Isotopes and the characterization of extrasolar planets

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1

Introduction

1.1 Search for exoplanets

How did we come into existence? Are we alone? The origin of life and the uniqueness of our position in the universe have been enduring quests of human beings. Despite speculations of the extrasolar planets and extra-terrestrial life for centuries, only three decades ago did astronomers start to peer into the diverse alien worlds beyond our own solar system. In 1992 Wolszczan & Frail (1992) first discovered planetary-mass objects orbiting the pulsar PSR B1257+12, which is a rapidly rotating neutron star. In contrast to the solar-system objects around our main sequence star, these planets were believed to be second generation products that formed in the debris disk after the catastrophic stellar evolution (Podsiadlowski et al., 1991). The first exoplanet around a main sequence star was discovered by Mayor & Queloz (1995), hallmarking the inception of exoplanetary science and awarded the Nobel Prize in Physics in 2019. This study detected a Jupiter-like gaseous planet orbiting the solar-type star 51 Pegasi. Strikingly, the planet 51 Pegasi b orbits its star at a separation of only 0.05 au (much smaller than Mercury's distance to the Sun), equating to an orbital period of 4.2 days. Ensuing the first breakthrough, a population of such close-in exoplanets has emerged, known as Hot Jupiters. Where did such planets form? How did they get there? Why are they so distinct from solar-system planets? These peculiar new worlds, with no analogs in our solar system, posed great challenges but also opened new windows to our understanding of planet formation and evolution.

Hitherto, over five thousand exoplanets have been discovered with various methods, including radial velocity, transit observations, and direct imaging. The planet mass versus semi-major axis diagram of the known exoplanet population is shown in Figure 1.1, illustrating the great diversity of exoplanets and large range in parameter space. The diagram reveals several classes that have no counterparts in the solar system, such as Hot Jupiters, super Jupiters (wide-orbit massive Jovian planets), and super-Earths and mini-Neptunes (planets with intermediate sizes between the Earth and the Neptune). Each detection technique has its own biases towards certain planet types as discussed below.

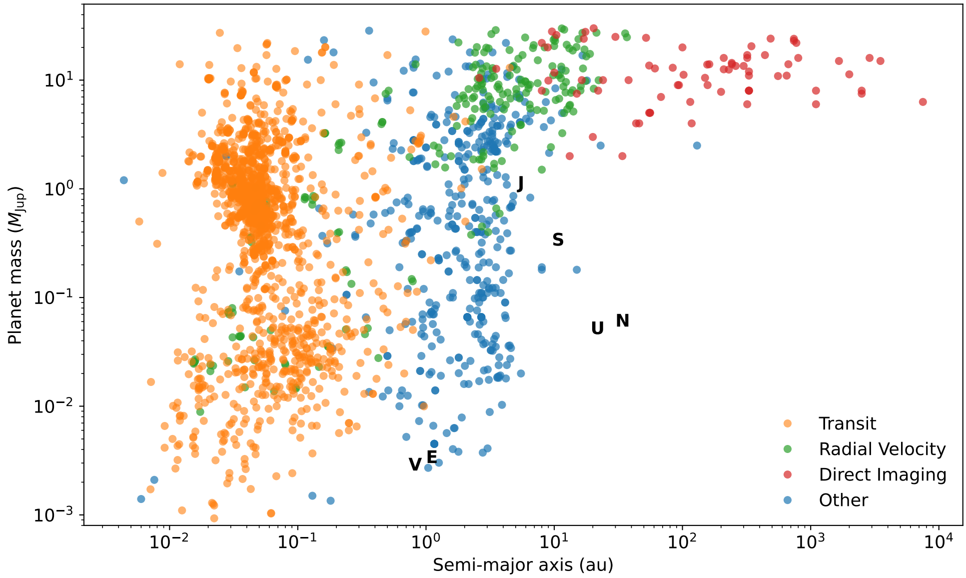

Figure 1.1: Planet mass versus semi-major axis of confirmed exoplanets, color-coded by detection method. The data were collected from the NASA Exoplanet Archive. The black letters denote the planets in the solar system.

Radial velocity

The radial velocity (RV) method makes use of the reflex motion of the host stars induced by the gravitational pull from the planets. These stellar wobbles result in periodic changes of the stellar velocity along the line of sight, which can be detected by measuring the Doppler shift of stellar spectral lines. The amplitude of the RV variation mainly depends on the planet mass and orbital distance as follows.

$$K \propto a^{-1/2} M_p \sin i \tag{1.1}$$

where K is the semi-amplitude of the RV variation, M_p is the planet mass, a is the semi-major axis of the planet orbit, and i is the orbital inclination. Therefore, the radial velocity method provides constraints on planet mass and it is most sensitive to massive planets at close-in orbits. For example, the first exoplanet 51 pegasi b was discovered by monitoring the RV change of $K \sim 60$ m s^{-1}. As the precision of RV measurements improves significantly over the past decades, the current-generation instrument such as ESO's VLT/ESPRESSO (Pepe et al., 2021) pushes to the limit of a few tens of cm s^{-1}, allowing for detection of rocky planets around low-mass stars, such as Proxima Centauri b and d (Anglada-Escudé et al., 2016, Faria et al., 2022) in the solar neighbourhood (4.2 light-years away from the Sun).

Transit observations

The transit method relies on a special geometry where the planetary orbit has an inclination close to 90° such that the planet passes in front of the host star and periodically blocks part of the stellar disc. This leads to periodic decrease in stellar flux during transit, which can be detected through photometric monitoring. The depth of the transit signal is proportional to the ratio of the planet-to-star disc area R_p^2/R_*^2. Therefore this method favors large planets at close-in orbits, as the probability of a planetary orbit aligned to the line of sight scales with the inverse of the orbital distance and thus the transit frequency is higher for close-in planets. Following the first observation of the hot Jupiter HD 209458 b (Charbonneau et al., 2000), the transit method has yielded by far the majority of exoplanet detection thanks to dedicated surveys from both ground and space, such as the Wide Angle Search for Planets (WASP; Pollacco et al., 2006), the Kepler space mission (Borucki et al., 2010), and the Transiting Exoplanet Survey Satellite (TESS; Ricker et al., 2015). Moreover, M dwarfs provide golden opportunities to search for terrestrial planets with the transit method due to their small stellar radii. One of the most intriguing examples is the TRAPPIST-1 system with seven Earth-sized planets around the M dwarf host star (Gillon et al., 2017), a few among which are expected to be located in the habitable zone and able to potentially sustain liquid water on their surface.

Transit detection is often complemented with radial velocity measurements. The combination of both techniques breaks the degeneracy of the planet mass and orbital inclination, allowing for constraints on the bulk density given their masses and radii. The mean density can be compared to theoretical models to constrain the bulk composition of exoplanets (Zeng et al., 2019). Furthermore, measuring radial velocity during transit can provide additional constraints on the projected angle between the planetary orbit and stellar spin axis using the Rossiter-McLaughlin (RM) effect (McLaughlin, 1924, Rossiter, 1924). This effect is the perturbation of stellar lines (hence the radial velocity) as a result of the planet blocking rotationally red-shifted or blue-shifted portions of the stellar disc during transit. It in particular depends on the projected spin-orbit angle, which can provide implications on the dynamical history of planetary systems. Therefore the synergy between the two methods plays an important role in understanding structure, formation, and evolution of exoplanets at population level.

Direct imaging

Direct detection of exoplanets is a highly challenging but rewarding way to probe exoplanets. It requires to overcome the small angular separation between the planet and the host star and the extreme planet-to-star brightness contrast. Therefore this method tends to detect wide-orbit massive giant planets that are still young and self-luminous due to the release of remaining internal energy from their formation processes. To approach deep contrast at small spatial separation, the high-contrast imaging method utilizes adaptive optics (correcting for wave-front aberrations caused by the turbulent Earth's atmosphere and pushing to the diffraction limit), coronagraphy (blocking on-axis starlight and boosting the contrast of off-axis objects, see e.g. Mawet et al.; 2012), and imaging/post-processing techniques for optimal subtraction of the stellar point spread function (e.g. Lagrange et al., 2009, Marois et al., 2006, Sparks & Ford, 2002).

The first direct detection of a planetary-mass companion was on 2M1207 b orbiting around a brown dwarf primary at an separation of >55 au (Chauvin et al., 2004). With the development of new instruments and data-processing techniques, more than 50 super Jupiters have been directly imaged so far, some of which are shown in Figure 1.2, such as the HR 8799 with four giant planets (Marois et al., 2010), PDS 70 with two newborn and accreting protoplanets (Haffert et al., 2019, Keppler et al., 2018). In the past decade, direct

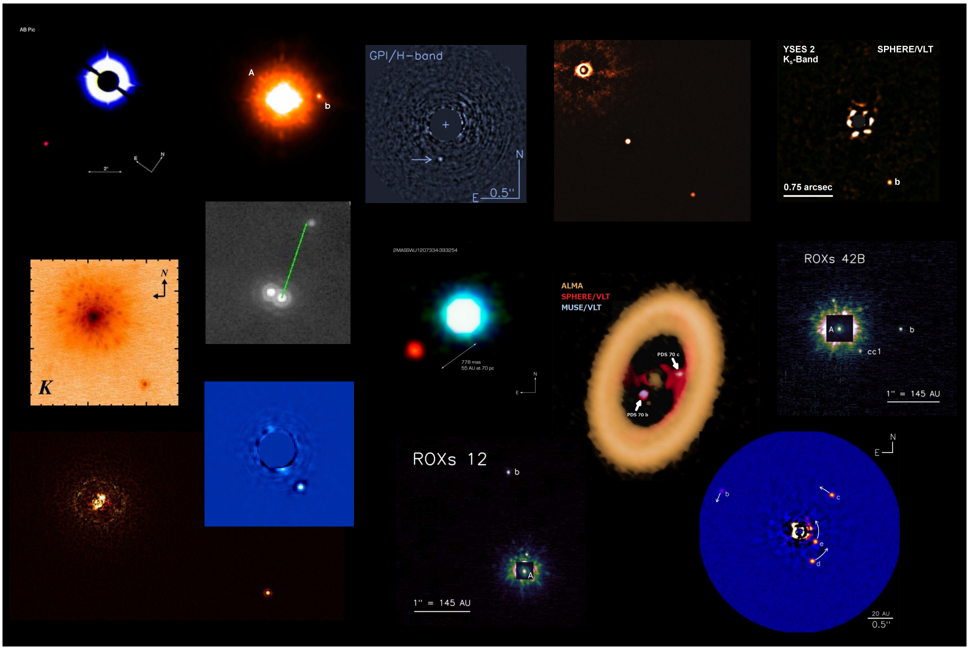

Figure 1.2: Gallery of wide-orbit directly imaged exoplanets collected from the literature (Bohn et al., 2021, 2020, Bowler et al., 2013, Chauvin et al., 2004, 2005, Janson et al., 2021, Keppler et al., 2018, Kraus et al., 2014, Lagrange et al., 2009, Macintosh et al., 2015, Marois et al., 2010, Neuhäuser et al., 2005).

imaging surveys have been delivering new discoveries of exoplanets as well as statistical results on the occurrence rates of super Jupiters, for instance, the Gemini PLanet Imager Exoplanet Survey (GPIES, Macintosh et al., 2014), the SpHere INfrared survey for Exoplanets (SHINE, Vigan et al., 2021), the Young Suns Exoplanet Survey (YSES, Bohn et al., 2020), and the Exoplanet Abundance Study (BEAST, Janson et al., 2021). These directly-imaged infant gas giants are excellent laboratories for understanding planet formation.

Direct imaging is powerful to unveil not only exoplanets, but also circumstellar disks, which were composed of gas and dust, and were believed to be the birthplaces of planets. Polarimetric differential imaging (PDI) is one of the most effective methods to capture scattered light from circumstellar disks. The reflected stellar light on dust grains gets polarized through scattering, while the emission from the unresolved central star is predominantly unpolarized. Therefore observing the polarized light assists to filter out the stellar speckle halo and reveal the circumstellar dust. PDI utilizes a polarizing beam splitter to record two orthogonal linear polarization states simultaneously on the detector (de Boer et al., 2020, Dohlen et al., 2008, van Holstein et al., 2020). Since the star exhibits only a low level of polarization, the starlight will be nearly identical in both beams and can be largely removed through the differential between two images, while the polarized scattered light from the disk will show up. A few dozens of circumstellar disks have been imaged in the near-infrared, showing a diverse range of morphological features such as rings, spirals, and shadows (Benisty et al., 2022). Scattered-light observations are suitable for tracing the surface shape, scale height, and flaring of disks (de Boer et al., 2016), the properties of dust grains as encoded in the intensity and degree of polarization as function of phase angles (Ginski et al. in prep.), providing valuable insights into the birth environment of planets.

1.2 Probing exoplanet atmospheres

As discussed in Section 1.1, it is possible to obtain an initial impression of exoplanet properties especially the bulk density by combining the transit and radial velocity methods. However, large degeneracies hinder detailed analysis of exoplanet compositions using solely planet mass and radius. Spectroscopic observations of exoplanet atmospheres open a critical avenue for a further level of characterization on atmospheric compositions, but also thermal structures and dynamics.

1.2.1 Transit spectroscopy

Transiting planets are ideal targets for atmospheric characterization using transit, secondary eclipse, and phase curve observations. As the planet passes in front of the host star, starlight filters through the terminator region of the planetary atmosphere and gets absorbed due to the opacity of different atoms or molecules. The presence of a certain species results in extra absorption at specific wavelengths, making the planet appear larger. With transmission spectroscopy, we effectively measure the apparent size of the planet as a function of wavelength. The shape of this spectrum depends on the atmospheric composition and other opacity sources such as clouds and hazes.

For example, sodium and water have been detected in exoplanet atmospheres (Charbonneau et al., 2002, Deming et al., 2013, Evans et al., 2016, Kreidberg et al., 2014b). Recently the successful operation of the James Webb Space Telescope (JWST) at infrared wavelengths opens up a new window to other molecules such as CO_2 and SO_2 for the first time (Rustamkulov et al., 2022). The ubiquitous presence of clouds and hazes in exoplanet atmospheres has been inferred by the muted spectral features and even completely featureless transmission spectra (Kreidberg et al., 2014a, Sing et al., 2016). The detection of hydrogen, helium, and ionic species in atmospheres that extend beyond several planetary radii provides direct probes of atmospheric escape by strong high energy stellar irradiation (Ehrenreich et al., 2015, Sing et al., 2019, Spake et al., 2018, Vidal-Madjar et al., 2003).

In addition to probing atmospheric constituents, secondary eclipses (when the planet is eclipsed by the star) and phase curves (the total flux from the system as function of planet orbital phase), probing direct thermal emission from exoplanets, provide constraints on vertical and longitudinal temperature structure, and atmospheric energy transport (Knutson et al., 2008, 2007).

1.2.2 Direct-imaging spectroscopy

Directly imaged planets in wide orbits provide unique opportunities for atmospheric characterization. In contrast to transiting planets, the emission spectra of super Jupiters are directly accessible at higher signal-to-noise (S/N) without significant contamination from their host stars. Spectral observations of direct-imaging planets was first achieved in HR 8799 planets using the medium-resolution ($\lambda/\Delta\lambda = \mathscr{R} \sim 4000$) integral field spectrograph

(IFS) Keck/OSIRIS, providing detection of CO and H_2O, and constraints on temperature and surface gravity (Barman et al., 2011, Konopacky et al., 2013). Another way of probing directly imaged planets with IFS is the molecular mapping method (Hoeijmakers et al., 2018) on β Pictoris b. It takes advantage of the distinct spectral features of the planet and the star to mitigate the starlight contamination and reveal CO and H_2O molecules in the planetary atmosphere. Furthermore, the application of interferometric observations with VLT/GRAVITY on exoplanets shows to be a powerful tool to perform spectroscopy of Jovian planets with small angular separation, such as β Pictoris b and PDS 70 planets (GRAVITY Collaboration et al., 2020, Kammerer et al., 2021, Wang et al., 2021b).

The ground-based spectral observations of directly-imaged planets have been mostly limited to the near-infrared wavelength as a result of exceedingly strong thermal background noise and telluric absorption towards longer wavelengths. Observations from space with JWST will play an important role in unlocking the full infrared spectra of wide-orbit super Jupiters. Recently the 1-20 μm spectrum of VHS 1256-1257b was observed with JWST, unveiling a plethora of spectral details to be exploited (Miles et al., 2022).

1.2.3 High-resolution spectroscopy

High-resolution spectroscopy ($\mathscr{R}$ > 10000) has proved to be an important way of studying exoplanet atmospheres. At high spectral resolution, spectral features of different species can be resolved into unique ensembles of individual lines, which allow for unambiguous identification of atoms or molecules and bypass the degeneracy among different absorbing species and clouds at low spectral resolution. However, as light is dispersed into a larger number of spectral channels, the S/N per channel decreases. To enhance the detection of the planetary atmosphere, the cross-correlation method is typically applied in the data analysis of high-resolution spectroscopy. The cross-correlation function (CCF) is calculated as

$$c(v,t) = \frac{\sum_i x_i(t) T_i(v)}{\sum_i T_i(v)}, \tag{1.2}$$

where $x_i(t)$ is the observation at time t and wavelength channel i. $T_i(v)$ is the spectral template of a certain species or atmospheric model shifted to a radial velocity v, such that the CCF effectively co-adds multiple spectral lines weighted by their strengths.

High-resolution spectroscopy can be utilized in parallel with both the aforementioned temporally (close-in exoplanets) and spatially (wide-orbit exoplanets) resolved techniques to provide unprecedented characterization of exoplanet atmospheres. Its first successful application was on the transiting hot Jupiter HD 209458b with VLT/CRIRES by Snellen et al. (2010), leading to the detection of carbon monoxide in the atmosphere and the orbital motion of the planet. This study also suggested the presence of day-to-night winds in the atmosphere of the hot Jupiter, which provides an important probe for the dynamics and energy transport in the highly-irradiated atmospheres. The orbital motion of close-in planets results in a planetary radial velocity variation by a few tens of km s^{-1} during transit. This doppler shift of planetary signal can be resolved with the high-resolution (~2 km s^{-1}) time-series spectroscopy (see Figure 1.3 for an illustration). The time-varying planetary signal can be disentangled from the relatively static stellar and telluric features using detrending methods such as airmass detrending, principle component analysis, and SYSREM (Birkby et al., 2013, Brogi et al., 2012, de Kok et al., 2013), leading to constraints on

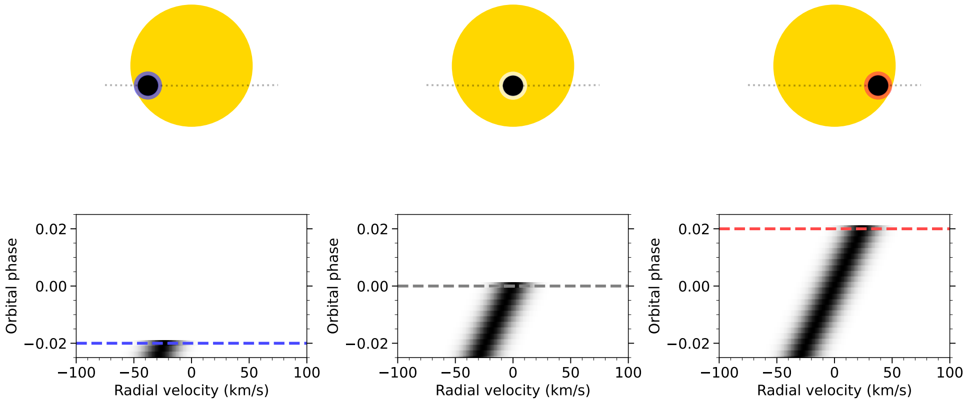

Figure 1.3: Schematic illustration of high-resolution transmission spectroscopy. The top panel comprises the yellow disc denoting the primary star, the black disc representing the transiting planet, and the colored ring showing the terminator region of the planetary atmosphere. Blue color denotes blue-shifted radial velocity of the planet, and red color means red-shifted motion. The bottom panel shows the time-series trace of the noise-free planetary absorption signal (in black shadow) during transit. The slanted planetary signature results from the orbital motion of the planet.

the semi-amplitude of planetary orbital velocity (K_p) and systemic velocity ($V_{\rm sys}$). Another advantage of the technique is the capability of probing non-transiting close-in exoplanets, such as τ Bootis b and 51 Pegasi b (Birkby et al., 2017, Brogi et al., 2014, 2012). Since then, it has been applied for various species at different wavelength ranges, from atomic to molecular species, from optical to infrared wavelengths (Giacobbe et al., 2021, Hoeijmakers et al., 2018, Prinoth et al., 2022), revealing intriguing physics in hot atmospheres such as the spatial asymmetry of iron absorption in WASP-76b possibly due to condensation of iron or clouds on the nightside (Ehrenreich et al., 2020, Kesseli & Snellen, 2021).

When it comes to the spatially resolved realm, high-resolution spectroscopy can be combined with the high contrast imaging to enhance the S/N (Snellen et al., 2015). The potential of the technique was demonstrated in Snellen et al. (2014), which measured the spin (via the rotational broadening of spectral lines) of the young super-Jupiter β Pictoris b taking advantage of both spatial and spectral distinctions between the planet and its host star (see also Bryan et al., 2018, Schwarz et al., 2016). With the current generation of instruments, efforts to combine high-contrast imaging and high-resolution spectroscopy have been made, such as the Keck Planet Imager and Characterizer (KPIC, Mawet et al., 2016) and High-Resolution Imaging and Spectroscopy of Exoplanets at the VLT (HiRISE, Vigan et al., 2018). This combination facilitates the spectral characterization of super Jovian companions at small angular separations ($<1''$) such as the HR 8799 planets (Wang et al., 2021a, Xuan et al., 2022). Next-generation facilities (such as ELT/METIS) will allow for probing terrestrial planets around nearby stars (Snellen et al., 2015).

1.2.4 Retrieval of exoplanet atmospheres

Atmospheric retrieval refers to constraining atmospheric properties of exoplanets given spectroscopic observations using inference methods (Madhusudhan, 2018). A retrieval framework is composed of a forward modeling of exoplanet atmospheres coupled with a Bayesian inference algorithm such as Markov chain Monte Carlo (MCMC) or Nested sampling to estimate the posterior distribution of model parameters given the spectral data. As the inference analysis involves over million times of model evaluations, the forward model is typically parametric, one-dimensional, and not self-consistent. The forward model comprises three major parts, the temperature-pressure (T-P) profile, the chemical abundances profile, and the cloud model, prescribing how the temperature, volume mixing ratios of various absorbing species and cloud species change as function of the altitude or pressure in the planetary atmosphere. Subsequently, a radiative transfer code is used to generate synthetic spectra to be compared to observations. In contrast to self-consistent models, the forward model in retrieval analysis provides a higher level of flexibility, therefore leading to better fit to observations, constraining a larger set of atmospheric parameters simultaneously, and further informing missing physical/chemical processes in modeling. Retrievals have been performed with both transmission and emission spectral observations to constrain atmospheric constituents and temperature structure of exoplanets (see e.g. Line et al., 2013, Madhusudhan et al., 2011, Mollière et al., 2020, Waldmann et al., 2015). Recently, retrieval analysis has also been developed for high-resolution spectroscopic observations, which are more sensitive and robust to the relative chemical abundances in atmospheres (Brogi & Line, 2019, Gandhi et al., 2019). The retrieval on the high-resolution spectra of the hot Jupiter WASP-77b provides tight constraints on its metallicity and carbon-to-oxygen ratio (Line et al., 2021) which provides implications on the formation history of this hot Jupiter.

1.3 Planet formation

1.3.1 Formation of gas giant planets

The rapidly growing number and diversity of exoplanets challenge our conventional understanding of planet formation, which had been predominantly established upon studies on the solar system. The routinely discovered super-Earths, mini-Neptunes, and hot Jupiters located in extremely close orbits indicate missing processes in the formation and evolution recipes. The wide-orbit, massive super Jupiters are on the other extreme, which usually straddle the mass boundary of planets and brown dwarfs, and cannot be easily reconciled with in-situ bottom-up formation pathways (Rafikov, 2011). The fundamental questions about gaseous planet formation remain unclear, while three major scenarios have been proposed (see the cartoon illustration in Figure 1.4).

1. Cloud fragmentation. The pre-stellar nebula may fragment and collapse into multiple objects, akin to the formation of multiple stellar systems (Chabrier, 2003, Kroupa, 2001).

2. Gravitational instability. The dense and self-gravitating regions in circumstellar disks may undergo top-down gravitational collapse due to instability (Boss, 1997, Kratter & Lodato, 2016).

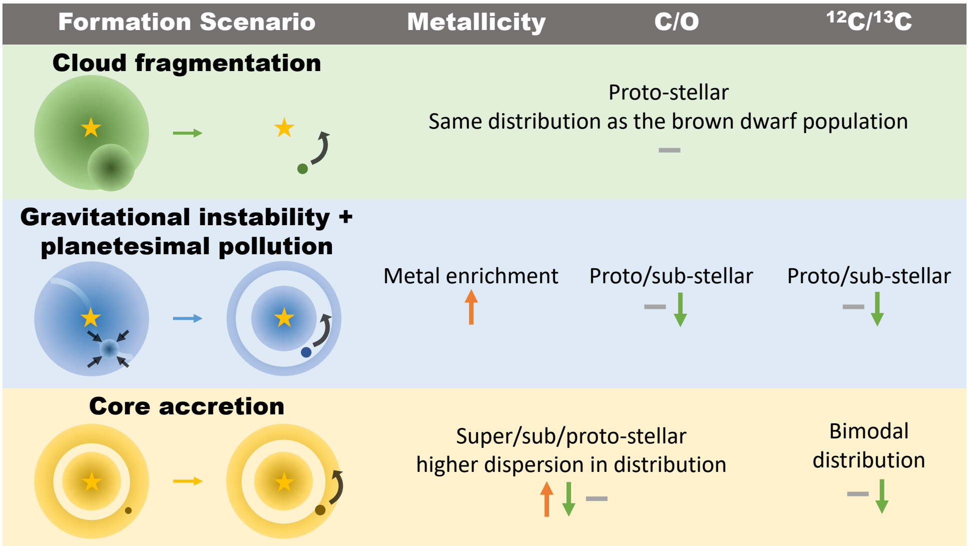

Figure 1.4: Schematic overview of possible formation scenarios of super Jupiters and expectation of the distribution of observational properties (metallicity, C/O, and carbon isotopic ratios) in comparison with the brown dwarf population.

3. Core accretion. The dust in protoplanetary disks coagulates and grows into planetesimals which further grow to form proto-planetary cores (via mutual collision or pebble accretion) that are massive enough to initiate runaway gas accretion (Lambrechts & Johansen, 2012, Pollack et al., 1996).

In addition to the unclear formation mechanisms, another complication lies in that planets do not form in isolation. The interactions of proto-planets with gas and dust in circumstellar disks, sibling planets, stellar companions and flybys play important roles in the outcome of planet formation. High angular resolution observations of circumstellar disks across a wide wavelength range reveal ubiquitous substructures (rings, spirals, and cavities) which may be carved by newborn planets (Andrews et al., 2018, Bae et al., 2018, Benisty et al., 2022, Lodato et al., 2019). The (areo)dynamical interactions with the disk can result in the transfer of angular momentum and hence planet migration (Lin & Papaloizou, 1986). This has been considered as one of the main mechanisms to explain the presence of hot Jupiters in close-in orbits (Lin et al., 1996). Planet-planet scattering may also cause migration of gas giant planets to large orbital distances beyond 100 au (Veras et al., 2009). It may account for some wide-orbit planets that are too massive to form in-situ via core accretion given the fast timescale of dust drift in the outer disks.

1.3.2 Observational probes of formation history

One important observational avenue of unraveling planet formation is to probe the chemical composition of planets. The atmospheric elemental abundance ratios such as carbon-to-oxygen (C/O) and nitrogen-to-carbon (N/C) have been proposed as important tracers. As the temperature decreases in protoplanetary disks with the distance to the central star, molecules will freeze out onto dust grains and get removed from the gas phase to the solid phase, which changes the elemental abundance ratios in the gas and solid reservoirs. Planets formed at different locations with respect to molecular icelines and/or incorporated different amounts of solids, are expected to show distinct chemical abundance ratios in atmospheres (Öberg et al., 2011, Turrini et al., 2021), therefore providing compelling implications on formation pathways, birth locations, and relative contributions of gas versus solid accretion. Observational constraints on C/O ratios in exoplanets, such as β Pic b, HR 8799e, and WASP-77b, allow for interpretation of the formation history. For instance, the substellar C/O ratio in β Pic b supports a core-accretion scenario with substantial planetesimal enrichment (GRAVITY Collaboration et al., 2020), while the HR 8799 planets with C/O ratios consistent with the stellar value may have formed outside the CO_2 or CO iceline (Mollière et al., 2020).

However, none of the single tracers is an unique indicator for planet formation. The process is complicated by intricate substructures, chemical and dust evolution in protoplanetary disks, let alone nuances in orbital migration of planets, evolution of planetary interior and envelope (Guillot & Hueso, 2006, Madhusudhan et al., 2014, Mordasini et al., 2016, van der Marel et al., 2021), making it challenging to draw the exact link between formation histories and observed atmospheric properties. Current studies have been focused on the most accessible probe, C/O ratios, in individual objects, including a few hot Jupiters and young massive super Jupiters. Whereas, the important lessons from the perspective of planet formation suggest that: i) combining multiple observational probes is essential for disentangling the degeneracy and subtlety of planet formation processes; ii) it is crucial to investigate the population-level trends of the observables with planetary properties.

1.4 This thesis

The work presented in this dissertation focuses on spectroscopic characterization of atmospheres in close-in hot Jupiters and wide-orbit super Jupiters. With medium and high-resolution spectroscopic observations, this research investigates a variety of topics on atmospheric compositions, structures, and dynamics of gas giant planets, forming an important step to link the spectral observations of exoplanet atmospheres to planet formation and evolution processes.

Chapter 2: First detection of minor isotopologue ^{13}CO in an exoplanet
Isotopes in exoplanet atmospheres have been proposed as interesting tracers of planet formation (Mollière & Snellen, 2019, Morley et al., 2019), as inspired by solar system measurements of deuterium-to-hydrogen (D/H) ratios, which show significant variations across different planets. This is believed to be linked to the varying isotope ratios in protoplanetary disks due to isotope selective processes (called fractionation) that are temperature dependent. Therefore, the location of planet formation, the relative contribution of gas or solid accretion, and the atmospheric loss (as heavy isotopes are less prone to escape from atmospheres) are expected to leave imprints in the planetary isotope ratios. This chapter presents the first detection of the minor isotopologue of carbon monoxide ^{13}CO in the atmosphere of the super Jupiter YSES-1 b using the near-infrared integral-field spectrograph SINFONI at the VLT, extending isotopic measurements to exoplanets for the first time. Through modeling of planetary atmospheres and Bayesian retrieval analyses, we deter-

mined the carbon isotope ratio in the planetary atmosphere to be ^{12}CO/^{13}CO~31, which means a factor of two enhancement of ^{13}C compared to the local interstellar medium (^{12}C/^{13}C~68). To explain this enhancement, we suggested that the planet was formed outside the CO iceline, so as to attain carbon contents mainly from accretion of ^{13}C-enriched ices.

Chapter 3: First detection of minor isotopologue ^{13}CO in a brown dwarf
Following the successful detection of ^{13}CO in the exoplanet YSES 1b, we applied the same method to an exoplanet analog 2M0355, which is a young, isolated brown dwarf with a similar mass and effective temperature as the super Jupiter companion. This study found no enrichment of ^{13}CO in the brown dwarf using archival observations taken with the high-resolution spectrograph NIRSPEC at the Keck observatory. The carbon isotope ratio in this brown dwarf (^{12}CO/^{13}CO~100) forms stark contrast to that in the exoplanet, hinting at distinct formation pathways. Recently, with follow-up observations of this benchmark brown dwarf taken with the upgraded state-of-the-art spectrograph CRIRES at the VLT, we confirmed the constraint on the carbon isotope ratio and further suggest that even the more challenging oxygen isotope (^{16}O/^{18}O) ratio is now accessible for brown dwarfs and bright super Jupiters with high-resolution spectroscopy.

Chapter 4: Search for He i airglow emission from hot Jupiter
The closeness of gaseous planets to their host stars can lead to drastic escape of their upper atmospheres due to high-energy stellar radiation, potentially driving the evolution of atmospheres (especially for planets smaller than Neptune). The near-infrared absorption by helium atoms in exoplanet atmospheres has been suggested to be a powerful probe of atmospheric escape in transiting gas giants (Oklopčić & Hirata, 2018, Seager & Sasselov, 2000). However, constraining the mass loss rate using helium in absorption alone remains inconclusive because of the degeneracy with the exospheric temperature. To break this degeneracy through combining the same transition in re-emission, we carried out the first search for helium airglow emission in the non-transiting hot Jupiter τ Bootis b with the near-infrared spectrograph CARMENES at the Calar Alto Observatory. This search resulted in a non-detection. We concluded that the current detection limit has not reached the contrast level of the helium emission, but next-generation telescopes will be able to measure this emission. Detecting the helium emission will be important for probing exospheric structure and mass loss rates, hence understanding the bulk-atmospheric evolution of close-in gaseous planets.

Chapter 5: Disentangle hydrostatic and exospheric regimes of ultra-hot Jupiters
The strong high-energy stellar irradiation on close-in hot Jupiters results in two distinct regimes in their atmospheres, the hydrostatic lower atmosphere and the hydrodynamic exosphere, that can be probed with different atoms or molecules. Measuring these species in action will provide essential insights into these unknown processes. The study in this chapter entails the characterization of the ultra-hot Jupiter MASCARA-4b (UHJ, with equilibrium temperatures above 2000 K) using transmission spectroscopic observations taken with the optical high-resolution spectrograph ESPRESSO at the VLT. In addition to detecting a profusion of absorbing species such as H i, Na i, Fe i, and Fe ii in the planetary atmosphere, we put the measurements in the context of a sample of seven ultra-hot Jupiters

and investigated the trend of these atomic absorption strengths. The comparison suggested that the neutral metal species trace the hydrostatic regime, while hydrogen and ionized metals probe the hydrodynamic exosphere and the atmospheric escape. This represents the first step towards the population-level analysis of high-resolution spectroscopic results, which enables disentangling different dynamic regimes of highly-irradiated atmospheres.

Chapter 6: Diverse outcomes of binary-disk interactions
To get insights into planet formation, we need to understand circumstellar disks, the cradle of planets. As about half of solar-type stars were born in multiple stellar systems, the presence of stellar companions can modify the morphology and evolution of disks, potentially affecting the outcomes of planet formation. In this chapter, we resolved circumstellar disks using polarimetric differential imaging with SPHERE/IRDIS at the VLT for three multiple systems, namely, CHX 22, S CrA, and HP Cha, as part of the Disk Evolution Study Through Imaging of Nearby Young Stars (DESTINYS) large program. The observed disk morphology in combination with astrometric and orbit analyses for the stellar companions allow for a better understanding of the interplay between disks and companions. The comparison of the three systems spans a wide range of binary separation (50 – 500 au) and illustrates the decreasing influence on disk structures with the distance of companions. This agrees with the statistical analysis of exoplanet population in binaries, that planet formation is likely obstructed around close binary systems, while it is not suppressed in wide binaries.

1.5 Outlook: unravel the origin of planets

Fundamental questions about when, where, and how gas giants form remain open. Do they form via bottom-up or top-down pathways? Do they form in-situ or undergo migration and scattering from a different birth-location? With the ability of reliably retrieving the formation tracers such as elemental and isotopic compositions from near-infrared high-resolution spectra, we will be able to address the questions through population-level analyses of young giant planets and brown dwarfs. Our team at Leiden is carrying out a large observational program with the newly upgraded high-resolution ($\mathscr{R} \sim 100\,000$) spectrograph VLT/CRIRES to survey over twenty super Jupiters, free-floating planets, and brown dwarfs (the **SupJup** Survey). This will provide the first homogeneous comparison of elemental and isotopic constituents in different classes of sub-stellar objects.

We will focus on disentangling formation pathways of planets and brown dwarfs by investigating the extent to which they are chemically and isotopically distinguishable. For instance, if the distribution of chemical properties (such as the median and dispersion of the C/O and carbon isotope ratios) are similar for super Jupiters and brown dwarfs, they may share the same star-like formation pathways (see Figure 1.4). Otherwise, it means that distinct formation scenarios apply to different classes of objects, and we can further explore the trends in elemental and isotopic ratios with stellar and planetary properties such as mass and orbital separation. Either the presence or lack of trends is crucial for assessing the plausibility of various formation scenarios. An interesting example is shown in Figure 1.5 where I compile the current knowledge of C/O and ^{12}CO/^{13}CO ratios in super Jupiters and brown dwarfs from our preliminary analysis of archival data and the

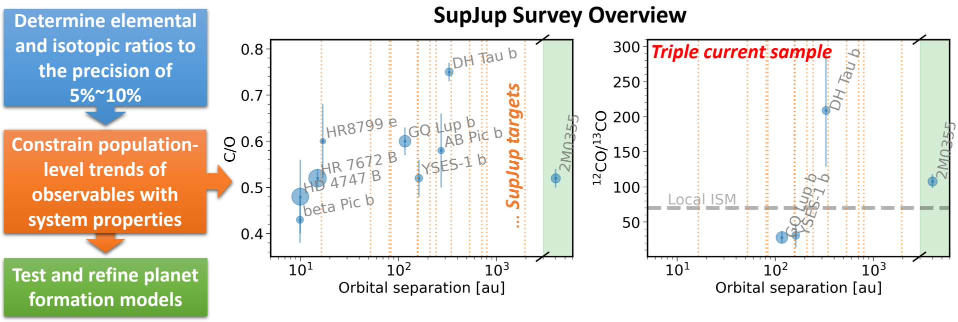

Figure 1.5: Atmospheric C/O and ^{12}CO/^{13}CO ratios against orbital separations of super Jupiters and brown dwarfs, suggesting a marginal trend of higher ratios at larger orbital distances. The size of the symbols indicates the estimated mass of the object. The vertical dotted lines suggest additional targets to be observed in the SupJup survey, which will triple the sample size, expand the coverage of the parameter space, and reveal a clearer picture of the presence or lack of trends.

literature (GRAVITY Collaboration et al., 2020, Mollière et al., 2020, Wang et al., 2022, Xuan et al., 2022, Zhang et al., 2021a,b). The marginal yet emerging trend of the ratios with orbital separations, which, as a key prediction of planet formation models, can be utilized for testing their validity. With the upcoming SupJup survey we will gain insights into such trends as we expand the sample size and improve the precision of measurements (see Figure 1.5). The census of chemical composition will contribute to bridging the gap between atmospheric observations and planet formation and evolution, and addressing the fundamental question of what distinguishes planets from brown dwarfs.

Furthermore, observations from space (JWST) with high sensitivity and unique wavelength coverage allow for filling the gap in the parameter space that is not accessible from the ground, such as studying colder gas giants on wide orbits and probing emission in the mid-infrared. The cross-validation and synergy between the space-based medium-resolution observations and the ground-based high-resolution data will provide complementary information on atmospheric properties (Brogi & Line, 2019) and mark an important step towards more accurate measurements of atmospheric constituents.

Looking further towards the future, the upcoming thirty-meter class telescopes such as the Extremely Large Telescope (ELT, first light expected in five years) and the next-generation flagship space telescope will routinely deliver characterization for smaller exoplanets with the potential of investigating atmospheric biosignatures and habitability (Kaltenegger, 2017, Meadows et al., 2018, Serindag & Snellen, 2019). The ELT will be promising for probing rare isotopes such as deuterium in exoplanets (Mollière & Snellen, 2019), which is one of the most informative tracers of planet formation and atmospheric evolution. Hopefully, we will be able to start answering the ultimate questions of how unique our solar system is and how we get here.