Spin misalignment of black hole binaries from young star clusters: implications for the origin of gravitational waves events

A. A. Trani 1,2, A. Tanikawa 1, M. S. Fujii 3, N. W. C. Leigh 4,5 and J. Kumamoto 3

1Department of Earth Science and Astronomy, College of Arts and Sciences, The University of Tokyo, 3-8-1 Komaba, Meguro-ku, Tokyo 153-8902, Japan
2Okinawa Institute of Science and Technology, Quantum Gravity unit, 1919-1 Tancha, Onna-son, Okinawa 904-0495, Japan
3Department of Astronomy, Graduate School of Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan
4Departamento de Astronomía, Facultad de Ciencias Físicas y Matemáticas, Universidad de Concepción, Concepción, Chile
5Department of Astrophysics, American Museum of Natural History, New York, NY 10024, USA

Accepted 2021 April 1. Received 2021 March 4; in original form 2021 January 26

ABSTRACT
Recent studies indicate that the progenitors of merging black hole (BH) binaries from young star clusters can undergo a common envelope phase just like isolated binaries. The stars emerge from the common envelope as naked cores, tidal interactions can efficiently synchronize their spins before they collapse into BHs. Contrary to the isolated case, these binary BHs can also undergo dynamical interactions with other BHs in the cluster before merging. The interactions can tilt the binary orbital plane, leading to spin–orbit misalignment. We estimate the spin properties of merging binary BHs undergoing this scenario by combining up-to-date binary population synthesis and accurate few-body simulations. We show that post-common envelope binary BHs are likely to undergo only a single encounter, due to the high binary recoil velocity and short coalescence times. Adopting conservative limits on the binary–single encounter rates, we obtain a local BH merger rate density of}$ \sim \frac{6}{8} \text{yr}^{-1}\text{Gpc}^{-3}$. Assuming low ($\lesssim 0.2$) natal BH spins, this scenario reproduces the trends in the distributions of effective spin $\chi_{\text{eff}}$ and precession parameters $\chi_p$ inferred from GWTC-2, including the peaks at $(\chi_{\text{eff}}, \chi_p) \sim (0.1, 0.2)$ and the tail at negative $\chi_{\text{eff}}$ values.

Key words: black hole physics – gravitational waves – methods: numerical – binaries: general.

1 INTRODUCTION
The origins of gravitational wave (GW) events from merging black hole (BH) binaries is still disputed. The numerous formation pathways that have been proposed so far can be organized into two broad categories: dynamically interacting binaries in dense environments and isolated binaries evolving due to stellar and binary evolution in the field.

The scenarios belonging to the first category include binaries dynamically assembled in globular clusters (GCs; e.g. Sigurdsson & Phinney 1995; Downing et al. 2010; Tanikawa 2013; Bae, Kim & Lee 2014; Leht et al. 2014b; Rodriguez, Chatterjee & Rasio 2016; Askar et al. 2017; Arca-Sedda & Gualandris 2018; Hong et al. 2018; Samsing, Askar & Giersz 2018; Antonini & Gieles 2020) and other dense stellar environments (open, young, and nuclear star clusters; e.g. Portegies Zwart & McMillan 2000; Ziosi et al. 2014; Banerjee 2017a, b; Fujii, Tanikawa & Makino 2017; Petrovich & Antonini 2017; Banerjee et al. 2018; Leht et al. 2018; Rastello et al. 2018; Rodriguez et al. 2018; Di Carlo et al. 2019; Michaela & Perets 2019; Hong et al. 2020; Mapelli et al. 2020; Rastello et al. 2020; Banerjee 2021), mergers mediated by dynamical interactions with a supermassive BH or an active galactic nucleus disk (e.g. Antonini & Perets 2012; Antonini & Rasio 2016; Leht et al. 2016b; Stone, Metzger & Haiman 2016; VanLardinghaim et al. 2016; Bartos et al. 2017; Hamers et al. 2018; Hoang et al. 2018; McKernan et al. 2018; Trani et al. 2019; Yang et al. 2019; Arca Sedda et al. 2020; McKernan, Ford & O'Shaughnessy 2020; Tagawa, Haiman & Kocsis 2020), and mergers in multiple stellar systems (e.g. Antonini, Murray & Mikkola 2014; Antonini, Toonen & Hamers 2017; Silsbee & Tremaine 2017; Rodriguez & Antonini 2018; Hamers & Safarzadeh 2020; Leht et al. 2020; Martinez et al. 2020).


The total number of events announced by Ligo-Virgo-KAGRA (hereafter LVK) collaboration amounts to 50: 11 from the O1/O2 observing runs (LIGO Scientific Collaboration & Virgo Collaboration 2019), and 39 from the first half of the O3 observing run (The LIGO

* E-mail: aatrani@gmail.com
Spin misalignment in black hole binaries

2 NUMERICAL SETUP

We perform direct N-body simulations of binary–single encounters using TSUNAMI (A.A.Trani et al., in preparation). TSUNAMI employs a combination of numerical techniques to ensure excellent accuracy over a wide dynamical range. First, we solve the equations of motion derived from a time-transformed Hamiltonian. Specifically, here we use a second order Leapfrog method from the regularized logarithmic Hamiltonian of Mikkola & Tanikawa (1999; see also Preto & Tremaine 1999). We then increase the accuracy of the integrator using the Bulirsch–Stoer extrapolation (Stoer & Bulirsch 1980).

Finally, the equations of motion are solved in a relative chain coordinate system, as in Mikkola & Aarseth (1993), in order to reduce round-off errors due to small interparticle distances far from the origin in the classical centre of mass coordinates. We also include post-Newtonian corrections to the equations of motion, specifically the 1PN, the 2PN, and 2.5PN terms (Blanchet 2014).

The initial setup is as follows: the binary centre-of-mass and the single lie on a hyperbolic (i.e. unbound) orbit with negative semimajor axis $a_{\text{in}}$ and eccentricity $e_{\text{in}}$. The mass of the binary members and the single are $m_1$, $m_2$, and $m_3$, respectively. The inner binary is on a (bound) elliptic orbit with semimajor axis $a_{\text{out}}$ and eccentricity $e_{\text{out}}$, and has a random orientation uniform on a sphere.

The orbital parameters and masses of the inner binary are taken from population synthesis simulations using a modified version of the BSE code (Hurley, Tout & Pols 2002). The initial conditions of the population synthesis simulations are the following. The initial mass function (IMF) of primary stars follows the (Kroupa 2001) IMF truncated from $10 M_\odot$ to $150 M_\odot$. The secondary-to-primary mass ratios are drawn from a flat distribution between 0 and 1, imposing a minimum mass of $10 M_\odot$ for the secondary star. The binary semimajor axes have a flat distribution in logarithmic scale from $1 R_\odot$ to $10^3 R_\odot$ (Andrews, Chanamé & Aguieros 2017), and their eccentricities follow a thermal distribution (Jeans 1919). The initial pericentre distances are set to be large enough to avoid the onset of Roche lobe overflow. Note that by simulating the binary stellar evolution in isolation we are neglecting common envelope events triggered by dynamical encounters, and therefore we might be underestimating the number of post-common envelope binaries.

We evolve three sets of different metallicities: 1, 0.1, and 0.01 $Z_\odot$ (where $Z_\odot = 0.02$), running $10^7$ realizations for each set. The stellar wind models and binary interaction model are the same as those in Tanikawa et al. (2021; see also Giacobbo, Mapelli & Spera 2018). We do not take into account BH natal kicks. Since there is no mechanism that can tilt BH spins from the orbital planes, the BH spins will be parallel to the orbital planes due to tidal synchronization (Hut 1981).

We select those binaries that are likely to have spinning BHs. Specifically, we select only those binaries whose separation is small enough to allow the tidal spin-up of the stars, after the binary exits the common envelope phase as a double Wolf–Rayet star. As shown by Kushnir et al. (2016; see also Safarzadeh & Hotokaza 2020), the value of the synchronization spin scales as $\dot{\chi} \propto d^{3/2}$, where $d$ is the binary separation. Given that the GW coalescence time-scale scales as $t_{\text{gw}} \propto d^3$, it follows that $\chi \propto t_{\text{gw}}^{-3/2}$, the shorter the coalescence time, the higher the dimensionless spin. Therefore, we select only those binaries that have a GW merging time-scale of $\lesssim 200$ Myr (before turning into BHs) and we exclude those binaries whose GW time-scales are too small ($<50$ Myr) to allow for encounters with other stars before their mergers.

The outer orbit is determined in the following way. The velocity at infinity $v_\infty$ of the outer orbit is drawn from a Maxwellian distribution with $\sigma_\infty$ dispersion. We consider two main environments in which the three-body encounters take place: open clusters (OCs) that have low velocity dispersions, and massive clusters with high velocity dispersions, such as globular and young massive star clusters. We set $\sigma_\infty \approx 1$ km s$^{-1}$ and $20$ km s$^{-1}$ for OC and GC simulations, respectively. Note that this represents the 3D velocity dispersion, rather than the commonly reported line-of-sight velocity dispersion, which is a factor of $\sqrt{3}$ smaller (Illingworth 1976; Harris 1996; Portegies Zwart, McMillan & Gieles 2010). Given $v_\infty$, the semimajor axis of the outer hyperbolic orbit is $a_{\text{out}} = -GM_{\text{tot}}/v_\infty^2$, where $M_{\text{tot}} = m_1 + m_2 + m_3$ is the total mass of the bodies. The eccentricity $e_{\text{out}}$ is instead calculated from the pericentre distance $p_{\text{out}} = a_{\text{out}}(1 - e_{\text{out}})$, which is drawn from a distribution uniform in $p_{\text{out}}^2$ between 0 and $2a_{\text{out}}$. This is chosen so as to minimize the number of flyby interactions, since numerical experiments have shown that the cross-section for resonant encounters drops for $p_{\text{out}} > 2a_{\text{out}}$ (e.g. Hut 1983, 1993; Hut & Bahcall 1983).

The mass of the third body is drawn from the stellar population synthesis code STAR, in accordance with the BSE simulations used for the inner binaries. It is well known that massive stars and binaries sink to the cores of star clusters faster than lighter stars, due to mass segregation and energy equipartition (e.g. Giersz & Heggie...
A. A. Trani et al.

Figure 1. Mass of the single body versus mass of the binary for each binary–single simulation. Blue squares: $Z = 10^{-2} Z_\odot$. Orange squares: $Z = 10^{-1} Z_\odot$. Green squares: $Z = Z_\odot$. The black dashed lines denote $m_1 + m_2 = m_3$. At low metallicities, the single BHs are more massive than the BHs in binaries, because they do not lose mass via binary interactions.

Table 1. Initial conditions.

<table>
<thead>
<tr>
<th>Set name</th>
<th>$\sigma_\infty$ [km s$^{-1}$]</th>
<th>$Z$ [$Z_\odot$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>GC Z2</td>
<td>1</td>
<td>0.01</td>
</tr>
<tr>
<td>GC Z2</td>
<td>20</td>
<td>0.01</td>
</tr>
<tr>
<td>GC Z1</td>
<td>1</td>
<td>0.1</td>
</tr>
<tr>
<td>GC Z1</td>
<td>20</td>
<td>0.1</td>
</tr>
<tr>
<td>GC Z0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>GC Z0</td>
<td>20</td>
<td>1</td>
</tr>
</tbody>
</table>

$\sigma_\infty$: dispersion of the Maxwellian distribution for $v_\infty$; $Z$: metallicity of the population synthesis simulations.

1996; Gürkan, Freitag & Rasio 2004; Khalisi, Amaro-Seoane & Spurzem 2007; Goswami et al. 2012; Tanikawa, Hut & Makino 2012; Tanikawa et al. 2013; Trani, Mapelli & Bressan 2014; Fuji & Zwart 2014; Spera, Mapelli & Jeffries 2016; Webb & Vesperini 2016; Pavlík 2020). We mimic this effect by pairing the most massive binaries to the most massive single body, as shown in Fig. 1. We combine three choices of stellar metallicity with two choices of velocity dispersion, for a total of six sets of simulations. Each set comprises of $10^5$ realizations, enough to sample the initial parameter space. Table 1 summarizes the initial conditions for each set.

The initial binary–single distance is set to $100 a_{\text{initial}}$, which is large enough so that the initial binary is unperturbed by the single. The simulations are run until either the three-body interaction is complete (with an outbound binary–single on a hyperbolic orbit), or there is a merger.

3 ENOUNTER OUTCOMES

A three-body encounter can be represented as a succession of strong chaotic interactions, wherein all three-bodies exchange energy, and long, regular excursions in which the single is ejected from the binary and forms a temporary hierarchical bound system (e.g. Stone & Leigh 2019). Eventually, assuming all point particles, the single will achieve a velocity above the escape velocity, and the encounter will end with an unbound binary–single. In the context of three-body interactions in the cores of stellar clusters, this process usually leads the binary semimajor axis to shrink, and it is therefore known as binary hardening (Heggie 1975).

Figure 2. Distribution of the misalignment angle $\Delta i$ for each of our simulation sets. Solid lines indicate GC initial conditions with $\sigma_\infty = 20$ km s$^{-1}$, while the dotted lines indicate OC initial conditions with $\sigma_\infty = 1$ km s$^{-1}$. Green lines: all binaries. Orange lines: original binaries. Blue lines: exchanged binaries. Top panel: $Z = 10^{-2} Z_\odot$. Middle panel: $Z = 10^{-1} Z_\odot$. Bottom panel: $Z = Z_\odot$. The grey shaded area shows the 90 per cent confidence interval of the distribution reconstructed from GWTC-2 (default spin model from The LIGO Scientific Collaboration & the Virgo Collaboration 2020b).

After the encounter is concluded, the orientation of the outgoing binary might be different than the initial one. This will cause spin-angle misalignment if initially the BH spins were aligned with the orbit. We measure the tilt angle $\Delta i$ between the initial binary plane and the final one, and check if one of the binary members was exchanged with the single BH. Hereafter, we refer to binaries that underwent an exchange as ‘exchanged binaries’, while the binaries that did not are termed ‘original binaries’.

Fig. 2 shows the distributions of $\cos \Delta i$ for all our sets. The distributions are essentially the same regardless of the initial velocity dispersion, indicating that encounters in OCs and GCs will lead to very similar tilt angles. This is because the initial binaries are very tight, and the single BH very massive, so that regardless of $\sigma_\infty$ we are in the regime of hard binary scatterings (Heggie 1975; Hut 1983, 1984). The tilt angle distribution of original binaries is strongly peaked at $\cos \Delta i = 1$, indicating that most original binaries retain their initial orientation. The peak at $\cos \Delta i = 1$ becomes more pronounced with increasing metallicity: about 15, 18, and 34 per cent of the binaries get misaligned by less than 15$^\circ$ at $Z = 0.01$, 0.1, and 1$Z_\odot$, respectively. The tilt angle distribution of exchanged binaries is
and OC sets, respectively. This results in the majority (about 60 per cent) of binaries escaping in the GC sets, while only about 40 per cent of the exchanged binaries escape in the OC sets. However, since original binaries have larger recoil velocities, 60 per cent of them escape from the cluster, compared to only 46 per cent of the exchanged binaries.

The distribution of the GW coalescence times $t_{\text{gw}}$ is shown in Fig. 4. We calculate the coalescence time using the following expression from Peters (1964):

$$t_{\text{gw}} = \frac{15c^5}{32G^3(m_1 + m_2)m_1m_2} f(e),$$

where $f(e)$ is a factor taking into account the orbital eccentricity that we evaluate numerically as

$$f(e) = \frac{(1 - e^2)^{4}}{e^{\frac{21}{4}} (e^2 + \frac{304}{121} x^2)^{\frac{11}{2}}} \int_0^\infty \left(1 - x^2\right)^{-\frac{1}{2}} dx.$$  

The peak coalescence time in the final distribution for all binaries becomes slightly shorter, at $\approx 10$ Myr after the encounter. At $Z = Z_\odot$, this peak is dominated by exchanged binaries: most of the original binaries have a much shorter coalescence time, peaked at $\approx 1$ Myr. At higher metallicity, the discrepancy in coalescence time between exchanged and original binaries lessens.

The reason for this is that at low metallicity, the original binaries have a shorter semimajor axis than the exchanged ones. Since at low metallicity the initial single star can be twice more massive than the binary (see Fig. 1), the binary needs to harden more in order to eject the single. On the other hand, if the initial single ejects one of the lower mass binary components, the binary can maintain a larger separation.

Table 2 summarizes the outcome fractions of the simulations. In the GC set, $\sim 40$ per cent of the final binaries are original binaries. However, since original binaries have larger recoil velocities, 60 per cent of them escape from the cluster, compared to only 46 per cent of the exchanged binaries.

The distribution of the GW coalescence times $t_{\text{gw}}$ is shown in Fig. 4. We calculate the coalescence time using the following expression from Peters (1964):

$$t_{\text{gw}} = \frac{15c^5}{32G^3(m_1 + m_2)m_1m_2} f(e),$$

where $f(e)$ is a factor taking into account the orbital eccentricity that we evaluate numerically as

$$f(e) = \frac{(1 - e^2)^{4}}{e^{\frac{21}{4}} (e^2 + \frac{304}{121} x^2)^{\frac{11}{2}}} \int_0^\infty \left(1 - x^2\right)^{-\frac{1}{2}} dx.$$  

The peak coalescence time in the final distribution for all binaries becomes slightly shorter, at $\approx 10$ Myr after the encounter. At $Z = Z_\odot$, this peak is dominated by exchanged binaries: most of the original binaries have a much shorter coalescence time, peaked at $\approx 1$ Myr. At higher metallicity, the discrepancy in coalescence time between exchanged and original binaries lessens.

The reason for this is that at low metallicity, the original binaries have a shorter semimajor axis than the exchanged ones. Since at low metallicity the initial single star can be twice more massive than the binary (see Fig. 1), the binary needs to harden more in order to eject the single. On the other hand, if the initial single ejects one of the lower mass binary components, the binary can maintain a larger separation.

Another way to phrase it is that the outcome distribution of binary binding energies $E_b = Gm_1m_2/2a$ of a three-body encounter is the same whether the final binary is the original or exchanged. Therefore, at the same $E_b$, a higher mass product $m_1m_2$ translates into a larger semimajor axis $a$, and vice versa (Valtonen & Karttunen 2005).

Table 2. Fractional outcomes of the simulation sets.

<table>
<thead>
<tr>
<th>Set name</th>
<th>$f_{\text{ori}}$</th>
<th>$f_{\text{ex}}$</th>
<th>$f_{\text{esc}}$</th>
<th>$f_{\text{ori, esc}}$</th>
<th>$f_{\text{ex, esc}}$</th>
<th>$f_{\text{merg}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>OC,$2Z_\odot$</td>
<td>0.410</td>
<td>0.578</td>
<td>0.986</td>
<td>0.409</td>
<td>0.577</td>
<td>0.011</td>
</tr>
<tr>
<td>GC,$2Z_\odot$</td>
<td>0.409</td>
<td>0.579</td>
<td>0.474</td>
<td>0.227</td>
<td>0.247</td>
<td>0.011</td>
</tr>
<tr>
<td>OC,$Z_\odot$</td>
<td>0.439</td>
<td>0.551</td>
<td>0.987</td>
<td>0.438</td>
<td>0.549</td>
<td>0.010</td>
</tr>
<tr>
<td>GC,$Z_\odot$</td>
<td>0.443</td>
<td>0.546</td>
<td>0.441</td>
<td>0.216</td>
<td>0.225</td>
<td>0.010</td>
</tr>
<tr>
<td>OC,$Z_\odot$</td>
<td>0.661</td>
<td>0.320</td>
<td>0.977</td>
<td>0.657</td>
<td>0.320</td>
<td>0.019</td>
</tr>
<tr>
<td>GC,$Z_\odot$</td>
<td>0.660</td>
<td>0.322</td>
<td>0.367</td>
<td>0.221</td>
<td>0.146</td>
<td>0.018</td>
</tr>
</tbody>
</table>

$f_{\text{ori}}$: fraction of original binaries; $f_{\text{ex}}$: fraction of exchanged binaries; $f_{\text{esc}}$: fraction of escaped binaries; $f_{\text{ori, esc}}$: fraction of original binaries that achieve the escape speed; $f_{\text{ex, esc}}$: fraction of exchanged binaries that achieve the escape speed; $f_{\text{merg}}$: fraction of mergers during the encounter.
where $\Gamma_1$ is the distance below which the binary–single can undergo a chaotic encounter that we conservatively set to $2\,\pi \, a$. This latter condition is always satisfied given the compactness of the binary.

The velocity dispersion depends on cluster size and mass via the virial relation $\sigma_1^2 = 0.45 G M_{\text{cl}}/r_h$, where $M_{\text{cl}}$ is the cluster mass and $r_h$ is the half-mass radius. We can eliminate the dependence on $r_h$ via the Marks–Kroupa relation (Marks et al. 2012; Leigh et al. 2013, 2015) that relates cluster mass at birth to its half-mass radius. Given an average stellar mass ($m$), we can re-express $N = M_{\text{cl}}/(m)$ and $n = r_h/m$, we obtain an encounter rate that depends only on cluster density, mass, and the relative fractions of objects undergoing the encounter

$$\Gamma_{\text{enc}}^2(M_{\text{cl}}) \simeq 30 \text{Myr}^{-1} f_{\text{bin}} f_{\text{sin}} \left( \frac{0.5 M_\odot}{m} \right)^2 \frac{\rho}{\left( 10^3 M_\odot \text{pc}^{-3} \right)^{0.565}} \left( \frac{M_{\text{cl}}}{M_\odot} \right) \frac{R_{\text{enc}}}{0.072 \text{au}} \left( \frac{M_{\text{cl}}}{60 M_\odot} \right) \left( \frac{m}{10^{-3} M_\odot} \right). \quad (4)$$

Here we have adopted the median values for our three-body simulations ($m_{\text{bin}} \simeq 60 M_\odot$, $a_{\text{bin}} \simeq 0.036 \text{au}$), and assumed that encounters occur mainly during the core collapse phase in stellar clusters, when the core density can peak at $>10^5-10^6 M_\odot \text{ pc}^{-3}$.

In the above equation, $f_{\text{bin}} \equiv f_{\text{CBBH}}$ is the fraction of post-common envelope binaries representative of our pre-encounter binary sample. This fraction can be estimated from our binary population synthesis simulations as the ratio between the number of selected binaries and the initial number of binary realizations. This fraction depends on the metallicity, and amounts to $7.6 \times 10^{-5}, 1.02 \times 10^{-3}$, and $2.17 \times 10^{-3}$ for $Z = 0.1, 0.01, 0$ Z$_\odot$, respectively. This is likely an underestimate of the number of compact binary BHs, because it considers only those formed from isolated evolution. The common envelope phase that leads to such compact binaries may be triggered by dynamical interactions therefore increasing the fraction $f_{\text{CBBH}}$ (Di Carlo et al. 2019; Kumamoto et al. 2019). The fraction of single black holes is instead $f_{\text{BH}} \simeq 0.028$, consistent with an evolving population of stars that follows a (Kroupa 2001) mass function between 0.8 and 150 solar masses.

Finally, we can obtain the encounter rate averaged over the star cluster mass function that follows a power-law of $\beta = -2$, as observed in massive clusters in the Galactic disk and starburst galaxies (Portegies Zwart et al. 2010)

$$\Gamma_{\text{enc}}^{2+1} = A_{\text{cl}} \int_{10^6 M_\odot}^{10^9 M_\odot} \Gamma_{\text{enc}}^2(M_{\text{cl}})^2 dM_{\text{cl}}, \quad (5)$$

where $A_{\text{cl}}$ is the normalization factor so that the cluster mass function normalizes to 1. The averaged encounter rate is then

$$\Gamma_{\text{enc}}^{2+1} \simeq 10^{-3} \text{Myr}^{-1} \left( \frac{f_{\text{CBBH}}}{10^{-3}} \right) \left( \frac{f_{\text{BH}}}{0.02} \right). \quad (6)$$

Given the short lives of OCS ($\sim 300 \text{ Myr}$; Portegies Zwart et al. 2010), it seems that OCS might only experience a few such binary–single encounters, if any. This low encounter rate justifies our assumption of considering only the effect of a single encounter.

On the other hand, the rate of binary–binary encounters in OCS dominates over that of binary–single encounters due to the abundance of wide stellar binaries (e.g. Leigh & Sills 2011; Leigh & Geller 2013; Geller & Leigh 2015). While we limit ourselves to simulating binary–single encounters, we do not expect the outcome of binary–binary encounters to be statistically different. The reason is that wide binaries in OCS have typically a semimajor axis much larger than 10 au that is $10^2-10^3$ larger then the hard binaries of our sample.

4 ENCOUNTER RATE ESTIMATES

The merger rate density for these kinds of events depends linearly on the encounter rate between the compact binary BHs and single BHs. Here we estimate and discuss the encounter rate for the three-body encounters considered in this work. The encounter rate of binary–single encounters $\Gamma_{\text{enc}}^{2+1}$ can be expressed as (Leigh & Sills 2011)

$$\Gamma_{\text{enc}}^{2+1} = N a_{\text{bin}} N a_{\text{sin}} \frac{3 \pi G m_{\text{tot}} R_{\text{esc}}}{\sigma_\infty} = f_{\text{bin}} f_{\text{sin}} N a_{\text{bin}} M_{\text{cl}} \frac{3 \pi G m_{\text{tot}} R_{\text{esc}}}{\sigma_\infty}, \quad (3)$$

where $n$ is the stellar number density, $N$ is the number of stars, $\sigma_\infty$ is the velocity dispersion, $m_{\text{tot}} = m_{\text{bin}} + m_{\text{bin}}$ is the mass of the binary plus single, $f_{\text{bin}}$ and $f_{\text{sin}}$ are the binary and single fractions, and $R_{\text{esc}}$ is the distance below which the binary–single can undergo a chaotic three-body encounter that we conservatively set to $2a_{\text{esc}}$. Here we have assumed that the cross-section is dominated by gravitational focusing, so that the Safronov number $\Theta = G m_{\text{tot}}/R_{\text{esc}} \sigma_\infty^2 \gg 1$ (Binney 2008). This latter condition is always satisfied given the compactness of the binary.

Figure 4. Distribution of the GW-coalescence time for each of our sets. Solid lines indicate GC initial conditions with $\sigma_\infty = 20 \text{ km} \text{s}^{-1}$, while dotted lines indicate OC initial conditions with $\sigma_\infty = 1 \text{ km} \text{s}^{-1}$. Green lines: all binaries. Orange lines: original binaries. Blue lines: exchanged binaries. Purple line: initial distribution. Top panel: $Z = 10^{-2} Z_\odot$. Middle panel: $Z = 10^{-1} Z_\odot$. Bottom panel: $Z = Z_\odot$. The inset shows the cumulative distribution.

However, at short coalescence times the distribution has a similar trend for both exchanged and original binaries.
(Raghavan et al. 2010). Such hard-soft binary encounters tend to quickly eject one of the wide binary members, and subsequently continue the evolution as a three-body encounter.

The binary–binary encounter rate is \( \Gamma_{\text{enc}}^{2+2} \) and can be calculated as

\[
\Gamma_{\text{enc}}^{2+2} = f_{\text{bin,a}} f_{\text{bin,b}} N_H \frac{8 \pi G m_{\text{tot}} R_{\text{enc}}}{\sigma_\infty}. \tag{7}
\]

Assuming the typical size of wide binaries, \( (R_{\text{enc}} = \sigma_{\text{WB}} = 30 \text{ au}; \) Raghavan et al. 2010), \( f_{\text{bin,a}} = f_{\text{BBH}} = 10^{-3} \), and a wide binary fraction of \( f_{\text{bin,b}} = f_{\text{WB}} = 0.5 \), equation (7) leads to a much higher encounter rate of \( \Gamma_{\text{enc}}^{2+2} \simeq 40 \text{ Myr}^{-1} \). However, only close passages between the compact binary BH with a binary member can lead to a meaningful encounter: given its compactness, the binary BH can simply pass through the wide binary without really interacting as a two-body object. Therefore, to estimate the binary BH-wide binary encounter rate we set \( R_{\text{enc}} \equiv 2 \sigma_{\text{WB}} \), and double the rate to take into account that each wide binary is composed of two objects. With this, the \( 2+2 \) encounter rate becomes \( \Gamma_{\text{enc}}^{2+2} \simeq 0.2 \text{ Myr}^{-1} \). In this assumptions we ignore that some of these encounters may end with the wide binary companion bound to the compact binary, forming a stable hierarchical triple. This triple would be too wide to affect the evolution of the compact binary via the von Zeipel–Kozai–Lidov mechanism (von Zeipel 1910; Lidov 1962; Kozai 1962), and would likely be disrupted via a subsequent interaction on a very short timescale.

Note that only encounters with wide binary BHs, rather than stellar wide binaries, can lead to a desirable outcome, that is tilting of the orbital plane of the binary BH. Most encounters with stellar objects will involve low-mass main sequence stars, because by the time the primordial binary has become a compact binary BH, massive stars have already collapsed into BHs. Such low-mass stars will have a limited impact on the more massive binary BH. To significantly affect the binary BH, the velocity kick from the passing star needs to be comparable to the orbital velocity of the binary BH, \( v_{\text{bin}} = \sqrt{GM_{\text{bin}}/D_{\text{bin}}} \). From conservation of linear momentum, this requires the star to approach one of the binary members by at least \( \sim a_{\text{bin}} (m_{\text{star}} + m_{\text{BH}}) / m_{\text{bin}} \). This distance is about 0.019 au for a 1 \( M_\odot \) star encountering a 40 \( M_\odot \) binary BH; this distance is dangerously close to the stellar tidal disruption radius \( R_{\text{tid}} (m_{\text{star}} / m_{\text{BH}})^{1/3} \sim 0.012 \text{ au} \). Hence most of the encounters between compact binary BHs and wide stellar binaries will result in either little impact on the binary BH or stellar tidal disruptions. We can then correct the binary–binary encounter rate by taking into account only encounters with wide binary BHs, whose fraction we can estimate as \( f_{\text{BHfWB}} \simeq 0.014 \). In this approximation we have neglected stellar binary interactions that are unlikely to occur in wide binaries. The total encounter rate is therefore \( \Gamma_{\text{enc}} = \Gamma_{\text{enc}}^{2+2} + \Gamma_{\text{enc}}^{2+1} \simeq 6.6 \times 10^{-3} \text{ Myr}^{-1} \).

This model assumes that most of the encounters will occur in the core, which may not be always correct. Barrera et al. (2021) find that the total integrated (i.e. over the entire volume of the cluster) encounter rate is underestimated by a factor of \( \sim 5 \) when compared to the core rate, as confirmed via N-body simulations. Barrera et al. (2021) found that of order 50 per cent of all interactions occur in the core, with a non-negligible additional contribution coming from interactions occurring just outside the core, and then drifting into the core due to mass segregation. Hence, the correction factor from the integrated rate calculation can simply be multiplied by the total core rate, in order to obtain a total rate for the entire cluster.

It is worth reminding that this cross-section estimate is rather simplistic because it neglects the role of global stellar cluster processes, such as core collapse, dynamical friction, and mass segregation, that tend to increase the frequency of encounters. The encounter rates outlined here are to be intended as a lower limit estimate. In other words, an enhanced rate of three-body encounters are an unavoidable consequence of the gravothermal instability of self-gravitating systems, and can accelerate the disruption of star clusters (Leigh et al. 2014a; Leigh, Shara & Geller 2016a).

## 5 MERGERS PROPERTIES

### 5.1 Local merger rate

To calculate the local merger rate density, we adopt the same approach as Kumamoto, Fujii & Tanikawa (2020). Particularly, we use their equation (16) to express the local merger rate density

\[
\Gamma_{\text{loc}}^{\text{GW}} = \frac{9 \times 10^{-4}}{4M_\odot} \ln 10 \int dZ \int d\eta \Psi(Z, \eta) \frac{D(Z, \eta_{\text{gw}})}{\eta} \frac{D(Z, \eta)}{dZ}, \tag{8}
\]

where \( D(Z, \eta_{\text{gw}}) \) is the merger rate of binary BHs originated from one cluster, \( \eta_{\text{gw}} \) is the lookback time, and \( \Psi(Z, \eta) \) is the comoving formation rate density of stars.

We calculate \( D(Z, \eta_{\text{gw}}) \) from the simulations, and include \( \Psi(Z, \eta) \) as estimated by Chruslinska & Nelemans (2019). We express \( D(Z, \eta_{\text{gw}}) \) as the product of the binary encounter rate \( \Gamma_{\text{enc}}(Z) \), and the density distribution of delay times \( B(Z, \eta_{\text{gw}}) \)

\[
D(Z, \eta_{\text{gw}}) = \Gamma_{\text{enc}}(Z) B(Z, \eta_{\text{gw}}). \tag{9}
\]

Here the encounter rate depends on the metallicity of the parent cluster through the compact binary BH fraction \( f_{\text{BBH}} \), as estimated as in Section 4 (\( \Gamma_{\text{enc}} \simeq 0.0005, 0.0066, \text{ and } 0.0143 \text{ Myr}^{-1} \) for \( Z = 1, 0.1, \text{ and } 0.001 Z_\odot \), respectively). The density distribution of delay times \( P(Z, \eta_{\text{gw}}) \) is obtained from the OC three-body simulations.

We consider three metallicity ranges: \( Z = 0.00632–0.1, 0.000632–0.00632, \text{ and } 0.00001–0.000632 \) for the simulations at 1, 0.1, and 0.01 \( Z_\odot \), respectively (i.e. equally spaced in logarithmic scale). Ultimately, the expression for the local merger rate reads as

\[
\Gamma_{\text{loc}}^{\text{GW}} = \frac{9 \times 10^{-4}}{4M_\odot} \ln 10 \sum_{1,2,3} \int D(Z, \eta_{\text{gw}} = \eta_{\text{gw}}) \Psi(Z, \eta_{\text{gw}}) d\eta_{\text{gw}}, \tag{10}
\]

where the summation is over the three ranges of metallicities, corresponding to the simulations at \( Z = 1, 0.1, \text{ and } 0.01 Z_\odot \), and \( \Psi(Z, \eta) \) is the star formation rate density \( d\Psi(Z, \eta) / dZ \) integrated over the three ranges (see equations 31–35 from Kumamoto et al. 2020).

We obtain a local merger rate of

\[
\Gamma_{\text{loc}}^{\text{GW}} \simeq 6.6 \text{ yr}^{-1} \text{ Gpc}^{-3}. \tag{11}
\]

Despite the higher abundance of compact binary BHs at \( Z = 0.001 Z_\odot (f_{\text{BBH}} \simeq 2 \times 10^{-3}) \), their contribution to the local merger rate is only \( \approx 2 \text{ yr}^{-1} \text{ Gpc}^{-3} \). The main reason is that most low-metallicity BHs are born at high redshift (see fig. 6 Chruslinska & Nelemans 2019), but they have a very short delay time (Fig. 4). Hence, the contribution to our estimated merger rate comes also from solar and moderately sub-solar metallicity binary BHs.

While our estimated merger rate lies at the lower limit inferred by GWTC-2 (The LIGO Scientific Collaboration & the Virgo Collaboration 2020b), it only applies to the subset of BH–BH mergers undergoing the pathway considered here. Our estimate indicates that such binaries may be already contributing to the current detection sample, and that they will likely emerge from the data after a few hundred detections.
5.2 $\chi_{\text{eff}}$ and $\chi_p$ distributions

The information on BH spin during the merger is encoded into two parameters, the effective spin parameter $\chi_{\text{eff}}$ and the effective precession parameter $\chi_p$. Both parameters describe the orientation of the spin vector with respect to the binary orbit: the effective spin $\chi_{\text{eff}}$ relates to the spin component parallel to the orbital angular momentum vector, while the effective precession $\chi_p$ relates to the orbital precession caused by the in-plane spin component.

Given the dimensionless spin $\chi$ and the spin obliquity $\theta$ (i.e. the angle between the spin vector and the orbital angular momentum vector), we can express $\chi_{\text{eff}}$ and $\chi_p$ as

$$\chi_{\text{eff}} = \frac{m_1 \chi_1 \cos \theta_1 + m_2 \chi_2 \cos \theta_2}{m_1 + m_2}$$

$$= \frac{(m_1 \chi_1 + m_2 \chi_2)}{m_1 + m_2} \cos \Delta \iota$$

$$\chi_p = \max \left[ \chi_1 \sin \theta_1, \chi_2 \sin \theta_2, \frac{4q + 3}{4 + 3q} \right]$$

$$= \max \left[ \chi_1, \chi_2, \frac{4q + 3}{4 + 3q} \right] \sin \Delta \iota,$$

where the indices $1$ and $2$ refer to the primary and secondary BHs, so that $m_1 > m_2$, and $q = m_2/m_1 \leq 1$ is the mass ratio. The last identity takes into account our initial setup, where both spins are initially aligned and $\theta_1 = \theta_2 = \Delta \iota$.

The dimensionless spin of BHs at birth is largely uncertain. Its precise value depends on the interplay between winds and tidal interactions of the progenitor binary, and on the physics of angular momentum transport during the last stages of core collapse (e.g. Qin et al. 2018; Bavera et al. 2020). These processes are largely uncertain, and they are commonly described by parametrized models. To avoid introducing further model degeneracies, we adopt three different phenomenological models for the dimensionless spin. In the MAXIMUM model, we assume that both BHs in the original binaries are born maximally spinning, i.e. $\chi_1 \equiv \chi_2 \equiv 1$. In the UNIFORM model, the spin of the BHs is instead randomly drawn from a uniform distribution between 0 and 1. In the BETA model, the spin is sampled from a beta distribution with scale parameters $(\alpha, \beta) = (2.3, 4)$. The beta distribution peaks at about $\chi \approx 0.2$ with a long tail at 0.3–0.7. The spin of the isolated BH can affect the effective spin distributions of exchanged binaries; it is assumed to be zero in all three models.

In physical terms, the BETA model is roughly consistent with a super-efficient angular momentum transport mechanism via the Tayler–Spruit magnetic dynamo (Spruit 1999, 2002; Fuller & Ma 2019; Fuller, Piro & Jermy 2019). In this model, all black holes are born with negligible spin ($\chi \simeq 10^{-5}$), unless their Wolf–Rayet progenitors are spin-up by tidal interactions.

Fig. 5 shows the cumulative distribution of $\chi_{\text{eff}}$ and $\chi_p$ for each simulated set. Because the outcome distributions are the same regardless of the initial velocity dispersion of the three-body encounter, we omit plotting the curves from the GC simulations.

In the MAXIMUM model, the $\chi_{\text{eff}}$ distributions are characterized by a peak at $\chi_{\text{eff}} \sim 1$, stronger at high metallicity. This peak is mainly composed of original binaries that experienced only weak encounters with moderate tilting. Hence, the peak at $\chi_{\text{eff}} \sim 1$ simply traces the distribution of $\chi_{\text{eff}}$ before the encounter, which is identical to 1 in the MAXIMUM model. The slope between $\chi_{\text{eff}} \sim -0.5, 0.5$ is composed of exchanged binaries, wherein the primary BH is the non-spinning, exchanged one. Overall, the slope in the MAXIMUM model is too shallow the one inferred from the observations.

Going from the MAXIMUM to the BETA model, the average dimensionless spin of the BHs decreases, and the cumulative distributions of $\chi_{\text{eff}}$ becomes more peaked at zero. Particularly, the distribution at $Z = 0.1$ and 0.01 $Z_\odot$ for the BETA model matches well the inferred distribution from GWTC-2.

The $\chi_p$ cumulative distribution has a similar trend, with the BETA model more peaked at zero, and the MAXIMUM model favouring larger $\chi_p$. Overall, the UNIFORM model matches better the $\chi_p$ constraints from the GWTC-2 data.

In addition to displaying the distribution of $\chi_{\text{eff}}$ and $\chi_p$ for each metallicity, we compute the local merger rate for different bins of $\chi_{\text{eff}}$ and $\chi_p$. Each domain range is divided in 25 uniform bins, and the procedure to calculate the local merger rate is repeated for each binary subset. Fig. 6 shows the obtained local merger rate as a function of $\chi_{\text{eff}}$ and $\chi_p$. The end result can be thought of as a combination of the distributions in Fig. 5, weighted by merger rate per metallicity range, plus second order effects from the correlations between effective spin and delay time.

The BETA spin model best matches the current observational data. The $\chi_{\text{eff}}$ distribution is compatible to the observed one, with a peak slightly above 0 and a tail at negative $\chi_{\text{eff}}$. The $\chi_p$ distribution has a broad peak at $\chi_p \sim 0.2$, in reasonable agreement with the GWTC-2 data (see fig. 9 of The LIGO Scientific Collaboration & the Virgo Collaboration 2020b).
On the other hand, models of isolated binary evolution with low natal kicks are not able to produce binaries with anti-aligned spins and consequently GW events with negative $\chi_{\text{eff}}$ (e.g. Bavera et al. 2020; Callister, Farr & Renzo 2020).

### 6 Caveats

We remind here the assumptions we made along this work. First, we have considered only compact binary BHs undergoing a single three-body encounter. This was justified in Section 4 and Section 3, by noting that the encounter rate of such binaries is small compared to cluster lifetimes and GW coalescence times. Moreover, the binaries get ejected from most stellar clusters due to the high recoil kicks from the encounters, preventing further encounters.

Another assumption of our work is that the BH spins are initially aligned with the orbit. This assumption is reflected in the choice of the initial conditions: all our binary BHs come from post-common-envelope evolution, and form a close Wolf–Rayet binary before collapsing into BHs. Our binary sample has a median period less than 1 d, so that tidal forces can efficiently align the spin of the progenitor stars (Kushnir et al. 2016; Hotokezaka & Piran 2017; Piran & Piran 2020). In general, this is not true for longer binary periods and stars that underwent significant mass transfer; however, this depends on the tidal efficiency and the angular-momentum transport within the stellar interiors, which are highly uncertain (Stegmann & Antonini 2021).

Finally, we neglected BH natal kicks that might tilt the binary plane and the stellar spins. In our case, the kick magnitude should be $>600 \text{ km s}^{-1}$ to affect the binary angular momentum, which is unlikely (Mandel 2016; Mirabel 2016; Wysocki et al. 2018).

### 7 Conclusions

We investigated the spin parameter distributions of post-common-envelope binaries that undergo dynamical encounters in stellar clusters. This binary formation pathway was identified by Kumamoto et al. (2019) and Di Carlo et al. (2020) in numerical simulations of young star clusters. Both studies showed that this pathway contributes significantly to the binary BH merger rate, especially at low metallicity.

We assume that binary BHs emerge from this evolutionary pathway with spins aligned with the orbital angular momentum, and subsequently undergo a three-body encounter with an isolated BH. The encounter can tilt the orbital plane of the binary, resulting in spin-orbit misalignment. The orbital tilt can therefore lead to GW signals with non-zero $\chi_p$ and negative $\chi_{\text{eff}}$, even if the BH spins remain aligned with each other. We consider only one single encounter, as justified by the high recoil velocity of the binary (Fig. 3) and by the low encounter rate of post-common-envelope binaries (Section 4).

We infer the distribution of orbital tilt angles $\Delta t$ after a single encounter by means of direct N-body integrations. We model the encounter with the highly accurate few-body code TSUNAMI, including post-Newtonian corrections to the equations of motion. Our binary initial conditions are drawn from an updated version of the population stellar synthesis code BSE (Tanikawa et al. 2021; see also Tanikawa et al. 2020b), considering three different metallicities: $Z = 1, 0.1,$ and $0.01 \text{ Z}_\odot$. We select only the binaries that survive common envelope evolution as Wolf–Rayet stars and that are spun-up by tidal interactions. The mass of the third BH is consistently selected from single stellar population synthesis. For the encounter properties, we consider both low velocity dispersion environments (corresponding
to open clusters) and high velocity dispersion environments (corresponding to globular and young massive star clusters). We show that the encounter outcome is the same regardless of the velocity dispersion, due to the compactness of the binaries.

While it is generally assumed that dynamical exchanges in star clusters result in an isotropic orbit-spin misalignment, we show that it is not the case for compact post-common envelope binaries that are limited to a single strong interaction. The orbital tilt angle distribution (Fig. 2) for exchanged binaries is not entirely flat, but still favours mild spin-orbit alignment. This results in a $\chi_{\text{eff}}$ distribution skewed towards positive values, in contrast to the symmetric distribution predicted by the dynamical assembly scenario.

We estimate the local merger rate considering the cosmic star formation rate density at different metallicities, taking into account the delay time of BH mergers and the binary encounter rates. We obtain a lower limit for the local merger rate of $\Gamma_{\text{loc}} \lesssim 6.6 \text{yr}^{-1} \text{Gpc}^{-3}$ that shows that this pathway might be contributing to the events detected so far.

We also estimate the differential merger rate for the effective $\chi_{\text{eff}}$ and precession $\chi_p$ spin parameters. Because the value of natal BH spins $\chi$ is subject to numerous uncertainties, we test three different phenomenological models.

Assuming low dimensionless spins $\chi \lesssim 0.2$ in binaries and non-spinning isolated BHs, our scenario qualitatively reproduces the $\chi_{\text{eff}}$ distribution skewed towards positive values, in contrast to the symmetric distribution predicted by the dynamical assembly scenario.

We estimate the local merger rate considering the cosmic star formation rate density at different metallicities, taking into account the delay time of BH mergers and the binary encounter rates. We obtain a lower limit for the local merger rate of $\Gamma_{\text{loc}} \lesssim 6.6 \text{yr}^{-1} \text{Gpc}^{-3}$ that shows that this pathway might be contributing to the events detected so far.

We also estimate the differential merger rate for the effective $\chi_{\text{eff}}$ and precession $\chi_p$ spin parameters. Because the value of natal BH spins $\chi$ is subject to numerous uncertainties, we test three different phenomenological models.

Assuming low dimensionless spins $\chi \lesssim 0.2$ in binaries and non-spinning isolated BHs, our scenario qualitatively reproduces the $\chi_{\text{eff}}$ distribution skewed towards positive values, in contrast to the symmetric distribution predicted by the dynamical assembly scenario.

We estimate the local merger rate considering the cosmic star formation rate density at different metallicities, taking into account the delay time of BH mergers and the binary encounter rates. We obtain a lower limit for the local merger rate of $\Gamma_{\text{loc}} \lesssim 6.6 \text{yr}^{-1} \text{Gpc}^{-3}$ that shows that this pathway might be contributing to the events detected so far.

We also estimate the differential merger rate for the effective $\chi_{\text{eff}}$ and precession $\chi_p$ spin parameters. Because the value of natal BH spins $\chi$ is subject to numerous uncertainties, we test three different phenomenological models.

Assuming low dimensionless spins $\chi \lesssim 0.2$ in binaries and non-spinning isolated BHs, our scenario qualitatively reproduces the $\chi_{\text{eff}}$ distribution skewed towards positive values, in contrast to the symmetric distribution predicted by the dynamical assembly scenario.

We estimate the local merger rate considering the cosmic star formation rate density at different metallicities, taking into account the delay time of BH mergers and the binary encounter rates. We obtain a lower limit for the local merger rate of $\Gamma_{\text{loc}} \lesssim 6.6 \text{yr}^{-1} \text{Gpc}^{-3}$ that shows that this pathway might be contributing to the events detected so far.

We also estimate the differential merger rate for the effective $\chi_{\text{eff}}$ and precession $\chi_p$ spin parameters. Because the value of natal BH spins $\chi$ is subject to numerous uncertainties, we test three different phenomenological models.

Assuming low dimensionless spins $\chi \lesssim 0.2$ in binaries and non-spinning isolated BHs, our scenario qualitatively reproduces the $\chi_{\text{eff}}$ distribution skewed towards positive values, in contrast to the symmetric distribution predicted by the dynamical assembly scenario.

We estimate the local merger rate considering the cosmic star formation rate density at different metallicities, taking into account the delay time of BH mergers and the binary encounter rates. We obtain a lower limit for the local merger rate of $\Gamma_{\text{loc}} \lesssim 6.6 \text{yr}^{-1} \text{Gpc}^{-3}$ that shows that this pathway might be contributing to the events detected so far.

We also estimate the differential merger rate for the effective $\chi_{\text{eff}}$ and precession $\chi_p$ spin parameters. Because the value of natal BH spins $\chi$ is subject to numerous uncertainties, we test three different phenomenological models.

Assuming low dimensionless spins $\chi \lesssim 0.2$ in binaries and non-spinning isolated BHs, our scenario qualitatively reproduces the $\chi_{\text{eff}}$ distribution skewed towards positive values, in contrast to the symmetric distribution predicted by the dynamical assembly scenario.
Spin misalignment in black hole binaries

Stegmann J., Antonini F., 2021, PhRvD, 103, 063007

This paper has been typeset from a TeX/\LaTeX file prepared by the author.