

Primordial Black Hole Seeds for Little Red Dots in $f(R)$ Gravity

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The discovery by the James Webb Space Telescope (JWST) of an abundant population of compact little red dots (LRDs) and supermassive black holes at high redshifts poses a severe timing challenge for standard Eddington-limited growth from stellar remnants. In this work, we present a unified hybrid assembly framework in which intermediate-mass seed black holes are formed via hierarchical primordial black hole (PBH) mergers within dense clusters in Hu-Sawicki $f(R)$ gravity, followed by galactic gas accretion. We demonstrate that the screened $f(R)$ fifth force nonlinearly accelerates early seed formation through a quadratic enhancement of the gravitational-wave radiation-capture kernel, while environmental chameleon screening dynamically self-regulates the growth. Because subsequent gas accretion scales multiplicatively with seed mass, the $f(R)$ seed enhancement is preserved throughout the accretion history, drastically reducing the time-averaged Eddington ratios required to assemble 10^6 - $10^9 M_\odot$ LRDs by cosmic dawn. Confronting our active mass functions with JWST data reveals that a small clustered PBH fraction ($f_{\text{PBH}} \lesssim 10^{-3}$) under a realistic active galactic nucleus duty cycle ($\delta \approx 10^{-2}$) naturally matches observed LRD space densities at $z \sim 5.5$ - 6.5 while remaining fully compliant with LIGO-Virgo-KAGRA limits, with modified gravity naturally driving the high-mass tail. Finally, we show that parameter degeneracies between modified gravity and cluster density can be cleanly broken by combining three multi-messenger diagnostics: remnant spin state signatures, a stochastic GW background cutoff, and a scale-dependent inversion in the PBH spatial correlation function.

I. INTRODUCTION

Deep near-infrared spectroscopy from the James Webb Space Telescope (JWST) has uncovered an unexpectedly abundant population of active black holes at high redshifts. Broad-line active galactic nuclei (AGN) and remarkably compact red continuum sources, now widely referred to as little red dots (LRDs), are observed in abundance at $z \sim 4$ - 9 , with virial black-hole masses inferred to lie in the range $M_{\text{BH}} \sim 10^6$ - $10^9 M_\odot$ [1–7]. The presence of such massive objects within the first gigayear of cosmic history further highlights a long-standing challenge for models of supermassive black-hole (SMBH) assembly [8–12]. Even with continuous Eddington-limited accretion, a $\sim 100 M_\odot$ Population III remnant [13, 14] cannot plausibly grow to $\sim 10^9 M_\odot$ by $z \sim 7$ without sustained super-Eddington accretion or highly idealized duty cycles. Heavy-seed scenarios can alleviate this timing problem to some extent, but they also face significant limitations. For example, direct-collapse black holes require pristine atomic-cooling halos exposed to an intense Lyman-Werner radiation field to suppress fragmentation [15–18], while runaway stellar collisions in dense nuclear clusters require finely tuned physical conditions [19, 20]. Moreover, these formation channels remain observationally unconfirmed and are expected to operate only in relatively rare environments. The apparent abundance of massive black holes at cosmic dawn therefore motivates alternative seed scenarios in which the characteristic seed mass and formation epoch are largely decoupled from the star-formation history.

Primordial black holes (PBHs), formed through the gravitational collapse of large-amplitude density perturbations during the radiation-dominated era, provide a nonstellar channel

for black-hole seeding [21–25]. Interest in PBHs was renewed following the LIGO-Virgo-KAGRA (LVK) detection of merging black holes with tens-of-solar-mass components [26–29]. Moreover, PBHs remain a viable dark-matter candidate over several mass ranges [30–34] and can provide black-hole seeds independently of conventional baryonic processes. An important feature for early structure formation is that PBHs need not form an approximately homogeneous Poisson distribution. Instead, primordial non-Gaussianity, spectator-field dynamics, and domain-wall or phase-transition mechanisms can generate significant spatial clustering at formation [35–40]. Consequently, a fraction of the PBH population may form within, or rapidly assemble into, dense virialized substructures. Under such conditions, the focus shifts from isolated binary formation [41–43] to the collective dynamical evolution of a self-gravitating PBH population, where close encounters, two-body relaxation, and gravitational-wave (GW) capture act concurrently.

The kinetics of PBH binary formation and mergers in virialized halos have been studied extensively over the past decade, both for the smooth cosmological PBH population and for populations embedded in dark-matter halos [27, 28, 44–49]. In parallel, it is shown that the predicted merger-rate density depends sensitively on the internal structure and collapse geometry of the host dark-matter halos. Ellipsoidal rather than spherical collapse can substantially enhance the merger rate [50], while self-interacting dark-matter profiles modify the probability of close encounters [51]. Furthermore, high-precision semianalytic mass functions can alter the abundance of potential host halos [52], whereas dense environments, such as dark-matter spikes around SMBHs and the interiors of cosmic voids, provide distinct dynamical settings for PBH capture [53, 54]. Consequently, the PBH merger rate and mass-growth efficiency depend not only on the intrinsic PBH abundance, but also on local environmental dynamics and the

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underlying theory of gravity.

This environmental dependence is especially pronounced in scalar-tensor theories of gravity, where an additional scalar field mediates a screened fifth force. In metric $f(R)$ gravity, the Hu-Sawicki model provides a canonical and observationally viable realization [55–58]. In this framework, the scalar field mediates a fifth force that enhances the effective gravitational coupling G_{eff} in low-density environments. At the same time, the chameleon mechanism suppresses this force in deep Newtonian potentials, allowing the theory to remain consistent with solar-system and laboratory constraints [59–62]. Since the thermally averaged cross section for GW radiation capture scales as $K_{ij} \propto G_{\text{eff}}^2$, even a moderate enhancement of G_{eff} within the allowed range can increase the capture rate. In particular, the PBH merger rate in $f(R)$ gravity has been shown to exhibit a robust enhancement relative to general relativity (GR), controlled by the background field amplitude $|f_{R0}|$ [63]. Furthermore, the merger dynamics of compact binaries has been investigated in both the Hu-Sawicki and normal-branch Dvali-Gabadadze-Porrati (DGP) models. In these models, modifications to the halo mass function, concentration, and velocity dispersion combine to produce a redshift-dependent enhancement of the merger rate [64, 65]. Therefore, given the properties of this class of modified gravity models, $f(R)$ gravity can provide a self-regulating framework in which environmental modifications enhance early black-hole assembly while remaining consistent with low-redshift constraints. Such a framework could, in turn, provide a dynamical basis for studying the subsequent coalescence and mass growth of early black holes and assessing their role as potential seeds of the LRDs observed by JWST.

Despite this progress, several aspects of PBH growth through repeated mergers remain to be explored. Many existing treatments focus on the merger rate for a prescribed PBH mass function rather than evolving the mass spectrum through successive merger generations [66–68]. Although the importance of multiple mergers depends on the initial mass function and can be subdominant in some scenarios [68], successive mergers can redistribute PBHs toward higher masses and therefore provide a natural channel for building a high-mass tail. Capturing this evolution requires following the full mass spectrum rather than a representative binary, for which the nonlinear Smoluchowski coagulation equation provides a natural kinetic framework [69, 70]. Moreover, the connection between modified-gravity effects and the kinetic evolution of the PBH population has not been systematically developed. In particular, previous work has not combined a full spectral coagulation solver with an environmentally screened effective coupling in a single framework. In addition, the connection between merger-driven PBH growth and the observed population of active black holes at $z \sim 5$ –7 remains comparatively unexplored. This connection is particularly relevant for assessing whether PBH mergers can contribute to the rapid emergence of massive black holes at high redshift. Also, the internal dynamical viability of dense PBH clusters must be established rather than assumed. Core collapse, two-body relaxation, mass segregation, and the retention or ejection of GW-recoiled merger remnants can all affect the efficiency of

hierarchical growth [71, 72].

In this work, we aim to clarify whether PBHs can provide viable seeds for the massive black holes powering LRDs at high redshift, and how their growth is influenced by the underlying gravitational dynamics. In this regard, the structure of this work is as follows. In Section II, we introduce the cosmological background, effective Hu-Sawicki $f(R)$ gravity, environmental screening, and dense PBH cluster dynamics. In Section III, we develop the hybrid mass-assembly model, including the GW radiation-capture kernel, Smoluchowski coagulation formalism, its numerical implementation, and the subsequent gas-accretion phase. In Section IV, we introduce the observables and diagnostics used to characterize the assembly history, including remnant spins, black-hole mass functions, the SGWB, and the PBH two-point correlation function. We present our results in Section V, and summarize our conclusions in Section VI.

II. THEORETICAL AND PHYSICAL FRAMEWORK

A. Cosmological Background

We consider a spatially flat Λ CDM cosmology to determine the cosmic time available for PBH mergers and subsequent black-hole growth. The cosmological background enters the calculation primarily through the relation between redshift and cosmic time. This relation sets the duration of the merger-coagulation phase and provides the time interval over which the resulting black-hole seeds can subsequently grow through gas accretion.

The Hubble expansion rate is given by

$$H(z) = H_0 \sqrt{\Omega_m(1+z)^3 + \Omega_\Lambda}, \quad (1)$$

where H_0 is the present-day Hubble constant, while Ω_m and Ω_Λ denote the present-day matter and dark-energy density parameters, respectively. We adopt the Planck 2018 best-fit values, $H_0 = 67.4 \text{ km s}^{-1} \text{ Mpc}^{-1}$, $\Omega_m = 0.3134$, and $\Omega_\Lambda = 1 - \Omega_m$ [73], since these determine the absolute cosmic-time budget available for PBH coagulation and set the overall normalization of the growth calculation that follows. The cosmic time corresponding to a given redshift is then obtained from

$$t(z) = \int_z^\infty \frac{dz'}{(1+z')H(z')}, \quad (2)$$

where z' is an integration variable.

The coagulation calculation is evolved from $z_{\text{ini}} = 11.5$ to $z_{\text{fin}} = 6.0$, a bracket chosen so that the lower bound coincides with the onset of the JWST spectroscopic redshift coverage used later for the black-hole mass function (BHMF) comparison (see, Sec. IV B), while the upper bound lies within the epoch commonly associated with Population III star formation and the assembly of the first dense stellar systems [13, 14]. For the adopted cosmology this interval corresponds to a cosmic-time budget of $\Delta t_{\text{merge}} \simeq 0.54 \text{ Gyr}$. Gas

accretion is *not* postponed until after $z = 6$. The BHMF comparison uses a time-averaged Eddington ratio over the full interval from z_{ini} to each observational snapshot z_{obs} , while the Smoluchowski solution isolates the dry-merger contribution to the mass spectrum over the same window. The two channels therefore operate as concurrent contributions to assembly rather than as a strictly sequential $z > 6$ then $z < 6$ history. The initial PBH mass is fixed at $m_{\text{PBH}}^{(0)} = 30 M_{\odot}$, matching the characteristic component mass of the stellar-mass binary black holes detected by LVK, which is also the mass scale for which PBHs have been most actively discussed as a dark-matter and seeding candidate [26–28].

We adopt a lognormal initial mass distribution

$$\frac{dN}{d \ln m} \propto \exp \left[-\frac{(\ln m - \ln m_{\text{PBH}}^{(0)})^2}{2\sigma_{\ln m}^2} \right], \quad (3)$$

where N denotes the number of PBHs and m is the PBH mass. The logarithmic width is set to $\sigma_{\ln m} = 0.40$, a value typical of the extended mass functions predicted by broad formation mechanisms such as curvaton-field or near-critical gravitational collapse scenarios, and is used here to avoid the artificial sharpness of a monochromatic spectrum in the coagulation calculation. The distribution is normalized to $N_{\text{cl}} = 10^5$ PBHs per cluster, a population large enough to yield a smooth, well-sampled statistical description of the merger hierarchy while remaining computationally tractable for the full mass-spectrum evolution described in Sec. III B. This initial population provides the starting point for the subsequent merger-coagulation evolution.

B. Hu-Sawicki $f(R)$ Gravity

In $f(R)$ gravity, the Einstein-Hilbert Lagrangian is generalized to a function of the Ricci scalar. The corresponding action is given by

$$S = \frac{1}{16\pi G} \int d^4x \sqrt{-g} f(R) + S_{\text{m}}[g_{\mu\nu}, \Psi], \quad (4)$$

where $g_{\mu\nu}$ is the spacetime metric, g is its determinant, R is the Ricci scalar, and S_{m} denotes the matter action with Ψ representing the matter fields. The additional gravitational degree of freedom, commonly referred to as the scalaron, is characterized by $f_R \equiv df/dR$. In this work, we adopt the Hu-Sawicki form [55],

$$f(R) = R - m^2 \frac{c_1(R/m^2)^n}{c_2(R/m^2)^n + 1}, \quad (5)$$

where m^2 sets the characteristic curvature scale, c_1 and c_2 are dimensionless model parameters, and n controls the curvature dependence of the modification. In the high-curvature regime, the Hu-Sawicki model approaches the GR limit while retaining a nontrivial scalar degree of freedom. We characterize the strength of the modification by the present-day background scalaron value, $f_{R0} \equiv f_R(z = 0)$, and use $|f_{R0}|$ to label the different modified-gravity cases considered below.

The scalaron can mediate an additional attractive force when it is sufficiently unscreened. In the Hu-Sawicki model, this fifth force is suppressed by the chameleon mechanism in sufficiently dense environments or in regions with deep gravitational potentials. Thus, the effective gravitational interaction depends on the surrounding environment. This environmental screening is central to PBHs residing in dense clusters, where the combined potential of the cluster and host halo regulates the local scalaron field.

For an isolated stationary black hole in vacuum, the no-hair property of $f(R)$ gravity implies a vanishing scalar charge, $q_s = 0$, and hence no leading-order scalar-mediated correction to the gravitational interaction relative to GR [74]. This result, however, does not directly apply to PBHs embedded in an extended matter distribution. In the present setting, the PBHs reside within a dense cluster and its host halo, whose gravitational environment can modify the local scalaron configuration and produce a nonvanishing spatial gradient, $\nabla f_R \neq 0$.

The relevant environmental depth is quantified by the dimensionless Newtonian potential associated with the PBH cluster

$$\Phi_{\text{cl}} = \frac{GM_{\text{cl}}}{R_{\text{cl}}c^2}, \quad (6)$$

where $M_{\text{cl}} = N_{\text{cl}}m_{\text{PBH}}^{(0)}$ is the total cluster mass, R_{cl} is the characteristic cluster radius, and c is the speed of light. The host halo contributes an additional term, $\Phi_{\text{host}} = v_{\text{host}}^2/c^2$, characterized by its circular velocity v_{host} . For a Milky-Way-like host halo this velocity is approximately $v_{\text{host}} \simeq 220 \text{ km s}^{-1}$, adopted here as a representative value for the galactic-scale environment in which the PBH cluster is embedded. In this regard, the total environmental potential entering the screening criterion is the sum $\Phi_{\text{tot}} = \Phi_{\text{cl}} + \Phi_{\text{host}}$.

The degree of chameleon screening can be related to the depth of the gravitational potential through the thin-shell condition. In the quasi-static limit, one can define the thin-shell ratio as

$$x_{\text{scr}} \equiv \frac{1.5 |f_{R0}|}{|\Phi_{\text{tot}}|}, \quad (7)$$

where the numerical prefactor of 1.5 is fixed by the Hu-Sawicki thin-shell relation. We adopt a smooth interpolation prescription that allows the effective coupling to vary continuously between the screened and unscreened regimes

$$f_{\text{scr}} = \frac{x_{\text{scr}}}{1 + x_{\text{scr}}}, \quad (8)$$

which reduces to $f_{\text{scr}} \simeq x_{\text{scr}}$ in the strongly screened regime $x_{\text{scr}} \ll 1$ and approaches unity asymptotically as x_{scr} increases. Thus, $f_{\text{scr}} \rightarrow 1$ corresponds to the unscreened limit, whereas $f_{\text{scr}} \rightarrow 0$ describes the strongly screened, GR-like regime. This prescription provides an effective description of the environmental suppression of the fifth force without requiring an explicit solution for the nonlinear scalaron profile within the PBH cluster.

In the absence of chameleon screening, the scalar contribution enhances the Newtonian gravitational coupling by a factor of $1/3$, such that $G_{\text{eff}} = 4G/3$. This well-known result follows from the extra scalar-mediated force carried by f_R in the weak-field limit of Hu-Sawicki gravity. Environmental screening suppresses this contribution according to the screening factor f_{scr} , so that the effective coupling relevant for the PBH encounter dynamics interpolates smoothly between the two limits,

$$G_{\text{eff}} = G \left(1 + \frac{1}{3} f_{\text{scr}} \right), \quad G \leq G_{\text{eff}} \leq \frac{4}{3} G. \quad (9)$$

This prescription applies to the long-range interaction governing PBH encounters and does not imply that the scalar field remains unscreened on horizon scales. Consequently, any suppression of the scalar-mediated interaction due to near-horizon dynamics leaves the macroscopic encounter dynamics consistent with the GR limit.

For concreteness, we consider Hu-Sawicki $f(R)$ models with $|f_{R0}| = 10^{-6}$, 10^{-5} , and 10^{-4} , corresponding to progressively stronger departures from the GR limit and defining the range of modified-gravity strengths explored in our analysis [55]. For the reference PBH cluster embedded in a Milky-Way-like host considered below, with $\Phi_{\text{tot}} \simeq 2.85 \times 10^{-6}$, Eqs. (7)-(9) give distinct effective gravitational couplings, listed in Table I. Consequently, each value of $|f_{R0}|$ enters the capture kernel through its corresponding G_{eff} .

TABLE I: Smooth thin-shell screening and the corresponding effective gravitational coupling for the reference PBH cluster embedded in a Milky-Way-like host. The adopted cluster parameters are $N_{\text{cl}} = 10^5$, $m_{\text{PBH}}^{(0)} = 30 M_{\odot}$, and $n_{\text{cl}} = 10^8 \text{ pc}^{-3}$, while the host has $v_{\text{host}} = 220 \text{ km s}^{-1}$, giving $\Phi_{\text{tot}} \simeq 2.85 \times 10^{-6}$.

Model	x_{scr}	f_{scr}	G_{eff}/G
GR	0	0	1.000
$ f_{R0} = 10^{-6}$	0.526	0.345	1.115
$ f_{R0} = 10^{-5}$	5.26	0.840	1.280
$ f_{R0} = 10^{-4}$	52.6	0.981	1.327

C. Cluster Dynamics and Retention

The efficiency of PBH coagulation is controlled not only by the gravitational interaction but also by the dynamical state of the host cluster. Repeated encounters require a sufficiently dense and long-lived system, while the remnants of successive mergers must remain bound to the cluster for hierarchical growth to proceed.

The cluster model is specified by the PBH number density n_{cl} and the total number of PBHs N_{cl} . For a spherical distribution with uniform number density, the cluster volume and

radius are

$$V_{\text{cl}} = \frac{N_{\text{cl}}}{n_{\text{cl}}}, \quad R_{\text{cl}} = \left(\frac{3N_{\text{cl}}}{4\pi n_{\text{cl}}} \right)^{1/3}, \quad (10)$$

where R_{cl} denotes the characteristic cluster radius. For the parameters considered throughout this work, this relation gives $R_{\text{cl}} \approx 0.062 \text{ pc}$. This density is representative of the cores of the densest known stellar systems, such as young massive and nuclear star clusters, and is adopted as an upper-end environment in which a clustered PBH sub-population could plausibly reside; as shown below, it is also the density regime for which the internal relaxation time is short enough for the cluster to remain dynamically active over the available cosmic-time budget.

For a virialized cluster we adopt the characteristic speed $v_{\text{vir}} \equiv \sqrt{GM_{\text{cl}}/R_{\text{cl}}} \approx 456 \text{ km s}^{-1}$ for the reference parameters above. Also, the corresponding escape velocity is $v_{\text{esc}} = \sqrt{2} v_{\text{vir}} \approx 645 \text{ km s}^{-1}$, which sets the velocity required for a merger remnant to leave the cluster within this description. The associated crossing time is

$$t_{\text{cross}} = \frac{R_{\text{cl}}}{v_{\text{vir}}} \approx 130 \text{ yr}, \quad (11)$$

while the two-body relaxation time is

$$t_{\text{relax}} \approx \frac{0.1 N_{\text{cl}}}{\ln N_{\text{cl}}} t_{\text{cross}} \approx 0.12 \text{ Myr}. \quad (12)$$

As evident from this relation, the relaxation time is much shorter than the available cosmic interval, $\Delta t_{\text{merge}} \simeq 0.54 \text{ Gyr}$. The PBH cluster can therefore undergo significant internal dynamical evolution during the merger epoch. In particular, two-body relaxation can redistribute the PBHs and drive the formation of a denser central region with $n_{\text{core}} > n_{\text{cl}}$, thereby enhancing the local encounter rate.

The retention of merger remnants is also an important consideration, since GW recoil can eject the remnant from the cluster. For comparable-mass binaries with modest spins, numerical-relativity studies typically find recoil velocities of tens to a few hundred km s^{-1} , while specially tuned spin configurations can produce kicks approaching or exceeding $\sim 10^3 \text{ km s}^{-1}$ [75–77]. For our reference cluster, with $v_{\text{esc}} \approx 645 \text{ km s}^{-1}$, the bulk of the isotropic, moderate-spin population considered in our Monte Carlo calculation remains gravitationally bound, with only the high-kick tail being susceptible to ejection. We therefore assume efficient remnant retention in the reference model and do not include a recoil-loss term in the coagulation equation. This approximation may require revision for systems with shallower gravitational potentials, where recoil ejections can become significant.

We formulate the coagulation dynamics using the characteristic cluster density n_{cl} specified by the initial configuration. We adopt this density as the environmental parameter entering the coagulation kernel, thereby providing a controlled description of the merger dynamics at fixed cluster conditions. The resulting framework isolates the effects of PBH coagulation and modified gravitational interactions for a given cluster environment, while the possible impact of subsequent structural evolution can be incorporated as an extension of the model.

III. HYBRID MASS ASSEMBLY MODEL

The assembly of massive black holes is modeled as a hybrid of two concurrent channels. Within a sufficiently dense cluster, PBHs undergo repeated binary formation and coalescence. The resulting evolution of the PBH mass distribution is described by the Smoluchowski coagulation equation, with the merger kernel determined by GW radiation capture. The same kernel also provides the merger-driven mass-growth rate of an individual tracked PBH. In parallel, radiatively efficient gas accretion can operate once seeds inhabit gas-rich galactic environments. Over the JWST redshift window the accretion channel dominates the bulk population amplitude used in the BHMF comparison, while coagulation controls the dry high-mass tail and the characteristic M_{max} tracks discussed below.

A. GW Radiation-Capture Merger Kernel

In a sufficiently dense PBH cluster, initially unbound PBHs can form bound binaries through GW radiation capture during close hyperbolic encounters. For two PBHs with masses m_i and m_j , the total and reduced masses are defined as

$$M_{ij} = m_i + m_j, \quad \mu_{ij} = \frac{m_i m_j}{m_i + m_j}. \quad (13)$$

Within the effective-coupling description of Hu-Sawicki $f(R)$ gravity adopted here, orbital dynamics and gravitational focusing are controlled by G_{eff} . We propagate this coupling into the capture estimate below as an effective model of the enhanced close-encounter rate. We will return to the physical justification and limitations of this step once the full kernel has been assembled. With that modeling choice, the energy radiated in GWs during an encounter with relative velocity v and pericenter distance r_p has the dependence

$$\Delta E_{\text{GW}} \propto \frac{G_{\text{eff}}^{7/2} \mu_{ij}^2 M_{ij}^{5/2}}{c^5 r_p^{7/2}}. \quad (14)$$

GW capture occurs when the radiated energy is sufficient to overcome the initial kinetic energy of the relative orbit,

$$\Delta E_{\text{GW}} \geq \frac{1}{2} \mu_{ij} v^2. \quad (15)$$

The equality in Eq. (15) determines the largest pericenter distance for which capture is possible. Combining Eqs. (14) and (15) gives

$$r_{p,\text{max}} \propto G_{\text{eff}} \mu_{ij}^{2/7} M_{ij}^{5/7} c^{-10/7} v^{-4/7}. \quad (16)$$

For the nonrelativistic encounters considered here, $v \ll c$, gravitational focusing dominates the relation between the impact parameter and the pericenter distance. In this regime,

$$b_{\text{max}}^2 \simeq \frac{2G_{\text{eff}} M_{ij} r_{p,\text{max}}}{v^2}, \quad (17)$$

and the corresponding capture cross section is $\sigma_{\text{cap}} = \pi b_{\text{max}}^2$. Substitution of Eq. (16) then yields

$$\sigma_{\text{cap}} \propto \frac{G_{\text{eff}}^2 M_{ij}^{12/7} \mu_{ij}^{2/7}}{c^{10/7} v^{18/7}}. \quad (18)$$

The dependence on G_{eff} propagated through Eqs. (14)–(18) should be interpreted as an environmental, mean-field effect, distinct from the modification of the horizon structure constrained by the no-hair result of Sec. II B. The latter restricts the scalar charge of an isolated, stationary vacuum solution and therefore does not directly constrain the effective coupling governing the relative dynamics of two PBHs embedded as dark-matter constituents in a sourced background with $\nabla f_R \neq 0$, generated by the cluster and host-halo potentials. Because the encounter timescale t_{cross} is short compared with the relaxation timescale of the ambient scalar field, one can treat this background, and hence G_{eff} , as quasi-static during an individual encounter. It therefore enters both the gravitational-focusing cross section, Eq. (17), and the quadrupole estimate, Eq. (14), consistently at the mean-field level.

The merger kernel entering the coagulation equation is the velocity-averaged capture rate, $K_{ij} = \langle \sigma_{\text{cap}} v \rangle$. For an isotropic three-dimensional Maxwellian distribution of relative velocities, this average gives

$$K_{ij} = C_{\text{GW}} \frac{G_{\text{eff}}^2 (m_i + m_j)^{10/7} m_i^{2/7} m_j^{2/7}}{c^{10/7} v_{\text{vir}}^{11/7}}, \quad (19)$$

where

$$C_{\text{GW}} = 2\pi \left(\frac{85\pi}{6\sqrt{2}} \right)^{2/7} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{14}\right) \left(\frac{4}{3}\right)^{-11/14}. \quad (20)$$

B. Smoluchowski Coagulation Formalism

The nonlinear evolution of the PBH mass distribution through repeated binary coalescences is described by the continuous Smoluchowski coagulation equation [69]. Let $n(m, t)$ denote the comoving number density of PBHs per unit mass at mass m and cosmic time t , and let $K(m_1, m_2)$ denote the merger kernel for a pair of PBHs with masses m_1 and m_2 . The mass distribution evolves according to

$$\begin{aligned} \frac{\partial n(m, t)}{\partial t} = & \frac{1}{2} \int_0^m K(m', m - m') n(m', t) n(m - m', t) dm' \\ & - n(m, t) \int_0^\infty K(m, m') n(m', t) dm'. \end{aligned} \quad (21)$$

The first term describes the formation of PBHs of mass m through mergers of lighter objects, whereas the second term accounts for the removal of PBHs of mass m through mergers with the rest of the population.

For the numerical evolution, the continuous mass distribution is discretized on N_{bins} logarithmically spaced mass nodes

$\{m_k\}$. The number of PBHs contained in mass bin k is denoted by N_k . For a cluster of volume V_{cl} , the merger-induced depletion rate of this bin is then

$$\left. \frac{dN_k}{dt} \right|_{\text{loss}} = -\frac{N_k}{V_{\text{cl}}} \sum_j K_{kj} N_j, \quad (22)$$

where $K_{kj} = K(m_k, m_j)$. The corresponding formation rate of merger pairs involving PBHs in bins i and j is

$$\dot{N}_{ij}^{\text{pair}} = \frac{1}{V_{\text{cl}}} \begin{cases} K_{ij} N_i N_j, & i \neq j, \\ \frac{1}{2} K_{ii} N_i^2, & i = j, \end{cases} \quad (23)$$

where the overdot denotes differentiation with respect to time, and the normalization of the interaction rates is fixed by Eq. (10).

A merger remnant has mass $m_{\text{new}} = m_i + m_j$, which in general does not coincide with a mass-grid node. For $m_k \leq m_{\text{new}} \leq m_{k+1}$, the remnant is therefore distributed between the two neighboring nodes according to the interpolation weights

$$w_k = \frac{m_{k+1} - m_{\text{new}}}{m_{k+1} - m_k}, \quad w_{k+1} = 1 - w_k. \quad (24)$$

These weights preserve the remnant mass exactly, since

$$w_k m_k + w_{k+1} m_{k+1} = m_{\text{new}}. \quad (25)$$

The discretized evolution therefore conserves the PBH mass within the resolved mass range. Consequently, merger remnants with $m_{\text{new}} > m_{N_{\text{bins}}}$ are recorded as flux through the upper mass boundary and excluded from the resolved mass distribution.

C. Merger-Driven Mass-Growth Rate

The coagulation equation describes the evolution of the entire PBH mass distribution, whereas the subsequent accretion model requires the mass growth rate of an individual PBH. This quantity can be obtained directly from the merger kernel. Consider a PBH of mass M embedded in the cluster. The rate at which it merges with PBHs in the mass interval $[m, m + dm]$ is

$$d\Gamma_{\text{merger}}(M, m, t) = K(M, m) n(m, t) dm. \quad (26)$$

Under the assumption adopted in the coagulation model that a merger between a PBH of mass M and a companion of mass m produces a remnant of mass $M + m$, the merger-driven mass-growth rate of a PBH of mass M is

$$\dot{M}_{\text{merger}}(M, t) = \int_0^\infty m K(M, m) n(m, t) dm. \quad (27)$$

The quantity $\dot{M}_{\text{merger}}$ denotes the per-object mass-growth rate, while the total cluster mass remains conserved under dry coalescences.

For the discretized mass distribution, Eq. (27) becomes

$$\dot{M}_{\text{merger},i} = \sum_j K_{ij} \frac{N_j}{V_{\text{cl}}} m_j, \quad (28)$$

where $\dot{M}_{\text{merger},i}$ is the merger-driven growth rate of a PBH with mass m_i . Equivalently, the corresponding merger timescale can be defined as

$$t_{\text{merger},i} = \frac{m_i}{\dot{M}_{\text{merger},i}}. \quad (29)$$

Consequently, the merger-driven growth rate is determined self-consistently from the same interaction kernel that governs the Smoluchowski evolution, maintaining consistency between the mass-growth and coagulation dynamics.

D. Numerical Implementation and Stability

Because the capture kernel has a superlinear mass dependence, $K_{ij} \sim M_{ij}^{10/7}$, the coagulation equations can become numerically stiff as the high-mass tail develops. We therefore solve the discretized Smoluchowski equation with an implicit, variable-order backward differentiation formula (BDF) scheme on a logarithmically spaced mass grid. We use 400 mass bins spanning $0.5 m_0$ to $10^7 m_0$, with relative and absolute tolerances of $\text{rtol} = 2 \times 10^{-7}$ and $\text{atol} = 10^{-10}$, respectively. The upper mass boundary is chosen sufficiently far from the masses reached during the evolution for the cluster parameters considered.

We monitor the numerical completeness of the mass distribution through the unresolved mass fraction

$$f_{\text{unres}}(t) = 1 - \frac{M_{\text{tot}}(t)}{M_{\text{tot}}(t_{\text{ini}})}, \quad M_{\text{tot}}(t) = \sum_k m_k N_k(t), \quad (30)$$

which measures the fraction of the initial cluster mass that crosses the upper mass boundary. We exclude parameter-space regions with $f_{\text{unres}} > 0.10$. In the retained parameter space, $f_{\text{unres}} < 10^{-5}$, so boundary losses are negligible. We also test the numerical convergence by varying the mass resolution, upper mass cutoff, and time-step control. These tests change the maximum assembled mass at $z = 6$ by less than 2%, demonstrating that the reported results are insensitive to the adopted numerical resolution.

E. Subsequent Gas-Accretion Formalism

Following the initial dynamical merger phase, we have modeled further growth through radiatively efficient gas accretion. The total mass-growth rate of a PBH is written as the sum of the merger and accretion contributions

$$\frac{dM}{dt} = \dot{M}_{\text{merger}} + \dot{M}_{\text{acc}}. \quad (31)$$

In this relation, the accretion contribution is parameterized by the Eddington ratio $\lambda_{\text{Edd}} \equiv L/L_{\text{Edd}}$ and the radiative efficiency ϵ :

$$\dot{M}_{\text{acc}} = \frac{1 - \epsilon}{\epsilon} \frac{\lambda_{\text{Edd}} M}{t_{\text{Edd}}}, \quad t_{\text{Edd}} \simeq 0.45 \text{ Gyr.} \quad (32)$$

where t_{Edd} is the Salpeter time. Here, the factor $(1 - \epsilon)/\epsilon$ accounts for the fraction of the accreted rest-mass energy that contributes to black-hole growth after radiative losses.

Combining Eqs. (27) and (32), one can rewrite Eq. (31) as

$$\frac{dM}{dt} = \int_0^\infty m K(M, m) n(m, t) dm + \frac{1 - \epsilon}{\epsilon} \frac{\lambda_{\text{Edd}} M}{t_{\text{Edd}}}. \quad (33)$$

This equation makes explicit the connection between the dynamical merger calculation and the subsequent accretion model.

When the merger contribution is subdominant relative to accretion, $\dot{M}_{\text{merger}} \rightarrow 0$ and Eq. (31) reduces to pure Eddington-limited growth. Assuming a constant Eddington ratio over a cosmic-time interval Δt , integration from a seed mass M_{seed} to a target mass M_{target} gives

$$M_{\text{target}} = M_{\text{seed}} \exp \left[\frac{1 - \epsilon}{\epsilon} \frac{\lambda_{\text{Edd}} \Delta t}{t_{\text{Edd}}} \right]. \quad (34)$$

Consequently, the Eddington ratio required to grow the merger-generated seed to a given target mass by a representative observation redshift z_{obs} is

$$\lambda_{\text{Edd, req}} = \frac{\epsilon}{1 - \epsilon} \frac{t_{\text{Edd}}}{\Delta t} \ln \left(\frac{M_{\text{target}}}{M_{\text{seed}}} \right). \quad (35)$$

Here, Δt denotes the cosmic time between the seed epoch and the target redshift. For the characteristic M_{max} tracks, we take $M_{\text{seed}} = M_{\text{max}}(z = 6)$ from the dry-coagulation calculation and evaluate Δt from $z_{\text{ini}} = 11.5$ to z_{obs} , providing the time available for subsequent accretion. This defines the seed for the accretion phase without double-counting the merger-driven growth.

IV. MULTI-MESSENGER OBSERVABLES AND DIAGNOSTICS

Gas accretion and GW-driven mergers can jointly shape the mass and spin distributions, SGWB, and spatial clustering of the evolving PBH population. In this section, we present the framework used to model these observables and the observational datasets used to constrain the underlying growth mechanisms and, where possible, assess the effective gravitational coupling.

A. Black Hole Spin Evolution

The spin vector of a black hole records its mass-assembly history. In dense cluster environments, seed PBHs grow

through gas accretion and hierarchical binary coalescences, each imparting characteristic torques whose imprint on the spin magnitude and orientation reflects the dominant channel. We first present the relativistic framework common to both channels, then describe how each regime drives spin evolution, and finally couple this framework to the cluster kinetics of Sec. III.

An isolated, stationary vacuum black hole is uniquely described by the Kerr metric, whose spin state is characterized by the dimensionless spin vector

$$\chi \equiv \frac{c \mathbf{S}}{GM^2}, \quad (36)$$

where $\mathbf{S}$ is the spin angular-momentum vector, $\chi \equiv |\chi|$ is bounded by $0 \leq \chi < 1$, and $\hat{\mathbf{S}} \equiv \mathbf{S}/|\mathbf{S}|$ is the unit orientation vector in the cluster frame.

The radiative efficiency and angular-momentum transfer of accreted matter can be set by the location of the innermost stable circular orbit (ISCO). In units of the gravitational radius $R_g \equiv GM/c^2$, the equatorial ISCO radius is [78]

$$r_{\text{ISCO}}(\chi) = 3 + Z_2 \mp \sqrt{(3 - Z_1)(3 + Z_1 + 2Z_2)}, \quad (37)$$

where the lower (upper) sign corresponds to prograde (retrograde) orbits, and

$$Z_1 \equiv 1 + (1 - \chi^2)^{1/3} \left[(1 + \chi)^{1/3} + (1 - \chi)^{1/3} \right], \quad (38)$$

$$Z_2 \equiv \sqrt{3\chi^2 + Z_1^2}. \quad (39)$$

The specific energy and angular momentum per unit rest mass carried across the horizon at the ISCO follow as

$$E_{\text{ISCO}}(\chi) = \frac{r_{\text{ISCO}}^{3/2} - 2r_{\text{ISCO}}^{1/2} \pm \chi}{r_{\text{ISCO}}^{3/4} \sqrt{r_{\text{ISCO}}^{3/2} - 3r_{\text{ISCO}}^{1/2} \pm 2\chi}}, \quad (40)$$

$$L_{\text{ISCO}}(\chi) = \pm \frac{GM}{c} \frac{r_{\text{ISCO}}^2 \mp 2\chi \sqrt{r_{\text{ISCO}}} + \chi^2}{r_{\text{ISCO}}^{3/4} \sqrt{r_{\text{ISCO}}^{3/2} - 3r_{\text{ISCO}}^{1/2} \pm 2\chi}}. \quad (41)$$

Based on this, one can obtain the Novikov-Thorne thin-disk accretion efficiency as $\eta(\chi) = 1 - E_{\text{ISCO}}(\chi)$ ¹.

The spin evolution can proceed through three physical regimes, depending on the gas-feeding geometry and cluster environment. When gas is supplied with a coherent, global angular momentum $\mathbf{J}_{\text{disk}}$, frame dragging exerts a Lense-Thirring torque on the misaligned accretion flow

$$\boldsymbol{\tau}_{\text{LT}} = \frac{2G}{c^2 r^3} (\mathbf{S} \times \mathbf{J}_{\text{disk}}), \quad (42)$$

¹ For a Schwarzschild black hole, $r_{\text{ISCO}} = 6 R_g$ and $\eta \approx 0.057$. For the extremal prograde limit, $r_{\text{ISCO}} \rightarrow R_g$ and $\eta \rightarrow 0.423$, while, for the extremal retrograde limit, $r_{\text{ISCO}} \rightarrow 9 R_g$ and $\eta \approx 0.038$. These limits bracket the accretion efficiencies and the spin-dependent electromagnetic signatures discussed in Sec. VC

which warps the inner disk and aligns $\hat{\mathbf{S}}$ with $\hat{\mathbf{J}}_{\text{disk}}$ via the Bardeen-Petterson effect [79] on a timescale much shorter than the mass-doubling time. Once aligned, prograde accretion drives the spin according to the Bardeen equation [80]:

$$\frac{d\chi}{d \ln M} = \frac{c L_{\text{ISCO}}(\chi)}{GM E_{\text{ISCO}}(\chi)} - 2\chi. \quad (43)$$

Under sustained accretion, the black hole is expected to approach Thorne's relativistic spin limit [81], $\chi_{\text{max}} \approx 0.998$, where the spin-up torque from accreted matter is balanced by the radiation-reaction torque due to disk photons captured by the horizon.

On the other hand, if gas is supplied through small, uncorrelated clouds with randomly oriented $\hat{\mathbf{J}}_{\text{cloud}}$, the black hole undergoes alternating prograde and retrograde accretion episodes [82, 83]. When individual clouds lack sufficient angular momentum to align the disk, the spin vector undergoes a three-dimensional random walk, leading to efficient spin-down. We model this chaotic-accretion regime phenomenologically as

$$\frac{d\chi}{d \ln M} = -\beta(\chi - \chi_{\text{eq}}), \quad (44)$$

where $\chi_{\text{eq}} \approx 0.18$ is the isotropic-accretion equilibrium spin [83] and $\beta \approx 1.8$ sets convergence within a mass growth of order unity in $\ln M$.

In gas-depleted environments, mass growth instead proceeds through GW-induced binary coalescences. Numerical-relativity simulations show that successive, isotropic, near-equal-mass mergers drive the spin toward a universal statistical attractor [84–87]:

$$\chi(M) = \chi_{\text{att}} - (\chi_{\text{att}} - \chi_0) \left(\frac{M_0}{M} \right)^\gamma, \quad (45)$$

where χ_0 is the spin at seed mass M_0 . The attractor value $\chi_{\text{att}} \approx 0.686$, dispersion $\sigma_\chi \approx 0.045$, and exponent $\gamma \approx 1.2$ are fixed by these population studies, are essentially independent of progenitor mass ratio and spin orientation, and largely erase the initial spin once $M/M_0 \gtrsim 3$.

To verify that this attractor is reproduced by the discrete merger sequences of our cluster model, we perform explicit Monte Carlo realizations of hierarchical mergers using numerical-relativity fitting formulas [75, 84, 88]. For a binary with masses m_1, m_2 , mass ratio $q \equiv m_2/m_1 \leq 1$, symmetric mass ratio $\kappa \equiv m_1 m_2 / (m_1 + m_2)^2$, and spin vectors χ_1, χ_2 , the remnant spin can be specified as

$$\chi_f = \frac{m_1^2 \chi_1 + m_2^2 \chi_2 + \ell_{\text{rem}} m_1 m_2 \hat{\mathbf{L}}}{(m_1 + m_2)^2}, \quad (46)$$

where $\hat{\mathbf{L}}$ is the orbital angular-momentum direction at merger and ℓ_{rem} is the specific orbital angular momentum feeding the final spin

$$\ell_{\text{rem}} = \frac{2.7456 + 1.2\kappa - 0.8\kappa^2}{1 - 0.4591\kappa \frac{s_{1,\parallel} + q^2 s_{2,\parallel}}{(1+q)^2}}, \quad (47)$$

with $s_{i,\parallel} \equiv \chi_i \cdot \hat{\mathbf{L}}$. We note that both the functional form and coefficients in Eq. (47) are fitted to numerical-relativity simulations [88]. Also, we evaluate $N_{\text{MC}} = 5000$ hierarchical merger chains, drawing initial spins uniformly from $[0, 0.3]$ and $\hat{\mathbf{L}}$ isotropically. This yields a Monte Carlo uncertainty below the intrinsic dispersion σ_χ , and the resulting mean remnant spin, $\langle \chi \rangle = 0.686 \pm 0.045$, agrees closely with χ_{att} in Eq. (45).

Having established the three regimes in isolation, we now couple them to the cluster kinetics of Sec. III, adopting the same parameters used throughout Secs. II and III. Binaries form via GW capture through the kernel K_{ij} [Eq. (19)], evaluated for both GR and $f(R)$ extensions. We integrate the continuous coagulation equation [Eq. (21)] from $z = 11.5$ to $z = 6.0$ using the BDF scheme of Sec. III D. We then extract the characteristic maximum mass $M_{\text{max}}(z)$, defined by $N(> M_{\text{max}}, z) = 1$ per cluster, and evolve it with Eq. (45) to trace the spin history under pure hierarchical mergers.

For accretion-driven channels, the mass-growth rate again follows the Eddington-limited form of Eq. (32), with $t_{\text{Edd}} \approx 0.451$ Gyr (Sec. III E). We set $\lambda_{\text{Edd}} = 1.0$ to isolate the intrinsic torque physics from any additional accretion-rate parameter and adopt $\epsilon = 0.10$, giving an e-folding growth time of $t_{\text{growth}} \approx 50.1$ Myr. This allows substantial spin evolution within the ~ 0.5 Gyr merger-to-accretion window of Sec. II A. With $A \equiv \lambda_{\text{Edd}}(1 - \epsilon)/(\epsilon t_{\text{Edd}}) \approx 20.0 \text{ Gyr}^{-1}$, the spin equations [Eqs. (43), (44)] take the time-derivative form

$$\frac{d\chi}{dt} = A \frac{d\chi}{d \ln M}, \quad (48)$$

integrated together with the mass-evolution equations from $z = 11.5$ to $z = 6.0$.

B. Black-Hole Mass Function and High-Redshift Data

The primary outcome of the coagulation and accretion solver is the normalized mass-weighted PBH distribution

$$\frac{df_{\text{PBH}}}{d \ln m}(m, z) = \frac{m N(m, z)}{\int_0^\infty m' N(m', z) d \ln m'}, \quad (49)$$

where $N(m, z)$ is the differential number density per mass bin within the cluster. The maximum black-hole mass $M_{\text{max}}(z)$ follows from the cumulative cluster population

$$N(> M_{\text{max}}, z) = \int_{M_{\text{max}}}^\infty N(m, z) dm = 1, \quad (50)$$

solved for $M_{\text{max}}(z)$ by log-linear interpolation.

To convert this cluster-level distribution into a cosmological active BHMF comparable with observations, we account for the global PBH abundance and duty cycles. The cosmological PBH number density is

$$n_{\text{PBH}}(z) = \frac{f_{\text{PBH}} \rho_{\text{DM}}}{\langle M \rangle(z)}, \quad (51)$$

where $\rho_{\text{DM}} = \Omega_{\text{DM}}\rho_{\text{crit},0} \approx 3.3 \times 10^{10} M_{\odot} \text{Mpc}^{-3}$ is the present-day dark-matter density [73], f_{PBH} the PBH dark-matter fraction, and $\langle M \rangle(z)$ the population-averaged mass. For an initial log-normal PBH mass function with dispersion $\sigma_{\ln m}$ undergoing concurrent Salpeter accretion

$$\langle M \rangle(z) = m_{\text{PBH}}^{(0)} \exp\left(\frac{\sigma_{\ln m}^2}{2}\right) f_{\text{acc}}(z), \quad (52)$$

with accretion growth factor

$$f_{\text{acc}}(z) = \exp\left[\frac{\lambda_{\text{Edd}}(1-\epsilon)}{\epsilon t_{\text{Edd}}} (t(z) - t_{\text{ini}})\right], \quad (53)$$

where $t(z)$ is cosmological time and $t_{\text{ini}} = t(z = 11.5)$ marks the onset of rapid growth.

The active BHMF per logarithmic mass interval is then

$$\Phi_{\text{active}}(M, z) = \delta f_{\text{cl}} n_{\text{PBH}}(z) \frac{df_{\text{PBH}}}{d \ln M}(M, z), \quad (54)$$

where $\delta \leq 1$ is the AGN duty cycle and $f_{\text{cl}} \in (0, 1]$ the fraction of PBHs in dense clusters where coagulation is efficient.

Until recently, observational tests of this prediction were limited, as few surveys had sufficient sensitivity to probe black holes in the 10^6 - $10^9 M_{\odot}$ range at $z \gtrsim 4$. Recent JWST spectroscopy has revealed an abundant population of compact, high-redshift broad-line sources, the so-called LRDs, with inferred black-hole masses of $M_{\text{BH}} \sim 10^6$ - $10^9 M_{\odot}$ at $z \gtrsim 4$ -7 [1, 4, 89, 90]. These sources therefore provide a direct observational test of the mass range predicted by our coagulation framework and of $\Phi_{\text{active}}(M, z)$ in Eq. (54). We compare our prediction with two independent, completeness-corrected BHMF measurements. The first is the broad-line H α active BHMF at $z = 4.2$ -5.5 from [4], based on 20 emitters from the EIGER and FRESCO surveys ($V_c = 5.7 \times 10^5 \text{ cMpc}^3$). The second is the broad-line AGN mass function at $z = 3.5$ -6.0 from [89], based on 62 CEERS and RUBIES NIRSpc detections ($V_c = 1.60 \times 10^6 \text{ cMpc}^3$). At $z = 6$ -7, where a complete BHMF is not yet available, we instead use the individual detections of [89] to derive empirical lower limits on the number density ($V_c \approx 4.4 \times 10^5 \text{ cMpc}^3$), and compare the high-mass tail of our prediction with the LRD mass estimates compiled by [90].

C. Stochastic Gravitational-Wave Background

Hierarchical coalescences of PBH binaries across cosmic time generate an unresolvable SGWB, with dimensionless spectral energy density [91]:

$$\Omega_{\text{GW}}(f) = \frac{f}{\rho_{\text{crit},0} c^2} \times \int_{z_{\text{min}}}^{z_{\text{max}}} \frac{\mathcal{R}_{\text{PBH}}(z, f_{R0})}{(1+z) H(z)} \frac{dE_{\text{GW}}}{df_s}(f_s) \mathcal{P}_{f(R)}(z) dz, \quad (55)$$

where $\rho_{\text{crit},0} = 3H_0^2/(8\pi G)$ is the present critical density, f the observer-frame frequency, $f_s = (1+z)f$ the source-frame frequency, $\mathcal{R}_{\text{PBH}}(z, f_{R0})$ is the intrinsic merger-rate

density, $\mathcal{P}_{f(R)}(z)$ denotes the propagation factor, and the integral spans the active merger epoch $z \in [6.0, 11.5]$.

For quasi-circular post-Newtonian inspirals, the angle-averaged energy spectrum per coalescence is [92]

$$\frac{dE_{\text{GW}}}{df_s}(f_s) = \frac{(\pi G)^{2/3}}{3} \mathcal{M}_c^{5/3} f_s^{-1/3}, \quad \text{for } f_s < f_{\text{ISCO}}, \quad (56)$$

where $\mathcal{M}_c \equiv (m_1 m_2)^{3/5}/(m_1 + m_2)^{1/5}$ is the chirp mass. The spectrum terminates at the source-frame ISCO frequency

$$f_{\text{ISCO}} = \frac{c^3}{6^{3/2} \pi G M_{\text{tot}}}. \quad (57)$$

This relation gives $f_{\text{ISCO}} \approx 73.3 \text{ Hz}$ for $M_{\text{tot}} = 60 M_{\odot}$, corresponding to an observed cut-off frequency of $f_{\text{ISCO}}^{\text{obs}} \approx 7.7 \text{ Hz}$ at the representative redshift $z = 8.5$, taken as the midpoint of the merger epoch.

The intrinsic merger-rate density $\mathcal{R}_{\text{PBH}}(z, f_{R0})$ comes directly from the coagulation calculation of Sec. III B. In standard GR, the rate is anchored to $\mathcal{R}_{\text{GR}}(z = 6) = 20 \text{ Gpc}^{-3} \text{ yr}^{-1}$, comparable to dynamical PBH-merger rate estimates for dense clusters [48], adopted as an illustrative normalization. Identical scaling factors are kept across all modified-gravity realizations, so any difference between curves reflects only the G_{eff} -driven enhancement of the coagulation kernel, which enters through the GW-capture cross section.

In metric $f(R)$ gravity, tensor perturbations propagate as $\ddot{h}_{ij} + (3 + \alpha_M) H \dot{h}_{ij} + (k^2/a^2) h_{ij} = 0$, with Planck-mass running rate $\alpha_M \equiv d \ln F / d \ln a$ and $F \equiv df/dR = 1 + f_R$ [93]. This introduces a ratio between electromagnetic and GW luminosity distances, the propagation factor [94, 95]

$$\mathcal{P}_{f(R)}(z) \equiv \left[\frac{d_L^{\text{EM}}(z)}{d_L^{\text{GW}}(z)} \right]^2 = \frac{F(z=0)}{F(z)} = \frac{1 + f_{R0}}{1 + f_R(z)}. \quad (58)$$

For observationally viable Hu-Sawicki models with $|f_{R0}| \leq 10^{-4}$, $|f_R(z)| \ll |f_{R0}| \ll 1$ at high redshift, so $\mathcal{P}_{f(R)}(z)$ deviates from unity by less than 0.01% across $z \in [6.0, 11.5]$. The dominant signature of modified gravity on $\Omega_{\text{GW}}(f)$ thus comes from the enhanced local merger rate $\mathcal{R}_{\text{PBH}}(z, f_{R0})$, not from propagation effects.

D. Spatial Clustering and the Correlation Function

In scalar-tensor theories such as the Hu-Sawicki $f(R)$ model [55], the additional scalar degree of freedom modifies the gravitational coupling on scales below its Compton wavelength. In the quasi-static linear regime, this scale dependence can be expressed through the effective gravitational coupling,

$$\mu(k, a) \equiv \frac{G_{\text{eff}}(k, a)}{G} = \frac{1 + \frac{4}{3} \left(\frac{k}{a, m_{f_R}(a)} \right)^2}{1 + \left(\frac{k}{a, m_{f_R}(a)} \right)^2}, \quad (59)$$

where $a = 1/(1+z)$ is the scale factor, $m_{f_R}(a)$ is the inverse physical Compton wavelength of the scalaron, $\lambda_C(a)$. For the Hu-Sawicki model with $n = 1$, the corresponding Compton wavelength is approximately

$$\lambda_C(a) \approx 32 \sqrt{\frac{|f_{R0}|}{10^{-4}}} \left(\frac{a}{a_0}\right)^2 \text{ Mpc}. \quad (60)$$

Thus, on scales well below the Compton wavelength, $k \gg a m_{f_R}$, the effective coupling approaches $\mu \rightarrow 4/3$, corresponding to the enhancement of gravity by $4/3$. On scales much larger than the Compton wavelength, $k \ll a m_{f_R}$, the scalar-mediated contribution is suppressed and the GR limit is recovered.

This scale dependence alters the coupling between large-scale density fluctuations and small-scale clustering modes. In the squeezed-limit bispectrum, the mode-coupling amplitude is modified as [96]

$$\eta(k_L, k_s) = K_{\text{GR}}(k_s) \frac{\mu(k_s)}{\mu(k_L)}, \quad (61)$$

where $K_{\text{GR}}(k_s) \equiv \frac{68}{21} - \frac{1}{3} [n_{\text{eff}}(k_s) - 3]$ is the standard GR squeezed-kernel amplitude, with $n_{\text{eff}}(k) \equiv d \ln P(k)/d \ln k$ the effective power-law index.

The resulting PBH spatial distribution follows the phenomenological cluster power spectrum

$$P_{\text{PBH}}(k) = A(k_L, k_s) \left(\frac{k}{k_0}\right)^{-2} \times \exp\left[-\left(\frac{k}{k_s}\right)^2\right] \exp\left[-\left(\frac{k_L}{k}\right)^2\right], \quad (62)$$

where k_0 is a pivot scale, k_L, k_s are large- and small-scale cut-offs. Also,

$$A(k_L, k_s) = A_0 \left[\frac{\eta(k_L, k_s)}{\eta_0}\right]^2 \mu^2(k_s), \quad (63)$$

with $A_0 = 0.90$, $\eta_0 = 14$, evaluated at $k_L = 0.05 \text{ Mpc}^{-1}$ and $k_s = 50 \text{ Mpc}^{-1}$.

Eventually, the isotropic real-space two-point correlation function follows from the spherical Bessel transform

$$\xi_{\text{PBH}}(r) = \frac{1}{2\pi^2} \int_0^\infty k^2 P_{\text{PBH}}(k) j_0(kr) dk, \quad (64)$$

where $j_0(x) \equiv \sin(x)/x$. Equation (64) therefore translates the scale-dependent clustering encoded in $P_{\text{PBH}}(k)$ into the real-space correlation function $\xi_{\text{PBH}}(r)$, providing a direct connection to spatial clustering observables of high-redshift black holes and their host galaxies.

V. RESULTS

Up to this point we have developed the theoretical and numerical framework for hierarchical PBH growth in environmentally screened Hu-Sawicki $f(R)$ gravity, including

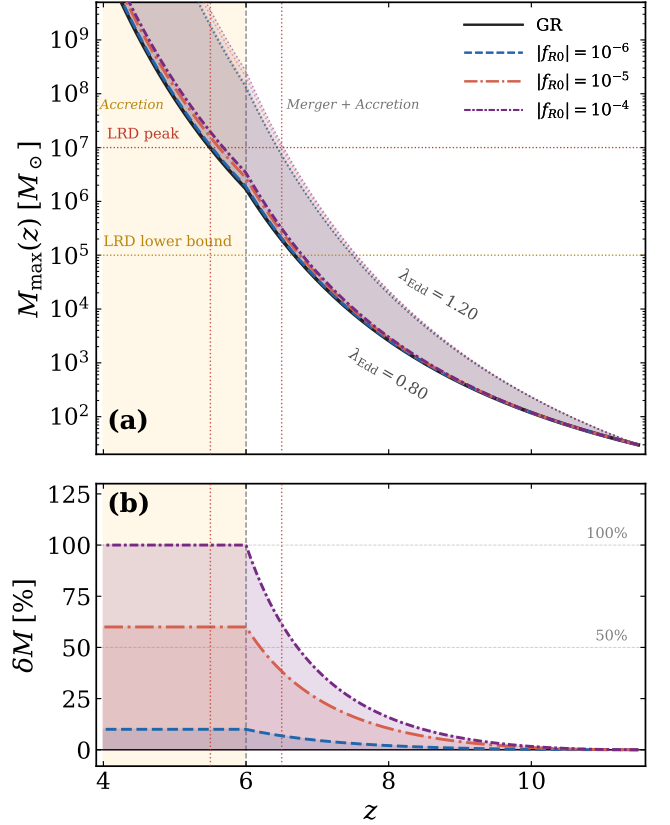


FIG. 1: Characteristic maximum black hole mass $M_{\text{max}}(z)$ from Eqs. (50) and (34) at cluster density $n_{\text{cl}} = 10^8 \text{ pc}^{-3}$ for GR and Hu-Sawicki $f(R)$ models ($|f_{R0}| = 10^{-6}, 10^{-5}, 10^{-4}$). White and yellow shaded background regions denote the dry merger phase with concurrent gas accretion ($z \geq 6.0$) and the pure gas accretion phase ($z < 6.0$), respectively. Vertical red dotted lines mark $z = 5.5$ and $z = 6.5$, indicating the snapshot redshifts selected for the black hole mass function comparison. **(a)** $M_{\text{max}}(z)$ evolution for time-averaged Eddington ratios $\lambda_{\text{Edd}} = 0.80$ and 1.20 . The horizontal dotted lines highlights the observed LRD lower bound and peak. **(b)** Fractional mass enhancement relative to GR evaluated along the $\lambda_{\text{Edd}} = 1.0$ evolution track.

the hybrid merger-accretion assembly model and the multi-messenger diagnostics used to characterize the resulting population. In this section we confront that framework with its quantitative predictions, following the same logical order as Secs. III and IV.

A. Seed Growth

In Fig. 1(a), we have shown the characteristic maximum mass $M_{\text{max}}(z)$ defined by Eq. (50), obtained by evolving the Smoluchowski equation (21) with the GW-capture kernel of Eq. (19) at $n_{\text{cl}} = 10^8 \text{ pc}^{-3}$. The plotted mass combines the hierarchical merger contribution with continuous Eddington-limited accretion. From $z = 11.5$ to $z = 6$, the Smolu-

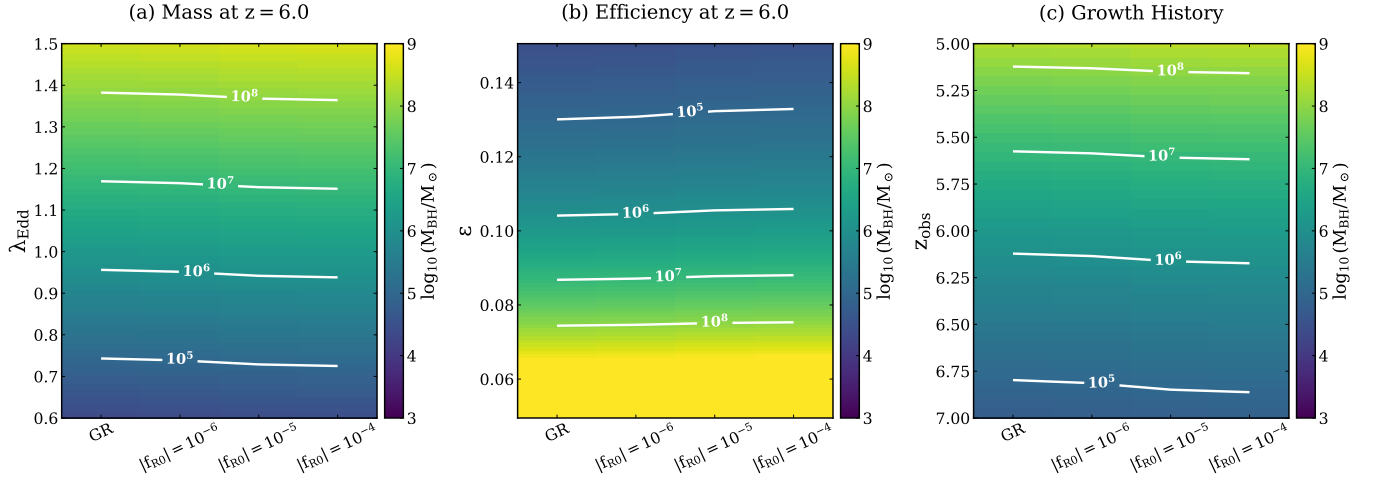


FIG. 2: Final black-hole mass $\log_{10}(M_{\text{BH}}/M_{\odot})$ from Eqs. (31) and (32) for GR and three models of Hu-Sawicki $f(R)$ gravity, $|f_{R0}| = 10^{-6}, 10^{-5}$, and 10^{-4} . **(a)** Mass at $z = 6$ versus λ_{Edd} at $\varepsilon = 0.10$. **(b)** Mass at $z = 6$ versus ε at $\lambda_{\text{Edd}} = 1$. **(c)** Mass versus z_{obs} at $\lambda_{\text{Edd}} = 1$ and $\varepsilon = 0.10$. Contours mark iso-mass lines of $\log_{10}(M/M_{\odot}) = 5, 6, 7$, and 8 .

chowski evolution builds the merger-driven seed while the Salpeter growth factor of Eq. (34) is applied concurrently, with $\epsilon = 0.10$ and $t_{\text{Edd}} = 0.45$ Gyr. At $z = 6$, the dry-merger calculation is terminated, and the resulting seed mass is subsequently evolved purely through accretion to lower redshifts. The two Eddington ratios, $\lambda_{\text{Edd}} = 0.80$ and $\lambda_{\text{Edd}} = 1.20$, are the time averages later used to match the observed BHMF at $z \approx 5.5$ and $z \approx 6.5$ (see, Fig. 5), respectively. We note that $\lambda_{\text{Edd}} = 1.20$ corresponds to mildly super-Eddington accretion. This value is required only for the earlier, $z \approx 6.5$ snapshot, where the shorter cosmic-time budget places a comparatively higher demand on the accretion channel, whereas the $z \approx 5.5$ match is achieved at a sub-Eddington rate. The corresponding accretion factors are applied from $z_{\text{ini}} = 11.5$ throughout the evolution shown in the figure.

In the merger-dominated interval, all models begin near the $30 M_{\odot}$ peak of the initial mass function of Eq. (3). Because $K_{ij} \propto G_{\text{eff}}^2$, the hierarchy of couplings in Table I is imprinted on the merger-driven seed growth. At $z = 6$, the underlying dry-merger solution reaches approximately $300 M_{\odot}$ in GR and $600 M_{\odot}$ for $|f_{R0}| = 10^{-4}$, with the $|f_{R0}| = 10^{-5}$ and 10^{-6} cases lying between these values. These dry-merger values are not shown as separate curves in Fig. 1(a). Instead, the plotted tracks include the concurrent accretion factor. Consequently, the plotted masses are already substantially larger than the corresponding dry seeds by $z = 6$. The dry-merger seeds nevertheless remain far below the LRD mass range, demonstrating that rapid accretion is required to reach $M_{\text{max}} \sim 10^7\text{--}10^8 M_{\odot}$ at the BHMF snapshot epochs.

In Fig. 1(b), we have also plotted the corresponding fractional enhancement $\delta M \equiv (M_{\text{max}}^{f(R)} - M_{\text{max}}^{\text{GR}})/M_{\text{max}}^{\text{GR}}$ along the $\lambda_{\text{Edd}} = 1.0$ track. As can be seen, during the evolution dominated by the mergers, δM grows from zero at $z = 11.5$ to approximately +10%, +60%, and +100% at $z = 6$ for $|f_{R0}| = 10^{-6}, 10^{-5}$, and 10^{-4} , respectively. Because the same accretion factor multiplies all gravity models, it cancels from

the mass ratio. The modified-gravity enhancement acquired during merger-driven seed assembly is therefore preserved during the subsequent accretion-dominated evolution, producing approximately constant fractional offsets below $z = 6$. Since $\Gamma_{\text{merge}} \propto n_{\text{cl}} G_{\text{eff}}^2$, the same hierarchy could in principle be reproduced in GR by increasing the cluster density. Thus, M_{max} alone cannot uniquely isolate $|f_{R0}|$ from n_{cl} . At the reference density, all four models satisfy $f_{\text{unres}} < 10^{-5}$ [Eq. (30)].

B. Accretion Parameter Space

In Fig. 2, we have mapped $\log_{10}(M_{\text{BH}}/M_{\odot})$, obtained from the hybrid growth equation (31), over the four gravity models and the accretion parameters entering Eq. (32). Each panel is a colour map spanning $3 \lesssim \log_{10}(M_{\text{BH}}/M_{\odot}) \lesssim 9$, with the gravity models GR and $|f_{R0}| = 10^{-6}, 10^{-5}, 10^{-4}$ arranged along the horizontal axis; white iso-mass contours have been overlaid at $\log_{10}(M/M_{\odot}) = 5, 6, 7$, and 8 to guide comparison across panels.

In Fig. 2(a), the Eddington ratio $\lambda_{\text{Edd}} \in [0.6, 1.5]$ is varied at $z = 6$, with $\varepsilon = 0.10$ held fixed. It can be seen that the colour gradient runs almost entirely along the vertical axis, confirming that λ_{Edd} is the dominant lever arm for the final mass at fixed epoch and efficiency, as expected from the linear dependence of Eq. (32) on the Eddington ratio. Correspondingly, the iso-mass contours are close to horizontal, with only a shallow downward tilt toward larger $|f_{R0}|$; this tilt is interpreted as encoding the heavier seed mass produced by the enhanced merger channel discussed in relation to Fig. 1. At fixed $\lambda_{\text{Edd}} = 1$, the final mass is $\approx 21\%$ larger for $|f_{R0}| = 10^{-4}$ than for GR, equivalent to a reduction $\Delta\lambda_{\text{Edd}} \approx 0.04$ in the accretion rate required by Eq. (35) to reach the same target mass.

In Fig. 2(b), the radiative efficiency ε is instead varied at

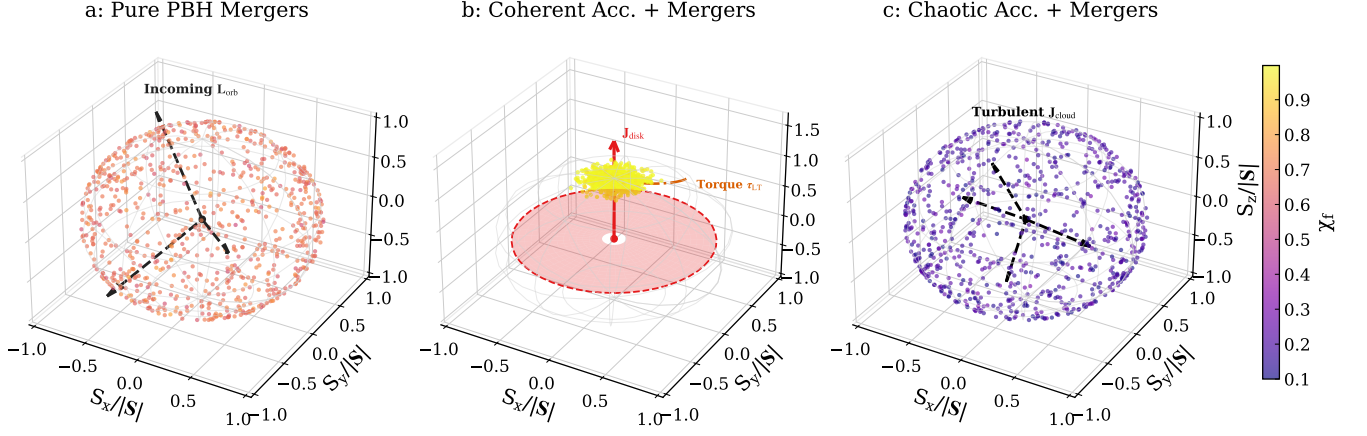


FIG. 3: Spin orientations on the unit sphere, coloured by remnant spin magnitude. **(a)** Pure PBH mergers: isotropic $\hat{\mathbf{S}}$ near $\chi_f \approx 0.686$ [Eq. (45)]. **(b)** Coherent accretion with mergers: polar alignment toward $\hat{\mathbf{J}}_{\text{disk}}$ with $\chi_f \rightarrow 0.998$. **(c)** Chaotic accretion with mergers: isotropic $\hat{\mathbf{S}}$ near $\chi_f \approx 0.18$ [Eq. (44)].

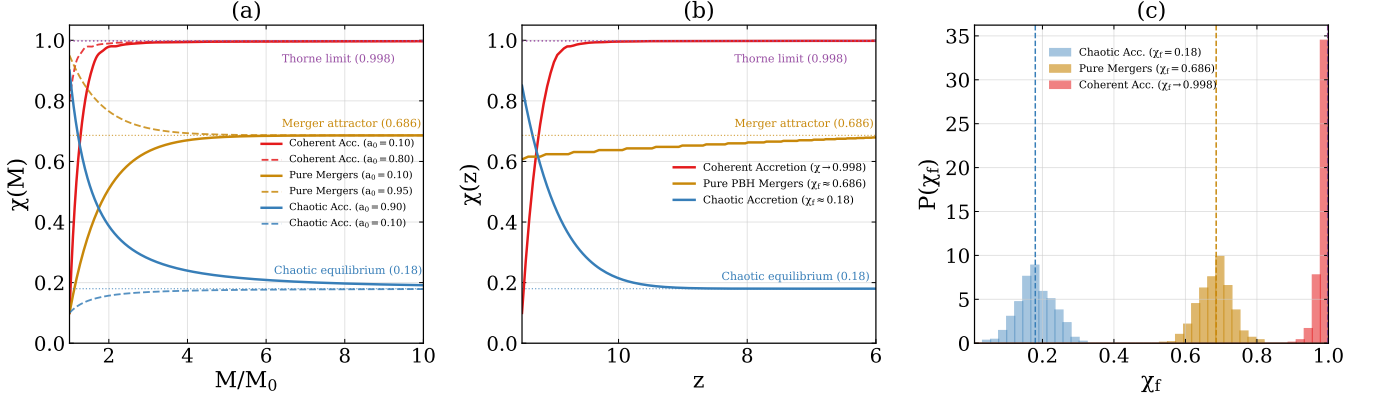


FIG. 4: Spin evolution for coherent accretion (red), pure PBH mergers (gold), and chaotic accretion (blue). **(a)** χ versus M/M_0 from Eqs. (43), (45), and (44). **(b)** $\chi(z)$ from $z = 11.5$ to $z = 6$ via Eq. (48). **(c)** Equilibrium distributions $P(\chi_f)$.

fixed $z = 6$ and $\lambda_{\text{Edd}} = 1$. Since a lower ε increases the retained rest-mass fraction $(1-\varepsilon)/\varepsilon$ in Eq. (32), the colour scale runs in the opposite sense to panel (a): it turns out that M_{BH} increases toward the *bottom* of the panel. Lowering ε from 0.15 to 0.06 moves the population from $\sim 10^6 M_\odot$ up to the 10^7 - $10^8 M_\odot$ range even under Eddington-limited accretion, showing that the efficiency is as important a driver of the final mass as the Eddington ratio itself. As in Fig. 2(a), the $f(R)$ enhancement is found to manifest as a small, nearly uniform upward shift of the contours with increasing $|f_{R0}|$: the efficiency required to reach a given mass is systematically lower in modified gravity than in GR by a comparable margin at every contour level, which is again attributed to the larger seed mass rather than to any modification of the accretion physics itself.

In Fig. 2(c), the growth history is shown, i.e. M_{BH} as a function of observation redshift $z_{\text{obs}} \in [5, 7]$ at fixed $\lambda_{\text{Edd}} = 1$ and $\varepsilon = 0.10$. Because a lower z_{obs} allows a longer integration time in Eq. (32), the final mass increases monotonically toward lower redshift for all four gravity models. It can be

seen that the hierarchy $\text{GR} < |f_{R0}| = 10^{-6} < |f_{R0}| = 10^{-5} < |f_{R0}| = 10^{-4}$ is already established by $z_{\text{obs}} = 7$ and is preserved down to $z_{\text{obs}} = 5$, with the separation between tracks remaining essentially constant in $\log_{10}(M_{\text{BH}})$ over the full redshift range. By $z_{\text{obs}} \sim 5$ -5.5, the 10^7 - $10^8 M_\odot$ tracks enter the mass range characteristic of the observed LRD population. It turns out that Eddington-limited accretion alone can potentially be sufficient to reach LRD-like masses by this epoch, without invoking episodic super-Eddington growth. However, at higher redshifts, larger values of λ_{Edd} might be required.

C. Remnant Spin Magnitudes and Orientation Distributions

In Fig. 3, we have illustrated the three-dimensional unit orientation vectors $\hat{\mathbf{S}} \equiv \mathbf{S}/|\mathbf{S}|$ for the black hole remnant spins alongside their spin magnitudes χ_f , providing a geometric comparison of the three assembly channels described in Sec. IV A. In Fig. 3(a) for pure PBH mergers, the isotropic

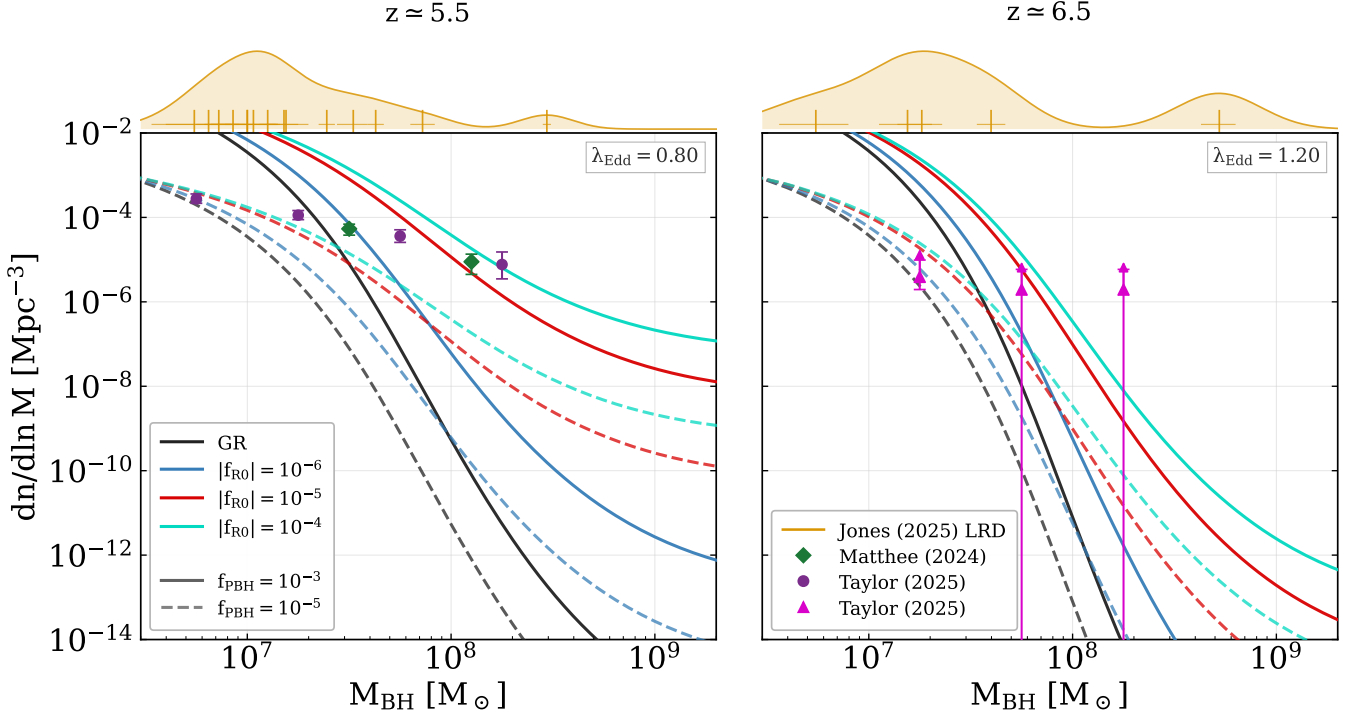


FIG. 5: Active black-hole mass function $\Phi_{\text{active}}(M, z)$ from Eq. (54) at $z \simeq 5.5$ with $\lambda_{\text{Edd}} = 0.80$ (**left**) and $z \simeq 6.5$ with $\lambda_{\text{Edd}} = 1.20$ (**right**), for GR and Hu-Sawicki $f(R)$ models ($|f_{R0}| = 10^{-6}, 10^{-5}, 10^{-4}$). Solid and dashed line styles denote initial PBH fractions of $f_{\text{PBH}} = 10^{-3}$ and 10^{-5} , respectively, under an active AGN duty cycle of $\delta = 10^{-2}$. Observational data include completeness-corrected measurements from [4] and [89] at $z \simeq 5.5$, empirical lower limits at $z \simeq 6.5$ from [89], and the LRD mass distribution from [90] (top kernel-density strips).

distribution of incoming orbital angular momentum vectors $\mathbf{L}_{\text{orb}}$ within dense clusters scatters the remnant spin orientations homogeneously across the unit sphere, while vector additions concentrate the spin magnitudes near the merger attractor value $\chi_{\text{att}} \approx 0.686$, see, Eq. (45). In Fig. 3(b), where coherent accretion is combined with mergers, the accretion disk establishes a preferred axis $\hat{\mathbf{J}}_{\text{disk}}$ along the $+\hat{z}$ -direction. The accompanying Lense-Thirring precession torque τ_{LT} , Eq. (42), efficiently drives the spin vector $\mathbf{S}$ toward the north pole ($S_z/|\mathbf{S}| \rightarrow 1$), while continuous co-rotating gas inflow drives the spin magnitude to the Thorne limit $\chi_f \rightarrow 0.998$. In Fig. 3(c), combining chaotic accretion with mergers yields isotropic spin orientations across the sphere due to the random directions of incoming turbulent gas clouds ($\mathbf{J}_{\text{cloud}}$). However, the alternating spin-up and spin-down episodes strongly damp the overall spin magnitude toward a low equilibrium value $\chi_{\text{eq}} \approx 0.18$, see, (44). Consequently, the joint distribution of spin orientation and magnitude provides a non-degenerate signature that uniquely distinguishes each growth channel.

In Fig. 4, we have also presented the corresponding evolutionary trajectories and final statistical distributions in mass growth, redshift, and spin parameter space. In Fig. 4(a), we have tracked the evolution of dimensionless spin $\chi(M)$ as a function of normalized mass growth M/M_0 , evaluated using Eq. (43) for coherent accretion, Eq. (44) for chaotic accre-

tion, and Eq. (45) for pure mergers. In every case, low-spin ($\chi_0 = 0.10$) and high-spin ($\chi_0 = 0.80 - 0.95$) initial conditions rapidly converge toward a single asymptotic attractor, effectively erasing progenitor spin memory within a few e-foldings of growth. Coherent accretion tracks exhibit the fastest convergence, rising to $\chi \rightarrow 0.998$ by $M/M_0 \approx 2$. Chaotic accretion tracks converge onto $\chi_{\text{eq}} \approx 0.18$ from both high and low initial states by $M/M_0 > 8$, while pure merger tracks approach $\chi_{\text{att}} \approx 0.686$ somewhat more gradually, fully converging by $M/M_0 \approx 4-6$.

In Fig. 4(b), we have mapped these trajectories to redshift evolution from $z = 11.5$ down to $z = 6$, highlighting the distinct physical timescales governing each growth channel. Chaotic accretion reaches its steady-state equilibrium value $\chi_{\text{eq}} \approx 0.18$ earliest, saturating by $z \approx 9.5$ due to the rapid ingestion of small, randomly oriented gas packets. Coherent accretion approaches the Thorne limit shortly thereafter, reaching $\chi \rightarrow 0.998$ by $z \approx 10.3$ under continuous gas supply. Conversely, the pure merger track exhibits a notably slower evolution, reaching $\chi_f \approx 0.686$ only around $z \approx 6.5$. This delayed saturation reflects the hierarchical timescales of cluster dynamics and the slower growth rate of the maximum host cluster mass $M_{\text{max}}(z)$, as shown in Fig. 1.

In Fig. 4(c), we have summarized the remnant spin probability density functions $P(\chi_f)$ at $z = 6$, generated via Monte Carlo sampling by integrating the underlying spin-evolution

differential Eqs. (43)-(45). The resulting distributions form three distinct, non-overlapping peaks: a narrow peak centered at $\chi_{\text{eq}} \approx 0.18$ for chaotic accretion, a Gaussian-like spread around $\chi_{\text{att}} \approx 0.686$ for pure mergers, and a sharp spike near the Thorne limit $\chi_f \rightarrow 0.998$ for coherent accretion. These spin regimes map directly to Novikov-Thorne radiative efficiencies, Eqs. (40)-(37) of $\eta \approx 0.06, 0.11$, and 0.32 , respectively, providing a decisive observational diagnostic for SMBH seed assembly at $z \geq 6$.

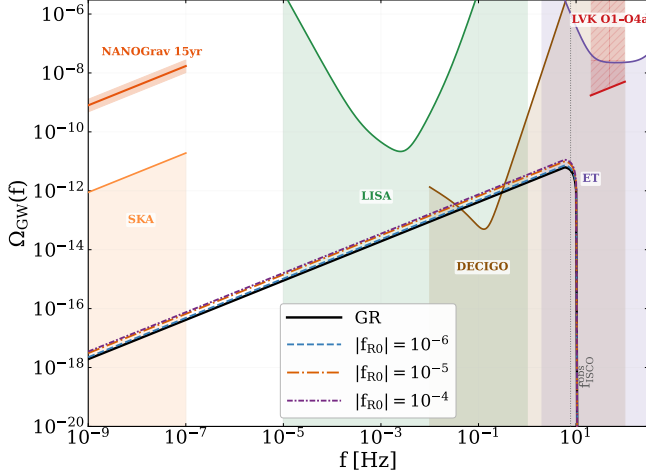


FIG. 6: Stochastic gravitational-wave background energy density spectrum $\Omega_{\text{GW}}(f)$ derived from Eq. (55) for GR and Hu-Sawicki $f(R)$ gravity models with $|f_{R0}| = 10^{-6}, 10^{-5}$, and 10^{-4} . The vertical dotted line indicates the observer-frame ISCO cutoff frequency at $f_{\text{ISCO}}^{\text{obs}} \approx 7.7$ Hz [Eq. (57)] for an equal-mass $M_{\text{tot}} = 60 M_{\odot}$ binary at mean formation redshift $\bar{z} = 8.5$. Observational constraints include the North American Nanohertz Observatory for Gravitational Waves (NANOGrav 15yr) [97] bounds, as well as the projected Square Kilometre Array (SKA) [98], Laser Interferometer Space Antenna (LISA) [99], LIGO-Virgo-KAGRA (LVK O1-O4a) [100] limits, the Decihertz Interferometer Gravitational wave Observatory (DECIGO) [101], and the Einstein Telescope (ET) [102].

D. Active Black-Hole Mass Function

In Fig. 5, we have compared the active black-hole mass function from Eq. 54 with JWST measurements at $z \simeq 5.5$ and $z \simeq 6.5$, assuming Eddington ratios of $\lambda_{\text{Edd}} = 0.80$ and $\lambda_{\text{Edd}} = 1.20$, respectively. Line colors distinguish GR from three Hu-Sawicki $f(R)$ gravity models ($|f_{R0}| = 10^{-6}, 10^{-5}, 10^{-4}$), while solid and dashed line styles represent PBH initial mass fractions of $f_{\text{PBH}} = 10^{-3}$ and 10^{-5} under an active AGN duty cycle of $\delta = 10^{-2}$. In Fig. 5(a), completeness-corrected measurements at $z \simeq 5.5$ from [4] and [89] are shown in the left panel, whereas in Fig. 5(b), $z = 6-7$ lower limits from [89] are presented in the right panel. Kernel-density distribution strips along the top indicate

the observed LRD mass sample from [90] across $M_{\text{BH}} = 10^7 - 10^9 M_{\odot}$.

The vertical amplitude of the active mass function is governed by the active number density from Eqs. (51)-(53), making it directly proportional to the product $f_{\text{PBH}} \times \delta$. With an active duty cycle of $\delta = 10^{-2}$, the solid curves for $f_{\text{PBH}} = 10^{-3}$ pass directly through the [4] and [89] measurements around $\log_{10}(M_{\text{BH}}/M_{\odot}) \simeq 7.5-8.0$. In contrast, the dashed curves for $f_{\text{PBH}} = 10^{-5}$ fall nearly two orders of magnitude below the observed space density. Consequently, an initial seed fraction of $f_{\text{PBH}} \approx 10^{-3}$ under a realistic duty cycle of $\delta = 10^{-2}$ naturally reproduces the observed JWST space densities at $z \simeq 5.5$, demonstrating that PBH seed models can account for the high-redshift active black hole population while remaining consistent with isotropic LVK upper limits ($f_{\text{PBH}} < 10^{-3}$).

At a fixed f_{PBH} , the four gravity models coincide at low black hole masses ($M_{\text{BH}} \sim 10^7 M_{\odot}$), where exponential gas accretion dominates the growth. However, at higher masses ($M_{\text{BH}} \gtrsim 10^8 M_{\odot}$), the models diverge significantly. Modified gravity enhances early halo structure formation and growth, producing a prominent high-mass tail in the active mass function. In particular, the $|f_{R0}| = 10^{-4}$ model (purple lines) predicts active space densities several orders of magnitude above GR (black lines) near $M_{\text{BH}} \sim 10^9 M_{\odot}$. While the observed LRD sample from [90] extends into this high-mass regime beyond $10^8 M_{\odot}$, larger spectroscopic samples and completeness-corrected space density measurements at $M_{\text{BH}} \gtrsim 10^8 M_{\odot}$ will be necessary to definitively constrain these modified gravity extensions.

E. Stochastic Gravitational-Wave Background

In Fig. 6, we have evaluated the SGWB energy density spectrum $\Omega_{\text{GW}}(f)$ across frequencies $f \in [10^{-9}, 10^2]$ Hz using Eq. (55). The underlying PBH merger rates are obtained from the Smoluchowski kinetic equation over redshifts $z \in [6.0, 11.5]$, with the GR baseline rate normalized to $\mathcal{R}_{\text{GR}}(z = 6) = 20 \text{ Gpc}^{-3} \text{ yr}^{-1}$. All four spectral curves exhibit the characteristic $f^{2/3}$ power-law slope across lower frequencies, corresponding to the un-redshifted quadrupole inspiral regime of equal-mass $M_{\text{seed}} = 30 M_{\odot}$ binaries ($M_{\text{tot}} = 60 M_{\odot}$, chirp mass $M_c \approx 26.1 M_{\odot}$). The spectra sharply terminate at the observer-frame ISCO frequency, Eq. (57), evaluated for $M_{\text{tot}} = 60 M_{\odot}$ at a mean redshift of $\bar{z} = 8.5$, indicated by the vertical dotted line. Because this cutoff occurs below 20 Hz, the SGWB signal terminates prior to entering the LVK O1-O4a sensitivity band ($f \gtrsim 20$ Hz).

The results show that the spectral amplitudes strictly follow the gravitational strength hierarchy: $\Omega_{\text{GW}}^{10^{-4}} > \Omega_{\text{GW}}^{10^{-5}} > \Omega_{\text{GW}}^{10^{-6}} > \Omega_{\text{GW}}^{\text{GR}}$. Under Hu-Sawicki $f(R)$ gravity, screening within dense cluster environments yields effective gravitational strength ratios of G_{eff}/G . Because the gravitational capture kernel scales as $K_{ij} \propto G_{\text{eff}}^2$, the intrinsic source-frame merger rates are enhanced relative to GR by factors of $(G_{\text{eff}}/G)^2 \approx 1.24, 1.63$, and 1.76 . Furthermore, the modified gravity GW propagation factor $P(z) = [1 + f_R(0)]/[1 +$

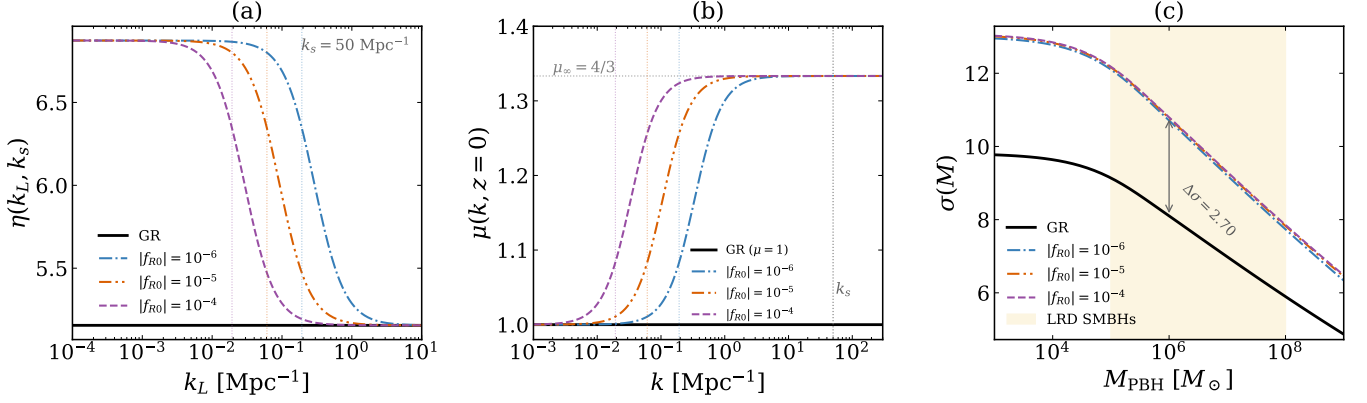


FIG. 7: Linear clustering diagnostics for GR and Hu-Sawicki $f(R)$ gravity models with $|f_{R0}| = 10^{-6}$, 10^{-5} , and 10^{-4} . **(a)** Squeezed-limit mode-coupling parameter $\eta(k_L, k_s)$ from Eq. (61) as a function of the long-mode wavenumber k_L , evaluated at a fixed short-mode wavenumber $k_s = 50 \text{ Mpc}^{-1}$ (vertical dotted line). **(b)** Scale-dependent Poisson modification factor $\mu(k)$ at $z = 0$ derived from Eq. (59), illustrating the smooth transition from Newtonian gravity ($\mu = 1$) at large scales ($k \ll k_*$) to the saturated scalar-tensor limit ($\mu_\infty = 4/3$, horizontal dotted line) at small scales ($k \gg k_*$). Vertical dotted line marks the short-mode reference scale k_s . **(c)** Linear rms mass variance $\sigma(M)$ at $z = 0$ as a function of PBH mass M_{PBH} . The three $f(R)$ curves overlap almost indistinguishably due to saturation on the $\mu = 4/3$ plateau, yielding a constant shift of $\Delta\sigma \approx 2.70$ above GR at $10^6 M_\odot$. The shaded gold region highlights the observed LRD SMBH mass interval 10^5 – $10^8 M_\odot$.

$f_R(z)$] [Eq. (58)] deviates from unity by less than 0.01% across $z \leq 11.5$. Consequently, the observed spectral enhancement is driven entirely by the boosted binary capture rate in the early Universe rather than wave-propagation effects.

Comparing these predictions with observational limits and sensitivity curves in Fig. 6, the signal lies several orders of magnitude below current pulsar timing array bounds from the North American Nanohertz Observatory for Gravitational Waves (NANOGrav 15-year) [97] as well as the projected Square Kilometre Array (SKA) [98], Laser Interferometer Space Antenna (LISA) [99], and LVK [100] limits. However, near its spectral peak ($\Omega_{\text{GW}} \sim 10^{-12} - 10^{-11}$) approaching representative $f_{\text{ISCO}}^{\text{obs}} \approx 7.7 \text{ Hz}$, the signal rises above the projected sensitivity threshold of the Decihertz Interferometer Gravitational wave Observatory (DECIGO) [101], while staying several orders of magnitude lower than the Einstein Telescope (ET) [102] threshold. Future deci-hertz observations with DECIGO measuring the peak amplitude ratio $\Omega_{\text{GW}}^{f(R)} / \Omega_{\text{GW}}^{\text{GR}}$ near $f \sim 0.1 - 7.7 \text{ Hz}$ will therefore provide a sensitive probe to constrain the modified gravity parameter $|f_{R0}|$ through primordial binary capture kinetics.

F. Clustering Signatures

In Fig. 7, we have evaluated the linear clustering quantities described in Sec. IV D that govern the amplitude of the spatial correlation function ξ_{PBH} . These quantities quantify the scale-dependent gravitational modification on sub-megaparsec scales without altering the PBH abundance calculation. In Fig. 7(a), we have presented the squeezed-limit coupling parameter $\eta(k_L, k_s)$ from Eq. (61) at a fixed short-mode wavenumber $k_s = 50 \text{ Mpc}^{-1}$, plotted as a function of the

long-mode wavenumber k_L . At large long-mode wavenumbers ($k_L \rightarrow 10 \text{ Mpc}^{-1}$), both modes lie inside the Compton scale, causing the coupling parameter for all Hu-Sawicki models to converge to the GR value of $\eta_{\text{GR}} \approx 5.16$. At small long-mode wavenumbers ($k_L \rightarrow 10^{-4} \text{ Mpc}^{-1}$), the coupling parameter reaches a maximum plateau of $\eta \rightarrow 6.87$, representing a 33% scale-independent enhancement in η across all $|f_{R0}|$ values. The transition wavenumber where $\eta(k_L, k_s)$ departs from the GR baseline is directly governed by the Compton scale λ_C from Eq. (60). Consequently, the model with $|f_{R0}| = 10^{-6}$ ($\lambda_C \approx 3 \text{ Mpc}$) exhibits a transition in η at a higher long-mode wavenumber k_L than $|f_{R0}| = 10^{-5}$ ($\lambda_C \approx 9.5 \text{ Mpc}$) and $|f_{R0}| = 10^{-4}$ ($\lambda_C \approx 30 \text{ Mpc}$).

In Fig. 7(b), we have also shown the scale-dependent modification to the Poisson equation $\mu(k, z = 0)$ derived from Eq. (59). Each Hu-Sawicki model smoothly interpolates from the Newtonian limit ($\mu = 1$) at large scales ($k \ll k_*$) to the scalar-tensor enhancement limit ($\mu_\infty = 4/3$) at small scales ($k \gg k_*$), where $k_* = (\sqrt{3} \lambda_C)^{-1}$ marks the characteristic transition scale. The short-mode reference scale $k_s = 50 \text{ Mpc}^{-1}$ resides firmly on the saturated $\mu = 4/3$ plateau for all three $f(R)$ models at $z = 0$. Because the background field magnitude $|f_R(z)|$ decreases at higher redshifts, the Compton scale λ_C contracts toward $z \sim 6$, pushing k_* to higher wavenumbers and making a larger fraction of the k -domain GR-like. Consequently, the $z = 0$ curves presented in Fig. 7(b) represent an upper envelope for the linear modified gravity enhancement.

Finally, in Fig. 7(c), we have mapped this modified gravitational slip into the linear mass variance $\sigma(M)$ by integrating $\mu^2(k) P_{\text{GR}}(k)$ against a top-hat window function in real space. Across the mass range shown ($M_{\text{PBH}} = 10^3 - 10^9 M_\odot$), the window function is dominated by modes sitting on the saturated $\mu = 4/3$ plateau. As a result, the three

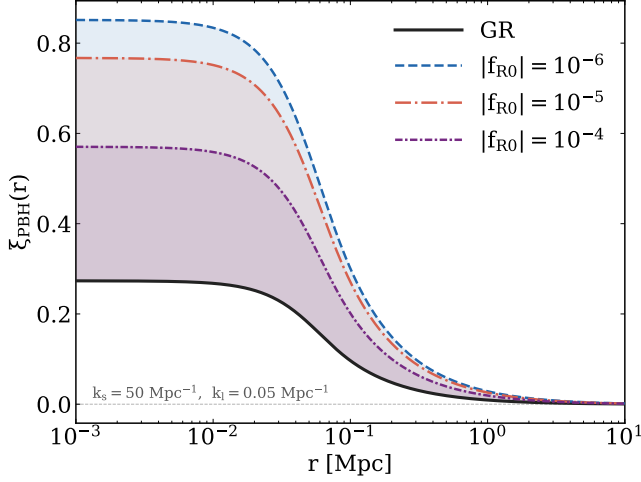


FIG. 8: Real-space PBH correlation function $\xi_{\text{PBH}}(r)$ at $z = 6$ from Eq. (64) for GR and Hu-Sawicki models with $|f_{R0}| = 10^{-6}$, 10^{-5} , and 10^{-4} , evaluated at $k_s = 50 \text{ Mpc}^{-1}$ and $k_L = 0.05 \text{ Mpc}^{-1}$.

Hu-Sawicki curves overlap almost indistinguishably, yielding a uniform amplification ratio of $\sigma_{\text{MG}}/\sigma_{\text{GR}} \approx 4/3$. At $M_{\text{PBH}} = 10^6 M_\odot$, the linear variance exhibits a constant shift from GR of $\Delta\sigma \approx 2.70$ (increasing from $\sigma \approx 8.1$ in GR to $\sigma \approx 10.8$ in modified gravity). The shaded gold region indicates the mass range of SMBHs observed in LRDs. This linear variance serves exclusively as a clustering diagnostic for the spatial distribution of existing objects rather than a primary seed formation constraint.

G. PBH Correlation Function

In Fig. 8, we have evaluated the real-space PBH spatial correlation function $\xi_{\text{PBH}}(r)$ at redshift $z = 6$, derived using Eq. (64) with the phenomenological power spectrum of Eq. (62) anchored at short- and long-mode wavenumbers $k_s = 50 \text{ Mpc}^{-1}$ and $k_L = 0.05 \text{ Mpc}^{-1}$. All four model profiles share a universal radial shape, exhibiting a constant small-scale plateau at $r \lesssim 0.01 \text{ Mpc}$, a steep power-law decline around $r \sim 0.1 \text{ Mpc}$, and a sharp large-scale cutoff at $r \gtrsim 1 \text{ Mpc}$ dictated by the long-mode pivot scale k_L . These spatial profiles differ solely through the overall clustering amplitude $A \propto \eta^2 \mu^2$ defined in Eq. (63).

GR establishes the baseline amplitude with $\eta_{\text{GR}} = 5.16$, $\mu = 1$, and $A = 0.122$. While every Hu-Sawicki model saturates to $\mu \rightarrow 4/3$ at the short-mode scale $k_s = 50 \text{ Mpc}^{-1}$ as shown in Fig. 7(b), the squeezed coupling $\eta(k_L, k_s)$ remains highly sensitive to $\mu(k_L)$ at the long-mode scale $k_L = 0.05 \text{ Mpc}^{-1}$. Because the smallest background field value $|f_{R0}| = 10^{-6}$ corresponds to the smallest Compton wavelength ($\lambda_C \approx 3 \text{ Mpc}$), the long mode $k_L = 0.05 \text{ Mpc}^{-1}$ penetrates deepest into its sub-Compton plateau, generating the largest squeezed coupling ($\eta = 6.82$, $A = 0.380$). Larger background field values yield smaller couplings: $\eta = 6.48$

($A = 0.342$) for $|f_{R0}| = 10^{-5}$, and $\eta = 5.58$ ($A = 0.255$) for $|f_{R0}| = 10^{-4}$. This establishes an inverted amplitude hierarchy, $\xi_{10^{-6}} > \xi_{10^{-5}} > \xi_{10^{-4}} > \xi_{\text{GR}}$, which is opposite to the host cluster growth-rate hierarchy shown in Fig. 1. Thus, weaker background field modifications produce stronger squeezed coupling at the pivot scale k_L used here.

At small separations ($r \lesssim 0.1 \text{ Mpc}$), the clustering enhancement ratios relative to GR reach $\xi_{\text{MG}}/\xi_{\text{GR}} \approx 3.11$, 2.81 , and 2.09 for $|f_{R0}| = 10^{-6}$, 10^{-5} , and 10^{-4} , respectively. These boosts significantly exceed the naive Poisson enhancement factor $\mu^2 \approx 1.78$ because the η^2 factor in Eq. (63) incorporates the additional non-linear long-short mode coupling. Physically, $\xi_{\text{PBH}}(r)$ characterizes the large-scale cosmological spatial clustering of the PBH population across 0.001 – 1 Mpc scales, operating independently of the local two-body cluster dynamics ($R_{\text{cl}} \approx 0.062 \text{ pc}$) governing coagulation kinetics.

VI. CONCLUSIONS

In this work, we have developed a kinetic framework to investigate whether the hierarchical coagulative growth of clustered PBHs in effective Hu-Sawicki $f(R)$ gravity can supply viable intermediate-mass seeds for the LRDs observed at cosmic dawn. By solving the continuous Smoluchowski coagulation equation with a mass-conserving numerical scheme, we have demonstrated that two-body radiation-capture mergers within dense primordial clusters can build an intermediate-mass seed population prior to the onset of primary quasar activity. Modified gravity nonlinearly accelerates this kinetic coagulation through an enhanced GW capture kernel, while environmental chameleon screening dynamically regulates the interaction strength, preventing runaway growth. Because subsequent gas accretion expands multiplicatively with initial seed mass, our findings indicate that the seed mass advantage gained during early dry mergers persists throughout the accretion history. This significantly alleviates the timing bottleneck for early SMBH assembly, reducing the required time-averaged Eddington ratios to plausible near-critical to mildly super-critical levels, with the modified-gravity enhancement manifesting as an equivalent, comparable-magnitude reduction in the radiative efficiency required to reach a given target mass.

By confronting our evolved active black hole mass functions with high-redshift JWST observations, our results show that a modest clustered PBH fraction combined with a realistic active AGN duty cycle can naturally reproduce the space densities of broad-line sources measured at $z \sim 5.5$ – 6.5 . Importantly, because the active population amplitude depends on the product of the seed abundance and the duty cycle, this mechanism accounts for the observed high-redshift black hole space density while requiring only a small fraction of dark matter in PBHs, keeping the scenario fully compatible with isotropic LVK merger-rate bounds. Furthermore, our calculations reveal that while modified gravity and GR produce similar mass function amplitudes at lower masses where gas accretion dominates, modified gravity significantly enhances structure for-

mation to generate a prominent high-mass tail that matches the upper envelope of the observed LRD population.

We have also demonstrated that potential parameter degeneracies between gravitational strength and cluster environment density can be broken by combining three complementary multi-messenger diagnostics. First, the remnant spin distribution provides a clear footprint of the growth channel: coherent accretion, chaotic accretion, and hierarchical dry mergers drive the black hole spin vectors toward distinct, non-overlapping magnitude and orientation states. Second, early binary coalescences produce an unresolvable SGWB featuring a characteristic $f^{2/3}$ inspiral spectrum with an observer-frame ISCO cutoff in the deci-Hertz band, offering a direct window into early binary capture kinetics accessible to future space-based detectors like DECIGO. Third, scale-dependent gravitational slip generates an inverted amplitude hierarchy in the sub-megaparsec spatial correlation function, providing a spatial diagnostic that cleanly separates modified gravity signatures from local cluster density effects.

Our findings demonstrate that effective $f(R)$ gravity can efficiently accelerate intermediate seed formation in dense clusters without violating local screening constraints, establishing a physically compelling and testable pathway toward assembling the massive black holes powering LRDs in the early Universe. However, several sources of uncertainty might point toward fruitful avenues for future research. In particular, our

environment-averaged thin-shell screening model could potentially be refined by incorporating full three-dimensional, non-linear scalaron field solutions within evolving cluster geometries. Additionally, internal cluster dynamics, including core collapse, mass segregation, two-body relaxation, and GW recoil ejections, may influence the long-term efficiency of hierarchical coagulation and could merit detailed N -body modeling. Furthermore, embedding this hybrid assembly picture within cosmological halo-occupation models can potentially help refine the spatial clustering predictions. These refinements can be considered as promising directions for future work.

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