1 Introduction

1.1 Black Holes: from mathematical concepts to astrophysical objects

There are not many objects in the Universe that are able to inspire the curiosity of astronomers and of the general public like Black Holes (BHs). From the mathematical point of view, these compact objects are solutions of Einstein's field equations of General Relativity (Einstein 1915). These equations link a distribution of mass and energy of an object to the shape of the spacetime curvature it generates, hence to the nature of the gravitational interaction between such object and the rest of the Universe. In particular, a BH is defined as a region of spacetime causally separated from the rest of the Universe. Physical objects can enter this region, but is then impossible for them to influence anything that is outside of it. The surface that delimits the boundary of a BH is called Event Horizon.

The fact that BHs represent exact solutions of Einstein's field equations was first demonstrated in the case of a spherically symmetric static source (Schwarzschild 1916), then in the case of a rotating axially symmetric one, either electrically uncharged (Kerr 1963), or charged (Newman et al. 1965). However, it is only since the second half of the 1960s that BHs have been considered also as astrophysical objects, and not only as mathematical concepts. The real existence of these extremely compact objects was suggested by the first observations of Quasistellar radio sources (Quasars), which emitted an amount of energy thought to be explainable only by the collapse of an object with a mass of the order of millions of Solar Masses ($M_\odot$) (Robinson et al. 1965). The theoretical confirmation of the fact that BHs could be astrophysical objects actually existing in the Universe came from results such as the one presented in Penrose (1965), where it was demonstrated that the gravitational collapse of a massive astrophysical object can indeed lead to the formation of a point-like singularity enclosed in an Event Horizon.

The first astrophysical object ever to be widely accepted to be a BH has been the galactic X-ray source Cygnus X-1, first observed in 1965 (Bowyer et al. 1965), and later confirmed to be a BH accreting mass from a blue supergiant star (Shipman 1975). The accretion process involves the conversion of the potential energy of material infalling onto the BH into thermal energy and luminosity emitted in the form of ElectroMagnetic (EM) waves. In the last 50 years, millions of accreting BHs have been detected. These objects can be divided into two main categories: stellar-mass BHs, and Super-Massive BHs (SMBHs). Stellar-mass BHs detected through EM waves have masses between approximately $3\mathrm{M}_\odot$ and $20\mathrm{M}_\odot$, and are the remnants of SuperNovae (SNe) events that marked the end of the core-burning phase of massive stars. The other category of detected BHs is characterised by masses between $10^6\mathrm{M}_\odot$ and $10^9\mathrm{M}_\odot$. These SMBHs can be found at the centre of galaxies and are the ones that power Active Galactic Nuclei (AGN). An AGN is a system formed by a central SMBH located at the centre of a gaseous disc, the material of which falls onto the compact object, causing the emission of a large amount of energy spread over a wide portion of the EM spectrum, from radio waves to gamma rays. The luminosity of an AGN usually out-shines the starlight emitted by the entirety of its host galaxy.

Measuring light coming from accretion is not the only way to use EM radiation to detect a BH. The position and the mass of compact objects can be calculated via the observations of microlensing events, when the path of the light coming from an object is perturbed by the passing of a BH between such object and the observer (Paczynski 1986, 1996). Another indirect way to infer the properties of a BH is by resolving the orbits of objects such as stars that are bound to it. This method has been used in the past to estimate the position and the mass of the SMBH that resides at the centre of the Milky Way (Schödel et al. 2002; Ghez et al. 2008) and of three stellar-mass BHs in its halo (El-Badry et al. 2023a,b; Gaia Collaboration et al. 2024).

1.2 Not only light: Binary Black Holes and Gravitational Waves

One of the biggest conceptual differences between Einstein's General Relativity and Isaac Newton's theory of gravitation (Newton 1687) is that, according to the former, the gravitational interaction between two objects travels at the same finite speed at which EM radiation travels in vacuum. In particular, when the mass distribution acting as source of spacetime curvature has a time-varying quadrupolar moment, it emits Gravitational Waves (GWs), which move from their source at the speed of light. A common way of conceptually and mathematically visualizing GWs is as travelling ripples, perturbations in the curvature of spacetime, the amplitude and the frequency of which depend on the characteristics of their originator.

Among the events that can emit detectable GWs there are the inspirals and mergers of binaries of compact objects. These waves can be detected by measuring the periodic variation of the proper distance between objects their passage cause. The relative amplitude of such variations is typically of the order of less than 10^{-20}, and it decreases linearly as a function of the distance from the source. However, the direct measurement of GWs coming from the merging binaries formed by stellar-mass BHs and/or Neutron Stars (NSs) has become a reality thanks to the laser interferometers of the LIGO-Virgo-KAGRA (LVK) collaboration (Acernese et al. 2015; LIGO Scientific Collaboration et al. 2015; Kagra Collaboration et al. 2019).

Almost ten year have passed since the first direct detection of GWs (Abbott et al. 2016), and since then three observing runs have been completed, while the fourth one is expected to last until June 9th, 2025. During the first three observing runs (O1, O2, and O3) a total of 90 mergers have been detected, most of them being of Binary Black Holes (BBHs) (Abbott et al. 2023b, 2024a). Figure 1.1 gives a visual representation of all these detected mergers in chronological order from left to right. On the vertical axis is the mass of the merging objects and of the remnant. Light blue dots represent BHs, orange one represent NSs, and objects the nature of which is uncertain are represented by half blue-half orange dots.

Merging BBHs are in general not expected to produce any EM radiation. Detecting the GWs they emit is therefore the only way to learn about them. The intrinsic properties of each binary that are possible to constrain with GW detections include the masses of the two components, and both the amplitude and the direction of their spins. Combining the information coming from all the single detections is possible to draw conclusion regarding the underlying astrophysical population of compact objects.

Figure 1.2, taken from The LIGO Scientific Collaboration et al. (2021b), shows the astrophysical mass spectrum for stellar-mass BHs inferred from the detections of the LVK collaboration. The differential merger rate is plotted as a function of the mass of the heavier component of the merging binaries m_1. While the black solid and dashed lines show the results obtained from all the events up to the first half of O3, the blue solid line and the light blue shaded region show the median and the 90 per cent credible interval of the posterior distribution inferred from all the events detected during the first three observing runs. The analytical model used for the fit consists of a truncated power-law, with a tapering at low masses and a Gaussian component. The vertical gray band in Figure 1.2 shows the 90 per cent credible interval on the position of the

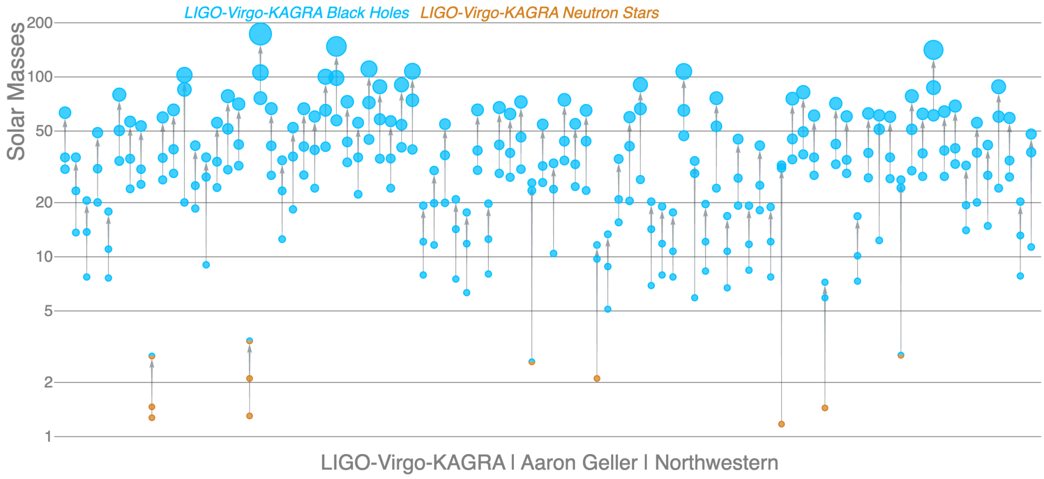

Figure 1.1: Visual representation of the 90 binary mergers detected by the interferometers of the LVK collaboration during their first three observing runs. The vertical axis indicates the rest-frame masses. In each group of three dots connected by an arrow, the bottom two represent the merging objects, while the top one represents the remnant. The mergers are chronologically ordered, from left to right. Light blue (orange) dots represent BHs (NSs). Objects the nature of which is uncertain are represented by symbols of both colors.

mean of such Gaussian component.

One conclusion of population analyses on BBHs that remains robust with respect to the analytical model that is assumed during the fit, is the fact that the mass spectrum of stellar-mass BHs extends to masses above $50\mathrm{M}_\odot$ (The LIGO Scientific Collaboration et al. 2021b). Objects with such masses were not present in the population inferred from observations of X-ray binaries, and their existence is not predicted by most of the models of stellar evolution (Heger & Woosley 2002; Belczynski et al. 2016). The presence of a gap between $50\mathrm{M}_\odot$ and $120\mathrm{M}_\odot$ in the mass distribution of the remnant of SuperNovae (SNe) events is expected because of the phenomenon of Pair Instability SuperNovae (PISNe) (Woosley 2019). These events represent the end of the life cycle of stars with an initial mass greater than approximately $150\mathrm{M}_\odot$, and consist in SNe where electron-positron pairs are created during the collapse of the stellar structure (Heger et al. 2003). The resulting runaway thermonuclear explosion is expected to leave no remnant (Fraley 1967).

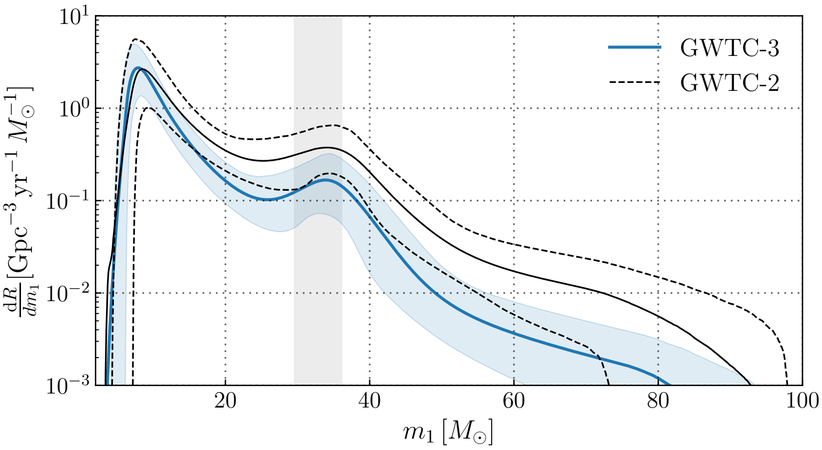

Figure 1.2: Differential merger rate as a function of the mass of the heavier component of BBHs. This astrophysical distribution of stellar-mass BH masses is the result of population analyses based on the GW detections performed by the LVK interferometers up to the first half of their third observing run (black solid and dashed lines), and including also the ones of the second half (blue line and shaded region). Solid lines indicate the median posterior distribution, and the shaded region and the dashed black lines indicate its 90 per cent credible interval. The models used for the fit is based on a truncated power law, with a tapering function at low masses, and a Gaussian component. The 90 per cent credible interval on the position of the mean of this Gaussian component is denoted by the vertical gray shaded region.

Observational evidences obtained thanks to the direct detection of GWs, such as the lack of a gap in the BH mass spectrum between $50\mathrm{M}_\odot$ and $120\mathrm{M}_\odot$, suggest the existence of BBH formation paths beyond the standard scenario of the evolution of an isolated binary stellar system. This remains valid even when taking into account that the position of the lower boundary of the so-called Pair Instability mass gap depends on the stellar model that is assumed, and on stellar properties such as the metallicity (Farag et al. 2022).

1.3 Formation of Binary Black Holes: isolated binaries and dynamically active environments

The physical origin of the binaries the mergers of which have been detected through GWs by the LVK collaboration remains elusive. In order for a binary of stellar-mass compact objects to emit energy in the form of GW radiation efficiently enough to be driven to merger within a Hubble time, its semi-major axis has to be of the order of 10^{-1} Astronomical Units (Mapelli 2021). Different formation paths for BBH that tight have been proposed, and they can be divided into two main categories: formation through the evolution of an isolated binary system of massive stars, and formation in dynamically dense environments, where encounters between stellar-mass objects are frequent (see Mapelli 2021, for a review of the possible binary formation paths).

In the case of a massive isolated stellar binary system a tight binary of compact objects can form after a Common Envelope (CE) phase (Ivanova et al. 2020). This occurs when one of the two stars incorporates the remnant of the other one within its own envelope, when entering the giant phase. If the CE is efficiently expelled because of the friction caused by the orbital motion of the two cores, the remaining binary can be tight enough to merge within a Hubble time an to be detected by the interferometers of the LVK collaboration. A schematic representation of the formation of a merging BBH through the CE channel is shown in Figure 1.3.

Another way for an isolated stellar binary system to create a BBH capable of merging within a Hubble time is through chemically homogeneous evolution (de Mink & Mandel 2016; Mandel & de Mink 2016). If a massive star is rotating fast and has a low metallicity, it might not develop a gradient of chemical composition in its interior. These chemically homogeneous stars have smaller radii compared to the slow rotating ones with the same mass, and can therefore form very tight binaries of compact objects without ever entering the CE phase (Marchant et al. 2016).

Alongside the evolution of isolated massive stellar binary systems, BBHs tight enough to be able to merge within a Hubble time can also form in dynamically active environments. A host environment is here referred to as "dynamically active" or "dynamically dense" if it has a density of approximately a thousand or more stellar-mass objects per cubic parsec. In such conditions, single objects or binary systems are expected to have strong gravitational interactions, that can lead to the formation of hard binaries. A binary is referred to as "hard" if its binding energy is larger than the average kinetic energy of the objects that are in its surroundings (Heggie 1973). Examples of dynamically dense environments are Globular Clusters (Gratton et al. 2019), Young Star Clusters (Lada & Lada 2003; Portegies Zwart et al. 2010), Nuclear Star Clusters (Ferrarese et al. 2006; Neumayer et al. 2020), and AGN accretion discs (McKernan et al. 2011a; Stone et al. 2017a).

In dense environments dynamical friction slows down objects on timescales

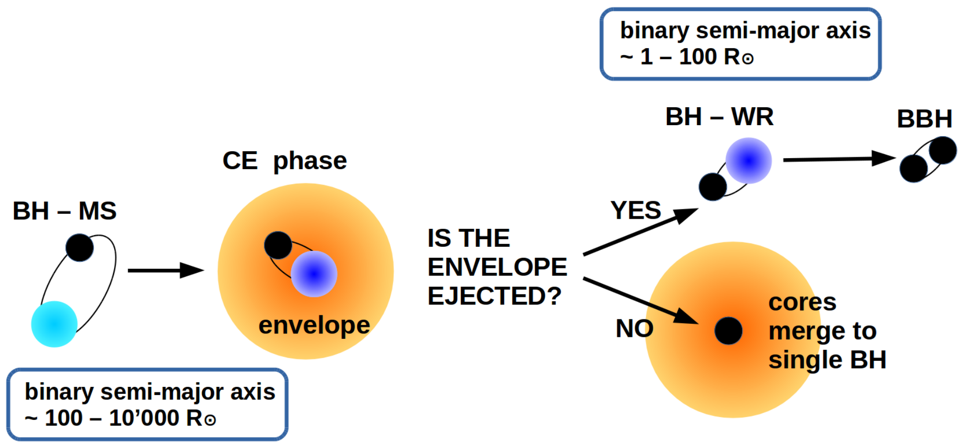

Figure 1.3: Representation of the formation of a merging BBH through the CE channel (taken form Mapelli (2021)). On the left it is shown a system formed by a star in the main sequence (light blue circle) and a BH, remnant of a SN event. When the star exits the main sequence and starts burning Helium in its core (blue circle), entering the giant phase, its envelope incorporates the BH. The binary system formed by the Helium-burning core and the BH gets tighter because of the drag exerted by the gas the envelope consists of. Part of the loss of orbital energy is turn into heat, which might cause the ejection of the envelope. If this happens, what is left is a tight binary formed by a BH and a naked stellar core, a Wolf-Rayet (WR) star. If the WR turns into a BH without disrupting the binary, the BBH that forms can be tight enough to emit detectable GWs efficiently and merge within a Hubble time. If the CE is not ejected, the Helium burning core and the BH merge inside of it, and no detectable GW is emitted.

inversely proportional to their mass (Chandrasekhar 1943). The more efficiently a massive object is slowed down the interaction with lighter ones surrounding it, the more quickly it sinks towards the gravitational centre of the host environment. This process leads to mass segregation, building up a population of heavy stellar-mass BHs and BBHs clustered in the inner regions of dense star clusters.

Beside dynamical friction, another class of gravitational interaction that is important to mention when talking about the formation of merging BBHs in dense environments is single-binary encounters. These processes involve a binary system of stellar-mass objects, and a single third object that can also be either a star or a compact object like a BH or a Neutron Star (NS). The encounter happens if the single object approaches the binary, reaching a distance from it comparable with its semi-major axis. The final product of this interaction is a binary which is in general harder than the original one, and that is formed by the two most massive objects that took part in the interaction. This is because if the intruder has a mass higher than at least one component of the original binary, than it has a probability close to one to take its place as part of the bound system, while the least massive object is ejected (Hills & Fullerton 1980). Hardening of binaries in these types of interactions takes place when part of the binary binding energy is transformed into kinetic energy of the ejected object.

Both dynamical friction and single-binary encounters happening in dynamically active environments are processes that can efficiently create binary systems composed by the heaviest objects that populate such environments (Ziosi et al. 2014). However, these processes cannot create binaries with BHs more massive than the ones that are already present in the initial population. They are therefore not sufficient to explain the observed evidences of merging BBHs with components that populate the Pair Instability gap in the stellar-mass BH spectrum.

One way of creating BHs with masses in the Pair Instability mass gap is through subsequent mergers, where at least one component of the merging binary is the remnant of a previous GW event. This hierarchical merger scenario is theoretically capable of creating objects with masses up to the Intermediate Mass BH (IMBH) regime (between $10^3\mathrm{M}_\odot$ and $10^6\mathrm{M}_\odot$) (Antonini et al. 2019; Mahapatra et al. 2024). However, in order for a remnant to have a non negligible chance to take part to a higher-generation event, it must be retained in the same environment that hosted the first merger, which is a reservoir of compact objects that can potentially act as components for the second one. When two compact objects merge the remnant undergoes the action of a recoil kick to guarantee the conservation of the total linear momentum of the binary system (Bonnor & Rotenberg 1961; Bekenstein 1973). Typical recoil kick velocities for the remnants of BBH mergers are of the order of $10^2\mathrm{km\ s}^{-1}$, but can reach reach values of thousands of kilometers per second for specific combinations of masses and spins of the binary components (Campanelli et al. 2007; Gerosa & Berti 2019). The hierarchical merger scenario, therefore, can only be efficient in very dense environments, whose escape velocity is large enough for most of the merger remnants to be retained. This is, for example, the case for Nuclear Star Clusters (Antonini & Rasio 2016; Mapelli et al. 2021).

Figure 1.4 shows a schematic representation of the interactions that are expected to take place in dynamically dense environments, resulting in the emission of detectable GWs.

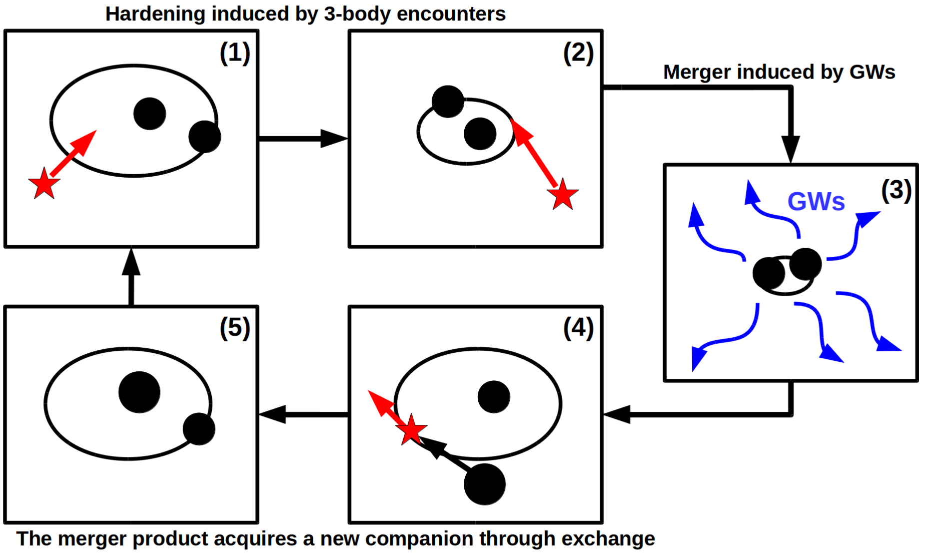

Figure 1.4: Schematic representation of the main processes that can take place in dynamically dense environments, concerning BBHs that merge emitting detectable GWs (taken from Mapelli (2021)). (1) A single stellar-mass object (red star) encounters a BBH both the components of which are more massive than the stellar-mass object itself. (2) The single-binary encounter hardens the bound system, reducing the size of its semi-major axis. (3) If the binary is tight enough, it starts to emit GWs efficiently. Such emission continues until the binary merges. This merger can be detected by the LVK interferometers. (4) The massive BH which is the remnant of the GW event gets retained in the host environment and encounters a binary system. The least massive of the three objects (red star) gets ejected and an exchange episode happens, in which the massive remnant takes its place in the binary system. (5) A new binary is formed, which can be hardened by a new single-binary encounter, and potentially merge in a higher-generation GW event.

Being the places in which processes like dynamical friction, single-binary encounters, and hierarchical mergers happen, dynamically dense environments have the potential of being the hosts of a significant fraction of the GW events detected so far by the LVK collaboration. More specifically this so-called "dynamical formation path" for merging BBHs is expected to be the channel that the most massive merging binaries more likely have followed, especially the ones with at least one component that has a mass in the Pair Instability gap predicted by stellar evolution models.

1.4 AGN discs as promising potential hosts of stellar-mass Binary Black Hole mergers

The two main characteristics that make AGN accretion discs different with respect to the other dynamically dense environments like Globular Clusters, Young Star Clusters, and Nuclear Star Clusters are their non-spherical shape, and that they are made of gas which interacts with the compact objects contained in the disc itself, modifying their orbits in a non-negligible way.

1.4.1 Disc captures

The moment in which a gaseous accretion disc forms around the SMBH which is at the centre of a galaxy marks the beginning of the AGN phase of such Nuclear Star Cluster. Stars and stellar-mass compact objects whose orbit around the central SMBH lies on the same plane of the newly-formed disc will start to interact dynamically with it. However, AGN accretion discs with a density larger than 10^{-10}g cm^{-3}, can capture objects that have a moderate ($< 15°$) initial orbital inclination with respect to the disc. These captures happen on timescales of the order of 10^6yr (Fabj et al. 2020) and are possible because of the exchange of energy and angular momentum between the disc and the orbiter, which takes place every time the latter passes through the former (Ostriker 1983; Syer et al. 1991).

Disc captures have been found to be more efficient in the case of retrograde orbiters (i.e. stellar-mass objects with orbits the angular momentum of which has an inclination with respect to the one of the disc larger than 90°) (Nasim et al. 2023). In the cases in which the disc capture mechanism turns out to be efficient, its final outcome is a increase in the density of stars and stellar-mass compact object in the accretion disc. In particular, this density is larger than the three-dimensional density the same objects would have in a spherical Nuclear Star Cluster without an AGN.

1.4.2 Migration

A compact object embedded in a gaseous disc interacts with it, suffering a net torque and exchanging energy and angular momentum (Armitage 2010; Paardekooper et al. 2010). This phenomenon takes place in systems of different scales, from protoplanetary discs to AGN accretion ones, and modifies the semi-major axis of the orbit of the interacting satellite around the central object, which consists of a protostar in the protoplanetary scenario or of a SMBH in the AGN one. If the mass ratio between the satellite object and the central one is of the order of 10^{-5} or smaller, this variation of semi-major axis is called Type I migration. This value of mass ratio is to be expected when considering the case of a stellar-mass BH (10^0 - $10^2 \mathrm{M}_\odot$) orbiting around a SMBH (10^6 - $10^9 \mathrm{M}_\odot$) located at the centre of an AGN. In regimes with a low turbulence level, Type I migration happens on a time-scale which is inversely proportional to the mass of the satellite objects, meaning that the heaviest stellar-mass BHs embedded in an AGN disc are the ones whose orbits change more rapidly due to the interaction with the gas (McKernan et al. 2011a).

While in general the migration of a stellar-mass compact object is expected to proceed inwards (Goldreich & Tremaine 1979), under the assumption of an adiabatic midplane of the disc, it can proceed outwards for specific ranges of radial distance between the orbiter and the central object (Paardekooper & Mellema 2006). On the border between a region in which migration is expected to proceed inwards, and a region in which it is expected to proceed outwards, there can be distances from the central object in which the net torque exerted by the gas of the disc on the satellite object is null. These peculiar radial positions are called migration traps. The presence of these traps in which orbiting objects are expected to halt their migration was proposed for the protoplanetary disc scenario by Lyra et al. (2010), and in Bellovary et al. (2016) it was found that they can exist also in AGN discs. They estimated that more than one migration trap can form in an accretion disc, and that their distance from the SMBH is of the order of 20 to 300 $\mathrm{R_g}$, where $\mathrm{R_g} = 2\mathrm{GM/c}^2$ is the gravitational radius of the central object, defined as a function of its mass (M), the gravitational constant (G), and the speed of light in the vacuum (c). Moreover, they found the position of the migration traps to be independent from the mass of the orbiter. This means that a high number of stellar-mass objects will pile-up around a very specific radial distance from the central SMBH, facilitating the formation of binary systems.

The presence of migration traps in the framework of Type I migration is nonetheless not guaranteed in every AGN. In particular, in Grishin et al. (2024) it is argued that using prescriptions calibrated from 3D simulations (Jiménez & Masset 2017), Type I torque is always negative-definite in the AGN discs they modelled. However, they find that migration traps can form due to thermal torques in AGN less luminous than $10^{44.5-45}$erg s^{-1}. These torques are caused by the thermal response of the gaseous disc to the accretion of the embedded stellar-mass BHs through their mini-discs.

Whether or not migration traps are developed in an AGN, inward radial motion of stellar-mass objects due to their interaction with the gaseous disc they are embedded in is expected to be able to cluster them in a small region. This can facilitate the gas-assisted binary genesis (Tagawa et al. 2020a; DeLaurentiis et al. 2023b; Rowan et al. 2023b) as well as the one the one from three-body encounters (Aarseth & Heggie 1976; Binney & Tremaine 2008) that are expected to take place inside AGN discs, therefore increasing the efficiency of the so-called "AGN channel" for the formation and evolution of the binaries whose mergers have been detected by the LVK collaboration. The main so far discussed mechanisms that act on the population of compact objects inside an AGN disc are visually summarised in Figure 1.5.

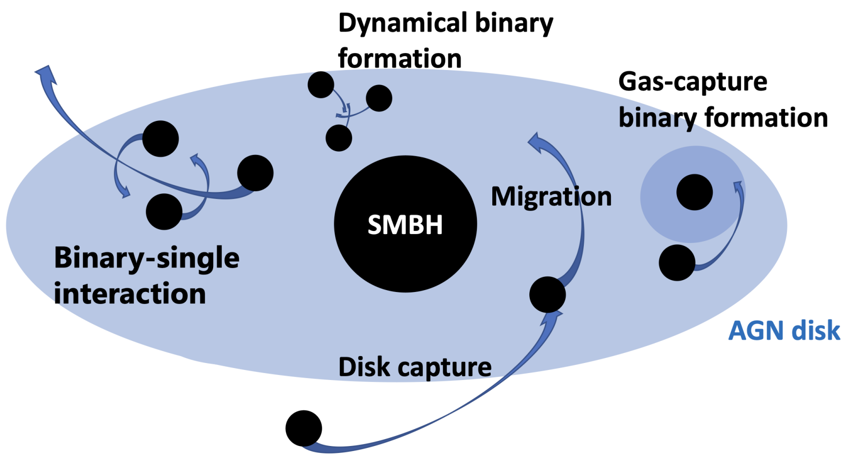

Figure 1.5: Visual representation of the main mechanisms that influence the population of compact objects inside and AGN disc, facilitating binary formation. Each of these processes has been presented in Section 1.4.1 or in Section 1.4.2. This Figure is adapted from Figure 3 of Tagawa et al. (2020a).

1.4.3 Characteristic observable signatures of BBHs merging in AGN discs

Binary systems formed and driven to merger inside an environment such as an AGN are expected to exhibit peculiar detectable features in the GW signal they emit. These features are caused by the interaction between the compact objects and the gas the accretion disc consists of. Their identification and the characterisation of their physical cause is a very important tool for the estimation of the fractional contribution of AGN binary formation channel to the total BBH merger rate.

1.4.3.1 Non-null eccentricity in the LVK band

When a binary is tight enough for the GW emission to be the dominant cause of the decrease in orbital energy, such emission is very efficient in driving the system towards a null value of eccentricity, circularising it (Peters 1964). For this reason, BBHs formed through the evolution of an isolated binary system are not expected to show any sign of eccentricity in their GW signal, when entering the LVK band, which extends approximately from 10^1 Hz to 10^4 Hz. However, hard binaries formed through repeated interactions like single-binary encounters, which are expected to happen in dynamically dense environments, can retain their eccentricity long enough to be detected (Samsing 2018; Calcino et al. 2023a).

The fraction of BBHs capable of exhibit a measurable eccentricity in the LVK band increases with respect to the general case of a dynamically dense scenario when an AGN disc-like host environment is considered. This is because in a pseudo-2D system it is likely that a single-binary encounter happens in the same plane of the of the orbit of the binary system, or on a plane with small inclination with respect to it (Samsing et al. 2022a; Trani et al. 2024). In such a configuration, the probability of the merger happening during a single-binary encounter, and not after it, is higher with respect to the probability of the same thing happening in a spherically symmetric environment. Binaries that merge during the encounter enter the LVK band while still retaining at least part of their eccentricity they originally had, which for BBHs dynamically assembled via co-planar interactions is distributed as $\mathcal{P}(e) \approx e/\sqrt{1-e^2}$ (Monaghan 1976; Stone & Leigh 2019).

The direct detection of a non-null eccentricity in a BBH merger is therefore to be considered as a smoking-gun signature of the dynamical origin of such binary, with a non-negligible chance for the host environment to be an AGN disc. Signs of eccentricity have been spotted for specific detected events (Romero-Shaw et al. 2021), but the systematic search of eccentric mergers is complicated by waveform systematics, and by the fact that residual eccentricity contained in the GW signal can act like a systematic uncertainty, generating biases in other intrinsic binary parameters like the spin directions of the two components (Fumagalli et al. 2024).

1.4.3.2 Anti-correlation between mass ratio and effective spin parameter

The mass-weighted projection of the spins of the components of a BBH onto the orbital angular momentum is referred to as "effective inspiral spin parameter", $\chi_{\rm eff}$. In the scenario in which a BBH is formed via repeated interactions in a generic dynamically dense environment, it is reasonable to assume that the directions of the spins of its components in the last phase of the inspiral and during the merger are randomly orientated with respect to each other. This is expected to be reflected in the $\chi_{\rm eff}$ distribution of the population of merging binaries coming from a dynamical formation scenario.

In Callister et al. (2021) it has been shown that at 98.7 per cent credibility it exist a relation between the value of $\chi_{\rm eff}$ for the detected binary mergers, and their value of the mass ratio $q = m_2/m_1$, where m_2 and m_1 are the mass of the lighter and of the heavier component, respectively. In particular, through a hierarchical Bayesian analysis on the 44 BBH merger detections listed in the second Gravitational Wave Transient Catalogue (GWTC-2), which contains the GW detections up until the first half of O3, they found that more unequal-mass binaries (low q) are more likely to have a larger $\chi_{\rm eff}$.

This anti-correlation has been observed also in the events contained in the third Gravitational Wave Transient Catalogue (GWTC-3), which contains also the events detected in the second half of O3 (see Figure 21 of The LIGO Scientific Collaboration et al. 2021b), and it has been identified as a potential hint of binary formation in a disc-like structure. In particular, assuming that the heaviest stellar-mass BHs whose orbit in a Nuclear Star Cluster have a small inclination with respect to the accretion disc of the AGN present in it are more quickly captured by it with respect to the lightest ones (Fabj et al. 2020), they will spend enough time in such gaseous environment to spin-up into alignment with respect to the angular momentum of disc. These heavier spin-aligned BHs might eventually merge with lighter ones that are captured by the gaseous disc at later times. This phenomenological model, in a scenario in which a dense disc and turbulent migration are involved, is expected to produce mergers that exhibit the detected $\chi_{\rm eff}$ - q anti-correlation (McKernan et al. 2022a).

The same relation between the effective inspiral spin parameter and the mass ratio of BBH binaries is to be expected also if these systems are formed and evolve in a axisymmetric disk-like environment that allows for hierarchical mergers to happen, without the need of any assumption regarding different disc capture time-scales for compact objects of different masses (Santini et al. 2023a).

1.5 The potential and the challenges of detecting EM counterparts of GW events

As mentioned at the beginning of Section 1.3, even after the direct detection through GWs of nearly 100 confirmed coalescence of binaries of compact objects, the fractional contribution to the total merger rate of the various binary formation paths is still unknown.

One possible way to answer this open question is to search in the GW signal of each individual event or in the properties of their overall population for specific signatures that can be explained preferentially by one specific formation channel. Examples of such smoking-gun signatures for the AGN channel are the ones described in Section 1.4.3. Another viable approach is to directly identify in which galaxies or in which type of galaxies the merger events happened. If, for example, it is found that the fraction of BBH mergers that took place in a galaxy that hosts an AGN is significantly higher than the estimated ratio between the number of such hosts with respect to the total number of galaxies in the Universe, this would suggest that the existence of a dense gaseous accretion disc might indeed facilitate the formation of binaries of compact objects that merge in the LVK band.

Being able to directly link GW events to the hosts in which they take place is not important to answer only astrophysical questions regarding the dynamics of BBHs, the evolution of binaries of massive stars, and the characteristics of dense star clusters and of AGN discs, but it has the potential of being relevant also from the cosmological point of view. When the interferometers of the LVK collaboration detect a GW signal, they directly measure the luminosity distance between the source and the Earth. If a one-to-one association is possible between a detected BBH event and its host galaxy, it is then possible to constrain the relation between the luminosity distance measured from the GW signal and redshift directly measured from the EM radiation. Constraining such relation means constraining cosmological parameters such has the Hubble constant. This method of putting constraints on the parameters that govern the Universe on cosmological scale is referred to as "standard sirens method" (Schutz 1986) and it has already been applied in the case of the first detected merger of a Binary Neutron Star system, GW170817 (Abbott et al. 2017).

If a direct one-to-one association between the GW signal and EM one is not available, it is still possible to measure cosmological parameters using the redshift estimates of all the galaxies that are within the localisation uncertainty of the detected merger. This is the so-called "dark sirens method" (Gair et al.

2023), and it has already been applied to the data collected during the first three observing runs of the LVK collaboration (Alfradique et al. 2024).

The main limiting factor that hampers analyses involving the connection between GW events and their EM counterparts is the large uncertainty that is typically associated by GW detectors to the position of a merger of binaries of compact objects, in particular to the one of a BBH merger. Figure 1.6 shows the Cumulative Distribution Function (CDF) of the sizes of the 90 per cent Credibility Level localisation volumes (V90) of the GW events detected during the first three observing runs. The median value of such distribution is of the order of $10^{8.5}$ cubic Megaparsecs. According to the redshift-dependent AGN luminosity function presented in Kulkarni et al. (2019) this median localisation volume might contain hundreds to thousands of AGN with a bolometric luminosity greater than 10^{45}erg s^{-1}, and even more regular galaxies that do not host an active nucleus. For this reason, consistently being able to confidently associate every GW event to its host environment is currently impossible.

1.5.1 Spatial correlation analyses with all-sky AGN catalogues

One way of estimating what fraction of the detected GW events took place in specific types of environments in through the analysis of the spatial correlation between the positions of such potential hosts and the GW sky maps of the measured mergers. The statistical constraining power of this approach depends on the number density of the potential hosts that are considered and on the completeness of the catalogues that are used. For this reason very luminous AGN represent an ideal class of objects of this type of studies, since all-sky catalogues with high levels of completeness are available. Two examples of such catalogues are the Million Quasars (Milliquas) catalogue (Flesch 2023) and Quaia (Storey-Fisher et al. 2024).

1.5.1.1 Milliquas

Milliquas is an AGN catalogue containing 1,021,800 objects in its latest version (Flesch 2023). It is presented as a collection of all the Quasars published up to June 30th, 2023. Figure 1.7 shows the mollweide projection of the sky distribution of such objects.

It is evident that, since Milliquas is an ensemble of several catalogues, its content is not uniformly distributed over the sky. In the northern sky in particular is noticeable that the region with the highest number of objects per square

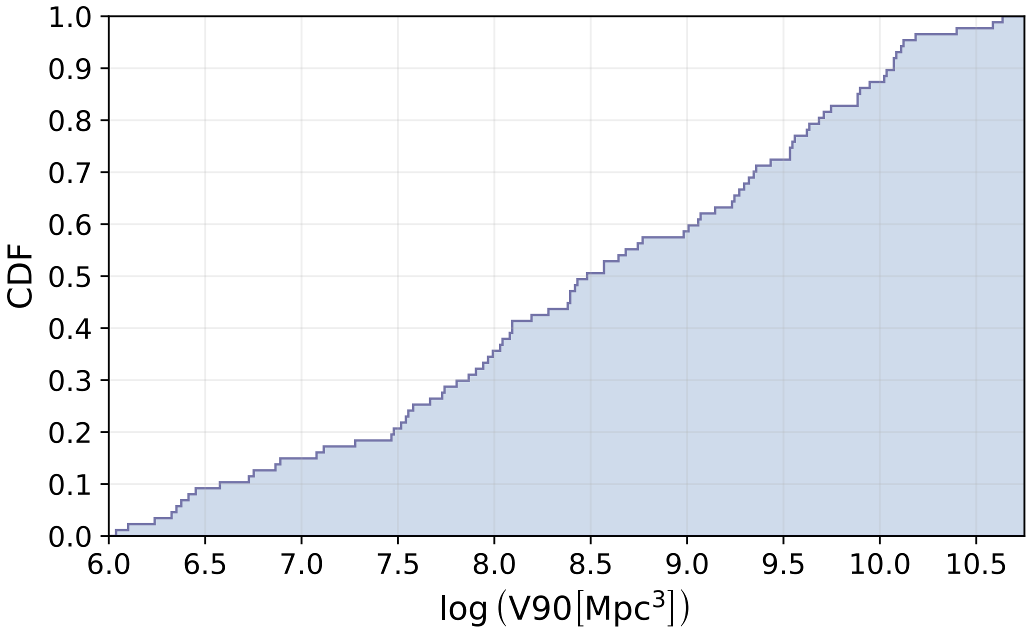

Figure 1.6: Cumulative Distribution Function of the sizes of the 90 per cent Credibility Level localisation volumes (V90) of the GW events detected by the LVK collaboration during the first three observing runs. From the shown distribution are excluded the localisation volumes of GW200308_173609 and of GW200322_091133, since these events are poorly-localised, and the available posterior samples do not allow for an estimation of their value of V90.

degree is the footprint of the Sloan Digital Sky Survey (SDSS) (Kollmeier et al. 2019), while the most crowded region in the southern sky is the footprint of the Two-degree-Field Galaxy Redshift Survey (Colless et al. 2001), which is visible in the figure as a stripe-shaped over-density of objects around an equatorial declination of $-30°$.

While the completeness of Milliquas in the most crowded regions can be close to unity, this is not in general the case for the other parts in the sky. Nonetheless, Milliquas consists of a valid tool to establish whether there is or not a spatial correlation between detected GW events and very luminous AGN in the Local Universe. In fact, while the all-sky average number density of spectroscopically identified AGN below $z = 0.3$ with a bolometric luminosity greater than 10^{45}erg s^{-1} is approximately the 48 per cent of the number density of the same objects in the SDSS footprint, this fraction reaches approximately

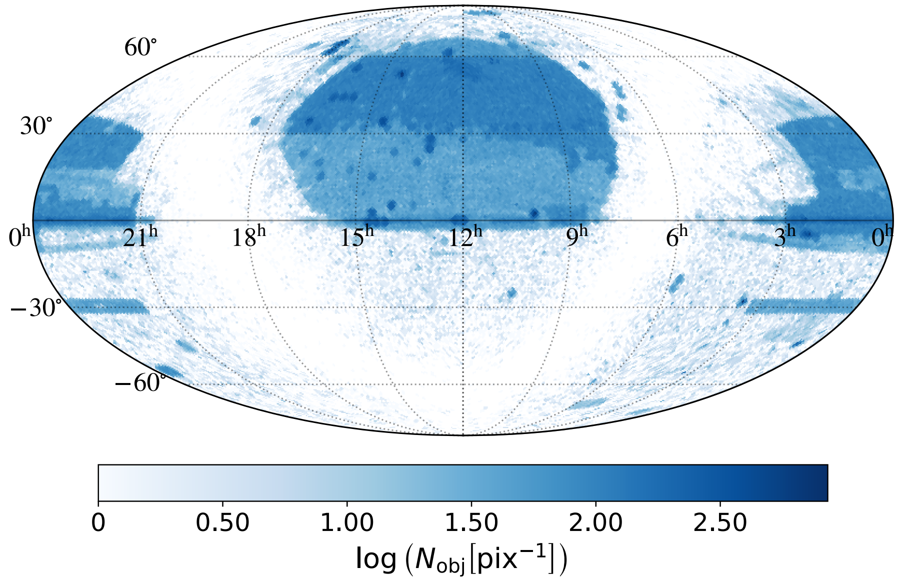

Figure 1.7: Mollweide projection of the latest version of the Milliquas catalogue (v8). The distribution of objects is displayed in a Healpix map with NSIDE=64. The colour of each pixel indicates the logarithm of the number of objects present in the catalogue in that sky position.

the 87 per cent when AGN brighter than 10^{46}erg s^{-1} are considered.

1.5.1.2 Quaia

Quaia (Storey-Fisher et al. 2024) is an all-sky AGN catalogue containing objects identified ad extra-galactic by the Gaia mission (Gaia Collaboration et al. 2016) in its third data release (Gaia Collaboration et al. 2023) that have a counterpart observed by the Wide-field Infrared Survey Explorer (WISE) (Wright et al. 2010) and contained in the unWISE catalogue (Lang 2014; Meisner et al. 2019).

All the objects in Quaia have passed a series of selections based on the proper motions and the colours of the objects, aimed to increase the purity of the sample. The final result is an all-sky catalogue which contains 1,295,502 quasars with a magnitude in the Gaia G band lower than 20.5. Their sky distribution is shown in Figure 1.8.

The redshift estimate for each object in Quaia is evaluated by training a k-Nearest Neighbor model using as training set the AGN in Quaia that have an available spectroscopic redshift estimate in SDSS. What makes Quaia an ideal

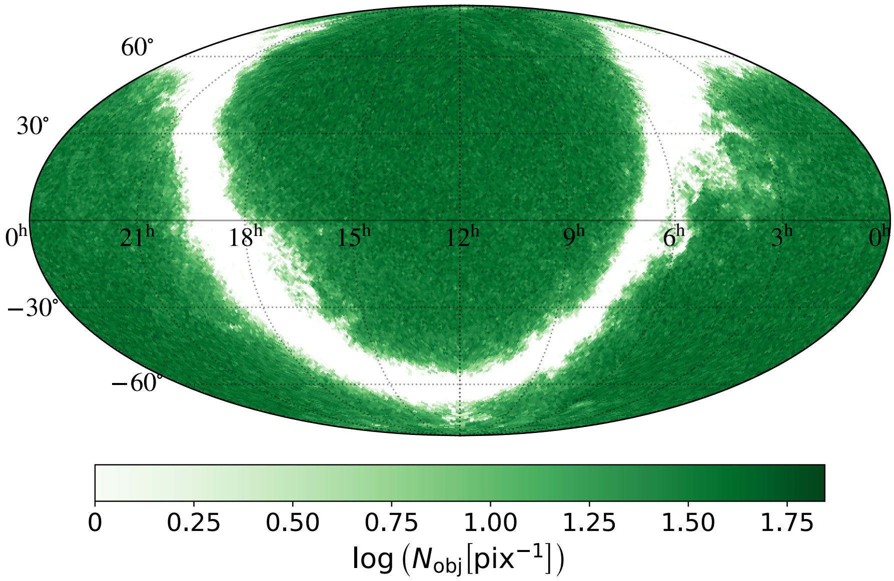

Figure 1.8: Mollweide projection of the all sky AGN catalogue Quaia. The distribution of objects is displayed in a Healpix map with NSIDE=64. The colour of each pixel indicates the logarithm of the number of objects present in the catalogue in that sky position. This Figure is also present in the work described in Chapter 4 of this thesis.

instrument for spatial correlation analyses is its remarkably uniform distribution of objects over the whole sky, once the region containing the galactic plane is excluded, together with its high level of completeness.

1.5.2 Spatial correlation analyses with unusual AGN flaring activities

Binary mergers happening in an AGN disc are expected to produce an EM counterpart, even if not always detectable, due to the interaction between the gas and the components of the binary or the remnant of the GW event (Bartos 2016a; McKernan et al. 2019a). In particular, it has been proposed that an observable flare coming from an AGN can be produced when the gas that interacts with the recoiled merger remnant which is traveling through the disc produces a shocked Bondi tail (Ostriker 1999; Antoni et al. 2019). Such flare is modeled to be manifest when the kicked BH reaches the surface of the disc with an optical depth of $\tau = 1$.

Recently, 20 AGN flares have been labeled by Graham et al. (2023a) as potential EM counterparts to the GW events detected during the third observing run of the LVK collaboration. These EM transients were found not compatible with being coming from SNe, Tidal Disruption Events, microlensing events, or regular AGN variability. They were found by analysing AGN light curves observed by the Zwicky Transient Facility (ZTF) (Bellm et al. 2019a; Graham et al. 2019a), a time-domain survey that since March 2018 covers the Northern sky every 2-3 nights, observing in the g and in the r band.

The sky distribution of the 20 selected flares is shown by the pink round markers in Figure 1.9.

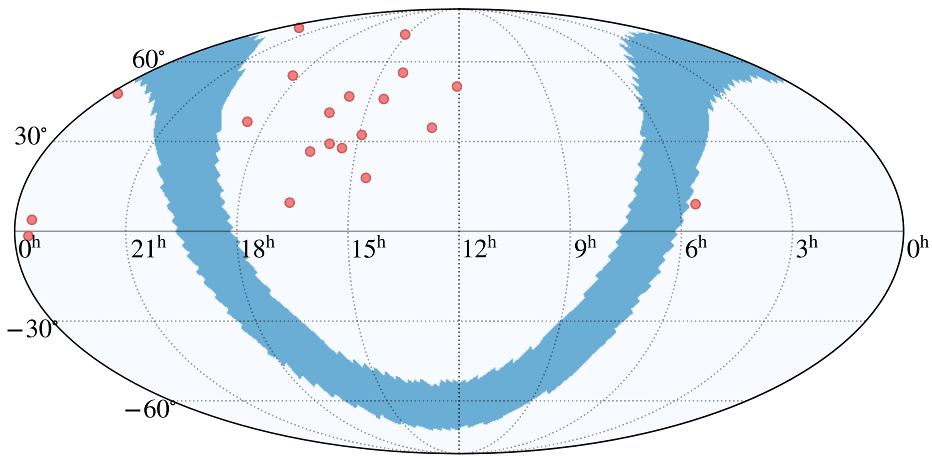

Figure 1.9: Mollweide projection of the positions of the 20 AGN flares identified in Graham et al. (2023a) as potential counterparts to BBH mergers (pick round markers). The distribution of objects is displayed in a Healpix map with NSIDE=32. The pixel corresponding to a galactic declination b between $-10°$ and $10°$ are in light-blue. This Figure is also present in the work described in Chapter 5 of this thesis.

The low volume number density of these unusual AGN flares, together with the fact that they are transient, not permanent EM signatures makes them ideal tools for spatial and temporal correlation analyses aimed to check whether it is plausible or not that a causal correlation exists with the mergers detected by the LVK collaboration. This is because the probability of having one of these flares matching by pure chance both spatially and in time with a BBH merger, without any physical causality relation between the two signals is typically low. For this reason, if such a causal connection exists, it should be possible to assess it confidently.

1.6 In this thesis

This thesis contains four studies I have conducted together with my co-authors. All of these works revolve around the investigation of the spatial correlation between AGN and GW events detected by the LVK collaboration. This analyses have required the creation and the characterisation of suitable all-sky AGN catalogues and the development of a statistical framework with a Likelihood function able to take into account the properties of such catalogues and of the sky maps of the detected mergers. The results this method consist of observational constraints on the efficiency of the AGN channel, which can be used as a proxy for constraining the properties of the accretion discs themselves.

In Chapter 2 I present the results of a Likelihood ratio method which applies the statistical framework presented in Bartos et al. (2017a) to O3-like sky GW detection I have simulated. This method is used to calculate the number of detections needed in order to be able to reject the hypothesis according to which there is no correlation between AGN and BBH mergers. We estimate to what fraction of the total merger rate the AGN binary formation channel has to contribute to have the possibility of rejecting the no-connection hypothesis with the number of detections obtained during O3. This is repeated varying the number density of the AGN that are considered as potential hosts. For example, we estimate that the number of detections performed in O3 potentially allows such a rejection with a 3σ confidence if rare (i.e. with number densities lower than $10^{-7.5}\mathrm{Mpc}^{-3}$) AGN are considered, and if the the accretion disc-assisted binary formation channel contributes to a significant fraction (30 per cent or more) of the total merger rate.

In Chapter 3 I first describe an updated version of the statistical method presented in Chapter 2. This consists of a new Likelihood function, the maximisation of which can of putting observational constraints on what fraction of the detected BBH mergers has originated in an AGN. In particular, this new statistical framework we developed is able to take into account the incompleteness of the AGN catalogue that uses, and the exact position of each potential host within the 90 per cent Credibility Level localisation volume of the GW detections. After testing its validity on mock data, we apply this method to the 30 BBH mergers detected during the first three observing runs of the LVK collaboration with a 90 per cent Credibility Interval on the luminosity distance entirely contained within $z = 0.3$. In particular we cross-match these events with three different catalogues of AGN in the same redshift range. These catalogues are created selecting objects from Milliquas that are also present in unWISE and that have a spectroscopic estimate of their redshift. What characterise each of these catalogues are the different thresholds on bolometric luminosity that have been used to create them. We find that the fraction of the detected BBH mergers that has originated in an AGN more luminous than $10^{45.5}$erg s^{-1} (10^{46} erg s^{-1}) is not greater than 49 (17) per cent at a 95 per cent Credibility Level. To our knowledge, these are the first observational constraints on the efficiency of the AGN channel for the formation of binaries systems that merge in the LVK waveband.

In Chapter 4 is presented a generalisation of the results described in Chapter 3. In particular we apply the same spatial correlation-based statistical approach to infer the fractional contribution of the AGN formation channel to the total merger rate, using as input data the Quaia all-sky AGN catalogue and the sky maps of all the GW events detected until the first half of the fourth observing run of the LVK collaboration (O4a). To do this we first estimate the bolometric luminosity of each object contained in Quaia up to $z = 1.5$. In the same range, we estimate for the first time the completeness of this catalogue as a function of redshift and luminosity. With respect to the work presented in Chapter 3 we therefore expand our dataset. We number of sky maps used go from 30 to 159 on the entire redshift range covered by the LVK interferometers. Moreover, the high level of completeness of Quaia allows us to put constraints on the relation between GW events and AGN over a wider range of bolometric luminosity. In particular we find that no more than the 23 (28) per cent of the detected mergers have happened in an AGN brighter than 10^{45}erg s^{-1} ($10^{45.5}$ erg s^{-1}) at a 95 per cent Credibility Level.

Finally, in Chapter 5 I present a spatial and temporal correlation analysis aimed to investigate whether there is or not a causal connection between the GW events detected during O3 and the 20 unusual AGN flares proposed in Graham et al. (2023a) as potential EM counterparts to binary mergers. We find that current data favour the hypothesis according to which there is no causal connection between such transients and the LVK detections. Performing Monte Carlo realisations of realistic catalogues of flares, we find that the number of spatial and temporal matches between the detected GW events and the observed EM transients is to be expected in the case of random-chance association, without any physical relation between the two types of signal. The BBH mergers the sky maps of which have a match with one of the 20 flares presented in Graham et al.

(2023a) are characterised by components that occupy the high-mass end of the stellar-mass BH mass spectrum inferred by (The LIGO Scientific Collaboration et al. 2021b). We find that this can be explained by the fact that these events are in general associated to large uncertainty on their position, therefore they have a high chance of having an AGN within their 90 per cent Credibility Level localisation volume just because of random association.

1.7 Future outlook

All the work presented in this thesis shows that the efficiency of the various formation paths proposed for merging stellar-mass BBHs can already be constrained with the data that has been so far collected. However, all the results of the spatial correlation analyses here described are purposely agnostic from the point of view of the underlying physical model. This means that in the statistical framework no prior knowledge is assumed regarding the distribution of the intrinsic binary parameters one should expect to measure in events coming from a specific formation channel, such as the AGN one.

Introducing physically-informed priors on parameters such as the eccentricity of the binaries, the masses of their components, and their spins will enable the possibility of performing a new type of spatial correlation-based investigation, which might lead to different constraints with respect to the ones described in the following chapters of this thesis. Moreover, physically-informed spatial correlation-based methods will also help to rank the different intrinsic properties of the merging binaries as a function of the amount of information that the assumption of a non-uniform prior on them is able to add to the analysis. This will consist of an indication regarding which are the binary parameters that are more tightly related to the host environment where the system has formed and evolved.

Another future development of spatial correlation analyses aimed to investigate the connection between BBH mergers and potential rare host environments is related to making forecasts on the constraining power of GW detectors that will start to operate in the next decade, like third-generation ground-based ones such as Einstein Telescope (ET) (Maggiore et al. 2020) and Cosmic Explorer (CE) (Reitze et al. 2019) and space-borne ones like the Laser Interferometer Space Antenna (LISA) (Amaro-Seoane et al. 2017). The sensitivity of ET and CE will be two orders of magnitude better with respect to the one of Advanced LIGO (Vitale & Evans 2017). However, the expected uncertainties on the sky positions and luminosity distances of the detected events are too large to allow a consistent one-to-one association between BBH mergers and their host galaxy (Pieroni et al. 2022). Nonetheless, analyses like the ones presented in this thesis will have their constraining power greatly enhanced by the fact that thousands of events every year are currently expected to be detected with an uncertainty on their position in the sky of 1 to few square degrees. Since these third-generation detectors are expected to identify BBH mergers up to $z \approx 30$ (Hall & Evans 2019), it will be possible to incorporate a redshift-dependence in the Likelihood function and then estimate the fractional contribution to the total BBH merger rate of the different proposed formation paths as a function of cosmic time.

Similar forecasts can be already made also concerning the mergers of binaries of Massive Black Holes with masses between $10^5 \mathrm{M}_\odot$ and $10^7 \mathrm{M}_\odot$ that will be observed by LISA. These mergers are expected to take place after the merger of two galaxies, if the two central BHs form a binary tight enough to efficiently lose orbital energy via GW emission, until they merge. The uncertainty on the sky position coming from LISA's detections is estimated to be of the order of one to 10 square degrees for mergers happening at $z = 1$ (Mangiagli et al. 2020). One strength of the statistical method presented in this thesis is that it can be applied to any kind of sky map and to any catalogue of potential hosts. Therefore no major adjustments to it are needed in order to make it applicable to LISA data. Cross-matching the sky maps of the detected Massive Black Hole binary mergers with catalogues of galaxies that are either currently observed as undergoing a merger event, or that are thought to have just experienced one, like starburst galaxies or E+A galaxies (Bekki et al. 2005), will help in putting constraints on the delay between the moment in which two galaxies start to merge and the moment in which their central Massive Black Holes coalesce. This constraint will be important to better understand the interactions between these massive objects and the stellar and gaseous content of galaxies, as well as the mechanisms that can bring binaries of SMBHs to be tight enough to make GW emission efficient.

Both in the case of ground based and of space-borne GW detectors, an important step of spatial correlation based methods to characterise the formation paths of GW events is to create the best possible catalogues of potential hosts and to characterise them. These catalogues should ideally be all-sky and complete. Future developments of this branch of GW astronomy therefore include the creation of these catalogues, and the mapping of their number density and completeness as a function of parameters like redshift, sky position, intrinsic luminosity, and accretion rate. This task is crucial for being able to put trustworthy constraints, but is not trivial, given the different properties and limitations of different surveys and the assumptions that have to be made when estimating the intrinsic properties of potential hosts, starting from observable. An example of this is that in order to calculate the bolometric luminosity of an AGN one has to assume the shape of its Spectral Energy Distribution (SED) and the bolometric correction needed to convert the luminosity emitted in a band of the EM spectrum into the bolometric one.