Formation pathway of Population III coalescing binary black holes through stable mass transfer

Kohei Inayoshi,1† Ryosuke Hirai,2 Tomoya Kinugawa3 and Kenta Hotokezaka4

1Department of Astronomy, Columbia University, 550 W. 120th Street, New York, NY 10027, USA
2Advanced Research Institute for Science and Engineering, Waseda University, 3-4-1, Okabo, Shinjuku, Tokyo 169-8555, Japan
3Institute for Cosmic Ray Research, The University of Tokyo, Chiba 277-8582, Japan
4Center for Computational Astrophysics, 162 5th Ave, New York, NY 10010, USA

ABSTRACT

We study the formation of stellar mass binary black holes (BBHs) originating from Population III (PopIII) stars, performing stellar evolution simulations for PopIII binaries with MESA. We find that a significant fraction of PopIII binaries form massive BBHs through stable mass transfer between two stars in a binary, without experiencing common envelope phases. We investigate necessary conditions required for PopIII binaries to form coalescing BBHs with a semi-analytical model calibrated by the stellar evolution simulations. The BBH formation efficiency is estimated for two different initial conditions for PopIII binaries with large and small separations, respectively. Consequently, in both models, ~10 per cent of the total PopIII binaries form BBHs only through stable mass transfer and ~10 per cent of these BBHs merge due to gravitational wave emission within the Hubble time. Furthermore, the chirp mass of merging BBHs has a flat distribution over $15 \lesssim M_{\text{chirp}}/M_{\odot} \lesssim 35$. This formation pathway of PopIII BBHs is presumably robust because stable mass transfer is less uncertain than common envelope evolution, which is the main formation channel for Population II BBHs. We also test the hypothesis that the BBH mergers detected by LIGO originate from PopIII stars using the total number of PopIII stars formed in the early universe as inferred from the optical depth measured by Planck. We conclude that the PopIII BBH formation scenario can explain the mass-weighted merger rate of the LIGO’s O1 events with the maximal PopIII formation efficiency inferred from the Planck measurement, even without BBHs formed by unstable mass transfer or common envelope phases.

Key words: black hole physics – gravitational waves – stars: Population III.

1 INTRODUCTION

Advanced LIGO (AdLIGO) has detected sources of gravitational waves (GWs). The sources, GW 150914, GW 151226 and LVT 151012, are inferred to be merging binary black holes (BBHs) with masses of $(36.2^{+8.8}_{-3.8} M_{\odot}, 29.1^{+4.2}_{-3.1} M_{\odot})$, $(14.2^{+8.3}_{-3.3} M_{\odot}, 7.5^{+2.7}_{-2.2} M_{\odot})$ and $(23^{+18}_{-16} M_{\odot}, 13^{+7}_{-6} M_{\odot})$ (Abbott et al. 2016b,d). The origin of such massive and compact BBHs and their formation pathways have been proposed (Abbott et al. 2016, references therein) through massive binary evolution (e.g. Belczynski, Bulik & Rudak 2004; Dominik et al. 2012; Kinugawa et al. 2014; Belczynski et al. 2016b) including rapid rotation and tides (Mandel & de Mink 2016; Marchant et al. 2016), and/or stellar dynamics in a dense cluster (e.g. Portegies Zwart & McMillan 2000; Mapelli 2016; O’Leary, Meiron & Kocsis 2016; Rodriguez, Chatterjee & Rasio 2016).

In the isolated binary scenario, metal-poor stars are generically required to form massive BHs because of inefficient stellar winds and smaller stellar radii. Many authors have investigated formation channels of BBHs via Population II (hereafter PopII) stars with $Z \lesssim 0.1 Z_{\odot}$ (e.g. Dominik et al. 2012; Belczynski et al. 2016b) and Population III (hereafter PopIII) with $Z \simeq 0$ stars (e.g. Kinugawa et al. 2014, 2016b; Belczynski et al. 2016a). The initial mass function (IMF) of PopII stars is expected to be less top-heavy (Omukai et al. 2005), whereas PopIII stars are thought to be typically as massive as ~10–300 $M_{\odot}$ (e.g. Hirano et al. 2014) and likely to evolve without losing their masses due to stellar winds (e.g. Baraffe, Heger & Woosley 2001; Inayoshi, Hosokawa & Omukai 2013). These scenarios may be distinguished in the future by the chirp mass distributions (Nakamura et al. 2016), where $M_{\text{chirp}} \equiv (M_1 M_2)^{3/5}/(M_1 + M_2)^{1/5}$ for a BBH with masses of $M_1$ and $M_2$, and stochastic GW backgrounds (GWBs; Abbott et al. 2016c;
Dvorkin et al. 2016; Hartwig et al. 2016; Inayoshi et al. 2016; Nakazato, Niino & Sago 2016).

In PopII BBH formation from isolated binaries, a significant fraction of the binaries experience unstable mass transfer (MT) during the binary evolution (e.g. Dominik et al. 2012; Belczynski et al. 2016b). The unstable MT makes the orbital separation shrink rapidly, which results in a common envelope (CE) phase (Paczynski 1976; Iben &Livio 1993; Taam &Sandquist 2000; Ivanova et al. 2013, references therein), where one of the stars plunges into the bloated envelope of the companion star and spirals inwards, losing its orbital energy and angular momentum. If the stellar envelope is successfully ejected due to the energy deposit and the spiral-in halts, a close binary system would be formed or else these stars would merge. To form BBHs that can merge within the Hubble time, PopII binaries should experience CE phases because their orbital separations tend to be wider due to mass-loss (e.g. stellar winds). Moreover, since PopII giant stars are likely to have convective stellar envelopes, the MT would be unstable. Because of uncertainties about relevant physical processes, however, the final outcome of binaries after unstable MT and CE phases is uncertain (e.g. Ivanova et al. 2013). In population synthesis models, in fact, merging rates of PopII BBHs vary by several orders of magnitude depending on the adopted prescriptions about the MT and CE (Belczynski et al. 2008; Dominik et al. 2012; Belczynski et al. 2016b; Eldridge & Stanway 2016).1

The CE phase also may play a crucial role for the PopIII binary evolution. Belczynski et al. (2016a) claimed that most of PopIII massive binaries merge in the CE phase thereby only a small fraction of them evolve to merging BBHs. However, as speculated by Kinugawa et al. (2014), there are PopIII binaries that can form BBHs with a coalescence time less than the Hubble time through stable MT and without experiencing any CE phases. This is because PopIII stars with certain masses evolve to compact blue giants with a radiative envelope instead of red giants with a convective envelope (e.g. Marigo et al. 2001; Ekström et al. 2008). The discrepancies between Kinugawa et al. (2014) and Belczynski et al. (2016a) come from the difference in models for PopIII single stellar evolution and their prescription to describe binary evolution during CE phases (e.g. stability conditions for MT and merger criteria in CE phases).

In this work, we address the following questions: (i) what conditions are required for the formation of merging PopIII BBHs to avoid the CE phases and (ii) what fraction of PopIII binaries evolve to merging BBHs without the CE phase. Then, we compare the total number of PopIII BBHs required from LIGO’s O1 merger rate and without experiencing any CE phases. This is because PopIII stars with certain masses evolve to compact blue giants with a radiative envelope instead of red giants with a convective envelope (e.g. Marigo et al. 2001; Ekström et al. 2008). The discrepancies between Kinugawa et al. (2014) and Belczynski et al. (2016a) come from the difference in models for PopIII single stellar evolution and their prescription to describe binary evolution during CE phases (e.g. stability conditions for MT and merger criteria in CE phases).

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1 Pavlovskii et al. (2017) have pointed out that massive stars with convective envelope could be more unlikely to experience unstable MT and CE than previously expected in PopII BBH formation (e.g. Belczynski et al. 2016b), considering a detailed model (Pavlovskii & Ivanova 2015). Although their model also might allow PopIII binaries to form more BBHs even via CE phase, we do not consider the effect to give a conservative discussion.
envelope during its lifetime (see their fig. 5). Note that properties of the stellar envelope are crucial to determine stability of MT (see Section 2.1.3).

Recently, Belczynski et al. (2016a) performed population synthesis calculations of PopIII binaries. They describe the time evolution of the stellar radius of PopIII stars, by adopting their lowest metallicity model (see Section 2.2.2).

The behaviour of the MT is determined by the response of the Roche radius and the stellar radius when it loses the material (Paczynski 1976). Assuming that the MT is conservative ($\beta = 1$), the radius of the Roche radius is approximately expressed as (Eggleton 1983)

$$R_{L,1} \simeq \frac{a}{M_1} \left[ 0.49 q_1^{\frac{1}{3}} + \ln \left( 1 + q_1^{\frac{1}{3}} \right) \right].$$

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$$\zeta_1 \equiv \frac{\mathrm{d} \ln R_{L,1}}{\mathrm{d} \ln M_1} \simeq 2.13 q_1 - 1.67$$

(Tout et al. 1997). For $\zeta_1 < \zeta^* = \ln(R_{L,1}/M_1)$, the stellar radius shrinks and becomes smaller than the Roche radius after the mass of the primary is transferred. On the other hand, for $\zeta_1 > \zeta^*$, the MT would proceed unstably and the two stars would either merge or experience a CE phase. The response of the stellar radius is automatically calculated in the stellar evolution calculations, while it is estimated with an analytical expression in our semi-analytical model (see Section 2.2.2).

We adopt the binary module in MESA to treat the MT process. When the Roche lobe is filled with stellar material ($R_L > R_{L,1}$), the MT rate is calculated by a method proposed by Kolb & Ritter (1990)

$$\dot{M}_1 = -2\pi F_1(q_2) R_{L,1}^3 \frac{GM_1}{M_1} \times \left[ \frac{k_B T_{\text{ph}}}{m_p \mu_{\text{ph}}} \right]^{3/2} \rho_{\text{ph}} \frac{\beta}{\sqrt{1 + \frac{\beta}{2}}} + \int_{r_{\text{ph}}}^{r_{\text{ph}}(\Gamma_1)} F_2(\Gamma_1) \left( \frac{k_B T}{m_p \mu} \right)^{1/2} dP ,$$

where $F_1(q_2) = 1.23 + 0.5\log q_2$, $F_2(\Gamma_1) = \Gamma_1^{1/2}[2/(\Gamma_1 + 1)]^{1/2} \Gamma_1^{1/2}[2/(\Gamma_1 + 1)]^{1/2} (\Gamma_1 + 1)^{-1}$, $\Gamma_1$ is the first adiabatic exponent, and $T_{\text{ph}}, \mu_{\text{ph}}, P_{\text{ph}}, P_{\text{ph}}$ and $P_{L,1}$ are the temperature, mean molecular weight, density and pressure at the photosphere and the radius of $R_{L,1}$, respectively. The first and second terms correspond to the MT rate for isothermal atmosphere (optically thin) and adiabatic atmosphere (optically thick).
thick), respectively. This rate is calculated self-consistently by considering properties of the donor star. Note that conservative MT, i.e. $J_{\text{orb}} = 0$ and $M = 0$ ($\beta = 1$) is assumed in our stellar evolution calculations.

### 2.1.4 Gravitational wave emission

A binary loses the orbital angular momentum and the energy due to emission of GWs following

$$\frac{J_{\text{orb}}}{J_{\text{orb}}} = -\frac{32G^3 M_1 M_2 M}{5c^2 a^3},$$

where $\epsilon = 0$ is assumed. From equation (7), the coalescence timescale due to GW emission is estimated as

$$t_{\text{GW}} = \frac{256G^3 M_1 M_2 M_{\text{tot}}}{5a^3 c^5},$$

$$\simeq 9.5 \frac{2q^2}{1 + q_1} \left(\frac{a}{0.2 \text{ au}}\right)^2 \left(\frac{M_1}{30 M_\odot}\right)^{-3} \text{ Gyr}.\quad (8)$$

### 2.2 Semi-analytical model

We describe the treatment of PopIII binary stars in our semi-analytical model. The differences from the detailed calculations of stellar structure are shown in the following. Since we do not follow the stellar evolution of binaries, instead we need to treat single stellar evolution (Section 2.2.1), the MT rate, and the response of the donor and accretor (Sections 2.2.2–2.2.5). The orbital evolution and GW emission from PopIII BBHs are calculated in the same way as in Sections 2.1.2 and 2.1.4.

#### 2.2.1 Single star evolution

We adopt fitting formulae for stellar radii and He-core mass of PopIII stars with masses of 10$M_\odot \leq M \leq 100 M_\odot$ as functions of the mass and time since the birth of the stars (Kinugawa et al. 2014). These are based on the results of the stellar evolution calculations for single PopIII stars by Marigo et al. (2001), where mass-loss due to the stellar wind and pulsation are not considered. Note that the time-averaged root-mean-square errors of the fitting formulae are within 6 per cent over the entire lifetime of PopIII stars. We set the critical mass required for BH formation to $M \geq 28 M_\odot$.

#### 2.2.2 Stability of MT

In our semi-analytical model, we evaluate stability of MT and estimate the transfer rate, instead of conducting stellar evolution calculations (Section 2.1). We obtain quantitative criteria for the stability of MT. In summary, PopIII binaries experience unstable MT and CE phases if any of the following conditions are satisfied during the evolution;

(A) either $M_1$ or $M_2$ exceeds 60$M_\odot$,

(B) $M_2/M_1 \leq 1/3$ at the first MT episode, and

(C) $M_2 > M_{\text{crit}} = (2 \times 10^{-2} M_\odot$ yr$^{-1}$).

In what follows, we explain these conditions in more detail.

(A) **Unstable MT due to convective envelope** – the stability of MT is determined by the response of the Roche radius $\xi_L$ and the stellar radius of the donor $\xi_*$ (Section 2.1.3). In our semi-analytical model, we adopt the analytical expressions for the value of $\xi_*$ as in population synthesis calculations (e.g. Hurley, Tout & Pols 2002; Belczynski et al. 2008).

At the early stage of the MT, mechanical equilibrium is restored in a dynamical time-scale and the star can be assumed to be at hydrostatic equilibrium at every time. That is, the response of the stellar radius occurs adiabatically. The value of $\xi_{\text{ad}, \text{conv}} = \frac{\partial \ln \rho}{\partial T}$ depends on whether the stellar envelope is convective or radiative. For a star with a core and a convective envelope, the value of $\xi_{\text{ad}, \text{conv}}$ is expressed as a function of the mass ratio $m_{1,1}$ between the core mass and the total mass in the primary (Hjellming & Webink 1987; Soberman, Phinney & van den Heuvel 1997). The value of $\xi_{\text{ad}, \text{conv}}$ increases with $m_{1,1}$ and approaches $-1/3$ for $m_{1,1} \rightarrow 0$, which corresponds to a fully convective star. As shown in Fig. 1, PopIII stars with $M_1 > 50 M_\odot$ have deep convective envelopes after the onset of He-core burning. From table 4 of Marigo et al. (2001), $m_{1,1} \simeq 0.45–0.5$ for 60 $M_\odot \leq M_1 \leq 100 M_\odot$, respectively. Thus, $\xi_{\text{ad}, \text{conv}} \simeq 0.44–0.56$ for the mass range, while $\xi_1 = 2.13 q_1^{-1} 1.67 \geq 0.46 (q_1 \geq 1$, see equation 5). Therefore, PopIII binaries that have components heavier than 60$M_\odot$ are likely to experience unstable MT unless the binary mass ratio is exactly unity or the MT occurs before the donor star reaches the Hayashi track because of a small initial separation. Here, to give a conservative argument, we simply impose that if either $M_1$ or $M_2$ exceeds 60$M_\odot$, the binary does not form a BBH because of unstable MT.

(B) **Delayed dynamical instability (DDI)** – for a star with a radiative envelope, the value of $\xi_{\text{ad}, \text{rad}}$ is generally positive. When the radiative envelope, which has a positive entropy gradient, is removed by MT, the layer with a lower entropy is exposed. Then, the density will increase to adjust its new hydrostatic equilibrium state with the same external pressure as before because $(\partial S/\partial \rho)_p = -(1/\rho^2) (\partial T/\partial \rho)_p < 0$. Thus, the donor’s radius shrinks in the dynamical time-scale. However, the situation in this case is more complicated. Even if the MT occurs stably at the early phase ($\xi_L < \xi_{\text{ad}, \text{rad}}$), the inner layer of the donor with a shallower entropy gradient can be exposed. If the entropy profile is shallow enough for the response of the stellar radius to be $\xi_L > \xi_{\text{ad}, \text{rad}}$, the MT would become unstable later due to the so-called DDI (Hjellming & Webink 1987). The critical mass ratio that leads to the DDI has been estimated as $q_{\text{crit},1} = 2–4$ for many kinds of donor stars (e.g. Hjellming 1989; Ge et al. 2010, 2015; Pavlovskii & Ivanova 2015). We note that the exact value of the critical mass ratio is still uncertain (e.g. treatment of superadiabatic layer; see discussions in Pavlovskii & Ivanova 2015), in particular, for metal-poor stars like PopIII stars. We here simply assume $q_{\text{crit},1} = 3$, which is the averaged value for PopI cases. Therefore, we assume that if the donor star is sufficiently massive ($M_1/M_2 \leq 1/3$), the MT will be unstable due to the DDI.

(C) **Expansion of accretors due to MT** – the fitting formulae we adopt are obtained by calculations of single stellar evolution, where the stellar structure is thermally relaxed. However, when the first episode of MT occurs, the secondary (main-sequence) star is away from its thermal equilibrium state. In fact, the main-sequence accretor could be bloated, depending on the MT rate. According to detailed stellar evolution calculations by Hosokawa et al. (2016), the accreting PopIII stars are unlikely to expand as long as the entropy hardly changes by emitting radiation within a dynamical time since the thermal time-scale of most parts of the envelope is longer than the dynamical time-scale.

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2 The fitting formula for the lifetime in the He-burning and He-shell burning phases were updated (Kinugawa, Nakamura & Nakano 2016a), which we adopt in this paper.

3 The entropy hardly changes by emitting radiation within a dynamical time since the thermal time-scale of most parts of the envelope is longer than the dynamical time-scale.
accretion rate is $\lesssim 10^{-2} M_\odot \text{yr}^{-1}$. The critical rate has also been estimated as a few $\times 10^{-2} M_\odot \text{yr}^{-1}$ (Hosokawa et al. 2012). The exact critical value is still unclear because it depends on treatment of the boundary conditions at the stellar surface. Here, we adopt the critical accretion rate of $\dot{M}_{\text{crit}} \approx 2 \times 10^{-2} M_\odot \text{yr}^{-1}$, above which the accretor would expand, fill its Roche lobe and might lead to unstable MT.

### 2.2.3 Mass transfer rate

In the following, we focus on cases with stable MT in the dynamical time-scale ($\xi_\text{L} < \xi_\text{th}$). Even in this case, the donor star gradually approaches its thermal equilibrium state, in which the response of the stellar radius can be satisfied with $\xi_\text{L} > \xi_\text{th} \equiv (\text{dln} R_1/\text{dln} M_1)|_{\text{th}}$ depending on the stellar structure. When the Roche lobe is filled with the stellar material due to thermal relaxation, MT occurs again in the Kelvin–Helmholtz (KH) time-scale ($t_{\text{KH}} \equiv GM_1^2/R_1L_1$). The MT rate is given by the overfilling of the donor’s Roche lobe, $\Delta R_{1} \equiv R_1 - R_{1,\text{th}}(\gtrsim 0)$, as

$$
\dot{M}_1 = - \frac{f(\mu)M_1}{\sqrt{R_1^2/GM_1}} \left(\frac{\Delta R_1}{R_1}\right)^3 d_{3/2},
$$

where

$$
f(\mu) = \frac{4\mu \sqrt{1 - \mu}}{(\sqrt{\mu + 1} - \mu)^3} \left(\frac{a}{R_1}\right)^3,
$$

$$
\mu = M_1/(M_1 + M_2) \quad \text{and} \quad d_{3/2} = 0.2203 \quad \text{(e.g. Paczyński & Sienkiewicz 1972; Savonije 1978; Edwards & Pringle 1987)}.
$$

Note that a polytropic equation of state with an index of $n = 3/2$ is assumed in equation (9). In fact, radial dependence of the adiabatic index affects the MT rate (see e.g. Kolb & Ritter 1990; Ge et al. 2010). However, we here adopt the simpler prescription because our semi-analytical model has a lack of thermal properties of the donor’s envelope.

The MT rate in equation (9) is high soon after the onset of the MT. However, the MT proceeds in the KH time-scale of the donor star. Thus, we set the maximum MT rate to $\dot{M}_{1,\text{max}} = \dot{M}_{1}(t_{\text{KH},1})$. Typically, $t_{\text{KH},1} \approx 4 \times 10^3 \text{yr}$ ($M_1/50 M_\odot)^2(R_1/20 R_\odot)^{-1}(L_1/10^6 L_\odot)^{-1}$ and then $\dot{M}_{1,\text{max}} \approx 1.25 \times 10^{-3} M_\odot \text{yr}^{-1}$. To estimate the KH time-scale, we adopt a fitting form of the stellar luminosity at the beginning of He-shell burning phase given by Kinugawa et al. (2014). In fact, since the stellar luminosity of the donor rapidly decreases during the MT (Paczynski 1967), we underestimate the value of $t_{\text{KH},1}$ and overestimate the maximum accretion rate. In other words, the condition (C) in Section 2.2.2 would be alleviated somewhat in detailed stellar evolution calculations.

### 2.2.4 Stellar radii during MT and rejuvenation

During an MT episode, the donor’s radius changes depending on how much of the mass is removed from the envelope. This process is generally complicated and difficult to be treated properly. For simplicity, we consider cases where the donor star is a giant in which He burning begins and the accretor is a main-sequence star. Note that MT between two main-sequence stars (the so-called case A) is not considered to avoid complicated situations.

The stellar radius of the donor during the MT is estimated using the fitting formulae for single star models as $R_i(M_i, t, t(M_i)) \rightarrow R_i(M_i + \delta M_i, t + \delta t_i(M_i))$, where $\delta t_i$ is the time after the onset of the MT, $\delta M_i = \int_{M_i}^{M_f} M_i \text{d}M (< 0)$ and $t_i(M_i)$ is the lifetime during He-core ($i = \text{He}$) and He-shell ($i = \text{HeS}$) burning phases. This prescription assumes that the core mass and the stellar age in the corresponding phase do not change during the MT because the MT occurs faster than the nuclear core and/or shell burning (see also the results with MESA shown in Figs 3 and 4).

The accretor is fed at a rate of $\dot{M}_2(\equiv -\dot{M}_1 > 0)$. Since unburnt hydrogen is supplied as fuel, we modify the stellar age (i.e. rejuvenation) following a method suggested by Tout et al. (1997) and Hurley et al. (2002). We approximate that the mass of H-burning core is proportional to $M_2 \times t/t_{\text{KH}}(M_2)$, where $t$ is the stellar age. Thus, we estimate a new stellar age due to rejuvenation as

$$
t' = \frac{M_2}{M_2 + \delta M_2} \frac{t_{\text{KH}}(M_2 + \delta M_2)}{t_{\text{KH}}(M_2)}.
$$

Using equation (11), we estimate the stellar radius of the accretor as $R_i(M_2 + \delta M_2, t', t_{\text{KH}}(M_2 + \delta M_2))$.

### 2.2.5 Termination of MT

The episode of MT terminates at the end of lifetime of the donor or when a large fraction of its hydrogen envelope is stripped from the donor. In the latter case, the donor’s radius rapidly shrinks when the He-core mass dominates its total mass. Note that we define the core boundary as the outermost part where the H mass fraction is lower than 0.01 and the He mass fraction is higher than 0.1. The critical ratio of the He core to the total mass is supposed to be $q_{\text{He,crit}} \approx 0.6$–0.8, above which the donor star evolves blueward in the HR diagram (Kippenhahn & Weigert 1990). In our semi-analytical model, we set $q_{\text{He,crit}} \approx 0.58$ so that the evolutionary tracks of the PopIII binaries agree with the results by the stellar evolution calculations.

### 3 POPULATION III BINARY BH FORMATION

In this section, we discuss the evolutionary paths of PopIII binaries. As an example, Fig 2 shows a schematic picture of the time evolution of a PopIII binary with the initial masses of $M_{1,0} = 50 M_\odot$ and $M_{2,0} = 25 M_\odot$, and the initial separation of $a_0 = 45 R_\odot$. This is a typical pathway of formation of PopIII BBHs without unstable MT and CE phases. In what follows, we first demonstrate two cases of binary evolution pathways calculated with MESA. Then, we compare these results with the semi-analytic formulae developed in the previous section.

#### 3.1 Evolution of individual PopIII binaries

##### 3.1.1 Stellar evolution calculations

We present the time evolution of two PopIII binaries with different initial conditions of $(M_{1,0}, M_{2,0}, a_0) = (50 M_\odot, 25 M_\odot, 45 R_\odot)$ in Fig. 3 and $(M_{1,0}, M_{2,0}, a_0) = (40 M_\odot, 25 M_\odot, 30 R_\odot)$ in Fig. 4, respectively. Red and blue curves show the evolution of the primary and secondary star, respectively. In each figure, the top panel shows the mass evolution of the two stars $M_{1,2}(t)$ (solid) and the H core of the primary star $M_{\text{H,crit}}(t)$ (dashed), and the bottom panel shows the evolution of the stellar radii $R_{1,2}(t)$ (solid), the Roche radii $R_{1,2}(t)$ (dashed) and the orbital separation $a(t)$ (black solid). Note that these results shown in Figs 3 and 4 are obtained by stellar evolution calculations with MESA. We follow the evolution of these binaries until just before the second episode of MT occurs because the MT (from the secondary star to a BH) is not conservative. Instead, the non-conservative MT is studied with our semi-analytical model, exploring the dependence of the results on the parameter $\beta$ (see Appendix A).
As shown in Fig. 3, after the two stars evolve from their ZAMS to post-main-sequence phases, their stellar radii expand. The primary star fills its Roche lobe after the end of the H-core burning and the first episode of MT begins at $t \simeq 4.39$ Myr. Since the mass ratio at the onset of the MT is larger than unity ($q_1 > 1$) and the MT is conservative ($M_1 = -M_2 > 0$), the separation initially shrinks (see equation 2). After the mass ratio becomes smaller than unity, the MT continues and thus the separation gets wider. Once the hydrogen-rich layer of the envelope is removed, the MT terminates at $t \simeq 4.6$ Myr due to the discrete change in the surface composition. This occurs just beneath the outermost convection zone in the hydrogen shell, where the helium abundance increases by a factor of $\sim 2$. By this time, the He-core mass occupies $\sim 65$ per cent of the total mass. The core mass of $\sim 22 M_\odot$ is massive enough to form a BH by direct collapse. Note that we do not calculate the evolution of the (primary) naked He star but the primary star is considered as a BH with $M_1 \simeq 22 M_\odot$ because of the absence of the wind mass-loss.

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but the accretor is a BH. Since the MT rate is estimated as
reproduce the plausible results by our simple model.

\[ \rho \text{,} \] than the actual values estimated in Section 3.1.1, but allows us to
form a BH.

The overall behaviours for the two cases shown in Figs 3 and 4
are similar. For both cases, the first episodes of MT terminate when the He-core mass of the primary stars occupies 65 (62) per cent of
their total mass.

3.1.2 Semi-analytical model

In Figs 5 and 6, we show the time evolution of two PopIII binaries
calculated by the semi-analytical model. The same initial conditions
are adopted for both cases as in Figs 3 and 4. The evolutionary tracks
until just before the second episodes of MT are very similar to those
of the stellar evolution calculations. Note that our semi-analytical
model does not replicate expansion phases of the secondary stars
during the first episodes of MT as shown in Figs 3 and 4. Here,
the critical core mass ratio is set to be \( q_{\text{He}, \text{crit}} = 0.58 \) in order to
determine the termination of the MT. This value is slightly smaller
than the actual values estimated in Section 3.1.1, but allows us to
reproduce the plausible results by our simple model.

In the second episode of MT, the donor is an ordinary star
but the accretor is a BH. Since the MT rate is estimated as
\[ |M_2| \sim 10^{-5} - 10^{-3} M_\odot \text{yr}^{-1}, \] the BH is fed at a super-Eddington
accretion rate of \[ |M_2|/M_{\text{Edd}, 1} \sim 10(1 - 10^2), \] where \( M_{\text{Edd}, 1} \equiv L_{\text{Edd}, 1}/(\epsilon c^2) \approx 6.9 \times 10^{-7} M_\odot \text{yr}^{-1} (M_1/30 M_\odot) (\epsilon/0.1)^{-1}, \]
\( L_{\text{Edd}, 1} \) is the Eddington luminosity and \( \epsilon \) is the radiative efficiency. Although one assumes that the accretion rate is limited
by the Eddington accretion, i.e., \( M_1 = \min(|M_2|, M_{\text{Edd}, 1}), \)
supercritical-Eddington accretion would be possible through an
optically thick accretion disc associated with outflows and/or jets
(e.g. Begelman 1978; Abramowicz et al. 1988; Ohsuga et al. 2005;
Jiang et al. 2014; Sadowski et al. 2015). We simply assume that a fraction \( \beta = M_1/|M_2| = 0.1 \) of the gas can accrete on to the BH
and the rest is ejected from the BH with a certain specific angular
momentum. We follow the orbital evolution using equation (3). Fi-
nally, the stellar envelope of the secondary star is stripped and the
second episode of MT terminates. The secondary (naked He star)
collapses into a BH and thus a binary BH system forms.

3.2 Parameter dependence on final states of PopIII binaries

Fig. 7 shows final fates of PopIII massive binaries with different initial conditions of the binary: \( M_{1,0} = 40 M_\odot, M_{2,0} = 25 M_\odot \)
and \( a_0 = 30 R_\odot, \) which are the same as in Fig. 4.

During the first episode of MT, the mass of the secondary star is increased to \( \approx 41 M_\odot. \) The maximum MT rate is estimated as
\[ 2 \times 10^{-3} M_\odot \text{yr}^{-1} \] at the early stage and drops to \( \lesssim 10^{-3} M_\odot \text{yr}^{-1} \)
later. After the MT, the secondary star becomes massive enough to
form a BH.

Figure 5. Time evolution of stellar masses, stellar radii and the orbital separation of a PopIII binary calculated by the semi-analytical model. The initial conditions are set to \( M_{1,0} = 50 M_\odot, M_{2,0} = 25 M_\odot \)
and \( a_0 = 45 R_\odot, \) which are the same as in Fig. 3.

Figure 6. Same as Fig. 5 (semi-analytical model), but different initial conditions of the binary: \( M_{1,0} = 40 M_\odot, M_{2,0} = 25 M_\odot \)
and \( a_0 = 30 R_\odot, \) which are the same as in Fig. 4.

In the top panel, the parameter dependence of the final fates of
PopIII massive binaries with different initial conditions of \( a_{1,0}/a_{1,0}, M_{1,0}/M_{2,0} \) and \( a_0 \) for three different primary
masses of \( M_{1,0} = 30 \) (top), 40 (middle) and 50 \( M_\odot \) (bottom),
respectively. Shaded regions indicate initial conditions for which
massive PopIII binaries form BBHs (blue), form neutron star (NS)-
BH binaries (green) and experience CE phases due to unstable MT
(red). With larger initial separations, stellar radii of the two stars
never exceed their Roche radii and they do not interact through
MT, indicated as ‘No RLOF’, where each of the stars evolve as a
single star. Dashed lines show boundaries, in the right-hand side
of which the binary can form a wide-separation BBH even with-
out binary interactions. It is worth noting that such wide-separation
BBHs formed in ‘No RLOF’ do not merge within the Hubble time.
On the other hand, with very small separations, the primary star fills
its Roche radius even during its main-sequence phase (the so-called
case A mass transfer). In this case, episodes of MT would be likely
to affect the evolution of the core mass because the core evolution
has not been decoupled yet from that of the total mass. Thus, our
treatment for the stellar evolution and its rejuvenation would not
work. In addition, the effects due to tidal force could be important
for such close binaries (see Section 6.2).

In the top panel, the parameter dependence of the final fates of
PopIII binaries with \( M_{1,0} = 30 M_\odot \) is shown. With smaller mass
For the highest primary mass ($M_{1,0} = 50 M_\odot$), the PopIII binary is more likely to experience CE phases for the two reasons described in Section 2.2.2. One is that the secondary star becomes more massive than $\approx 60 M_\odot$ via the first episode of MT. Thus, when the secondary star fills its Roche lobe and undergoes the second episode of MT, the MT is unstable because its stellar envelope is convective. Another reason is that the MT rate from the primary to the secondary can be higher than the critical value of $M_{\text{crit},2}$, above which the secondary stellar radius would be bloated. As a result, in this case ($M_{1,0} = 50 M_\odot$), PopIII binaries with smaller ($\sim 0.2$ au) or lager ($\sim 4$ au) separations can form BBHs via stable MT without experiencing CE phases.

In summary, we find that there are regions in the parameter space where merging BBHs are formed from PopIII binaries without experiencing CE phases. We consider these pathways are robust to form PopIII merging BBHs. In the following discussion, we focus only on such a population because the outcome of the CE phases of PopIII binaries is uncertain. In this sense, our argument on the event rate of BBH mergers is somewhat conservative.

### 4 Formation Efficiency and Population of PopIII Binary BHs

In the previous section, we discussed formation pathways of PopIII BBHs, in particular, focusing on those with or without unstable MT and CE phases. Applying the results, we estimate efficiency of PopIII BBH formation for given initial conditions of PopIII binaries. In the following, we discuss the BBH formation efficiency with an analytical argument in Section 4.1. As we will see, this estimate gives reasonable BBH formation efficiencies and the delay time distribution. We also build population synthesis models for two types of binary initial conditions as examples (see Sections 4.2 and 4.3). The initial conditions of $N_{\text{tot}}$ binaries are generated with the Monte Carlo method and then the evolution is followed by the semi-analytic formula developed in Section 2.2. The convergence of the results has been checked for $N_{\text{tot}} = 10^5$ and $10^6$. Note that we focus only on PopIII BBH formation through stable MT, i.e. without experiencing any case A MT and CE phases. If BBHs formed via these processes, the efficiency of BBH formation could be higher.

#### 4.1 Analytical estimate

Here, we estimate analytically the number fraction of PopIII BBHs coalescing within the Hubble time to the total number of PopIII binaries, $f_{\text{BH}} = I/J$, where

$$I = \int_{M_{\text{min},1}}^{M_{\text{max},2}} dM_1 \Psi(M_1) \int_{q_{\text{min}}}^{q_{\text{max}}} dq \Phi(q) \int_{a_{\text{min}}}^{a_{\text{max}}} da \Gamma(a),$$

and

$$J = \int_{M_{\text{min},1}}^{M_{\text{max}}} dM_1 \Psi(M_1) \int_{q_{\text{min}}}^{q_{\text{max}}} dq \Phi(q) \int_{a_{\text{min}}}^{a_{\text{max}}} da \Gamma(a).$$

Here, $\Psi(M_1)$ is the IMF for the primary star with $M_{\text{min},1} \leq M_1 \leq M_{\text{max},1}$. $\Phi(q)$ is the initial mass-ratio distribution with $q_{\text{min}} = M_{\text{min},1}/M_1 \leq q \leq 1$. $\Gamma(a)$ is the initial distribution of binary separations with $a_{\text{min}} \leq a \leq a_{\text{max}}$. For a primary star with $M_1 > M_{\text{crit},1}$, it forms a BH by direct collapse. For $M_1 > M_{\text{crit},2}$, the primary evolves a red giant with a deep convective envelope, resulting in unstable MT and a CE phase (see Section 2.2.2). We here set $M_{\text{crit},1} = 28 M_\odot$ and $M_{\text{crit},2} = 60 M_\odot$, respectively. We define $q_{\text{crit}} = \max[q_{\text{min}}, q_{\text{CE}}]$, where $q_{\text{CE}} = 1/3$ is the critical mass ratio below which a binary could evolve through

\[\text{Figure 7.} \text{ Dependence of final states of PopIII binaries on the initial conditions of the mass ratio } q_{1,0} = M_{2,0}/M_{1,0} \text{ and the orbital separation } a_0. \text{ Shaded regions indicate conditions for which BBHs form (blue), NS-BH form (green) and PopIII binaries experience CE phases (red). For } q_{1,0} \leq 1/3, \text{ the binaries experience the DDI. For } M_{1,0} = 50 M_\odot, \text{ the binaries are likely to experience CE phases during either the first or second episode of MT. For other cases, compact binaries (BBH or NS-BH) are formed as remnants only via stable MTs. Even for an initially less massive primary, its mass can increase via MT to } \gtrsim M_{\text{crit},1} (\sim 28 M_\odot), \text{ above which the star collapses directly into a BH without explosions. In other words, the MT from the massive primary allows the secondary to become massive enough to form a BH. For higher initial primary mass } (M_{1,0} = 40 M_\odot), \text{ the overall result is similar to that for } M_{1,0} = 30 M_\odot, \text{ but BBHs can form for a wider range of initial conditions of binaries.} \]
a CE phase due to the DDI. As shown in Section 3.1.2 (Figs 5 and 6), the orbital separation after forming a BBH hardly changes from the initial separation. The critical separation for a formed BBH required to merge within the Hubble time is estimated as $a_{GW} \simeq 0.22 \text{ au} \left( M_1 / 30 M_\odot \right)^{1/4}$, where formed BBHs are assumed to be equal-mass binaries (see Figs 5 and 6). The value of $a_{\text{crit}} \simeq 0.1 \text{ au}$ is adopted so that PopIII binaries do not experience (case A) MT during their main-sequence phases (see Fig. 7). As long as $\Gamma(a)$ is not a steep function at $0.1 \lesssim a / \text{au} \lesssim 0.3$, therefore, equation (12) can be approximated as

$$I \simeq \int_{a_{\text{crit},0}}^{a_{GW,0}} da \Gamma(a) \times \int_{M_{\text{crit},1}}^{M_{\text{max},1}} dM_1 \Psi(M_1) \int_0^1 dq \Phi(q), \quad (14)$$

where $a_{GW,0} = 0.22 \text{ au}$ and $a_{\text{crit},0} = 0.1 \text{ au}$. Using equations (13) and (14), and assuming $\Gamma(a) \propto a^{-\gamma}$, we can estimate

$$f_{\text{BBH}} \simeq \frac{\int_{M_{\text{crit},1}}^{M_{\text{max},1}} dM_1 \Psi(M_1) \int_0^1 dq \Phi(q)}{\int_{M_{\text{min}}}^{M_{\text{max}}} dM_1 \Psi(M_1) \int_0^1 dq \Phi(q)} \times \left\{ \begin{array}{ll} \frac{\int_{a_{GW,0}}^{a_{\text{crit},0}} da \Gamma(a)}{a_{GW,0}^{(\gamma - 3)/4}} & (\gamma = -1), \\ \frac{\int_{a_{\text{crit},0}}^{a_{GW,0}} da \Gamma(a)}{a_{\text{crit},0}^{(\gamma - 3)/4}} & (\gamma \neq -1). \end{array} \right. \quad (15)$$

In addition, we can estimate the number of PopIII BBHs which merge in coalescence time-scales of $t_{GW}$ as

$$\frac{dN}{dt_{GW}} = \frac{dN}{da} \left. \frac{da}{dt_{GW}} \simeq \Gamma(a) \frac{a}{t_{GW}} \propto t_{GW}^{(-3\gamma)/4}, \right. \quad (16)$$

where we use $dN/da \simeq \Gamma(a) \propto a^{-\gamma}$ and $t_{GW} \propto a^{\gamma}$ (see equation 8). Note that the coalescence time distribution is not sensitive to the choice of $\gamma$. It is worthy estimating the efficiency of BBH formation which allows pathways even through unstable MT and CE phases. The efficiency can be roughly estimated as $f_{\text{BBH}, \text{max}} = K / J$, where

$$K \simeq \int_{a_{\text{crit},0}}^{a_{GW,0}} da \Gamma(a) \times \int_{M_{\text{crit},1}}^{M_{\text{max}}} dM_1 \Psi(M_1) \int_0^1 dq \Phi(q), \quad (17)$$

Here, the conditions (A) and (B) shown in Section 2.2.2 are removed, i.e. $M_{\text{crit},1} \rightarrow M_{\text{max}}$ and $q_{\text{crit}} \rightarrow q_{\text{min}}$. We also allow rapid MT to form BBHs (see condition C in Section 2.2.2) and thus set $a_{\text{crit},0} \simeq 1 \text{ au}$ (see bottom panel in Fig. 7).

### 4.2 Two types of binary initial conditions

PopIII binaries formed in a circumstellar disc at $\sim 1$–100 au (Machida et al. 2008; Clark et al. 2011; Greif et al. 2012; Hosokawa et al. 2016) and/or at larger scales of $\sim 10^3$ au (Turk, Abel & O’Shea 2009; Stacy & Bromm 2013). In addition, massive PopIII stars emit strong UV radiation (Hosokawa et al. 2011; Stacy, Greif & Bromm 2012), which affects gas accretion on to the protostellar and the final masses. Susa, Hasegawa & Tominaga (2014) have studied statistical properties of PopIII binaries in $\sim 60$ minihaloes, performing radiation hydrodynamical simulations with a spatial resolution of $\sim 10$ au. As a result, the binary fraction is $\sim 50$ per cent and the separation is $10^{11}$ au. Stacy, Bromm & Lee (2016) have performed a cosmological simulation including radiative feedback with a very high resolution of $\sim 1$ au. They studied star formation in one minihalo and found that a close massive PopIII binary forms with $13 + 15 M_\odot$ and $a \sim 5$ au.

#### 4.2.1 Wide-binary model

As an example, we consider the same initial conditions as in Kinugawa et al. (2014), where a classical model for initial conditions of field binaries (e.g. Hurley et al. 2002) is applied for PopIII binaries. Namely, we adopt a flat IMF, $\Psi(M_1) \propto const.$, for the primary star with $10 \leq M_1 / M_\odot \leq 100$, a flat mass-ratio distribution, $\Phi(q) \propto const.$, with $q_{\text{max}} = 10 M_\odot / M_1 \leq q \leq 1$, and a log-flat distribution for the orbital separation, $\Gamma(a) \propto a^{-\gamma}$. The minimum separation is set so that the binary does not fill its Roche radius from the beginning. We set $a_{\text{max}} = 10^3 R_\odot$ ($\simeq 4.6 \times 10^3$ au). In this model, the number fraction of PopIII BBHs formed by stable MT is estimated from equation (15) as

$$f_{\text{BBH}} \simeq \frac{\ln \left( \frac{a_{GW,0}}{a_{\text{crit},0}} \right)}{\ln \left( \frac{a_{\text{max}}}{a_{\text{min}}} \right)} \times \frac{2}{3} \left( M_{\text{crit},1} - M_{\text{crit},1} \right) \left( M_{\text{max}} - M_{\text{min}} \right). \quad (18)$$

Note that this equation is valid for $M_{\text{min}} \leq M_{\text{crit},1}/3 \simeq 9.3 M_\odot$. Adopting the values of the initial conditions, we estimate $f_{\text{BBH}} \simeq 0.02$ from equation (18), where we adopt $a_{\text{min}} \simeq 3 R_\odot \simeq 7 R_\odot$.

In this condition, adding to $f_{\text{BBH}} \simeq 0.02$ the possibility that BBHs are also formed by unstable MT, equation (17) gives a maximum formation efficiency $f_{\text{BBH}, \text{max}} \sim 0.1$, which is consistent with that by Kinugawa et al. (2014).

#### 4.2.2 Close-binary model

Different initial conditions have been suggested by Belczynski et al. (2016a) for close Pop III binaries (close-binary model). These initial conditions are motivated by $N$-body simulations by Ryu, Tanaka & Perna (2016), who follow the time evolution of multiple systems in a star-forming cloud in a minihalo. They considered that PopIII stars form due to disc fragmentation around 10–20 au and these stars lose their angular momentum by dynamical friction with the ambient gas, resulting in formation of stable close binaries. The distribution of the initial separation is given by a Gaussian function with the average of $a_{\odot} \simeq 0.4 \text{ au}$ and the dispersion of $\sigma_a \simeq 0.34 \text{ au}$. The primary mass and mass ratio in this model have bimodal distributions, respectively (see table 2 of Belczynski et al. 2016a in detail).

### 4.3 Resultant distribution functions

Fig. 8 presents the chirp mass distribution of PopIII BBHs for the wide-binary (red) and close-binary (blue) models, respectively. Note that the chirp mass is a physical quantity to determine the leading-order amplitude and frequency evolution of the GW signal. The values of $y$-axis is normalized by the total number of PopIII binaries $N_{\text{tot}}$. PopIII BBHs formed through stable MT (dashed) and PopIII BBHs coalescing within the cosmic age, $t_{GW} < 13.8$ Gyr (solid). For the wide-binary model, 0.8 per cent of the PopIII binaries form BBHs through stable MT and can merge due to GW emission within the Hubble time. This result is consistent with the analytical estimate of the fraction shown in Section 4.1, where $f_{\text{BBH}}$

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4 Ryu et al. (2016) assumed a uniform density distribution of the ambient gas ($n_{\text{gas}} = 10^5 \text{ cm}^{-3}$) at 10–20 au, and neglected radiative feedback. Since the gas density at such small scales is $> 10^4 \text{ cm}^{-3}$ (Greif et al. 2012), however, the effect of dynamical friction would be underestimated. Moreover, radiation from the formed binaries would determine their final properties as shown in Stacy et al. (2016).
for the PopIII BBHs to merge in the LIGO detection horizon of stable MT (dashed) and PopIII BBHs coalescing within the cosmic age, tGW < 13.8 Gyr (solid) are shown.

Figure 9 shows the distribution of the coalescence time of PopIII BBHs for the wide-binary (red) and close-binary (blue) models, respectively. PopIII BBHs formed through stable MT can merge due GW emission within the Hubble time is at least 1 per cent, i.e. fGW ≳ 0.01. In this model, the initial separation distribution has a peak at a0 ≃ 100 R⊙ (≃ 0.5 au) and a tail towards smaller separations. Thus, a significant fraction of PopIII binaries can form BBHs only via stable MT (see Fig. 7).

Fig. 9 shows the distribution of the coalescence time of PopIII BBHs for the wide-binary model (red), the coalescence time distribution follows dN/dtGW ∝ tGW because of the separation distribution is approximated as (1 + a) → a0 + tGW, the coalescence time distribution is approximated as dN/dtGW ∝ tGW−0.7. Since most PopIII BBHs form at z ≳ 10, which corresponds to the cosmic age of tSF ≃ 1 Gyr, we require 10.8 Gyr ≲ tGW + tSF ≲ 13.8 Gyr for the PopIII BBHs to merge in the LIGO detection horizon (0 ≤ z ≤ 0.2, the corresponding time duration is ∼3 Gyr). From the distribution shown in Fig. 9, the fraction of merging PopIII BBHs detectable by LIGO (i.e. 9.8 ≲ tGW/Gyr ≲ 12.8) is estimated as fGW ≃ 0.17 for both models and thus fGW/fGW ≃ 1.7 × 10−3 is obtained.

5 OBSERVATIONAL CONSTRAINTS ON POPIII BBH FORMATION SCENARIO

In this section, we discuss the possibility that PopIII stars can be the progenitors of the three BBH mergers detected by AdLIGO, GW 150914 (Abbott et al. 2016b), GW 151226 and LVT 151012 (Abbott et al. 2016d) based on the formation efficiencies obtained in the previous section and the total number of PopIII stars inferred from Planck’s result.

From the LIGO’s detections, the stellar mass BBH merger rate is estimated as R ≃ 5.5 × 10−14 Gpc−3 yr−1 (Abbott et al. 2016a). Assuming that the MW mass function of coalescing binaries follows

\[ \Psi(M_1) \propto M_1^{-\alpha}, \]

with Mmin ≤ M1 ≤ M1 + M2 ≤ 100 M⊙, and a uniform distribution on the secondary mass between Mmin = 5 M⊙ and M1, the power-law index is inferred as \( \alpha \approx 2.5^{+1.5}_{-0.5} \) (Abbott et al. 2016a).

Let us suppose that all the LIGO events originate from PopIII BHs. We can evaluate the merger rate from the PopIII star formation rate as

\[ \langle M_{\odot} \rangle R \approx \dot{\rho}_{\star,\text{III}} \frac{2 f_{\text{bin}}}{1 + f_{\text{bin}}} f_{\text{BBH}} f_{\text{delay}}, \]

where \( \dot{\rho}_{\star,\text{III}} \) is the PopIII star formation rate (SFR), fbin (≃ 0.7) is the binary fraction, fBBH is the number fraction of merging BHs within the Hubble time to the total number of PopIII stars and fdelay is the number fraction of BBHs that merge in the LIGO detection horizon to the total number of merging PopIII BHs. Here, the mean mass of BHs is \( \langle M_{\odot} \rangle \approx 30 M_{\odot} \) for \( \alpha = 2.5 \). Therefore, the PopIII SFR required to explain all the LIGO events is

\[ \dot{\rho}_{\star,\text{III}} \approx 1.3 \times 10^{-3} M_{\odot} \text{yr}^{-1} \text{Mpc}^{-3} \left( \frac{f_{\text{bin}}}{0.4} \right) \left( \frac{R}{60 \text{Gpc}^{-3} \text{yr}^{-1}} \right) \left( \frac{f_{\text{BBH}}}{0.01} \right) \left( \frac{f_{\text{delay}}}{0.2} \right)^{-1}, \]

where we have used fBBH obtained in Section 4, i.e. the efficiency of BH formation only via stable MT, which we consider as the lower limit. For the two models for initial conditions of PopIII binaries, the number fraction of formed coalescing PopIII BHs within the Hubble time is at least 1 per cent, i.e. fGW ≳ 0.01. In this sense, the estimated PopIII SFR can be lower by a factor of a few. When we consider only GW 150914, which has \( \langle M_{\odot} \rangle \approx 65.3 M_{\odot} \) and \( R = 3.4^{+5.8}_{-3.8} \text{Gpc}^{-3} \text{yr}^{-1} \), the required PopIII SFR is

\[ \dot{\rho}_{\star,\text{III}} \approx 0.15 \times 10^{-3} M_{\odot} \text{yr}^{-1} \text{Mpc}^{-3}. \]

Now we compare directly the PopIII SFR of equation (21) with the constraint by the Planck measurement of the optical depth of the universe to electron scattering, which arises due to ionizing photons emitted from PopIII stars and other sources (e.g. accreting BHs). Thus, assuming that all the photons required to explain the observed optical depth are produced only by PopIII stars, the upper limit for the cumulative (comoving) mass density of PopIII stars is given by

\[ \rho_{\star,\text{III}} \lesssim 8.2 \times 10^2 M_{\odot} \text{Mpc}^{-3} \times \left( \frac{\eta_{\text{ion}}}{5 \times 10^4} \right) \left( \frac{f_{\text{esc}}}{0.1} \right)^{-1} \left( \frac{\tau_\text{e}}{0.066} \right) \left( \frac{\Delta \tau_\text{e}}{\Delta \tau_\text{e}} \right). \]
The value of the escape fraction for the flat (Salpeter) IMF with a mass range of $10^{-4} \leq M/M_\odot \leq 100$ (Schaerer 2002). The value of the escape fraction $f_{\text{esc}} \simeq 0.1$ corresponds to dark matter haloes with masses of $\gtrsim 10^7 M_\odot$ (Wise et al. 2014), where most of the PopIII stars would form (see also Inayoshi et al. 2016). We here set our fiducial value to $\tau_e = 0.066 \pm \Delta \tau_e$, where $\Delta \tau_e = 0.016$ is the 1σ error (Planck Collaboration XIII 2016). The PopIII SFR peaks at $z \simeq 10$ corresponding to the time-scale of $\sim 0.5$ Gyr so that the upper bound of PopIII SFR is

$$\dot{\rho}_{\text{III}} \lesssim 1.3 \times 10^{-3} M_\odot \text{yr}^{-1} \text{Mpc}^{-3}. \quad (23)$$

This upper limit is consistent with the most probable value of the rate of all three events (see equation 21). Therefore, we conclude that the PopIII BH formation scenario can explain all the three BBH mergers detected in LIGO’s O1 run with the maximal PopIII formation efficiency inferred from the Planck measurement, even without BBHs formed by unstable MT or CE phases.

6 DISCUSSIONS

6.1 Gravitational wave background

A stochastic GWB from unresolved PopIII BBH mergers is a useful probe for the existence of massive BBH populations at higher redshifts (Dvorkin et al. 2016; Hartwig et al. 2016; Inayoshi et al. 2016; Nakazato et al. 2016). Inayoshi et al. (2016) have estimated the amplitude of the PopIII GWB adopting a PopIII SFR whose normalization is consistent with the Planck measurement of the electron scattering optical depth (see equation 22). However, they also assume the merging rate of PopIII BBHs obtained by Kimura et al. (2014), which include BBHs formed by unstable MT and CE phases. According to the model by Kimura et al. (2014), 12 (2.6) per cent of PopIII binaries form BBHs coalescing within the Hubble time for the flat (Salpeter) IMF with $10 \leq M/M_\odot \leq 100$ and $37 (55)$ per cent of such BBHs [i.e. $4.2 (1.4)$ per cent of the total binaries] are formed without experiencing CE phases. On the other hand, the lower limit we estimate in Section 4 is only $\sim 1$ per cent of total binaries. Therefore, the GWB amplitude produced by merging PopIII BBHs formed only by stable MT is several times smaller than that estimated by Inayoshi et al. (2016), but gives a lower limit of the GWB. The detectability of the PopIII GWB in the future observing run in AdLIGO/Virgo in five years depends on physical parameters relevant to reionization and high-redshift galaxies shown in equation (22).

6.2 Tidal force and stellar spins

In this paper, we neglect effects of stellar rotation on the evolution so far. As we discussed, non-rotating PopIII stars are likely to evolve to compact blue giants and thus can avoid unstable MT and CE phases during their lifetime. However, stellar rotation may change the evolution of Pop III stars because of hydrodynamical instabilities induced by rotation (e.g. meridional circulations). For a slow-rotating PopIII star with $v_{\text{Kep}} \sim 0.2 v_{\text{Kep}}$ ($v_{\text{Kep}}$ is the Keplerian velocity of the star), the effective temperature at the end of the main-sequence phase tends to be lower than for a non-rotating PopIII star with the same mass, because unburnt hydrogen is supplied to the core of the rotating PopIII star due to the mixing (Ekström et al. 2008; Takahashi, Umeda & Yoshida 2014). Furthermore, mixing of heavy elements would increase the opacity of the stellar envelope (Joggerst & Whalen 2011). Therefore, the rotating PopIII star tends to evolve to red giants instead of blue giants expected for the non-rotation case. Since a red giant has a bloated stellar convective envelope, the stellar radius is more likely to fill its Roche lobe and lead to unstable MT, which would result in CE phase. On the other hand, a fast-rotating PopIII star with $v_{\text{Kep}} \gtrsim 0.5 v_{\text{Kep}}$, would experience chemically homogeneous evolution due to strong mixing effects and then become bluer without any redwards evolution (e.g. Yoon & Langer 2005; Woosley & Heger 2006; de Mink et al. 2009; Song et al. 2016). In this case, the PopIII stars can avoid unstable MT and CE phases.

The rotation period of a star in a close binary system is likely to be the same as the orbital period because of the tidal torque. This synchronization time-scale of massive main-sequence stars is estimated as (Kushnir et al. 2016a,b; see also Zahn 1975)

$$t_{\text{sync}} \simeq 2 \text{Myr} \left(1 + q \right)^{31/24} \left(\frac{r_g}{2q} \right)^{17/8} \left(\frac{M}{10^2 M_\odot} \right)^{109/24} \left(\frac{M_\text{con}}{24 M_\odot} \right)^{4/3}, \quad (24)$$

where $R_\text{con}$ and $M_\text{con}$ are the size and mass of the convective core, $r_g$ is the gyration radius of the star. Here, the fiducial values are adopted from data calculated with the MESA code and approximate $R_\text{con}/M_\text{con} \simeq 0.5$. PopIII main-sequence stars in binaries are likely to be synchronized at orbital separations where the coalescence time is shorter than the Hubble time. Note that this estimate is very sensitive to the convective-core radius and the mass of the star.

Importantly, when they are tidally synchronized at the separation where the coalescence time corresponds to the Hubble time, the rotational velocity of synchronized PopIII main-sequence stars is quite slow as $v_{\text{Kep}} < (0.01-0.1) \times v_{\text{Kep}}$. Therefore, the stellar rotation does not play important roles irrespective of the initial spin. Of course, binaries with smaller separations, i.e. shorter coalescence times, the stellar rotation might play important roles. However, BBHs formed in such systems merge in the early universe and they are not observable by LIGO.

6.3 Remnants after common envelope phases

Throughout the paper, we do not discuss the outcome of PopIII binaries that experience CE phases, in order to give conservative arguments. Many previous studies concluded that possible outcomes after CE evolution are tight binaries and/or stellar mergers, but the bifurcation conditions are highly uncertain (e.g. Iben & Livio 1993; Taam & Sandquist 2000; Ivanova et al. 2013). Even for PopIII binaries, CE evolution would occur for massive stars with $M > 50 M_\odot$ because (1) the accretor expands due to violent MT from the donor or (2) the MT would be unstable when the donor has a deep convective envelope in the late stage of its evolution (see bottom panel in Fig. 7). If the CE evolution of such binaries does not lead to stellar mergers, possible types of the remnants would be binaries of a He star ($\gtrsim 20 M_\odot$) with a main-sequence star ($\gtrsim 40 M_\odot$) or a BH ($\gtrsim 30 M_\odot$) after the first/second episodes of MT. Subsequently, if any, they form massive BBHs coalescing due to GW emission within the Hubble time. In order to discuss the outcome after CE evolution of PopIII binaries, we need to understand basic properties of the stellar dynamics in the CE phases, e.g. the energy budget...
during the CE phases more precisely using stellar evolution calculations as studied for stars with $0.0004 \leq Z \leq 0.02$ (e.g. Kruckow et al. 2016).

7 SUMMARY

We study formation of stellar mass BBHs originating from PopIII stars, performing stellar evolution simulations for PopIII binaries with a public code MESA. We find that a significant fraction of PopIII binaries form massive BBHs through stable MT without experiencing CE phases. The formation efficiency of coalescing PopIII BBHs is estimated for two different initial conditions for PopIII binaries with large and small separations, respectively. As a result, $\sim$10 per cent of the total PopIII binaries form BBHs only through stable MT and $\sim$10 per cent of these BBHs merge due to GW emission within the Hubble time. Furthermore, the chirp mass of merging BBHs has a flat distribution over $15 \lesssim M_{\text{chirp}}/M_\odot \lesssim 35$. This formation pathway of PopIII BBHs is presumably robust because stable MT is less uncertain than CE evolution, which is the main formation channel for PopIII BBHs. We then test the hypothesis that the BBH mergers detected by LIGO originate from PopIII stars using our result and the upper limit on the total number of PopIII stars formed in the early universe as inferred from the optical depth measured by Planck. We conclude that the PopIII BBH formation scenario can explain the mass-weighted merger rate of the LIGO’s O1 events with the maximal PopIII formation efficiency inferred from the Planck measurement, even without PopIII BBHs formed by unstable MT or CE phases.

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APPENDIX A: NON-CONSERVATIVE MASS TRANSFER: THE DEPENDENCE ON $\beta$

Through the paper, we set the value of $\beta$, which is a parameter to describe the efficiency of non-conservative MT. We adopt $\beta = 0.1$ as our fiducial value. In this appendix, we briefly discuss the dependence of the choice of $\beta$ on the results. The orbital evolution is described by equation (3). Integrating this equation over the second episode of MT, where the donor is a star with $M_1$ and the accretor is a BH with $M_2$, the orbital separation after the MT is given by

$$a_f = \left( \frac{M_1}{M_{1f}} \right)^2 \left( \frac{M_2}{M_{2f}} \right)^{2/\beta} \left( \frac{M_1 + M_2}{M_{1f} + M_{2f}} \right) a_i, \quad (A1)$$

where the subscript $i$ and $f$ indicate the values before and after the MT, respectively, and $M_{2f} = M_{2i} + \beta(M_{1i} - M_{1f})$. For $\beta = 0$, $M_2$ does not change via the MT, we obtain

$$a_f = \left( \frac{M_{1i}}{M_{1f}} \right)^2 \left( \frac{M_{1i} + M_2}{M_{1f} + M_{2f}} \right) e^{2(1-q_1)\alpha_i}. \quad (A2)$$

Fig. A1 presents the time evolution of the orbital separation and the BH (accretor) mass with the same initial conditions as shown in Figs 3 and 5 for different values of $\beta$. For $\beta \lesssim 0.1$, the resultant track of the separation and the BH (accretor) mass do not change significantly since the final separation can be written by equation (A2) for smaller $\beta$. For conservative MT ($\beta = 1$), the final orbital separation is similar to those for $\beta \lesssim 0.1$, but the BH mass becomes higher. However, a significant fraction of the transferred mass would be ejected from the system because the accretion flow on to the BH releases a huge amount of energy as radiation and/or outflows (e.g. Blandford & Begelman 1999; Ohsuga et al. 2005; Jiang et al. 2014; Sadowski et al. 2015).

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