Lava worlds: characterising atmospheres of impossible nature

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ENGLISH SUMMARY

Just 30 years ago, our understanding of worlds other than Earth was tied to the Solar System. When astronomers began to look for exoplanets in 1980s, there was great scepticism that these even existed. The outlook changed dramatically in 1992, when the first unambiguous detection of two Earth-sized planets around a remnant of a star was made. If dead stars can have planets, surely the Milky Way must be filled with them. The search for distant worlds was on, and just three years later, the first planet orbiting a star entirely like the Sun was found. It was not just any kind of planet, it was a gas giant with an orbital period of 4.2 days, which is over 7 times closer to its star than Mercury to Sun. Astronomers have discovered an entirely new class of worlds that do not exist in the Solar System - hot Jupiters. As little sense as that made theoretically, it was clear that our knowledge of planetary systems was lacking.

At this point the exoplanets field would take off with explosive power. New instruments and techniques were quickly developed, now resulting in over 5000 confirmed exoplanets. New estimates show that there are at least as many planets in the Milky Way as there are stars, hundreds of billions if not trillions. The discovery of a hot Jupiter was just the beginning of the diversity that we would encounter. Soon, discoveries of super-Earths, lava worlds, warm-Neptunes, sub-Neptunes, and planets that are so hot that they slowly erode into dust, would be made. The majority of the discovered planetary systems did not look like the Solar System at all. Most contain short-period planets that are larger than Earth and closer to Neptune; some, like TRAPPIST-1 have 7 Earth sized worlds, all within an orbital period of 19 days; and some even orbit multiple stars. In the 30 years, as we went from 8 known planets to over 5000, our perception has expanded to a boundless variety of worlds. It was now evident that the Solar System is but one outcome of the stellar genesis, and that the cosmos is filled with worlds stranger than strange.

To find planets, astronomers developed a number of highly-efficient techniques. One of the first and most successful methods was to use radial velocity shifts. A presence of a planet around a star causes both objects to orbit a common centre of mass. The induced periodic motion of the star results in the observed spectrum features being shifted to different wavelengths. More massive planets induce larger shifts, and thus by using radial velocity one can determine not only the presence of a planet, but also its mass. Using this technique astronomers found almost a thousand planets, but it was quickly overshadowed by the photometric transit method. Transit photometry relies on the orbiting planet to obstruct

a small percentage of the observed starlight. This dimming is visible even with "backyard" telescopes. The method was so successful that several space telescopes were launched to survey the sky. Lo and behold, in just two years of monitoring NASA's Kepler telescope found more than two thousand planetary candidates, including first Earth-like planets orbiting a Sun-like star. With over 2600 confirmed planets to date, the transit technique is responsible for the majority of the discoveries. In the recent years, it also became possible to spatially resolve planets from their host star. This astonishing method is known as direct imaging, and while still in its infancy, it already has resulted in a few dozen young systems being photographed. Jupiter-sized planets can be directly seen orbiting distant stars. With the next generation of telescopes, such as ELT, direct imaging may provide first ever photographs of Earth-like worlds orbiting nearby stars.

Determining the mass and radius of a planet allows us to estimate its bulk properties, however, we truly wish to characterise it further, to know the composition of its atmosphere, surface, interior and even how and where it formed. Currently, one of the only viable ways to do this is to probe a planet's atmosphere using spectroscopy. Transmission spectroscopy has long been used in studying the Solar System, and was quickly adapted to measure atmospheres of exoplanets. Unlike photometry, spectroscopy relies on observing the planet at varying wavelengths. When a planet transits a star, its atmosphere acts as an altitude- and wavelength-dependant filter. Certain wavelengths are absorbed by the chemical inventory of the atmosphere and thus appear diminished. Each unique atom and molecule has their own spectroscopic opacity, which has allowed astronomers to single out a multitude of species in exoplanets; now over 20 elements of the periodic table, including molecules of H_2O, CO, NH_3, CH_4, HCN, TiO and several others. While most of these were found on gas giants, the sensitivity and spectral coverage required to characterise rocky worlds has just been achieved with the James Webb Space Telescope (JWST).

The transmission method has inherit downsides, with the biggest issue being the inability to probe compact atmospheres. Because a significant number of discovered exoplanets are strongly irradiated, enough so that they emit detectable light (or reflect), a supplementary method of probing their atmospheres was developed - emission spectroscopy. The planet is observed just before and during the eclipse by the star. Taking the difference between the spectra gives us the emission of just the planet. Because the signal comes from the chemical species emitting at different temperatures, this allows us to probe not only the vertical thermal structure of an atmosphere, but even create longitudinal maps called phase curves. The very first phase curve of a rocky world outside the Solar System was obtained in 2016, of a super-Earth named 55 Cancri e. Observations revealed a hotspot that is likely only explained via heat transport by a substantial atmosphere. Dayside temperatures on 55 Cancri e reach over 2700 K, thus it is considered to be a lava world, possibly covered with oceans of molten silicates. Current theory predicts that lava worlds have tenuous silicate-rich atmospheres that are sustained by the outgassing of the underlying magma. Though no unambiguous detections of atmospheres on lava worlds have been made, JWST may soon confirm or deny their presence.

We only truly understand a planet's atmosphere if we can reproduce the observed results with computational models. With our understanding of physical processes improving, we gain the knowledge necessary to build accurate simulations that mimic observations. These days, it is even feasible to simulate full 3-D climates of some planets, but the computational power required to run such models is expensive and time consuming. Since our general understanding of exoplanets is still in its infancy, a better approach to the problem is to use faster and more flexible, one-dimensional models. 1-D models rely on the fact that the averaged properties of a planet are well represented by just vertical variation, and indeed they have proven to be invaluable in predicting and explaining many observed phenomenon. In recent years, the community has shifted the focus towards statistical methods, relying on data-driven simulations. While such are extremely good at deducing planetary properties from observations, they still depend on the accuracy of full forward models.

Building a consistent 1-D atmospheric model only requires two components, a radiative-transfer climate model and a chemical or a photochemical model. The basic principle of a climate model is to solve the propagating stellar flux in the atmosphere and obtain a temperature-pressure profile and the planet's spectrum. Using various approximations, the structure can be solved in a plane-parallel fashion, taking into account only the vertical axis. The entirety of flux propagation in atmosphere is dictated by its chemical species absorbing and emitting certain frequencies of light. For an accurate model, as many as fifty or even more species are included, many containing billions of unique spectral lines. While at full scale this a computational nightmare, methods have been developed to approximate spectral lines in more compact tables, all without losing too much accuracy and making 1-D models fast and efficient.

Solving the chemistry comes in two main flavours, thermochemical equilibrium and photochemical kinetics. The first method is rather straightforward and involves minimising the Gibbs free energy of the system. Equilibrium chemistry usually takes into account thousands of different molecules, as the only input required are experimentally or computationally derived thermodynamical properties of each individual species. Because of how fast equilibrium calculations are, the method is adapted to the majority of exoplanet observations. This is especially true for statistical models, which require millions of individual cases to be computed. However, for a more detailed analysis a photochemical approach is necessary. Unlike equilibrium chemistry, which assumes that chemical timescales are much shorter than dynamical, photochemical codes take reaction rates into account. In reality, chemical reactions occur at vastly different periods of time, and not spontaneously, as equilibrium chemistry assumes. Not only that, but chemistry is heavily affected by the dynamics of the atmosphere, as well as by stellar irradiation. While photochemical models are much more accurate, they do have inherit downsides of being computationally slow and requiring reaction rate coefficients, which are especially lacking for high temperatures and generally difficult to determine experimentally. Because in most cases the the involved chemistry is incredibly complex, it is a major source of uncertainties. That said, both equilibrium and photochemical models are invaluable assets to exoplanet studies.

Even when approximated in 1-D, these accurately predict and explain many of the observations.

The work in this thesis heavily focuses on using 1-D chemistry and radiative-transfer codes to simulate atmospheres that may surround strongly irradiated super-Earths. The main goal is to guide observers to potentially detectable species that would help us gain insight into many of the drawn assumptions, allowing us to build better and more consistent models. Most of the presented results are applicable to low-resolution infrared spectroscopy, especially suitable for observations with JWST.

In Chapter 2 we simulate volatile atmospheric compositions surrounding a super-Earth 55 Cancri e. We take Titan's atmosphere as our starting point and use chemical kinetics with analytical temperature profiles to model a wide range of possible compositions. To assess observability, we additionally generate emission and transmission spectra applicable to the JWST wavelength range. The results indicate that species such as HCN, CN or CO could be observed and would likely indicate an atmosphere enriched in carbon.

Chapter 3 continues the topic of volatile atmospheres, but additionally adds radiative-transfer models that compute the temperature structure. The work is focused more on the ability of shortwave absorption to cause temperature inversions that would effect the observed spectrum. Indeed we find that the presence of CN can result in deep inversions in atmospheres with temperatures > 2000 K. Carbon-rich or hydrogen-depleted atmospheres around short-period super-Earths may be especially prone to this.

In Chapter 4, we move away from volatile compositions and explore silicate-rich atmospheres, outgassed from magma oceans residing on super-Earths. In addition to radiative-transfer and atmospheric chemical models, we make use of an outgassing code that determines the chemical budget. The thermal structure, including the temperature of the surface, are solved self-consistently with the chemistry for all currently known lava planets. As with previous works, we additionally simulate emission spectra. The results show that SiO and SiO_2 are likely to be the easiest to characterise in silicate atmospheres. We suggest that for a number of targets these could be detected using JWST's MIRI instrument. In this study we also find additional species, such as TiO, that may be heavily linked to the composition of the melt and surface-interior dynamics.

Finally, in Chapter 5 we combine all of the previous papers to model observability of volatile atmospheres around super-Earths and sub-Neptunes that may be contaminated by the outgassing of an underlying melt. The work is heavily based on predictions that magma oceans can store large reservoirs of volatile material that buffer atmospheres against stellar erosion. The models focus on atmospheres of H, C and N that are enriched in silicates. The results indicate that silicate contamination may be detectable with JWST through the presence of the 5 and 9 μm SiO features, however, these are expected to be strongly diminished by the presence of the residing volatiles. We also find that outgassing can cause deep thermal inversions, even in thick volatile atmospheres, affecting observability of all species. Detecting SiO in a volatile-rich atmosphere could indicate that the planet has an underlying melt that efficiently supplies the atmosphere with silicates.

And thus we conclude by saying that while in only 30 years the exoplanets field has revealed an astonishing diversity of worlds, it is truly only the beginning of what the future holds. Spectroscopy is a powerful tool that has allowed astronomers to glimpse into the atmospheres of distant planets. As of yet, there are no unambiguous evidence of super-Earths or lava worlds possessing atmospheres. However, JWST will shortly observe several irradiated rocky worlds in the hopes of finding chemical signatures. The next generation of telescopes and computational models will likely allow us to gain knowledge of exoplanets better than of many planets in the Solar System. It is not unfeasible that soon we will be mapping continents and oceans of distant Earths and maybe even discovering signs of biological presence. We hope that the work done in this thesis will provide at least some guidance for future observations and modelling efforts.