Tight Constraint on the Maximum Mass of Stellar-origin Binary Black Holes and Evidence for Hierarchical Mergers in Gravitational Wave Observations

Yuan-Zhu Wang,1 Yin-Jie Li,2 Jorick S. Vink,3 Yi-Zhong Fan,1 Shaopeng Tang,1 Ying Qin,4,5 and Da-Ming Wei1,2

1Key Laboratory of Dark Matter and Space Astronomy, Purple Mountain Observatory, Chinese Academy of Sciences, Nanjing 210033, People’s Republic of China.
2School of Astronomy and Space Science, University of Science and Technology of China, Hefei, Anhui 230026, People’s Republic of China.
3Armagh Observatory and Planetarium
4Department of Physics, Anhui Normal University, Wuhu, Anhui 241000, People’s Republic of China.
5Guangxi Key Laboratory for Relativistic Astrophysics, Nanning 530004, People’s Republic of China.

(Dated: August 26, 2022)

ABSTRACT

The origins of the coalescing binary black holes (BBHs) detected by the advanced LIGO/Virgo are still under debate, and clues may present in the joint mass-spin distribution of these merger events. Here we construct phenomenological models to investigate the BBH population detected in gravitational observations. The data can be well explained by the members originated from two different channels: one is the evolution of field binaries, and the other is the dynamical assembly. We obtain a tight constraint on the maximum mass for events of the stellar-origin, which is $m_{\text{max}} = 39.4^{+2.6}_{-2.5}\, M_\odot$ at 90% credibility. This mass cutoff likely arises from the (pulsational) pair-instability supernova explosion and/or stellar winds. We also find that a fraction of $4-17\%$ of dynamical events were hierarchical mergers, and these BHs had an average spin magnitude significantly larger than the first-generation mergers, with $d\mu_a > 0.4$ at 99% credibility.

1. INTRODUCTION

With the help of the Advanced LIGO and Virgo detector network, the number of observed binary black hole (BBH) mergers is rapidly growing. To date, more than 90 BBH merger candidates have been released with the current catalogs of compact binary coalescences (GWTC-3) (Abbott et al. 2019a, 2021a; The LIGO Scientific Collaboration et al. 2021a). The origins of these compact objects are still unclear. Various formation channels have been proposed, including, for instance, the isolated binary evolution, dynamical capture, and the AGN enhancement (see Refs. Mapelli 2021 and Gerosa & Fishbach 2021 for recent reviews).

Formation channels may leave their ‘fingerprints’ in the final population of BHs. Of all various channels, the leading scenario for the progenitor of BBHs is a close binary system composed of a BH and a helium star, which can be the outcome of the classical isolated binary evolution (Belczynski et al. 2016a) through the common envelope (Ivanova et al. 2013). From the point of view of stellar evolution theory, the BH masses are expected to fall outside a gap starting at $\sim 40-65\, M_\odot$ and ending at $\sim 125\, M_\odot$ due to (pulsational) pair-instability supernovae ((P)PISNe) (Belczynski et al. 2016b; Woosley 2017; Spera & Mapelli 2017; Stevenson et al. 2019; Mapelli et al. 2020). The BH spins are generally small (Qin et al. 2018; Fuller et al. 2019; Belczynski et al. 2020) under the assumption of efficient angular momentum transport within their progenitors. On the other hand, in the chain of hierarchical mergers, BHs inside the (P)PISNe mass gap can appear in the second or higher-generation mergers, and large spin magnitudes are expected (Miller & Hamilton 2002; Giersz et al. 2015; Fishbach et al. 2017; Gerosa & Berti 2017; Rodriguez et al. 2019; Arca Sedda et al. 2021; Mapelli et al. 2021; Gerosa & Fishbach 2021). More specifically, for the hierarchical mergers happened in the AGN disk, BHs may align their orbits and component spins with the disk, leading to a broad effective spin ($\chi_{\text{eff}}$) distribution with positive mean value (Yang et al. 2019b; Tagawa et al. 2021). These characteristics, however, are not clearly revealed in the data, as shown by the recent study of The LIGO Scientific Collaboration et al. (2021b). One solution to this discrepancy is that the observed events may originate from multiple channels (Kimball et al. 2021;
Galudage et al. 2021; Wang et al. 2021; Bouffanais et al. 2021; Zevin et al. 2021; Wong et al. 2021; Roulet et al. 2021), thus the key features of particular channels are covered up by the mixing of events with different channels.

Population studies were carried out with phenomenological models guided by theoretical concerns (Kimball et al. 2020; Abbott et al. 2021b; Wang et al. 2021; Li et al. 2021a), simulations (Baxter et al. 2021; Bavera et al. 2020a) or non-parametric approaches (Li et al. 2021b; Rinaldi & Del Pozzo 2021) to recover the astrophysical distributions of BBHs. There are evidence for features/substructures in the primary mass function (Abbott et al. 2021b; Wang et al. 2021; Tiwari 2021; Li et al. 2021b), spin distribution (Galudage et al. 2021), mass ratio distribution (Li et al. 2022), and potential correlations (Callister et al. 2021; Safarzadeh & Wysocki 2021; Tang et al. 2021).

In this work, we search for additional clues for sub-populations in the GWTC-3 events. We introduce paring functions into our phenomenological models and aim to construct simple models with astrophysical motivations to describe the mass and spin distributions self-consistently. The paper is arranged as follows: in Sec. 2, we describe our models; in Sec. 3, we introduce the statistical method; the analysis results are presented in Sec. 4, and we give further implication and discussions on our results in Sec. 5 and Sec. 6, respectively.

2. POPULATION MODELS

One way to model the distribution of the component masses \((m_1, m_2)\) of the merging BBHs is to construct the marginal primary mass distribution and the conditional secondary mass distribution (Abbott et al. 2019b):

\[
p(m_1, m_2 | A_m) = p(m_1 | A_m)p(m_2 | m_1, A_m),
\]

where \(A_m\) is the hyper-parameters governing the exact shape of the distribution. A form of \(p(m_2 | m_1, A_m) \propto m_2^\beta\) is generally considered in the literature (Abbott et al. 2019b, 2021b; The LIGO Scientific Collaboration et al. 2021b) to reflect the dependency between \(m_1\) and \(m_2\). On the other hand, Fishbach & Holz (2020) introduced the ‘paring function’ to study the mass distribution. Following their method, the distribution can be written as

\[
p(m_1, m_2 | A_{m_1}, A_{m_2}, A_p) \propto \begin{cases} p(m_1 | A_{m_1})p(m_2 | A_{m_2})w(m_1, m_2 | A_p), & \text{for } m_2 < m_1, \\ 0, & \text{for } m_2 > m_1. \end{cases}
\]

which can be interpreted as follows: the primary and secondary masses are separately drawn from independent distributions \(p(m_1 | A_{m_1})\) and \(p(m_2 | A_{m_2})\), and the probability of two masses belonging to a merging binary is given by the paring function \(w(m_1, m_2 | A_p)\) (Fishbach & Holz 2020). We find it convenient to use the paring function to address diverse preferences for the combination of component masses in multiple channels, so our following modeling is based on Eq. (2).

We consider the distribution model consisting of two sub-populations: one forms through the evolution of field binaries (labeled with ‘field’) and the other forms dynamically (labeled with ‘dyn’). The model that contains both the mass and spin parameters \((\Theta = (m_1, m_2, a_1, a_2, \cos \theta_1, \cos \theta_2))\) can be expressed as

\[
p(\Theta | A_{\text{field}}, A_{\text{dyn}}, f_{\text{dyn}}) = (1 - f_{\text{dyn}}) p_{\text{field}}(\Theta | A_{\text{field}}) + f_{\text{dyn}} p_{\text{dyn}}(\Theta | A_{\text{dyn}}),
\]

where \(A_{\text{field}}\) and \(A_{\text{dyn}}\) are the hyper-parameters for the field and dynamical sub-population respectively, and \(f_{\text{dyn}}\) is the mixing fraction of the dynamically formed BBHs. Assuming the component BHs in a merging binary are drawn from the same underlying distribution, we extend Eq. (2) to model each sub-population:

\[
p_x(\Theta | A_x) \propto \prod_i^2 \pi_x(m_i, a_i, \cos \theta_i | A_x) w_x(\Theta | A_x),
\]

where \(x\) represents ‘field’ or ‘dyn’. \(\pi_x\) is the underlying joint distribution, and we assume that it consists of two independent parts:

\[
\pi_x(m_i, a_i, \cos \theta_i | A_x) = \pi_{m,x}(m_i | A_{m,x})\pi_{s,x}(a_i, \cos \theta_i | A_{s,x}),
\]

in which \(\pi_{m,x}\) is the underlying mass distribution and \(\pi_{s,x}\) is the spin distribution for the underlying BHs if they pair to become a component of merging system.

For the ‘field’ channel,

\[
\pi_{m,\text{field}}(m_i | A_{\text{field}}) = P(m_i | a, m_{\text{min}}, m_{\text{max}}, \delta_m),
\]

...
and,

\[ \pi_{\text{field}}(a_i, \cos \theta_i ; \mathbf{A}_{\text{field}}) = \mathcal{G}(a_i ; \mu_{a,\text{field}}, \sigma_{a,\text{field}}) \mathcal{G}'(\cos \theta_i ; \mu_{\text{ct,field}}, \sigma_{\text{ct,field}}), \]

where \( \mathcal{P} \) is a truncated power-law with a smooth tail at low mass as described in Abbott et al. (2019b); \( \mathcal{G} \) and \( \mathcal{G}' \) are Gaussian distributions truncated at \([0, 1]\) and \([-1, 1]\) respectively. Specifically, under the assumptions of efficient angular momentum transport in stellar evolution (Spruit 2002; Fuller et al. 2019), one would expect \( \mu_{a,\text{field}} \ll 1 \) and \( \mu_{\text{ct,field}} \sim 1 \) (Qin et al. 2018; Fuller et al. 2019; Belczynski et al. 2020) for the binaries formed through the common envelope phase, and the \( m_{\text{max}} \) should be consistent with the lower edge of PPISN gap (Belczynski et al. 2016b). To approximate the preference for symmetric systems in the binary evolution channel, we consider a paring function of

\[ w_{\text{field}}(m_1, m_2 ; \mathbf{A}_{\text{field}}) \propto \left( \frac{m_2}{m_1} \right)^{\beta_{\text{field}}}. \]

For the dynamical channel, building phenomenological distribution model is more challenging, as the formation of binaries may happen in different environments and there might be contributions from hierarchical mergers. To avoid our model being too complicated and redundant, we only consider hierarchical mergers up to the second generation. We first consider a relatively simple case, in which the first generation (1G) dynamical BBHs share the same underlying mass distribution with those originated from field binaries, i.e., \( \pi_{\text{m,1G}}(m_i) = \pi_{\text{m,field}}(m_i) \). The spin distribution of 1G dynamical BBHs is modeled as

\[ \pi_{\text{a,1G}}(m_i, a_i, \cos \theta_i ; \mathbf{A}_{\text{field}}) = \mathcal{G}(a_i ; \mu_{a,1G}, \sigma_{a,1G}) \mathcal{G}'(\cos \theta_i ; \mu_{\text{ct,1G}}, \sigma_{\text{ct,1G}}). \]

Assuming the component BHs are the remnants of single star evolution, under the efficient angular momentum transport assumption, their spin magnitudes will also be small as the field BBHs (hereafter we use ‘stellar BHs’ to represent field and 1G dynamical BHs); therefore, we let \( \mu_{a,1G} \equiv \mu_{a,\text{field}} \equiv \mu_{a,\text{ste}} \) and \( \sigma_{a,1G} \equiv \sigma_{a,\text{field}} \equiv \sigma_{a,\text{ste}} \) to simplify our model. Guided by the results of some simulations for dynamical processes (O’Leary et al. 2016; Yang et al. 2019a), we consider a paring function that depends on both the mass ratio and the total mass:

\[ w_{\text{dyn}}(m_1, m_2 ; \mathbf{A}_{\text{dyn}}) \propto \left( \frac{m_2}{m_1} \right)^{\beta_{\text{dyn}}}(m_1 + m_2)^{\gamma_{\text{dyn}}}. \]

In general, dynamical captures in environments such as globular, nuclear, and young star clusters expect isotropic spin orientation (\( \sigma_{\text{dyn}} \gg 0 \)) (Mandel & O’Shaughnessy 2010; Rodriguez et al. 2016; Mapelli et al. 2022), while the evolution of BBHs in AGN disks may lead to certain degrees of alignment, depending on the details of the dynamics in the disk (McKernan et al. 2018, 2020; Tagawa et al. 2020; Vajpeyi et al. 2022; Mapelli et al. 2022).

The underlying mass distribution of 2G dynamical BBHs can be approximated by the total mass distribution of 1G mergers, which can be calculated by

\[ \pi_{\text{m,2G}}(m_i ; \mathbf{A}_{\text{m,2G}}) \propto \int_{m_{\text{min}}}^{m_{\text{max}}} \int_{m_{\text{min}}}^{m_{\text{max}}} \mathcal{P}(m_{i}^*, m_{i}^* - m_2) \mathcal{P}(m_2) w_{\text{dyn}}(m_{i}^* - m_2, m_2) \mathcal{H}(\frac{m_{i}^*}{2} - m_2), \]

where \( \mathbf{A}_{\text{m,2G}} = (\alpha, m_{\text{min}}, m_{\text{max}}, \delta_{\alpha}, \beta_{\text{dyn}}, \gamma_{\text{dyn}}) \), and we set \( m_{i}^* = 1.05m_2 \) to approximate the loss of gravitational mass during the coalescence. The underlying joint distribution for 2G mergers can then be written as

\[ \pi_{\text{2G}}(m_i, a_i, \cos \theta_i ; \mathbf{A}_{\text{2G}}) = \pi_{\text{m,2G}}(m_i ; \mathbf{A}_{\text{m,2G}}) \mathcal{G}(a_i ; \mu_{a,2G}, \sigma_{a,2G}) \mathcal{G}'(\cos \theta_i ; \mu_{\text{ct,2G}}, \sigma_{\text{ct,2G}}). \]

By introducing a parameter \( r_{2G} \) to describe the fraction of 2G underlying BHs, the overall 1G+2G underlying distribution for dynamical channel is

\[ \pi_{\text{dyn}}(m_i, a_i, \cos \theta_i ; \mathbf{A}_{\text{dyn}}) = (1 - r_{2G})\pi_{\text{1G}}(m_i, a_i, \cos \theta_i ; \mathbf{A}_{\text{1G}}) + r_{2G}\pi_{\text{2G}}(m_i, a_i, \cos \theta_i ; \mathbf{A}_{\text{2G}}). \]

We take the spin tilt hyper-parameters \( \mu_{\text{ct,field}} \equiv \mu_{\text{ct,1G}} \equiv \mu_{\text{ct,2G}} \equiv 1 \) in our analysis, because a half Gaussian that peaks at 1 and truncates at -1 can approximate both the aligned case (with \( \sigma \sim 0 \)) and the isotropic case (with \( \sigma \gg 0 \)).

\(^1\) Although the second-born BH may spin fast due to tidal acceleration, the vast majority of BHs observed in LIGO’s horizon will have small spins as demonstrated in Bavera et al. (2020b).
Meanwhile, we also assume that $\sigma_{ct,1G} \equiv \sigma_{ct,2G} \equiv \sigma_{ct,dyn}$ in this work. The hyper-parameters of the model and their meanings are summarised in Tab. 1.

In addition to the fiducial model (namely the OnePL model) described above, we also consider five additional models for comparison: 1) a Gaussian component representing the pile-up of remnants BHs whose progenitors underwent PPISN is added to the underlying mass distributions (Talbot & Thrane 2018) of ‘field’ BBHs and 1G ‘dyn’ BBHs (Model PPISN Peak); 2) the 1G ‘dyn’ BHs have a different underlying power-law mass distribution (Model TwoPL); 3) an isotropic spin orientation model for the dynamical channel (Model IsoDyn); 4) the Power-law + Peak mass model and the Default spin model in The LIGO Scientific Collaboration et al. (2021b) (Model PP & Default); 5) having the same mass model as the OnePL model but with the Default spin model (Model OnePL & Default). The details of these models are shown in Appendix. A.

### 3. HIERARCHICAL BAYESIAN INFERENCE

We perform hierarchical Bayesian inference to constrain our model parameters. The likelihood for the inference is constructed based on Poisson process. For a series of measurements of $N_{\text{obs}}$ events $\vec{d}$, assuming a redshift evolving merger rate of $R \propto (1 + z)^{2.7}$ (as inferred by The LIGO Scientific Collaboration et al. (2021b)), the likelihood for the hyper-parameters $\Lambda$ can be inferred via (Thrane & Talbot 2019; Abbott et al. 2021b)

$$
\mathcal{L}(\vec{d} \mid \Lambda) = N^{N_{\text{obs}}} \exp(-N\eta(\Lambda)) \prod_{i} Z_{\tilde{\varnothing}}(d_{i}) \frac{1}{n_{i}} \sum_{k}^{n_{i}} p(\theta_{i}^{k} \mid \varnothing) p(\theta_{i}^{k} \mid \Lambda),
$$

where $N$ is the expected number of mergers during the observation period and can be derived by integrating the merger rate over the co-moving space-time volume. $\eta(\Lambda)$ is the detection efficiency, following the procedures described in the SensitivityTutorial in LIGO Public Document Database, we use the injection campaign released in The LIGO Scientific Collaboration et al. (2021b) to estimated this quantity. The $n_{i}$ posterior samples for the $i$-th event, the evidence $Z_{\tilde{\varnothing}}(d_{i})$ as well as the default prior $\pi(\theta_{i} \mid \varnothing)$ are obtained from the released data accompanying with (Abbott et al. 2019a, 2021c; The LIGO Scientific Collaboration et al. 2021a). We use the same criteria that define the detectable events as The LIGO Scientific Collaboration et al. (2021b), i.e., FAR $< 1/\text{yr}^{2}$. For each event, we use 1000 random draws from its parameter estimation result in the inference.

Finally, we use the python package Bilby and PyMultinest sampler to obtain the Bayesian evidence and posteriors of the hyper-parameters for each model.

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2 A stricter criterion of FAR $< 0.25/\text{yr}$ are also adopted in the inference for comparison, and it yields consistent results.
Table 1. Hyperparameters, their descriptions, and choices of priors for the fiducial model in this Work

| Models                  | parameters | descriptions                                      | priors       |
|-------------------------|------------|---------------------------------------------------|--------------|
| Mass distribution       | $\alpha$  | slope of the power-law underlying mass distribution of stellar BHs | U(0,8)       |
|                         | $m_{\text{min}}$ | minimum mass of stellar-formed BHs               | U(2,10)     |
|                         | $m_{\text{max}}$ | maximum mass of stellar-formed BHs               | U(30,100)   |
|                         | $\delta_{m}$ | width of mass range that smoothing function impact on | U(0,10)     |
|                         | $\beta_{\text{field}}$ | power-law index in the paring function of field BBHs | U(0,6)      |
|                         | $\beta_{\text{dyn}}$ | power-law index for mass ratio in the paring function of dynamical BBHs | U(0,6)      |
|                         | $\gamma_{\text{dyn}}$ | power-law index for total mass in the paring function of dynamical BBHs | U(-4,12)    |
|                         | $f_{\text{dyn}}$ | the mixing fraction of the dynamically formed BBHs | U(0,1)      |
|                         | $\log_{10} r_{2G}$ | logarithm of the underlying fraction of the 2nd generation BHs | U(-4,0)     |
| Spin distribution       | $\mu_{a,\text{ste}}$ | the Gaussian mean value for spin magnitude of stellar BHs | U(0,1)      |
|                         | $\sigma_{a,\text{ste}}$ | the Gaussian width for spin magnitude of stellar BHs | U(0.05,0.5) |
|                         | $\mu_{a,\text{2G}}$ | the Gaussian mean value for spin magnitude of 2nd generation BHs | U(0,1)      |
|                         | $\sigma_{a,\text{2G}}$ | the Gaussian width for spin magnitude of 2nd generation BHs | U(0.05,0.5) |
|                         | $\sigma_{\text{ct,field}}$ | the Gaussian width for spin orientation of the field BBHs | U(0.1,4)   |
|                         | $\sigma_{\text{ct,dyn}}$ | the Gaussian width for spin orientation of the dynamical BBHs | U(0.1,4)   |

Note. Here, ‘U’ means the uniform distribution.

4. RESULTS

We summarize in Tab. 2 the (logarithmic) Bayes factors of the models compared to OnePL model. We interpret $\ln B > 3.5$ ($\ln B < -3.5$) as a strong evidence for the corresponding model being more (less) supported by the data than the OnePL model. We also adopt the Akaike information criterion (AIC=$2n - 2\ln L_{\text{max}}$; Akaike 1981) in the model comparison. The smaller the AIC, the greater the data’s preference for the model, and values of $\Delta\text{AIC} > 6$ are considered significant for model selection (Liddle 2009). The results show more supports for the OnePL model, the TwoPL model, and the PPISN model over the others, and their constraints on the hyper-parameters are shown in Appendix. C.

Table 2. Model comparison results

| Models                  | $\ln B$ | $\Delta\text{AIC}$ |
|-------------------------|---------|---------------------|
| OnePL                   | 0       | 0                   |
| TwoPL                   | 0.7     | 2.8                 |
| PPISN Peak              | 0.8     | 2.8                 |
| OnePL & IsoDyn          | -4.4    | 14                  |
| OnePL & Default         | -11     | 18.6                |
| PP & Default            | -12     | 26.2                |

Note. ‘IsoDyn’ means the model with isotropic spin orientation distribution for dynamical assembly; Default means the Default spin model used in Abbott et al. (2021b).

One intriguing result is that the $m_{\text{max}}$ is tightly constrained in the inference. As demonstrated in Fig. 1, the marginal posterior distributions of $m_{\text{max}}$ are consistent with each other across the four models. Combining the four posterior sample sets, we obtain an overall constraint of $m_{\text{max}} = 39.3^{+2.3}_{-2.5} M_\odot$ at 90% credibility. Such tight and consistent constraints may originate from the fact that our models effectively utilize the information of the secondary masses of BBHs, which are also forbidden from the high mass gap. We also investigate the possibility that $m_{\text{max}}$ is mainly constrained by the measurement of the heaviest sample (GW190521), whose primary mass is about twice as large as $m_{\text{max}}$. By leaving GW190521 out of the inference, we find that the change on the $m_{\text{max}}$ posterior distribution is
Figure 1. The marginal posterior distributions for the maximum mass of field BBHs (left) and the difference between the mean values of spin magnitudes for the stellar-originated BHs and dynamical 2G BHs (right).

Figure 2. The reconstructed astrophysical primary mass distribution for the OnePL model. The shaded areas indicate the 90% credible regions for different components.

negligible. Thus, the constraints may come from the overall trend of data rather than a particular event. In addition to the inference by modeling both mass and spin data, we also conduct an analysis with less dependency on the mass distribution (see Appendix B for details). This analysis also demonstrates that the BBHs can be divided into two groups according to a division mass \( M_d \gtrsim 40M_\odot \). The BHs with a mass lower than \( M_d \) have an average spin magnitude significantly smaller than those with higher masses.
Figure 3. Posterior predicted check for the reconstructed primary mass distribution and the mass ratio distribution.

To compare with the results in Abbott et al. (2021d), we plot the marginalized primary mass distribution in Fig. 2. Different from the $m_1$ distribution as shown in Fig. 10 of The LIGO Scientific Collaboration et al. (2021b), the distribution inferred with our model shows a clearly sharp decay in $m_1 \sim 40M_{\odot}$. The shallow bump extended to a higher mass is contributed by the 2G dynamical BHs. Similar $m_1$ spectral shapes are also obtained in some studies using different approaches (Wang et al. 2021; Wong et al. 2021; Baxter et al. 2021). To avoid model misspecification (Romero-Shaw et al. 2022), we perform posterior predicted checks following the procedures described in Abbott et al. (2021d). As shown in Fig. 3, the observed accumulated distribution of primary mass and mass ratio are within the predicted region of the model.

The inference also reveals a significant difference between the spin magnitude of the 2G dynamical BHs and stellar-origin BHs. For the OnePL model, we inferred that $\mu_{a,\text{ste}} = 0.15^{+0.08}_{-0.13}$ and $\mu_{a,2G} = 0.87^{+0.11}_{-0.21}$; these two parameters have consistent constraints in other models. We plot the difference between $\mu_{a,2G}$ and $\mu_{a,2G}$ in Fig. 1. Accounting for all models we have considered, the constraint on the difference is $d\mu_a > 0.4$ at 99% credibility. We note that for $\mu_{a,\text{ste}}$, the posterior support does not go down to zero for $\mu_{a,\text{ste}} = 0$, while for $\mu_{a,2G}$, the case of having an average spin of $\sim 0.7$ (which is the case for the remnant of a coalescing system with non-spinning equal-mass components) is within its 90% credible interval. We plot the 90% credible region of the spin amplitude distribution in red for the field + 1G ‘dyn’ mergers and in blue for the 2G ‘dyn’ mergers in Fig. 4. We also demonstrate the reconstructed distributions of $\cos \theta_i$ (which is governed by $\sigma_{ct,i}$) of the field and dynamical mergers. For both channels, the case of perfect alignment is not supported by the posterior distributions. The Bayes factor of the IsoDyn model compared to the OnePL model indicates that the isotropically tilted case for the dynamical BHs is also strongly disfavored.

We address some caveats in interpreting the spin results: first, some astrophysical models predict more complex spin distributions (see Sec. 5 for more discussions), and hence the simple truncated Gaussian has a limitation on recovering the exact shape of the distributions; however, our empirical model can still reflect the rough central tendency of data.
Second, we have utilized parameter estimation samples derived with the default prior (Uniform distributions for $a_i$ and $\cos \theta_i$) for individual events. Thus our inference has limitations in identifying sub-populations with negligible spins, as demonstrated in Galandage et al. (2021). We leave further investigation on this issue in future work since it will not change our current conclusion.

The existence of a distinct underlying mass distribution for the dynamical BHs is ambiguous. The logarithmic Bayes factor of the TwoPL model compared to the OnePL model is 0.7, indicating the introduction of the additional parameter, $\alpha_{\text{dyn}}$, does not significantly improve the model in describing the data. The posterior distribution of $\alpha_{\text{dyn}}$ implies the underlying mass spectrum of this sub-population may be much flatter than that of the field BBHs, though their 90% credible intervals overlap with each other in the range of $3^{+24}_{-20.80}$.

The results also reveal different paring functions between the ‘field’ BHs and ‘dyn’ BHs. For the OnePL model, we infer $\gamma_{\text{dyn}} = 8.11^{+1.98}_{-2.70}$, for the TwoPL model, the constraint is much weaker and $\gamma_{\text{dyn}}$ is strongly correlated with $\alpha_{\text{dyn}}$ and $\log_{10} r_{2G}$ in the inference. We show the corner plot for these parameters in Fig. 5 to illustrate the degeneracy.

We further use the results to derive branch ratios for different types of mergers. Combing the posterior distributions from OnePL, TwoPL, and PPISN model, we obtain $f_{\text{dyn}} = 0.18^{+0.16}_{-0.08}$, which means $\sim 20\%$ of the astrophysical mergers could form through the dynamical process. The parameter $\log_{10} r_{2G}$ describes the fraction of underlying 2G BHs in the dynamical environments. Its posterior distribution for the TwoPL model deviates from the results of the OnePL model and the PPISN model due to its degeneracy with $\beta_M$ and $\alpha_{\text{dyn}}$. We further translate the constraint on $r_{2G}$ into the fraction of mergers that contain at least one 2G BH in the dynamical sup-population, and the result is shown in Fig. 5. Combing the constraints in different models, the fraction is $0.09^{+0.08}_{-0.05}$ at 90% credible level.

5. ASTROPHYSICAL IMPLICATION

We discuss the astrophysical implications of our results under the hypothesis of our models (i.e., the BBHs consist of the field and dynamical sub-populations).

In principle, the position of the maximum BH mass can be explained by a combination of PI physics at low metallicities ($Z$) and Fe-dependent Wolf-Rayet (WR) mass loss at high $Z$ without needing to change the uncertain nuclear reaction rate. As shown in Farmer et al. (2019), a $M_{\text{max}} \sim 40M_\odot$ can be attained by varying the $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$ thermonuclear reaction rate within its 1$\sigma$ uncertainties for the progenitors with $Z \leq 3 \times 10^{-3}$. On the other hand, at higher $Z$, iron (Fe) dependent WR winds (Vink & de Koter 2005; Sander & Vink 2020) could be the leading factor.
models by Higgins et al. (2021), it was found (Fig. 13 in that paper) that above \( Z/Z_\odot \) was of order 40 \( \mu \), that decides \( M \), and close to the maximum BH mass uncovered by our phenomenological model.

When a more complex function of the (maximum) BH masses becomes available as a function of \( Z \) and redshift \( z \), the issue of constraining the \( ^{12}\text{C}(\alpha, \gamma)^{16}\text{O} \) thermonuclear reaction rate could be revisited. In addition, the sub-population of very hot WR stars and the WO stars could help constrain this elusive nuclear reaction rate (Tramper et al. 2015). In other words, multi-messenger astrophysics, including both GW events and electromagnetic (EM) information, could be combined to determine both the \( ^{12}\text{C}(\alpha, \gamma)^{16}\text{O} \) rate as well as stellar wind physics, by disentangling high \( Z \) and low \( Z \) GW events.

The BH spins have been widely considered to distinguish the BBH formation channels. In the isolated evolution of massive stars via common-envelope phase (Ivanova et al. 2013), the first-born BH originating from an initially massive star has negligible/small spin due to the standard angular momentum transport (Qin et al. 2018; Fuller et al. 2019; Belczynski et al. 2020); the second-born BH from the less massive star can have spin from zero to maximally spinning due to tidal spin-up (Qin et al. 2018; Hu et al. 2022), while this effect is limited within the horizon of current gravitational-wave detectors (Bavera et al. 2020b, 2022). These predictions seem to be in line with our inferred result which allows for the ‘field’ sub-population to have \( \mu_{\alpha,\text{ste}} \sim \sigma_{\alpha,\text{ste}} \sim 0.1 \). Nevertheless, within their 90\% credible region, \( \mu_{\alpha,\text{ste}} \) and \( \sigma_{\alpha,\text{ste}} \) have more posterior supports at slightly larger values. Higher spins in isolated binary evolution can be attained by various processes, like the tidal spin-up of two He stars following the double-core common envelope phases (Olejak & Belczynski 2021), the Eddington-limited accretion onto BHs, the efficient angular momentum transport within massive stars (Qin et al. 2022; Zevin & Bavera 2022), and the chemically homogeneous evolution (de Mink & Mandel 2016; Marchant et al. 2016). In addition, the spins may be tossed due to the supernova kicks during their formation process in the core collapse of massive stars (Tauris 2022).

We have inferred a total local (\( z = 0 \)) BBH merger rate of \( 18.2^{+7.65}_{-5.4} \) Gpc\(^{-1}\)yr\(^{-1}\), consisting with the result in The LIGO Scientific Collaboration et al. (2021b). Our models enable us to derive branch ratios for different sub-populations. The analysis has shown that the dynamical channel contributes to 10\% – 34\% of the mergers, in agreement with the expectations of some dynamical environments (Gerosa & Fishbach 2021). The investigation of spin distributions in this work sheds light on the details of dynamical environments. Dynamical assembly in dense stellar environments like globular clusters predict isotropic spins, while the features for the mergers in the AGN disks can change in a variety of ranges depending on the properties of the disk (Vajpeyi et al. 2022) and the dynamics in play (Tagawa et al. 2020). Our analysis disfavors both the perfectly alignment case and the isotropically tilted case of the spin, implying that not all of the dynamical mergers happen in old, dense AGNs, or, young, dilute AGNs/globular cluster (Benacquista & Downing 2013; Vajpeyi et al. 2022); however, it is likely that the AGN disk environment has contributions to the ‘dyn’ mergers. The reconstructed spin amplitude distribution for the 2G BBHs has \( \mu_{\alpha,2G} \gg 0 \), which can be explained by the inheritance of orbital angular momentum of 1G mergers in the framework of our model. For a coalescing system with non-spinning equal-mass components, the remnant will have spin amplitude \( \sim 0.7 \); On the one hand, non-zero and isotropically distributed spins of 1G BHs (due to, e.g., natal kicks) will increase the dispersion of spin amplitude distribution of 2G mergers; on the other hand, if the component spins and orbital angular momentum were aligned by the accretion torque and co-rotation torques in the AGN disk, the remnants could have larger spins.

The paring function for the dynamical sub-population prefers systems with higher total mass, though large systematical differences are presented in the posterior distributions of \( \gamma_{\text{dyn}} \) between the OnePL and the TwoPL model. O’Leary et al. (2016) found that dynamical interactions can enhance the merger rate of BBHs by a boost factor \( \propto M_{\text{tot}}^{\gamma} \), with \( \gamma \geq 4 \), which is consistent with the constraints on \( \gamma_{\text{dyn}} \) in our model. It is interesting to point out Yang et al. (2019a) addressed the AGN disk will also harden the mass distribution of BBHs, and the power-law index of the mass spectrum will change by \( \Delta \alpha_{\text{dyn}} \sim 1.3 \). This possibility is included in the results for the TwoPL model, considering the statistical uncertainties. More theoretical and statistical investigations about how dynamical BHs are paired in different environments are needed in the future.

6. SUMMARY AND DISCUSSION

In this work, we study the joint mass-spin distribution of coalescing binary black holes by incorporating the paring functions into the hierarchical Bayesian inference. With astrophysical concerns, we propose a model consisting of two subpopulations: one with a paring function preferring equal mass systems (representing the systems with field origin), and the other with a paring function preferring equal mass and higher total mass systems (representing the
systems with dynamical origin). We find that this model can well explain the current population of BBHs observed by LIGO/Virgo/KAGRA. Under the framework of our model, some key features of different formation channels are revealed and well constrained in the analysis. For the field binaries and 1G dynamical binaries, we obtain a tight constraint on the maximum mass of \( m_{\text{max}} = 39.3^{+2.3}_{-2.5} M_\odot \); we also infer that the 2G dynamical mergers have an average spin magnitude that is significantly larger than other kinds of mergers, with \( d \mu_A > 0.4 \) at 99% credibility. As we have discussed in Sec. 5., the inferred values of hyper-parameters in our phenomenological model can be naturally explained by current astrophysical theories, and in turn, can help to distinguish the acting mechanisms during the formation of field BBHs, as well as the environments of dynamical BBHs assuming our model is correct.

Our model considers the trade-off between accuracy and complexity, and can capture the rough features in the distributions of field binaries and dynamical binaries if they exist. It has limitations in identifying sub-classes under each sub-populations. Very massive BHs lying in the conventional PI gap can also be formed through the preserve of large H envelope for progenitor stars with reduced metallicity (\( Z < 0.1 Z_\odot \) or below) (Vink et al. 2021), and could be responsible for some events like GW 190521. Further studies with additional considerations on these channels are needed to clarify their existence and branch ratios in the GW events.

With more events from future observations, the redshift evolution of mass function and spin distributions might be well modeled, and there are already some studies (Fishbach et al. 2021; Biscoveanu et al. 2022) attempting to reveal the trends with current data. Employing the paring functions in the investigation may bring unique insights to uncover the nature of coalescing black holes.

ACKNOWLEDGMENTS

This work was supported in part by NSFC under grants of No. 11921003, No. 11773078, and No. 11933010. YQ acknowledges the support from the National Natural Science Foundation of China (Grant Nos. 12003002, 12192220, 12192221) and the Natural Science Foundation of Universities in Anhui Province (Grant No. KJ2021A0106).

Software: Bilby (Ashton et al. 2019, version 1.1.4, ascl:1901.011, https://git.ligo.org/lscsoft/bilby/), PyMultiNest (Buchner 2016, version 2.11, ascl:1606.005, https://github.com/JohannesBuchner/PyMultiNest).

REFERENCES

Abbott, B. P., Abbott, R., Abbott, T. D., et al. 2019a, Physical Review X, 9, 031040, doi: 10.1103/PhysRevX.9.031040
—. 2019b, ApJL, 882, L24, doi: 10.3847/2041-8213/ab3800
Abbott, R., Abbott, T. D., Abraham, S., et al. 2021a, Physical Review X, 11, 021053, doi: 10.1103/PhysRevX.11.021053
—. 2021b, ApJL, 913, L7, doi: 10.3847/2041-8213/abe949
Abbott, R., Abbott, T. D., Abernathy, C., et al. 2021c, arXiv e-prints, arXiv:2108.01045. https://arxiv.org/abs/2108.01045
Abbott, R., Abbott, T. D., Abraham, S., et al. 2021d, ApJL, 913, L7, doi: 10.3847/2041-8213/abe949
Akaike, H. 1981, Journal of Econometrics, 16, 3
Arca Sedda, M., Amaro-Seoane, P., & Chen, X. 2021, A&A, 652, A54, doi: 10.1051/0004-6361/202037785
Ashton, G., Hübner, M., Lasky, P. D., et al. 2019, Bilby: Bayesian inference library, Astrophysics Source Code Library, record ascl:1901.011. http://ascl.net/1901.011
Bavera, S. S., Fishbach, M., Zevin, M., Zapartas, E., & Fragos, T. 2022, arXiv e-prints, arXiv:2204.02619. https://arxiv.org/abs/2204.02619
Bavera, S. S., Fragos, T., Qin, Y., et al. 2020a, A&A, 635, A97, doi: 10.1051/0004-6361/201936204
—. 2020b, A&A, 635, A97, doi: 10.1051/0004-6361/201936204
Baxter, E. J., Croon, D., McDermott, S. D., & Sakstein, J. 2021, ApJL, 916, L16, doi: 10.3847/2041-8213/ac11fc
Belczynski, K., Holz, D. E., Bulik, T., & O’Shaughnessy, R. 2016a, Nature, 534, 512, doi: 10.1038/nature18322
Belczynski, K., Heger, A., Gladysz, W., et al. 2016b, A&A, 594, A97, doi: 10.1051/0004-6361/201628980
Belczynski, K., Klenczyki, P., Fields, C. E., et al. 2020, A&A, 636, A104, doi: 10.1051/0004-6361/201936528
Benacquista, M. J., & Downing, J. M. B. 2013, Living Reviews in Relativity, 16, 4, doi: 10.12942/lrr-2013-4
Biscoveanu, S., Callister, T. A., Haster, C.-J., et al. 2022, ApJL, 932, L19, doi: 10.3847/2041-8213/ac71a8
A. MODIFICATIONS OF POPULATION MODELS WITH ASTROPHYSICAL CONCERNS

We also try to take some widely concerned astrophysical motivation into our population models. Firstly, we consider the pile-up at the high-mass cutoff of the BH mass spectrum that results from the PPISNe (labeled ’PPISN Peak’) (Talbot & Thrane 2018),

$$
\pi_{ste,m}(m_i|\Delta_{ste}) = \mathcal{P}(m_i|\alpha, m_{\text{min}}, m_{\text{max}}, \delta_m) * (1 - r) + r * \mathcal{G}(m_i|\mu, \sigma, m_{\text{min}}, m_{\text{max}}),
$$

$$
r = \int_{m_{\text{max}}}^{m_{\text{max}} + \Delta_m} \text{d}m \mathcal{P}(m|\alpha, m_{\text{min}}, m_{\text{max}} + \Delta_m, \delta_m)
$$  \hspace{1cm} (A1)

where $\mathcal{P}$ is the normalized power law with smoothing treatment on the low-mass cutoff, so $r$ represents the fraction of the underlying BHs that could have been in the range of $\Delta_m$ above $m_{\text{max}}$, but appeared below $m_{\text{max}}$ because of the PPISN. Note that $\Delta_m$ should be smaller than the width of the high-mass gap caused by the (P)PISN. Therefore, we set the prior of $\Delta_m$ to be uniformly distributed in $(0, 100)M_\odot$, $\Delta_m = 100M_\odot$, which is wider than the widely expected mass gap (Spera & Mapelli 2017). As presented in the Fig. 6, the contribution of PPISN channel is negligible, and the high-mass cutoff is still tightly constrained, as shown in Fig.1. However, the $\Delta_m$ is not well constrained (i.e., is similar to the prior distribution, and $\Delta_m = 0M_\odot$ ($\Delta_m = 100M_\odot$) can not be ruled out).

The BHs formed through different formation channels/environments may follow different spectrum indexes. Therefore, we introduce the second modified model (labeled ‘TwoPL’), in which we consider another power-law index $\alpha_{\text{dyn}}$ for the mass function of first-generation BHs in the dynamical assembly.

**Table 3.** The additional hyper-parameters, and Chosen Priors for the modified model

| Models       | parameters | descriptions                                | priors       |
|--------------|------------|---------------------------------------------|--------------|
| PPISN Peak   | $\Delta_m$ | the mass range above $m_{\text{max}}$ that contribute to the PPISN peak | $U(0,100)$   |
|              | $\mu$      | the Gaussian central value of the PPISN peak | $U(20,50)$   |
|              | $\sigma$   | the Gaussian width of the PPISN peak         | $U(1,10)$    |

*Note. Here, ‘U’ means the uniform distribution.*

Finally, we concern that the spin orientation of BBHs formed by the dynamical capture may have isotropic distribution, therefore in the modified model (labeled ‘IsoDyn’), we assume that $\pi_{\text{dyn}}(\cos \theta_{1,2}) = 1/2$, for $\cos \theta_{1,2} \in (-1,1)$, i.e., $\cos \theta_{1,2}$ uniformly distributed in (-1,1). However, as summarised in Tab.2, such scenario is not favored by the GW observation.

B. ANALYSING THE SPIN DISTRIBUTION ALONE

It’s shown in our results that the stellar-origin BHs are not likely to have masses above $\sim 40M_\odot$, and the BHs present in the mass range $\gtrsim 40M_\odot$ should be formed through the merger of the ancestors BBHs. As is known that the spin magnitudes of the second-generation BHs should be distinguished from that of the stellar-formed BHs Information encoded in gravitational-wave signals (see Gerosa & Fishbach 2021, and the Refs.). Therefore, we create a simplified model (see below) for the spin distribution of BHs to test the validation of our findings. We assume that the BHs with masses above a certain criticality ($m_{\text{cut}}$) have a different spin distribution from that of BHs below $m_{\text{cut}}$,

$$
\pi_s(a_i, \cos \theta_i|m_i, m_{\text{cut}}; \Lambda_s) = \begin{cases} 
\mathcal{G}(a_i|\mu_{a,1}, \sigma_{a,1}) \mathcal{G}'(\cos \theta_i|1, \sigma_{ct,1}) & \text{for } m_i < m_{\text{cut}} \\
\mathcal{G}(a_i|\mu_{a,2}, \sigma_{a,2}) \mathcal{G}'(\cos \theta_i|1, \sigma_{ct,2}) & \text{for } m_i > m_{\text{cut}} 
\end{cases}
$$  \hspace{1cm} (B2)

all the parameters, their descriptions, and the chosen priors are summarized in Tab. B. Note that both BHs in one BBH follow the same model (i.e., Eq. B2). Though the second-generation BHs may also present below $m_{\text{cut}}$, the fraction is relatively small. Therefore it will make rather small influence for the BHs in the low-mass range, and will
Figure 6. The same as Fig.2, but for the PPISN Peak model.

Table 4. Hyperparameters, Their Descriptions, and Chosen Priors for the Spin model described by Eq. (B2)

| parameters       | descriptions                                                                 | priors                       |
|------------------|-----------------------------------------------------------------------------|------------------------------|
| $m_{\text{cut}}[M_\odot]$ | the demarcation point in the mass range that diving the two subpopulations | $U(20,70)$                   |
| $\mu_{a,1}$    | the Gaussian mean value for spin magnitude of the BHs below $m_{\text{cut}}$ | $U(0,1)$                    |
| $\sigma_{a,1}$ | the Gaussian width for spin magnitude of stellar the BHs below $m_{\text{cut}}$ | $U(0.05,0.5)$               |
| $\sigma_{\alpha,1}$ | the Gaussian width for spin orientation of the BHs below $m_{\text{cut}}$   | $U(0.1,4)$                  |
| $\mu_{a,2}$    | the Gaussian mean value for spin magnitude of the BHs above $m_{\text{cut}}$ | $U(0,1)$                    |
| $\sigma_{a,2}$ | the Gaussian width for spin magnitude of the BHs above $m_{\text{cut}}$     | $U(0.05,0.5)$               |
| $\sigma_{\alpha,2}$ | the Gaussian width for spin orientation of the BHs above $m_{\text{cut}}$ | $U(0.1,4)$                  |

Note. Here, ‘U’ means the uniform distribution.

not affect the spin distribution of BHs in the high-mass range. Though the model is simplified, the inferred parameters ($\mu_{a,1}, \sigma_{a,1}, \sigma_{\alpha,1}, \mu_{a,2}, \sigma_{a,2}, \sigma_{\alpha,2}$) are similar to ($\mu_{a,1G}, \sigma_{a,1G}, \sigma_{\alpha,1G}$, $\mu_{a,2G}, \sigma_{a,2G}, \sigma_{\alpha,2G}$) obtained by the synthesis models in the main text, as shown in Fig.7 and Fig.8. The demarcation point $m_{\text{cut}}$ is constrained to $46.14^{+6.79}_{-5.76}M_\odot$ at 90% credible level, this value is closed to the $m_{\text{max}}$ obtained by the synthesis models. Therefore it’s clear that there must be a subpopulation of BHs above the maximum mass of stellar-formed BHs, and their distinguished spin magnitudes ($\sim 0.7$) make them associated with the remnants of previous mergers.

C. THE POSTERIOR DISTRIBUTIONS COMPARISON

We compare the inferred parameters obtained by the OnePL model and the TwoPL model as described in Appendix A, as shown in Fig. 8. The PPISN Peak model has similar constraints for the overlapping parameters with the OnePL model. We find that the most parameters are nearly identical in both models expect for $\gamma_{\text{dyn}}, \log_{10} r_{2G}$, which are strongly degenerate with $\alpha_{\text{dyn}}$. Fortunately, the fraction of the BBHs that involve at least one 2nd-generation BH is well constrained, though the constraint of $\log_{10} r_{2G}$ is not optimistic as shown in Fig. 5.
Figure 7. posterior distributions of parameters of the spin model described by Eq.(B2), the dashed lines represent the 90% credible intervals.
Figure 8. Posterior distribution of all the parameters that obtained by the OnePL and the TwoPL models; the dashed lines in the marginal distribution represent the 90% credible intervals.