Appendix A 1.

Before discussing the specifics of the collider searches, we elucidate a few representative benchmark points, as outlined in Table II. These benchmarks satisfy all relevant constraints, including the correct relic density for the permitted temperatures (T_r). As already discussed, lower T_r implies a faster Universe expansion rate, as per Eq. (3.3). Corresponding decay lengths of the VLQ are provided in the final column of Table II. For a clear comparison, one reference benchmark point (BP0) is also added considering the standard radiation-dominated (or $n = 0$) background, which clearly demonstrates the usefulness of a probe with a long-lived particle or displaced vertex signature. However, such a recipe is ineffective for the remaining BPs with alternative cosmology ($n > 0$), which is our primary motivation for finding alternative signatures in this study.

V. PROBING DARK SECTOR AT THE LHC

The presence of a VLQ and its stronger Yukawa interaction with the FIMP candidate opens up intriguing opportunities for exploring the dark sector through an

TABLE II. A list of benchmark points (BP1–BP3) is presented with the corresponding parameters chosen for our study on the freeze-in dark matter model under the influence of nonstandard cosmology. For an explicit comparison, one additional reference benchmark point (BP0) is added for the standard radiation-dominated (or $n = 0$) background. Note the remarkably tiny coupling needed in BP0 to satisfy the correct relic density and demonstrate the usefulness of a probe with a long-lived particle or displaced vertex signature in this case. But that is ineffective for the rest of the BPs with alternative cosmology ($n > 0$), and we propose an alternative search strategy in the present work.

Benchmark points	$\tilde{y}_t$	m_ψ [GeV]	m_S [KeV]	n	T_r [GeV]	$\Omega_S h^2$	Γ_ψ [GeV]	$c\tau_\psi$ [mm]
BP0	2.25×10^{-8}	1000	12	0	...	0.12	5.03×10^{-15}	39.35
BP1	1.0×10^{-6}	800	12	2	0.095	0.12	7.94×10^{-12}	0.025
BP2	3.0×10^{-7}	1080	12	2	1.929	0.12	9.66×10^{-13}	0.205
BP3	5.0×10^{-7}	1500	12	2	1.339	0.12	3.73×10^{-12}	0.053

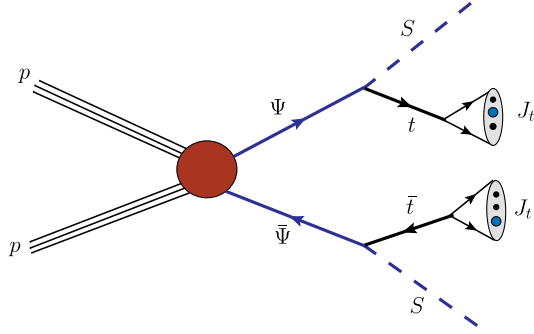


FIG. 2. A diagrammatic representation of two toplike fatjets and MET signature through pair production of vectorlike quarks at the LHC. Many a times, one or both of these fatjets can be mimicked by the QCD radiation, especially for the background processes.

alternative approach at the collider. The colored $2/3e$ electromagnetic charged VLQ, in principle, can interact with all up-type standard model quarks and dark matter via Yukawa interactions. As a Z_2 -odd particle, the VLQ does not mix with SM quarks. We focus on a scenario where the VLQ couples predominantly to the top quark, while its interactions with lighter up and charm quarks are either absent or negligibly small. Due to this top-philic nature, VLQ production at the LHC occurs primarily through pair production, making their searches at the LHC largely model independent.⁵ The production of VLQ with dark matter at the LHC is not feasible in this top-philic scenario.⁶ The leading-order (LO) production channels, illustrated in the top row of Fig. 3, depend solely on the strong coupling constant (α_S) and the mass of the VLQ.

Hence, displaced vertex searches at the LHC have been a primary approach for probing FIMP dark matter models. However, in our alternative cosmological scenario, the requirement for a comparatively larger Yukawa coupling reduces the decay length of the VLQ. The decay length in all sample benchmark points is less than a centimeter, indicating prompt decay. This suggests that, for a significant mass gap between the VLQ and dark matter, prompt searches for FIMP dark matter models at the LHC are feasible under this modified cosmology. Such searches could offer better sensitivity compared to displaced vertex searches. To further improve the reach of our analysis,

⁵Please note that in case the VLQ couples to the first two generation SM quarks, a DM-mediated t-channel process via quark-antiquark annihilation can also contribute to VLQ pair production, consequently imparting the BSM model dependence in the production cross section.

⁶If the VLQ has nonzero interaction with light SM quarks, then associated production of VLQ with the DM is possible. The production cross section is $\sigma(pp \rightarrow \Psi S)_{\text{LO}} \sim \mathcal{O}(\alpha_S \tilde{y}_t^2)$. Given that $\tilde{y}_t \ll 1$, the contribution of associated production remains negligible compared to the dominant pair production cross section of the VLQ.

TABLE III. The cross section for the VLQ pair production at the 14 TeV LHC at the LO and NLO with integrated K-factor are shown for 14 TeV LHC. The superscripts and subscripts indicate the theoretical scale uncertainties (in percentages) of the total cross section considering an envelope of renormalization (μ_R) and factorization (μ_F) scale variation around the central scale, as discussed in the text.

	m_Ψ [GeV]	$\sigma(pp \rightarrow \Psi\bar{\Psi})$ (fb)		
		LO, $\mathcal{O}(\alpha_S^2)$	NLO, $\mathcal{O}(\alpha_S^3)$	K-fac
BP1	800	$129.7^{+28.6\%}_{-20.8\%}$	$187.9^{+8.8\%}_{-10.6\%}$	1.45
BP2	1080	$18.95^{+28.7\%}_{-20.9\%}$	$26.62^{+10.0\%}_{-11.3\%}$	1.40
BP3	1500	$1.787^{+29.2\%}_{-21.3\%}$	$2.327^{+10.9\%}_{-11.9\%}$	1.30

we will employ jet substructure techniques and advanced multivariate analysis methods to enhance the signal.

To investigate this model at the LHC, we focus on producing the VLQ pair. After production, each VLQ decays into a top quark and a dark matter particle. Consequently, the final state consists of two top quarks and a pair of dark matter candidates. The signal topology is as follows:

$$pp \rightarrow \Psi\bar{\Psi} \rightarrow (t, S), (\bar{t}, S) \equiv 2J_t + \text{MET}. \quad (5.1)$$

The noninteracting DM particles do not leave any detectable traces in the detector, contributing to some measurable signature, termed missing transverse momentum (also customarily labeled as MET), from the momentum imbalance of all the visible products at the detector. If the mass gap between the VLQ and the DM is substantial, produced top quarks from the decay of heavy VLQs are highly boosted, causing their hadronic outcomes to form large-radius, three-prong fatjets. Thus, the final signature includes two such toplike fatjets and significant MET⁷ (see Fig. 2 for a diagrammatic representation). The LO cross section for VLQ pair production is presented in Table III. To improve the precision of our estimate, we also account for one-loop QCD corrections to the VLQ pair production processes, providing more accurate cross sections and differential distributions of various kinematic observables. Some representative virtual one-loop QCD-corrected Feynman diagrams are shown in the last two rows of Fig. 3.

The total next-to-leading-order (NLO) QCD cross section is also provided in Table III for the central choices of renormalization (μ_R) and factorization (μ_F) scales. μ_R and μ_F are fictitious scales that appear through higher-order

⁷Interested readers can find that the same final state can be realized in other BSM scenarios, such as searches for heavy scalar leptoquark [86,87]. A comprehensive collider analysis, combined with polarization variables, is utilized to exclude some model parameters and distinguish between different scalar leptoquark models.

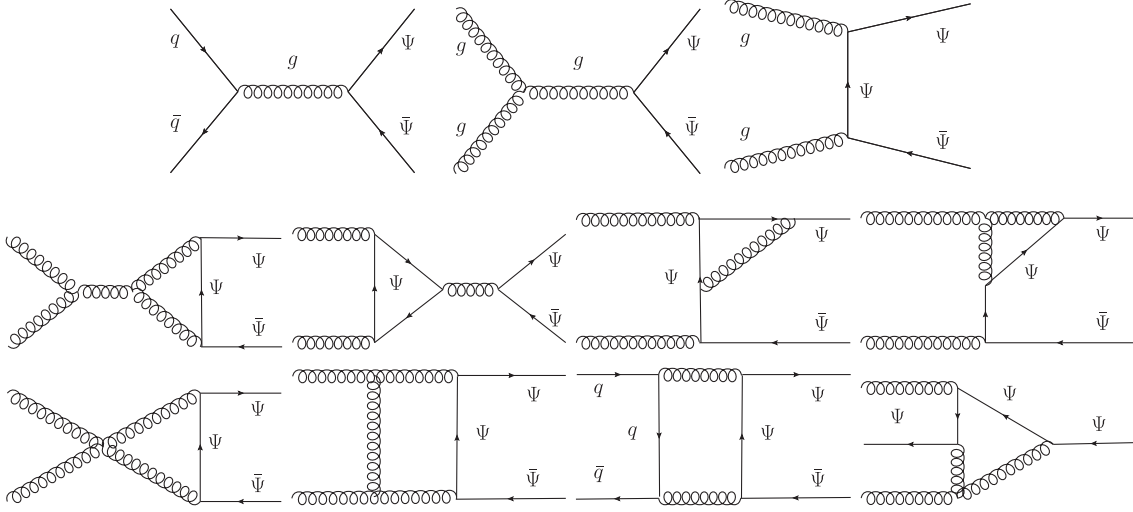


FIG. 3. The upper row displays the parton level leading-order Feynman diagrams for VLQ pair production. In our study, we consider one-loop correction in α_s of all these diagrams, and some of the representative virtual diagrams are shown in the lower two rows.

calculations and parton distribution functions. The central choice is set at the dynamical partonic center-of-mass energy scale of the process, i.e., $\mu_R = \mu_F = \sqrt{\hat{s}}$. The scales are further varied as $\mu_R = \zeta_1 \sqrt{\hat{s}}$ and $\mu_F = \zeta_2 \sqrt{\hat{s}}$, with ζ_1 and ζ_2 taking values from the set $\{1/2, 1, 2\}$, generating a total of nine datasets around the central scale. The superscripts and subscripts in the cross sections represent the envelope of these nine datasets, denoting the theoretical scale uncertainty associated with each cross section. As shown in Table III, the NLO cross section is substantially higher than the LO prediction, and the scale uncertainties are significantly reduced by implementing the NLO calculation. The K-factor, defined as the NLO to LO cross section ratio, is also provided in Table III.

A. Simulation details and backgrounds

We implement the extended standard model, as represented in different terms of the Lagrangian, in Eqs. (2.1) and (2.6) in FeynRules [88] and use the NLOCT [89] package to generate the UV and R_2 counterterms and generate the NLO Universal FeynRules Output (UFO) model file. The signal and background events are generated utilizing the MadGraph5_aMC@NLO [90] environment. Our analysis includes all background processes that can mimic the signal. Background events are generated with two to four additional QCD jets using the MLM matching [91,92] scheme. All standard model backgrounds are further scaled using available higher-order QCD cross sections. The generated parton level events are further passed through Pythia8 [93,94] for parton showering, fragmentation, and hadronization. The NNPDF3.0 [95] LO and NLO parton distribution function (PDF) sets are utilized to generate leading-order and next-to-leading-order events, respectively. These showered events are also processed through Delphes3 [96] to simulate detector effects. Jets with a radius

parameter of 0.4 are constructed using the anti- k_T [97] clustering algorithm. Fatjets are formed using Delphes towers with a radius of 1.5, clustered with the anti- k_T algorithm. The radius parameter, R , of a fatjet scales approximately as $R = \frac{2M_J}{p_T(J)}$, where M_J is the fatjet mass (top quark mass in our case), and $p_T(J)$ is its transverse momentum. Fastjet 3.2.2 [98] is used for clustering, requiring each fatjet to have a minimum transverse momentum of $p_T \geq 200$ GeV. Subsequently, we further recluster the constituents of each fatjet using the Cambridge-Aachen (CA) algorithm [99] to perform pairwise clustering for the soft drop procedure [100]. Soft drop grooming eliminates soft and wide-angle unassociated constituents of the fatjets. Finally, we utilize the adaptive boosted decision tree (BDT) algorithm [101–103] for multivariate analysis (MVA) within the Toolkit for Multivariate Analysis (TMVA) framework [104].

The primary standard model background for the signal arises from semileptonic top quark pair production $t\bar{t} + \text{jets}$. In semileptonic decay, one top quark decays hadronically, resulting in a fatjet, while the other decays leptonically. The misidentified charged lepton and the neutrino from the top decay contribute to the MET. Conversely, when both top quarks decay hadronically, producing two fatjets, the requirement for high missing transverse momentum reduces this background significantly. This reduction occurs because the MET, in this case, primarily arises from jet mismeasurements, and imposing a cut of $\text{MET} \geq 150$ GeV further diminishes the background. The semileptonic $t\bar{t} + \text{jets}$ background is generated with two additional QCD jets using an MLM matching scheme, with one of these QCD jets mimicking another fatjet.

Other significant backgrounds include $V + \text{jets}$, where V represents either the Z or $W^\pm$ boson. In the case of $Z + \text{jets}$, two neutrinos from the invisible decay of the Z boson contribute to a large MET. In contrast, for $W + \text{jets}$, the

MET arises from the neutrino and the misidentified charged lepton produced in the leptonic decay of the W boson. A generation-level cut on $\text{MET} > 80$ GeV is applied to both backgrounds. Additionally, each background is generated with four extra QCD jets using an MLM matching scheme, and these QCD jets imitate fatjets in both cases.

$tW + \text{jets}$ provides another significant SM background that mimics the signal. In this process, either the top quark or the W boson decays leptonically, resulting in a large MET, while the other decays hadronically and is reconstructed as a fatjet. This background is generated with up to two additional jets using MLM matching, and the second fatjet arises from these QCD jets.

We also consider the diboson + jets background, which includes $pp \rightarrow W^\pm Z, W^+W^-$, and ZZ productions. In these processes, one of the weak bosons decays either invisibly or leptonically, leading to a significant MET, while the other boson decays hadronically, forming a fatjet. All diboson backgrounds are generated with two additional QCD jets using an MLM matching scheme. The second fatjet arises from these QCD jets.

All the backgrounds mentioned above are normalized using the available higher-order QCD-corrected cross sections [105–109].

B. High-level variables

We now define some of the reconstructed variables that probe the internal structure within the fatjets and thus have a close connection with the original colored particle from which these final state hadrons originated. They are immensely powerful in reducing the unassociated soft and wide-angle QCD contributions, leading to improved prediction of fatjet properties and masses.

N -subjettiness ratio: in the previous section, we noted that one or more QCD radiation mimics fatjets in the background. At the same time, for the signal, both fatjets are the result of the hadronic decay of boosted top quarks. Therefore, analyzing how the constituents of a fatjet are distributed within both the leading and subleading fatjets can help distinguish the signal from the background. N -subjettiness is one such powerful variable employed for this purpose. It seeks to identify N lobes within a boosted fatjet that correspond to N -subjets. For example, let J be a boosted fatjet and $a_1, a_2, \dots, a_N$ are sets of N -axes within the fatjet. The un-normalized N -subjettiness [110] is then defined as follows:

$$\tau_n = \sum_i p_{T_i} \min\{\Delta R_{i,1}^\beta, \Delta R_{i,2}^\beta, \dots, \Delta R_{i,n}^\beta\}. \quad (5.2)$$

The summation includes all constituent particles within the fatjet, with p_{T_i} representing the transverse momentum of the i th constituent. $\Delta R_{i,j}$ denotes the separation of the i th constituent from the j th axis in the rapidity-azimuth plane. The minimization in Eq. (5.2) is performed by varying the

axis directions. The choice of axes is not unique—one minimization procedure that uses a variant of the k -means clustering algorithm is described in Ref. [111]. For our analysis, we consider winner-takes-all k_T -axes [112–114] and choose $\beta = 1.0$ in Eq. (5.2). We define two variables for each fatjet: τ_{32} and τ_{21} . τ_{32} is the ratio of τ_3 to τ_2 and is particularly effective in distinguishing three-prong toplike fatjets from those with one or two prongs [115].

Soft drop: jet mass is another good variable for discrimination between the toplike fatjets from the QCD jets. The large radius fatjets are pronged to capture soft and wide-angle constituents that are not part of the original jet. Soft drop grooming/tagging [100] is a procedure to groom away those unassociated constituents and correctly predict the fatjet mass. We use a soft drop grooming method to remove those contaminants. We construct fatjets of radius $R_0 = 1.5$ using the anti- k_T algorithm. After that, we recluster the constituents of each fatjet with the CA algorithm to create a pairwise angular-ordered clustering tree. The subsequent steps involve applying the soft drop algorithm as follows:

- (1) After clustering the jet, j , using the CA algorithm, decluster its last recombination stage and label them as two subjets, j_1 and j_2 .
- (2) Now check the following condition:

$$\frac{\min\{p_{T_{j_1}}, p_{T_{j_2}}\}}{p_{T_{j_1}} + p_{T_{j_2}}} > z_{\text{cut}} \left(\frac{\Delta R(j_1, j_2)}{R_0} \right)^\beta, \quad (5.3)$$

where $p_{T_{j_1}}$ and $p_{T_{j_2}}$ are the subjets' transverse momentum, and their distance in the rapidity-azimuth plane is $\Delta R(j_1, j_2) = \sqrt{(y_1 - y_2)^2 + (\phi_1 - \phi_2)^2}$.

- (3) If the condition is satisfied, set the jet j as a final soft drop jet. If not, discard the softer subjet and prompt the harder subjet as j . Iterate the procedure from step 1.

The soft drop procedure relies on two parameters: a soft threshold, z_{cut} , and an angular exponent, β . The procedure returns the original ungroomed jet when $z_{\text{cut}} \rightarrow 0$ or $\beta \rightarrow \infty$. Soft drop grooming mode is infrared and collinear safe for $\beta > 0$. In our analysis, we set $\beta = 1.0$ and $z_{\text{cut}} = 0.1$ [100]. For $\beta = 0$, the method reduces to the modified mass drop tagger. In this scenario, grooming depends exclusively on the momentum fraction z_{cut} and is independent of the angular separation. However, as β increases, greater emphasis is placed on wide-angle radiations, whereas smaller values of β suppress their influence.

C. Event selection

The following baseline selection criteria are used to select the events for our analysis:

- (1) Each event must contain at least two fatjets of radius 1.5, having substantial transverse momentum $p_T(J_0), p_T(J_1) > 200$ GeV within a rapidity range

of $|\eta| < 2.5$. J_0 and J_1 are leading and subleading fatjets, respectively.

- (2) Events contain considerable missing transverse momentum, $\text{MET} > 80$ GeV.
- (3) To reduce the impact of jet mismeasurements on the missing transverse momentum, event selection criteria are applied on the azimuthal separation between any fatjet and the MET, $\Delta\phi(J_i, \text{MET}) > 0.2$ ($i = 0, 1$).

In addition to these baseline selection criteria, we applied the following additional event selection criteria to reduce overwhelming backgrounds before the MVA:

- (4) A lepton veto is applied since no isolated lepton is expected from the signal. We discard any event that contains a lepton ($l = e^\pm, \mu^\pm$) with $p_T \geq 10$ GeV and within $|\eta_e| < 2.1$ and $|\eta_\mu| < 2.4$.
- (5) The signal consists of two top quarks in the final state, each decaying into a b quark and hadronic products from W boson. Tagging a b -jet within either fatjet enhances the signal-to-background ratio. We require a b -tagged subjet within the leading or subleading fatjet (J_0 or J_1), utilizing the default b -tagging efficiency provided by the Delphes CMS card, as described in Ref. [116].
- (6) MET has further increased from 80 to 150 GeV.
- (7) Since both the fatjets in the signal originate from the top quarks, we demand a larger soft drop jet (defined in Sec. VB) mass for both fatjets, $M_{J_0}, M_{J_1} > 100$ GeV.

Table IV presents the cut flow for the signal (BP1 and BP2) and all SM background processes, including the cut efficiency and the number of events at an integrated luminosity of 300 fb^{-1} at the 14 TeV LHC. Notably, the cut efficiencies for BP3 and BP2 are nearly identical. From the table, the following observations can be made:

- (i) The lepton veto cut significantly reduces the $t\bar{t}$ + jets, W + jets, and WW + jets' backgrounds while preserving nearly 100% of the signal.
- (ii) A stringent MET cut further suppresses the background effectively.
- (iii) B -tagging within a fatjet substantially reduces the V + jets and VV + jets' backgrounds ($V = Z, W$).
- (iv) Cuts on the soft drop mass of the two leading fatjets further suppress backgrounds that do not originate from top-quark decays.

Figure 4 presents the normalized distributions of certain kinematic variables for the signal (BP1, solid red) and background after applying all the event selection criteria, as discussed before. The filled blue, olive, orange, black, and magenta areas represent contributions from different background processes: $t\bar{t}$ + jets, Z + jets, W + jets, tW + jets, and diboson + jets, respectively. After applying the baseline selection cuts (outlined at the beginning of Sec. VC), some of these kinematic variables are shown in Appendix A 2 in Fig. 9.

The missing transverse momentum distribution is shown in Fig. 4(a). The background decreases sharply at high MET values while the signal distribution remains relatively flat. The source of MET in the signal arises from two dark matter particles produced in the cascade decay of a heavy VLQ pair. This allows the dark matter particles to avail nearly the entire phase space, resulting in a nearly uniform MET distribution up to a certain range. The soft drop mass distributions for the leading and subleading fatjets are presented in Figs. 4(b) and 4(c), respectively. In both distributions, the signal exhibits a peak near the top-quark mass. In contrast, the background shows a peak near the top mass for the leading fatjet, while the subleading fatjet does not exhibit a similar peak. This absence indicates that the subleading fatjet primarily

TABLE IV. After applying the corresponding cuts, the expected number of events and the cut flow for both signal (BP1 and BP2) and background processes for an integrated luminosity of 300 fb^{-1} are presented. The total background is given in the last column.

Cuts	BP1	BP2	$t\bar{t}$ + jets	Z + jets	W + jets	tW + jets	WZ + jets	WW + jets	ZZ + jets	total BG
2 fatjets, $ \eta_i < 2.5$	15411.3	2546	1.2×10^7	6.94×10^6	9.0×10^6	3.3×10^6	105196	491801	30503	3.16×10^7
$p_T(J_i) \geq 200$ GeV ($i = 0, 1$)	[100%]	[100%]	[100%]	[100%]	[100%]	[100%]	[100%]	[100%]	[100%]	[100%]
Lepton veto	15394.3	2543.5	4.27×10^6	6.94×10^6	3.14×10^6	2.67×10^6	105151	154454	30493	1.73×10^7
	[99.9%]	[99.9%]	[36.2%]	[99.9%]	[34.9%]	[81.7%]	[99.9%]	[31.4%]	[99.9%]	[54.7%]
MET > 80 GeV	14853	2492.4	1.91×10^6	6.3×10^6	2.6×10^6	528670	74475	58003	20401	1.16×10^7
	[96.4%]	[97.9%]	[16.2%]	[90.7%]	[29.9%]	[16.2%]	[70.8%]	[11.8%]	[66.9%]	[36.6%]
$\Delta\phi(J_i, \text{MET}) > 0.2$	14255.5	2395.5	1.59×10^6	5.8×10^6	2.35×10^6	385210	66241	46757	18331	1.03×10^7
	[92.5%]	[94.1%]	[13.5%]	[83.5%]	[26.1%]	[11.8%]	[62.9%]	[9.5%]	[60.1%]	[32.5%]
1 b -tagging (within J_0 or J_1)	12029	2006.3	1.28×10^6	1.04×10^6	419492	290469	13799	9643	3471.5	3.06×10^6
	[78.1%]	[78.8%]	[10.9%]	[15.0%]	[4.66%]	[8.91%]	[13.1%]	[1.96%]	[11.4%]	[9.67%]
MET > 150 GeV	11130	1918	410084	633069	194518	88681	8072	3298.5	1935	1.34×10^6
	[72.2%]	[75.3%]	[3.48%]	[9.11%]	[2.16%]	[2.72%]	[7.67%]	[0.67%]	[6.34%]	[4.24%]
SD mass	6852	1233	175971	142991	52094.3	29635.4	1382	765.5	382	403221
$M_{J_i} \geq 100$ GeV	[44.5%]	[48.4%]	[1.5%]	[2.0%]	[0.58%]	[0.9%]	[1.3%]	[0.16%]	[1.3%]	[1.27%]

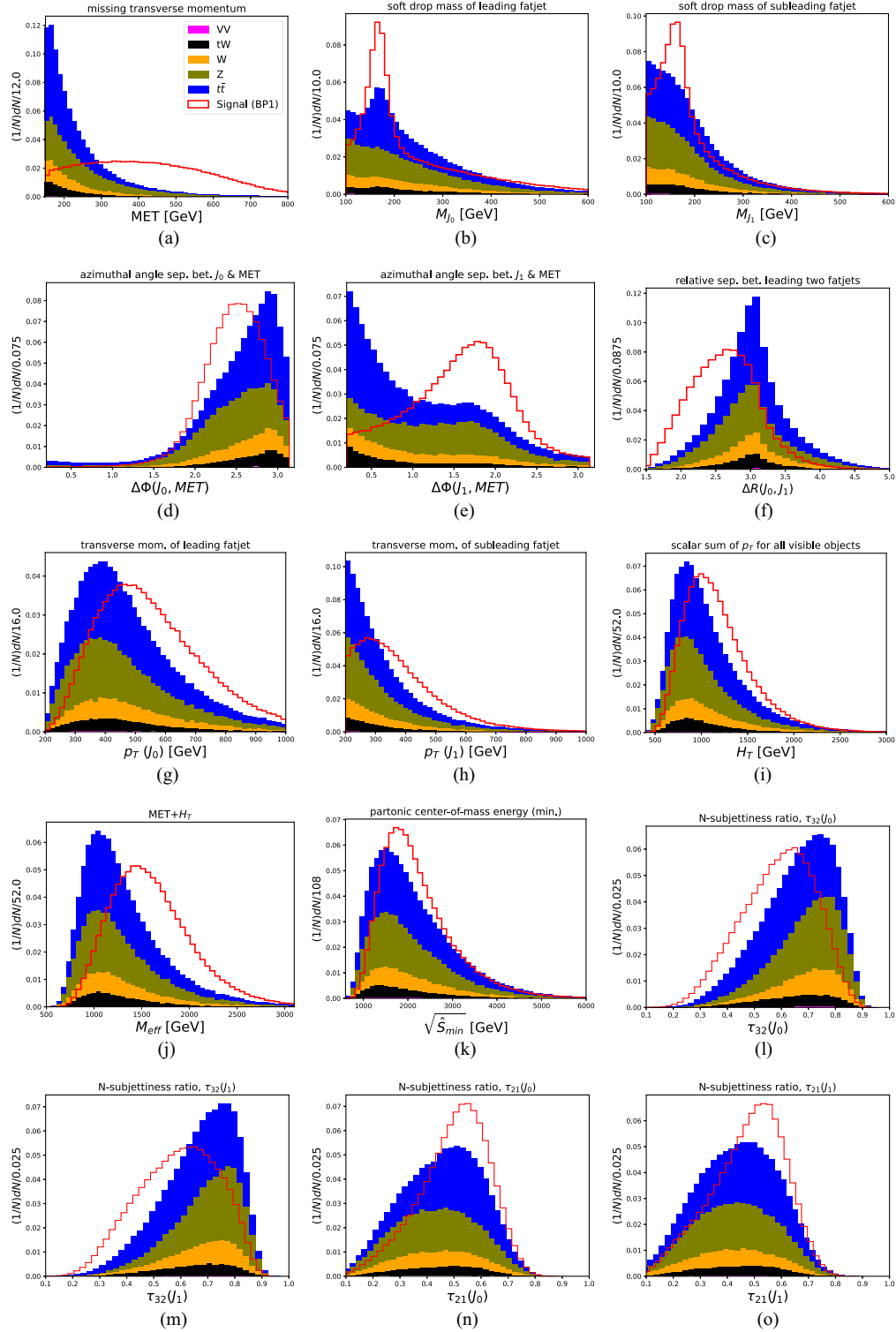


FIG. 4. Stacked histograms of various kinematic observables for SM backgrounds and the signal (BP1) in the fatjets plus the MET final state are shown after applying all the event selection criteria, as discussed in the text. The subfigures show normalized distributions of key kinematic variables: (a) missing transverse momentum, soft drop mass distributions for the (b) leading and (c) subleading fatjets, (d) azimuthal separations between leading fatjet and MET, (e) azimuthal separations between subleading fatjet and MET, (f) the distance between the two fatjets in the $\eta - \phi$ plane, transverse momentum distributions of the (g) leading and (h) subleading fatjets, (i) H_T , (j) M_{eff} , (k) $\sqrt{\hat{s}_{\text{min}}}$, (l) N-subjettiness ratio τ_{32} of the leading fatjet, (m) τ_{32} of the subleading fatjet, (n) τ_{21} of the leading fatjet, and (o) τ_{21} of the subleading fatjet.

originates from QCD radiation in most events. The azimuthal separations between each fatjet and MET are shown in Figs. 4(d) and 4(e), while Fig. 4(f) illustrates the distance between the two fatjets in the $\eta - \phi$ plane, $\Delta R(J_0, J_1) = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$. From these distributions, we observe that the two fatjets are nearly back-to-back in most background events, which is not the case for the signal.

The transverse momentum distributions of the fatjets are illustrated in Figs. 4(g) and 4(h). The distributions of other inclusive variables, H_T , M_{eff} , and $\sqrt{\hat{s}_{\text{min}}}$, are presented in Figs. 4(i)–4(k), respectively, with their definitions provided below:

$$H_T = \sum_{i \in \text{visible}} |\vec{p}_{T_i}|, \quad (5.4)$$

$$M_{\text{eff}} = \text{MET} + \sum_{i \in \text{visible}} |\vec{p}_{T_i}|, \quad (5.5)$$

$$\sqrt{\hat{s}_{\text{min}}} = \sqrt{E^2 - P_Z^2} + \text{MET}. \quad (5.6)$$

Here, p_{T_i} is the transverse momentum of the i th AK4 jet, and the summation runs over all visible jets in the event. E and P_Z represent the total energy and longitudinal momentum component of all visible jets in the event. The distributions of the N-subjettiness ratios $\tau_{32} = \tau_3/\tau_2$ and $\tau_{21} = \tau_2/\tau_1$ for both leading and subleading fatjets are shown in Figs. 4(l)–4(o). As expected, the signal yields a smaller τ_{32} value than the background. N-subjettiness, τ_n , defined in Sec. V B, quantifies the number of subjets within a fatjet. Signal fatjets are predominantly three-pronged, yielding a low τ_3 and high τ_2 values, thus a smaller τ_{32} ratio. In contrast, background fatjets

often appear one- or two-pronged, leading to lower τ_3 and τ_2 values and, consequently, a higher τ_{32} ratio than the signal. As a result, τ_{32} can be a good variable for signal-background discrimination. In contrast, τ_{21} is less effective for this purpose, as signal fatjets are predominantly three-pronged.

The expected number of signals and total background events that survive after applying all the cuts discussed in Sec. V C are presented in the second column of Table VI for the 14 TeV LHC with an integrated luminosity of 300 fb⁻¹. The event yields for individual background processes can be found in the last row of Table IV. The last column of Table VI shows the statistical significance achieved through this traditional cut-and-count search method. Although refining kinematic cuts could enhance statistical significance, we prioritize MVA in the next section, where more sophisticated techniques will be employed for better signal-background discrimination.

D. Analysis based on the multivariate gradient boosting technique

We perform a multivariate analysis utilizing a gradient BDT method to enhance our collider search. Several characteristics of the reconstructed fatjets and the missing transverse momentum are employed as inputs for the BDT. Those variables include the transverse momentum of the fatjets after soft drop, $p_T(J_i)$ ($i = 0, 1$), and their corresponding masses, M_{J_i} , MET, the azimuthal separation between each fatjet and the MET, $\Delta\phi(J_i, \text{MET})$, the separation between fatjets in the rapidity-azimuth plane, $\Delta R(J_0, J_1)$, transverse momentum of the b-jet [$p_T(b)$] that is tagged inside J_0 or J_1 , N-subjettiness ratio $\tau_{32}(J_i)$, $\tau_{21}(J_i)$, and other inclusive variables, H_T , M_{eff} , and $\sqrt{\hat{s}_{\text{min}}}$.

TABLE V. Method unspecific relative ranking of input variables based on their separation power in discriminating the signal (BP1) class from the background before MVA. The same variables are used in all other benchmark scenarios.

	MET	M_{eff}	$\Delta R(J_0, J_1)$	$\Delta\phi(J_1, \text{MET})$	$\tau_{32}(J_0)$	$\tau_{32}(J_1)$	$\Delta\phi(J_0, \text{MET})$	$\tau_{21}(J_0)$	M_{J_0}	$\tau_{21}(J_1)$	M_{J_1}
BP1	34.62	14.28	13.33	12.92	7.39	7.10	5.26	3.16	2.34	2.21	1.55

TABLE VI. The table presents the effectiveness of the search in terms of statistical significance for signal over background at different benchmark points. N_S and N_B indicate the total surviving signal and background events after an optimal BDT cut. The fourth and fifth columns indicate the efficiencies for the signal and background, respectively. The second-to-last column represents the statistical significance of the MVA for 300 fb⁻¹ integrated luminosity. The last column, which represents the statistical significance of cut-and-count searches, is provided for comparison.

	Events before BDT	Optimal BDT cut	Signal efficiency	Background efficiency	N_S	N_B	$\frac{N_S}{N_B}$	Significance ($\frac{N_S}{\sqrt{N_S+N_B}}$)	Significance (cut and count)
BP1	6852	0.356	0.378	7.356×10^{-3}	2585	2966	0.87	34.69	10.7
BP2	1233	0.594	0.205	5.042×10^{-4}	253	203	1.24	11.84	1.94
BP3	106	0.683	0.130	1.292×10^{-4}	14	52	0.27	1.72	0.17
BG	403221								

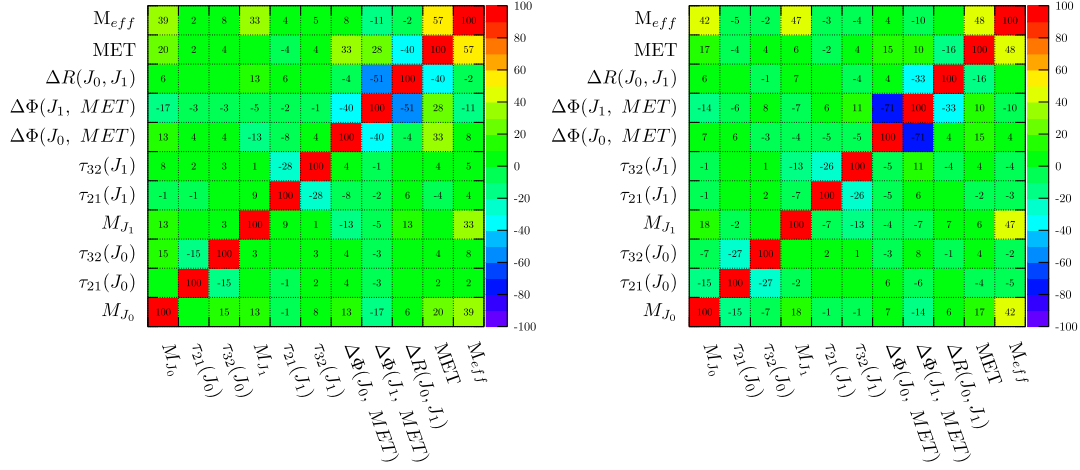


FIG. 5. Linear correlation coefficients (expressed as percentages) between various kinematic variables for the signal (BP1, left panel) and background (right panel). Missing values indicate a negligible correlation or anticorrelation, less than one. Positive coefficients show a correlation, while negative coefficients indicate an anticorrelation.

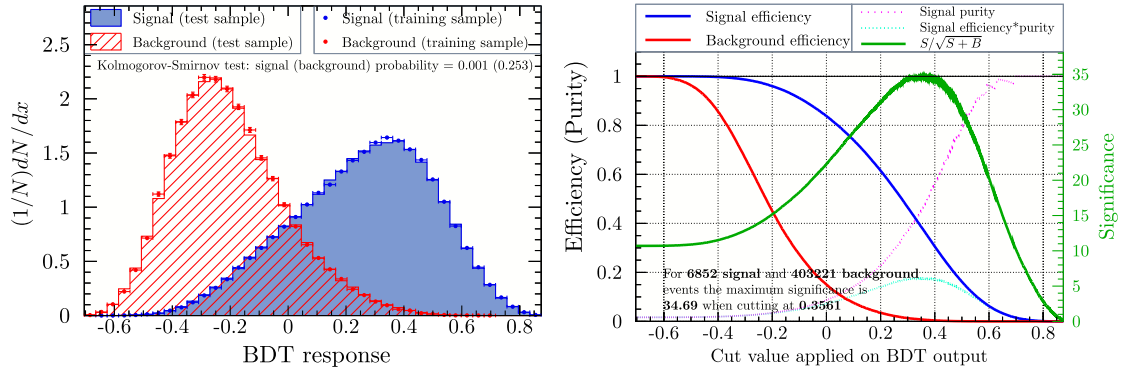


FIG. 6. Left panel: the normalized distribution of the BDT response is shown for both signal (blue, BP1) and background (red). Dotted histograms represent training samples, while solid histograms denote testing samples. Right panel: the efficiency of the signal (blue) and background (red), along with the signal's statistical significance (green), are plotted as functions of the BDT output cut applied.

Not all of the variables discussed above are included in the multivariate analysis, as some exhibit significant (anti) correlations with one another. It is important to note that using variables with high (anti)correlation does not enhance efficiency. Therefore, we carefully select only those with low to moderate (anti)correlation. For example, M_{eff} and $\sqrt{\hat{s}_{\text{min}}}$, defined in Eqs. (5.5) and (5.6), are highly correlated in both signal and background classes. Similarly, M_{eff} and $p_T(J_1)$ also show a strong correlation in both classes. We retain M_{eff} while excluding $p_T(J_1)$ and $\sqrt{\hat{s}_{\text{min}}}$, as M_{eff} demonstrates greater relative separation power between the signal and background classes. This relative separation power indicates that the variable is more effective in discriminating between the two classes than the others. The background represents the weighted sum of the individual background processes discussed in Sec. VA. The final set of variables utilized in our MVA is presented in Table V, along with their relative separation power in distinguishing between signal and background.

The correlation between the variables for the signal (considering benchmark point BP1) and background classes is illustrated in the left and right panels of Fig. 5, respectively. Most of these variables exhibit low (anti)correlations. However, M_{eff} and MET display a moderate correlation in both signal and background classes, and we retain both variables due to their significant relative separation power. In contrast, the azimuthal separations $\Delta\phi(J_0, \text{MET})$ and $\Delta\phi(J_1, \text{MET})$ show strong anticorrelations in the background yet only moderate anticorrelations in the signal. Consequently, we include both variables in our analysis.

Figure 6(a) displays the normalized distributions of the BDT response for both the signal and background classes, encompassing both training and testing samples. The distributions for these two datasets align closely, and there is also a distinct separation between the signal and background classes. The parameters used for training the boosted decision tree are outlined in Appendix A 3. We optimize our training separately for each benchmark point. Although

BDT is a robust classifier, it can be susceptible to over-training. To confirm that the BDT model is not overtrained, we assessed the Kolmogorov-Smirnov probability, a statistical test that measures the difference between the cumulative distribution functions of two datasets (test and train samples), presented in Fig. 6(a).

In the right panel of Fig. 6, we illustrate how the signal (solid blue) and background (solid red) efficiencies change with respect to the cut applied to the BDT response. Signal (background) efficiency is defined as the ratio of the number of signal (background) events that survive after applying a specific cut on the BDT output to the total number of signal (background) events in the sample. The solid green line represents the variation in statistical significance as a function of the cut on the BDT output. This statistical significance is calculated as $\frac{N_S}{\sqrt{N_S+N_B}}$, where N_S and N_B are the numbers of signal and background events, respectively, that survive after the cuts. The dotted magenta line indicates the signal purity, defined as $\frac{N_S}{N_S+N_B}$. At the far left of the figure, we observe that the signal purity is very low due to the high number of background events relative to the signal. However, as the cut value on the BDT output increases, our model demonstrates its effectiveness, as the signal purity improves significantly.

VI. RESULTS

As outlined in the model section, the independent parameters of our simplified model include the mass of the vectorlike quark (m_Ψ), the coupling ($\tilde{y}_t$), and the dark matter mass (m_S). For the fixed dark matter mass $m_S = 12$ KeV, the model's parameter space is represented by a plane with parameters $\tilde{y}_t$ and m_Ψ . We have selected three nonstandard benchmark points, as presented in Table II, to demonstrate the effectiveness of our BDT analysis in different regions of the parameter space. Table VI summarizes the results of the multivariate analysis for these three representative benchmark points. The second column contains the number of signal events for all benchmark scenarios and total background events before doing MVA. The immediate next column is the optimal BDT cut value that should be applied to the BDT response to get the optimal statistical significance. The following columns contain the signal and background efficiencies and the number of the signal (N_S) and background (N_B) events that survived after applying the optimal BDT cut. The signal-to-background ratio is presented in the eighth column. The second-to-last column shows the statistical significance of the MVA for an integrated luminosity of 300 fb^{-1} . To give a comparison, the last column provides the corresponding value for the traditional cut-and-count search. The MVA achieves a significant improvement over the cut-and-count method.

Figure 7 illustrates the exclusion contours in the $\tilde{y}_t$ vs m_Ψ plane from our prompt search analyses at the LHC. The

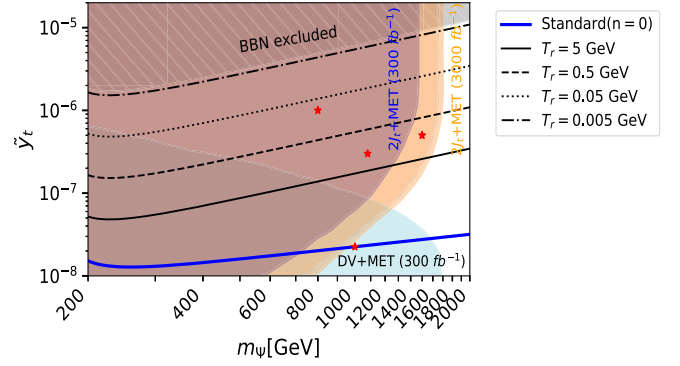


FIG. 7. Excluded regions at a 95% CL are shown in the Yukawa coupling ($\tilde{y}_t$) and vectorlike quark mass m_Ψ plane for the freeze-in dark matter model. Baseline contours satisfy the dark matter relic density constraint $\Omega h^2 = 0.12$ for different early Universe cosmological evolution scenarios, as discussed in Fig. 1. Model spaces within the blue (orange) region can be excluded for an integrated luminosity 300 fb^{-1} (3000 fb^{-1}) at the LHC, considering a nonstandard cosmological scenario. The orange dashed dot contour shows the exclusion contour at 3000 fb^{-1} integrated luminosity considering 10% systematics. The cyan-shaded region shows exclusions from the displaced vertex search (300 fb^{-1}) at the LHC. The gray-shaded region is ruled out since any T_r lower than BBN ($\approx 4 \text{ MeV}$) conflicts with the cosmological observation.

projected reach can be better appreciated along with contours that satisfy the dark matter relic density constraint for different early Universe cosmological evolution scenarios. The 2σ exclusion contours for the simplified FIMP model are shown in the blue-shaded region for an integrated luminosity of 300 fb^{-1} and in the orange-shaded region for the projected reach at the 14 TeV High-Luminosity LHC (HL-LHC) with 3 ab^{-1} . The dashed-dotted orange contour represents the HL-LHC exclusion reach when a 10% systematic uncertainty is considered. At 300 fb^{-1} , the discovery (5σ) and exclusion (2σ) reach for the vectorlike quark mass extend up to approximately 1305 and 1470 GeV, respectively. The HL-LHC exclusion reach extends up to 1700 GeV. However, when 10% systematics are included, the exclusion sensitivity at HL-LHC reduces, reaching up to 1655 GeV.

Note that, as long as the BSM coupling $\tilde{y}_t$ is large enough, the demonstrated exclusion contours in Fig. 7 are primarily insensitive to the coupling due to the model-independent nature of our study. One can follow Footnotes 1 and 5 for further discussion. However, this heavy vectorlike quark, after its QCD production, can be long-lived if $\tilde{y}_t$ is substantially small when its decay occurs from a secondary vertex, a few millimeters to meters away from the original primary production vertex, depending upon the smallness of the coupling. For reference, we listed displaced distance before decay for all BP points in Table II. The crucial point remains that the calorimeter energy deposits in the latter case are not associated with tracks

from the hard scattering primary vertex, unlike prompt QCD production. Hence, such hadronic deposits cannot be reconstructed as a (boosted) hadronic jet from the primary vertex and part of our signal. Thus, despite the VLQ having a single decay mode, the exclusion significance reduces their sensitivity with the minuscule coupling values when Ψ fails to decay promptly from the primary vertex. We approximated this reduction in sensitivity by a mathematical function, as discussed in Appendix A 4. We find that if the coupling is considerably large to trigger the prompt decay of the vectorlike quark, our collider analysis is capable of probing a broad region of the parameter space. Conversely, if the coupling is small, the displaced vertex + MET search [117] can explore higher VLQ masses (lower right of Fig. 7). In contrast, our complementary search can probe larger VLQ masses when the coupling is more significant (top right of Fig. 7), which is the case for the FIMP scenario with alternative cosmology.

CMS and ATLAS collaborations have extensively searched for supersymmetric particles. A close comparison can be drawn between our search and stop pair production at the LHC. The stop, the superpartner of the SM top quark, arises from the mixing of left- and right-handed top squarks, forming the lighter and heavier mass eigenstates $\tilde{t}_1$ and $\tilde{t}_2$. At the LHC, the production of light stop pairs is widely studied through their decay into SM top quarks and neutralinos [118–124]. However, a direct comparison between stop and vectorlike quark searches may not yield accurate results due to their production mechanisms and spin differences. The leading-order partonic diagrams for stop pair production resemble those in Fig. 3 (upper row)—an additional gluon-gluon annihilation process via a contact interaction is present for stops. Furthermore, stops are color scalars (spin-0), whereas VLQs are color fermions (spin-1/2). The difference in mass dimension of the fields (1 for stop field, 3/2 for VLQ) also leads to distinct Feynman vertex structures. Nonetheless, the result of the stop search can be recast in the VLQ context to derive meaningful constraints.

A recent analysis by ATLAS collaboration [123] considers stop pair production resulting in a final state with two hadronically decaying top quarks and a pair of neutralinos, leading to significant missing transverse momentum and no leptons in the final state. The study uses data collected at the 13 TeV LHC with an integrated luminosity of 139 fb^{-1} . This final state is identical to the one considered in our search. We reinterpret the ATLAS results using CheckMATE2 [125–127] and find that the 95% CL exclusion reach for the VLQ mass extends to 1230 GeV. In contrast, our dedicated analysis for the 13 TeV LHC with 139 fb^{-1} of integrated luminosity achieves an exclusion reach of up to 1320 GeV. When a 10% systematic uncertainty is included, the reach slightly decreases to 1292 GeV. The details about this recasting procedure are provided in Appendix A 5. Our analysis provides improved

sensitivity over the reinterpretation of stop searches, highlighting the need for dedicated optimization in VLQ searches.

A significant number of vectorlike quark (top partner [128,129]) searches have also been conducted at the LHC [130–132]. In these searches, the VLQ is typically Z_2 even, allowing it to mix with the SM top quark. As a result, ATLAS and CMS primarily focus on VLQ pair or single production, followed by decays into channels such as tZ , th , bW , or tg . In contrast, our model features a Z_2 -odd VLQ, which does not mix with the SM top quark. Instead, it interacts with SM quarks and dark matter through a Yukawa interaction.

VII. SUMMARY AND CONCLUSION

In this work, we examine a simplified FIMP model where the freeze-in production of dark matter relies on the decay of vectorlike quark Ψ into a dark matter particle (S) and an up-type quark through a feeble coupling. DM, being a pure singlet, Ψ , is forced to have the same gauge quantum number as the SM particle—in particular, the mediator poses the same gauge charge as the right-handed quark since we consider the top-philic model. During the evolution of the early Universe, the parent particle Ψ thermalizes with the primordial soup due to considerable gauge interaction. However, the DM can never become part of the thermal bath owing to the smallness of the Yukawa coupling, and its generation takes place from the decay of Ψ via the freeze-in mechanism.

Since the vectorlike quark mediator is already constrained to be rather heavy while the dark matter can be light, it requires an approximate range of Yukawa coupling $\sim(10^{-7}\text{--}10^{-13})$ to guarantee the observed dark matter relic through the freeze-in process, considering the standard radiation-dominated early Universe. Hence, the long-lived particle searches and displaced vertex signature typically play an essential role in constraining this kind of picture at the LHC. On top of that, the typical $\mathcal{O}(10)$ keV dark matter can resolve the small-scale crisis of the Λ CDM model by putting down the structure formation at that scale due to the warmness, in addition to offering the platform to be probed at various astrophysical and cosmological experiments.

However, there is no direct measurement of the Universe’s energy budget in the pre-BBN era, so looking at possible alternative background cosmologies is prudent. Here, we adopt a particular scenario with a pre-BBN fast expansion picture, such as a well-motivated quintessence fluid. It alters the dark matter phenomenology and the collider signature by demanding a significant increase in interaction strength compared to the standard radiation-dominated assumption to achieve the DM abundance in the correct ballpark. The characteristic LLP searches and DV signatures fall short of effectively constraining such a scenario. This analysis shows the extended parameter space

due to modified cosmology, satisfying the relic density constraint. We built a suitable search strategy at the LHC to significantly incarcerate a large part of newly opened regions.

Finally, the generous pair production of vectorlike quarks is expected at the LHC owing to its strong interaction and promptly decays into the dark matter along with the SM quarks. The production of light dark matter particles from the decay of heavy VLQ ensures the output of topline boosted fatjets. We exploit the inherent features of these jets and their substructures to construct our search strategy and probe this channel over a vast QCD backdrop. With a precision estimate of the signal at the next-to-leading-order QCD, particle level event simulation, the inclusion of detector effect, and multivariate analysis based on the boosted decision tree and boosted jet variables, a comprehensive computation is done to showcase the possible reach of this model. In this study, our collider analysis explores a broad parameter space of the model in the Yukawa coupling and VLQ mass plane. Our search strategy provides a complementary way to constrain the extended region parameter space for the dark matter, where most regions remain inaccessible to the traditional long-lived particle or displaced vertex searches.

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DATA AVAILABILITY

This study uses simulated data from standard HEP packages. The details of generating the simulated data supporting these findings are available within this article. Any additional information is available from the authors upon reasonable request.

APPENDIX

1. Upper bound on $\tilde{y}_t$ from DM thermalization for fast expanding universe

To understand the theoretical validity of Yukawa coupling $\tilde{y}_t$ for a given VLQ mass, one is required to calculate the ratio between the corresponding interaction rate with the Hubble expansion rate, i.e., $\langle\Gamma_\Psi\rangle/H$, and check whether

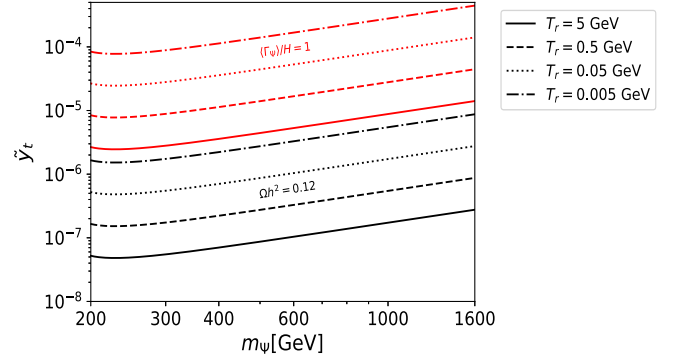


FIG. 8. Thermalization contours (defined by the interaction rate equal to the Hubble rate) for different reference temperatures with a fixed value of $n(=2)$ are shown in red in Yukawa coupling vs mediator mass plane. The set of black lines at the bottom represent the relic-density-satisfied contours for the same fixed values of T_r and n . The corresponding DM is not thermalized (gets thermalized) for a parameter region below (above) each contour.

this ratio exceeds 1. The DM thermalizes for a ratio larger than or equal to 1. In Fig. 8, we have shown the contours with the ratio $\langle\Gamma_\Psi\rangle/H = 1$ with the red color lines. This contour for a particular T_r sets a conservative upper bound on $\tilde{y}_t$ to realize nonthermal DM. Clearly, relic-satisfied points are well within this limit.

2. Distributions after baseline selection

After applying only the baseline selection criteria, normalized distributions of various kinematic observables for the signal (BP1) and backgrounds are presented in Fig. 9. At the baseline selection, the dominant background comes from the $W + \text{jets}$ channel, with $Z + \text{jets}$ and $t\bar{t} + \text{jets}$ providing the second and third most significant contributions. After applying the full event selection criteria detailed in Sec. VC, the primary background shifts to $t\bar{t} + \text{jets}$, followed by $Z + \text{jets}$ and $W + \text{jets}$, as shown in Table IV.

Figure 9 reveals that both fatjets from the signal exhibit a second soft drop mass peak around the masses of the W boson, along with one at the top quark. This low mass peak arises when the fatjets are moderately boosted, capturing only the subjets corresponding to the W boson decay rather than all three subjets of the top quark. Additionally, a small shift of the peaks in $\sqrt{\hat{s}_{\min}}$, $\Delta\Phi(J_i, \text{MET})$, and $\tau_{21}(J_i)$ distributions is observed between Figs. 9 and 4 (after applying all event selection cuts).

3. BDT hyperparameters

To enhance the better performance in signal-background discrimination, we perform a multivariate analysis utilizing a gradient BDT method, where several characteristics of the reconstructed fatjets and the missing transverse momentum are employed as inputs for the BDT. In Table VII, we list the hyperparameters used in adaptive BDT analysis.

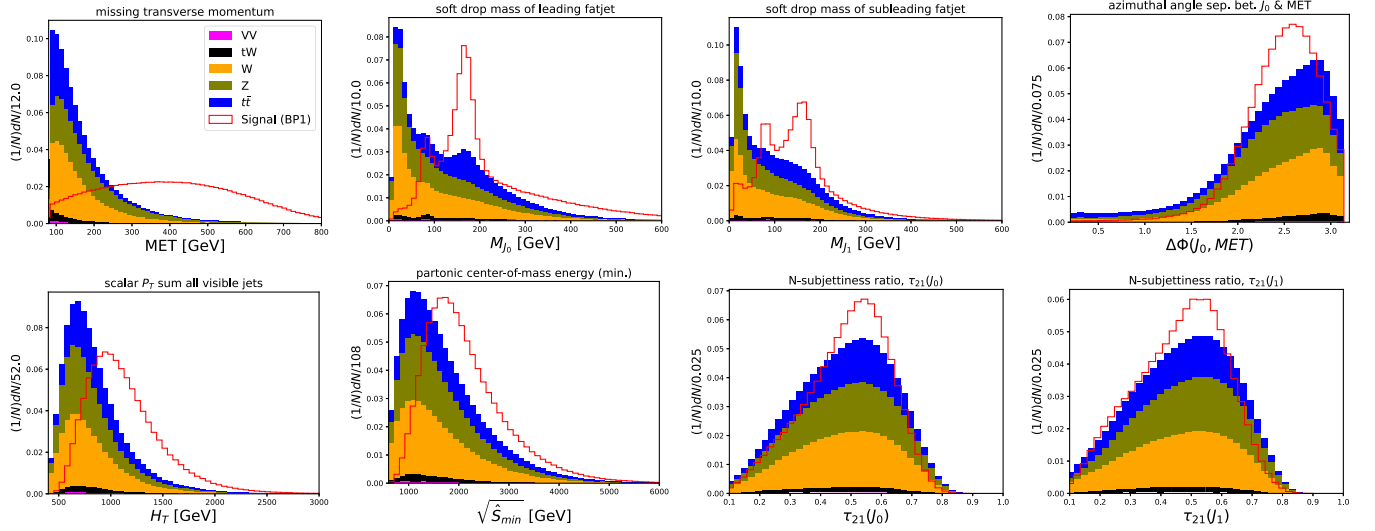


FIG. 9. Some of the normalized stacked histograms of various kinematic observables for the SM backgrounds and the signal (BP1) are presented after applying only the baseline selection criteria: at least two fatjets with $p_T(J_i) > 200$ GeV, $MET > 80$ GeV, and $\Delta\phi(J_i, MET) > 0.2$ ($i = 0, 1$).

4. Exclusion reach as a function of coupling

As discussed in the main text, our collider analysis is based on the prompt decay of the vectorlike quark (Ψ) into the dark matter and the top quark. In our simplified model, Ψ has only one decay channel, and its decay lifetime depends on the coupling $\tilde{y}_t$ and its mass. The decay length of the VLQ in its rest frame is given below:

$$c\tau = \frac{1.98 \times 10^{-13}}{\Gamma_\Psi(\tilde{y}_t, m_\Psi)} mm. \quad (A1)$$

Here, $\Gamma_\Psi(\tilde{y}_t, m_\Psi)$ represents the decay width of the VLQ in its rest frame, defined in Eq. (4.2). For our prompt search analysis, estimating the fraction of the Ψ that decays within the tracking system at the LHC is necessary, which can provide us with the boosted fatjet signature. The probability that Ψ can traverse a distance x in the detector from the primary vertex without decaying is given by

$$P(x) = \exp(-x/\gamma\beta c\tau). \quad (A2)$$

TABLE VII. Hyperparameters used in adaptive BDT analysis. The number of trees (NTrees) is specified for BP1, BP2, and BP3, respectively.

BDT hyperparameters	Optimal selection
BoostType	AdaBoost
AdaBoostBeta	0.3
NTrees	400, 250, 210
MinNodeSize	5.0%
MaxDepth	4
UseBaggedBoost	True
BaggedSampleFraction	0.6
SeparationType	GiniIndex
nCuts	20

Here, $\gamma = \frac{1}{\sqrt{1-\beta^2}}$ represents the Lorentz factor, and $\beta = v/c$. In natural units ($\hbar = c = 1$), some useful relations for the rotation-free Lorentz transformation are

$$\gamma = \frac{E_\Psi}{m_\Psi} \quad \text{and} \quad \beta = \frac{|\vec{p}_\Psi|}{E_\Psi}. \quad (A3)$$

The momentum of the VLQ, $|\vec{p}_\Psi|$, depends on the partonic center-of-mass energy, $\sqrt{\hat{s}}$, which typically lies above the production threshold, $\sqrt{\hat{s}} \gtrsim 2m_\Psi$, for VLQ pair production. If Ψ possesses a long lifetime, we must rescale the pair production cross section of the vectorlike quark for our prompt search as an effective cross section,

$$\sigma_{\text{eff}} = \sigma(1 - P(x)). \quad (A4)$$

The surviving probabilities for prompt search $[1 - P(x)]$ increase for larger values of x . Hence, for our prompt search, one can get a conservative estimate by setting the detecting scale at one millimeter and boost factor $\gamma\beta = 1.0$. That would reproduce the $\tilde{y}_t$ dependence of the exclusion contour, especially for lower values. In principle, since we know the exact $\sqrt{\hat{s}}$ distributions of our simulated events (for a given mass), the exact distribution of $\gamma\beta$ can be computed trivially to derive this contour. However, this approximation should work equally well, especially since our analysis is not optimized for this region—instead, displaced vertex search is expected to take care of this region.

5. Reinterpreting the stop searches at ATLAS

We performed a detailed reinterpretation based on the existing 13 TeV LHC data with an integrated luminosity of 139 fb^{-1} . A search for top squarks in the all-hadronic final

state with a top-antitop pair and missing transverse momentum has been presented by ATLAS collaboration. The analysis is based on 139 fb^{-1} of proton-proton collision data at a center-of-mass energy of 13 TeV, collected with the ATLAS detector at the LHC [123]. We reinterpret this analysis in the context of our top-philic dark matter model using the CheckMATE2 framework [125–127].

The ATLAS analysis defines multiple signal regions (SRs), labeled SRA to SRD, based on the stop’s two- to four-body decay topologies. The SRA regions are specifically optimized for scenarios with two-body stop decays, large mass gaps between the top squarks and the neutralino dark matter candidate, and stop masses above 1 TeV. Since our model features a VLQ with a mass at the TeV scale and a light dark matter candidate, we concentrate on the SRA region. In these regions, the dominant background is typically $Z + \text{jets}$, where the Z -boson decays invisibly into neutrinos. However, our analysis reveals that the two main background processes— $Z(\text{inv}) + \text{jets}$ and semileptonic $t\bar{t} + \text{jets}$ —contribute comparably to the total background. In fact, the semileptonic $t\bar{t} + \text{jets}$ channel contributes a larger number of background events than $Z(\text{inv}) + \text{jets}$. The ATLAS analysis models the stop pair production signal at LO in QCD.

In the SRA region, the leading reconstructed fatjet ($R = 1.2$) is required to have a mass greater than 120 GeV and a b -jet is tagged within leading fatjet. Based on the mass of the second fatjet, the SRA region is further divided into three subregions:

- (i) SRA-TT: second fatjet mass > 120 GeV, and a b -jet is tagged within the subleading fatjet.
- (ii) SRA-TW: second fatjet mass between 60 GeV and 120 GeV.
- (iii) SRA-T0: second fatjet mass < 60 GeV.

We recast our VLQ signal and obtain a 2σ reach using the signal regions SRA-TT and SRA-TW. For the recasting, the VLQ signal is generated at the 13 TeV LHC using the NNPDF2.3 parton distribution function, consistent with the ATLAS analysis. For a benchmark dark matter mass of 12 keV, the 95% confidence level exclusion limits obtained from this reinterpretation are summarized below:

- (1) When using NLO cross sections and NLO signal distributions, the results exclude VLQ masses up to 1230 and 1210 GeV in the SRA-TT and SRA-TW signal regions, respectively.
- (2) When using LO cross sections while retaining NLO signal distributions, the exclusion reach extends up to 1190 and 1145 GeV in the SRA-TT and SRA-TW signal regions, respectively.

In comparison, our independent analysis with NLO signal events at $\sqrt{s} = 13$ TeV LHC with 139 fb^{-1} , incorporating all the optimization strategies and kinematic observables discussed in our manuscript, shows that VLQ masses up to 1320 GeV can be excluded. When a 10% systematic uncertainty is included, the exclusion reach slightly reduces to 1292 GeV.

Even though existing stop searches in the all-hadronic final state can be recast for the VLQ case, our collider analysis aids the following. In existing searches, the dominant background in the SRA-TT and SRA-TW scenarios is $Z(\text{inv}) + \text{jets}$. However, our analysis shows that semileptonic $t\bar{t} + \text{jets}$ contribute a comparable—and in fact larger—number of background events compared to $Z(\text{inv}) + \text{jets}$. Therefore, the VLQ signal model requires a different optimization strategy compared to stop searches. Furthermore, using NLO cross sections and signal distributions leads to a more stringent bound on the VLQ mass. Finally, our proposed analysis achieves a better reach on the VLQ mass compared to the recasted stop analysis.

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