Simulating (Sub)Millimeter Observations of Exoplanet Atmospheres in Search of Water

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Abstract

Context: Spectroscopic characterization of exoplanetary atmospheres is a field still in its infancy. The detection of molecular spectral features in the atmosphere of several hot-Jupiters and hot-Neptunes has led to the preliminary identification of atmospheric H$_2$O. The Atacama Large Millimeter/Submillimeter Array is particularly well suited in the search for extraterrestrial water, considering its wavelength coverage, sensitivity, resolving power and spectral resolution.

Aims: Our aim is to determine the detectability of various spectroscopic signatures of H$_2$O in the (sub)millimeter by a range of current and future observatories and the suitability of (sub)millimeter astronomy for the detection and characterization of exoplanets.

Methods: We have created an atmospheric modeling framework based on the HAPI radiative transfer code. We have generated planetary spectra in the (sub)millimeter regime, covering a wide variety of possible exoplanet properties and atmospheric compositions. We have set limits on the detectability of these spectral features and of the planets themselves with emphasis on ALMA. We estimate the capabilities required to study exoplanet atmospheres directly in the (sub)millimeter by using a custom sensitivity calculator.

Results: Even trace abundances of atmospheric water vapor can cause high-contrast spectral absorption features in (sub)millimeter transmission spectra of exoplanets, however stellar (sub) millimeter brightness is insufficient for transit spectroscopy with modern instruments. Excess stellar (sub) millimeter emission due to activity is unlikely to significantly enhance the detectability of planets in transit except in select pre-main-sequence stars.

Thermal emission from known exoplanets is too weak for the successful detection of atmospheric water vapor with ALMA. Mature exoplanets will remain difficult to directly detect with ALMA, even gas giants in the nearest star systems.

Contaminating telluric lines pose a challenge to ground based observation of Earth-like exoplanet atmospheres, requiring hot (T > 1500K) planets with water lines found in the high transmission bands of the millimeter wavelength range.

Conclusion: State of the art (sub)millimeter arrays require a 1-3 order of magnitude improvement in sensitivity to allow for the direct detection of nearby exoplanets within reasonable observational constraints. An interferometer with 40,000 12 m antennae could make 3σ detections of water lines in Hot Jupiters at distances less than 25 pc in a single day of observation.
Acknowledgements

I would like to thank my parents for supporting me unconditionally without whom I could not have made it this far. I would like to thank Silke for her wonderful encouragement and care. I would like to thank my supervisor Floris van der Tak for providing this engaging topic, for the fruitful discussions and suggestions, for his patience with my struggles, and for his thorough review and attention to detail. I would like to thank Michael ‘Migo’ Müller and Rien van de Weijgaert for gladly accepting my requests for them to review this thesis. Finally I would like to thank the residents of the Masterkamer for often, if not always, being there.
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1 Introduction

The search for life beyond the Earth has inspired much astronomical research over the centuries. The discovery and application of spectroscopy opened the planetary atmospheres of the Solar System to remote study. The first spectroscopic observations of Mars were interpreted as evidence for a water-bearing Earth-like atmosphere (Huggins, 1867), followed by multiple confirmations (Vogel, 1876), all of which were spurious detections of the Earth’s intervening atmospheric water vapor. These claims fueled much speculation as to Mars’ habitability. When carefully controlled observations resulted in nondetections the early results were put into question (Campbell, 1894). Mars was eventually revealed to be a comparatively barren world (Adams and St. John, 1926). This cautionary tale of the difficulty of interpreting ground-based spectra in the search for extraterrestrial water vapor is still relevant today.

The search for water now continues beyond the solar system with the study of planets orbiting stars other than the Sun. Exoplanets with insolation and dimensions that fall within a theoretically habitable parameter space have already been detected (Torres et al., 2017). Atmospheric spectroscopy of exoplanets pushes onward to smaller and cooler planets (Wakeford et al., 2017) approaching the limits of stellar variability (Zhang et al., 2018). While potential biosignature gases have already been discussed (Seager et al., 2005, 2016), water is seen as a basic requirement for any environment to be potentially habitable to life as we know it.

1.1 Exoplanets

Illusory signals and retracted claims plagued exoplanet research for more than a century before the first confirmed detection. Bessel was the first to use astrometry to detect unseen stellar mass companions around Sirius and Procyon (Bessel, 1844). His success in the indirect detection of dark massive objects led to the first scientific claim of an extrasolar planet when Capt. W. S. Jacob proposed a 3-body solution to his astrometric observations of 70 Ophiuchi (Jacob, 1855) yet the proposed orbital arrangement was found to be unstable (Moulton, 1899). Knowing that a massive planet would have a larger gravitational influence on a star of lower mass, Peter van de Kamp studied nearby M-dwarfs and claimed an astrometric detection of a 1.6 M_J planet orbiting Barnard’s Star (van de Kamp, 1963; Gizis, 1997) which was later demonstrated to be the result of instrumental effects (Hershey, 1973).

In 1988 a spectroscopic survey of solar-type stars led to the tentative detection of a planetary mass object orbiting the primary component of the γ Cephei binary. (Campbell et al., 1988). Reflex motion of the star due to gravitational interactions with the planet induced a detectable periodic oscillation in the measured stellar radial velocity. The planetary nature of the γ Cephei Ab claim was retracted in 1992 only to be confirmed in 2003 (Hatzes et al., 2003) disqualifying it as the first unambiguously confirmed detection. Similarly the $M\sin(i) = 11$ M_J planet candidate HD 114762b was discovered in 1989 but was identified as a probable brown dwarf, its minimum mass lies near the deuterium-fusion limit 13 M_J (Latham et al., 1989).

The first confirmed detection of an exoplanet occurred in 1992 when timing observations of the millisecond pulsar PSR B1257+12 revealed a periodicity best explained by a 2 or 3 body Keplerian fit (Wolszczan and Frail, 1992) (Wolszczan, 1994). The detection technique was sensitive to planets far below the mass range accessible to contemporary high-precision spectrographs. The planets range in mass from 0.02-4.3 M_⊕ on semi-major axes 0.19-0.46 au.

The first confirmed detection of a planetary mass object orbiting a main sequence star occurred in 1995 via Doppler spectroscopy. The planet 51 Pegasi b was discovered by observations of periodic oscillations in the host star’s radial velocity (Mayor and Queloz, 1995). With an orbital period of 4.23 days and a mass of 0.476 M_J it represented a new class of planet with no solar system analog; the Hot...
Jupiter. Since this discovery 78% of the known exoplanets have been detected via transit photometry, with most of the remainder detected by Doppler spectroscopy and to a much lesser extent gravitational microlensing and direct imaging (Perryman 2014; Deeg and Alonso 2018). As of July 2018, there are 3774 confirmed exoplanets and 4496 candidate exoplanets in the NASA Exoplanet Archive (Akeson et al., 2013).

To date there have been several successful detections of molecules in exoplanet atmospheres (Burrows, 2014a; Crossfield, 2015). Atomic or molecular line detection has occurred via both spectroscopy and broadband photometry. For planets with equilibrium atmospheres and initially solar abundances, CO and H$_2$O are expected to be the most abundant and spectroscopically active molecules (Burrows and Sharp, 1999). CO has been observed to be abundant in Hot Jupiter atmospheres through high dispersion spectroscopy and at lower dispersion in directly imaged exoplanets (Snellen et al., 2010; Konopacky et al., 2013). High CO/CH$_4$ ratios are taken as evidence of strong vertical mixing in the atmosphere of Hot Jupiters (Crossfield, 2015) with direct implications for the vertical H$_2$O abundance. H$_2$O is also detected in low dispersion spectroscopy of transiting systems (Deming et al., 2013) (see §1.2.1).

Future observatories such as the James Webb Space Telescope (JWST) will open the possibility of atmospheric characterization of smaller and cooler terrestrial exoplanets (Barstow and Irwin, 2016), and hence the detection of molecular species and possibly even gaseous biosignatures in their atmospheres (Beichman et al., 2014; Greene et al., 2016).

1.1.1 Observational Techniques

Transit Method

The *Kepler* space telescope is responsible for the majority of exoplanet detections to date. *Kepler*, and its extended *K2* mission, utilizes the transit photometry technique to detect exoplanets. *Kepler* performed white-light photometry on $\sim$150000 targets simultaneously with a photometric stability of 29 ppm. A planet is said to transit when it orbits in a plane that intersects the stellar disk. To first order, the probability that a given planet in a circular orbit will transit $p$ is

$$p = \frac{R_\star + R_p}{a}$$

(1)

Where $R_\star$ is the stellar radius, $R_p$ the planetary radius, and $a$ the planet’s orbital semi-major axis (Borucki and Summers, 1984). From this we can estimate the transit probability for a planet with $a = 1$ au orbiting a star with radius $R_\star = R_\odot$ as 0.46%. For a habitable zone planet around the M8V dwarf TRAPPIST-1 ($R_\star = 0.121 R_\odot$, $a \sim 0.02$ au) we find a probability of $\sim 2\%$ (Schmidt et al., 2007; Van Grootel et al., 2018). The light which is occluded by the opaque planet during the transit produces a potentially detectable photometric signature. The resulting phases of ingress, transit, and egress result in a characteristic light curve profile. The four primary observables are the period of the transit, the transit depth $\Delta F$, the interval between first and fourth contact $t_T$, and the interval between second and third contacts $t_F$. With the approximations that $a << R_\star$, $M_p << M_\star$, and that the orbit is circular, the planetary orbital period $P$, the stellar density $\rho_\star$, the impact parameter $b$ (the projected distance between centers of the star and planet), the planetary orbital radius $a$, and the planet’s orbital inclination $i$ can all be derived from the shape of the transit light curve. The resulting change in observed flux $\Delta F$ can be predicted to first order via the ratio of the areas of the planetary to stellar disks

$$\Delta F = F_\star \frac{R_p^2}{R_\star^2}$$

(2)

where $F_\star$ is the stellar flux, $R_p$ the planetary radius, and $R_\star$ the stellar radius. Accordingly, a greater stellar flux results in higher signal-to-noise ratio, as does a larger planet or smaller star. A high temporal sampling rate is required to derive the exoplanet parameters with confidence. Exoplanet transit durations are found to occur on the order of 1 hour while the ingress and egress phases last only minutes, yet the observation of this phase is needed for the characterization of the exoplanet parameters. A partial

[1]https://exoplanetarchive.ipac.caltech.edu/
detection of a transit event reveals only $\Delta F$. Stellar rotation complicates atmospheric retrieval with implications for multi-epoch observations (Zhang et al., 2018). The duration of planet transit sets a limit on observational integration time per transit. The duration of the transit event $t_T$ can be derived via

$$t_T = \frac{P}{\pi} \sin^{-1} \left( \frac{R_\ast \sqrt{(1 + R_p/R_\ast)^2 - (a/R_\ast \cos i)^2}}{a \sin i} \right)$$

(3)

where $P$ is the period of its orbit, $i$ is the orbital inclination and $a$ is the planet orbit semi-major axis.

During the transit event, the planetary atmosphere will also contribute to the occlusion of stellar light. This fortuitous arrangement allow for the spectroscopy of planetary atmospheres (Seager and Sasselov, 2000). A fraction of the light emitted by the exoplanet’s host star passes through an annulus of the atmosphere and spectral absorption features are introduced into the signal. The contribution of the atmospheric signal $\delta$ is

$$\delta = \frac{2 R_p H}{R_\ast^2}$$

(4)

where $H$ the atmospheric scale height (see Eq.19). For the Earth and Sun $\delta = 1.13$ parts-per-million (ppm). Through subtraction of the stellar spectrum and with sufficiently high photometric precision and spectral resolution, the contribution of the planetary atmospheric absorption to the transit signal can be detected. Due to frequency dependent opacity in the planet atmosphere a transit will appear to result in different apparent planetary radii at differing frequencies. In this way broadband photometry can act as an ersatz spectrum. The interpretation of atmospheric absorption features detected by transmission spectroscopy is confounded by the potential presence of clouds, aerosols, hazes, temperature inversions, and condensation and other non-equilibrium phenomena occurring on the terminator of the exoplanet (Burrows, 2014b).

A transiting planet will also be occluded by its star on each orbit. This alignment is known as the secondary eclipse. The secondary eclipse offers the opportunity to study the spectrum of the host star alone while the planet is occluded. Subtracting the stellar spectrum from the combined spectrum leaves a potentially detectable residual signal.

Emission Spectroscopy

Planetary emission spectra are multi-component. Solar system planets were first identified in antiquity by their reflected (rather than intrinsic) emission. Incident solar radiation will only be partially absorbed by the planet and the rest reflected as a function of planetary albedo. The planet itself will have an intrinsic thermal emission. Spectral features will be imprinted in the reflected solar light by its absorption as it enters the planetary atmosphere, again as it is partially absorbed and reflected by the planetary surface, and finally once more as it is scattered back out of the planetary atmosphere. The planetary thermal emission will also have absorption features introduced by the planet’s atmosphere and the atmosphere itself may introduce its own lines in emission.

Exoplanets have been found in orbits ranging in semi-major axis from 0.0058-6900 au have been found (Deacon et al., 2016; Smith et al., 2018), unambiguously around stars of spectral classes from M to A. The resulting diversity of radiation field intensity in which planets are embedded results in a calculated range of equilibrium temperature from $\sim$40-2000 K. The planet equilibrium temperature $T_{eq}$ is a theoretical description of an isothermal planet in complete equilibrium with the radiation field of its host star. $T_{eq}$ can be derived from the energy balance between the energy emitted and absorbed by the planet in the case of no greenhouse effect:

$$T_{eq} = T_* \left( \frac{R_\ast}{a} \right)^{1/2} (1 - A_B)^{1/4}$$

(5)

where $T_*$ is the stellar effective temperature, $R_\ast$ is the stellar radius, $a$ is the planet orbital radius, and $A_B$ is the Bond albedo. The Bond albedo is the fraction of radiation which is emitted back into space
by the planet, measuring its departure from a black body radiator. Values of $A_B$ for the solar system planets are shown in Table 1.

<table>
<thead>
<tr>
<th>Planet</th>
<th>$A_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mercury</td>
<td>0.068</td>
</tr>
<tr>
<td>Venus</td>
<td>0.770</td>
</tr>
<tr>
<td>Earth</td>
<td>0.306</td>
</tr>
<tr>
<td>Mars</td>
<td>0.250</td>
</tr>
<tr>
<td>Jupiter</td>
<td>0.343</td>
</tr>
<tr>
<td>Saturn</td>
<td>0.342</td>
</tr>
<tr>
<td>Uranus</td>
<td>0.300</td>
</tr>
<tr>
<td>Neptune</td>
<td>0.290</td>
</tr>
</tbody>
</table>

Table 1: Bond Albedo of the Planets. A value of 0 represents total absorption of incident radiation and a value of 1 represents total scattering of all incident radiation back into space.

Objects which emit as blackbodies follow Planck’s law. The spectral radiance $B_\nu$ (emitted power per unit area per unit frequency per unit solid angle at some temperature $T$) of a black body is

$$B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1}$$

(6)

Where $h$ and $k$ are the Planck and Boltzmann constants respectively. The luminosity $L$ can be calculated by integrating $B_\nu$ over the frequency range $d\nu$ and the solid angle $d\Omega$ to find the radiated power. Knowing the distance $D$ to the emitting object and its emitting area we can calculate an observed flux $F = L/(4\pi D^2)$. Note however that the observed quantity brightness temperature $T_b$ is frequency dependent, and corresponds to the temperature of a blackbody with the same flux within some frequency range.

$$T_b(\nu) = \left( \frac{F}{\sigma R^2} \right)^{1/4}$$

(7)

While exoplanetary temperature estimates can be informed by equilibrium temperature calculations, these require assumptions regarding albedo and planetary greenhouse effect, both of which can cause significant departure from the idealized relation. The large deviation of the true Venus surface temperature from the equilibrium temperature calculation is caused by its CO$_2$ driven greenhouse effect which traps heat near the surface by the absorption of re-emitted surface infrared radiation. In the case of Venus instead of a temperate but warm $T_{eq} = 315$ K, we find an uninhabitable 700 K at the surface [Avduevskij et al., 1971]. Massive young planets which have not yet dissipated their heat of formation also deviate from the relation. A frequency dependent star/planet thermal flux ratio can be derived as

$$\frac{F_{o,p}}{F_{o,*}} = \frac{F_{e,p} R_p^2}{F_{e,*} R_\star^2} = \left( \frac{\nu^{h\nu/kT_p} - 1}{\nu^{h\nu/kT_\star} - 1} \right) \left( \frac{R_p^2}{R_\star^2} \right)$$

(8)

where $F_{o,p}$ and $F_{o,*}$ are the observed planetary and stellar fluxes, $F_{e,p}$ and $F_{e,*}$ are the emitted planetary and stellar fluxes, $R_p$ and $R_\star$ are the planetary and stellar radii, $\nu$ is the frequency, $T_p$ and $T_\star$ are the planetary equilibrium effective temperature and the stellar temperature [Seager, 2010]. Typical star/planet flux ratios in the (sub)millimeter are $10^4 - 10^6$ (see §3.2).

**Direct Imaging**

Directly imaged planets are spatially resolved from their host stars and are detected via their intrinsic thermal emission or by reflected stellar light. This technique has thus far favored planets at large angular (and thus orbital) separation from their host stars, and protoplanets which have not yet completely cooled to reach equilibrium after their formation [Marois et al., 2008]. Only 44 exoplanets have been directly...
imaged as of July 2018, 6 of which have an angular separation from their star > 10000 milliarcseconds (mas), and 15 greater > 1000 mas.

Direct detection is challenging due to the small angular size of the more typical exoplanet orbits. The nearest star Proxima Centauri hosts a planet with a semi-major axis of 0.0485 au. At a distance of 1.295 pc this results in a maximum separation of 0.019". The (sub)millimeter interferometer ALMA’s angular resolution (see §1.3.2) is described by

$$\theta = 0.02'' \left( \frac{\lambda}{1\text{ mm}} \right) \left( \frac{10\text{ km}}{\text{max-baseline}} \right)$$

which for a wavelength of 0.3 mm and a maximum baseline of 15 km results in a maximum angular resolution of ~0.004". Submillimeter interferometry thus offers a chance to observe planets very close in to their host star given that the planet signal is detectable. The extreme contrast ratio between stars and planets further complicates observations. The ratio of star-planet reflected light can be written as

$$\frac{f_p}{f_\star} = p(\lambda) \frac{R_p}{a} g(\alpha)$$

where $p(\lambda)$ is the wavelength dependent geometric albedo (ranging from 0-1), $a$ is the semi major axis (typical values of 0.01-100 au), and $g(\alpha)$ is a function dependent on phase; $g(\alpha) = \frac{\sin(\alpha) + (\pi - \alpha)\cos\alpha}{\pi}$ and $\cos\alpha = -\sin i \sin(2\pi\phi)$ where $i \in [0,\pi/2]$ is the inclination and $\phi \in [0,1]$ is the orbital phase such that $\alpha \in [0,\pi]$ and $g(\alpha) \in [0,1]$. The ratio is $10^{-9}$ for Jupiter and the Sun at maximum elongation when seen from 10 pc and $10^{-4}$ for the Hot Jupiter τ Boötis. Diffracted light from telescope optics and scattered light from wavefront aberrations cause a residual signal (Perryman, 2014).

**High Dispersion Spectroscopy**

An emerging technique is the use of high resolution spectrographs to trace the radial velocity shift of a planet’s molecular lines during an orbit (Snellen et al., 2010). Ground-based telescopes can be equipped with instruments of spectral resolution $R = \lambda/\Delta\lambda > 30000$. A synthetic spectrum can then be cross-correlated with the resulting radial velocity shift of possible planetary orbital parameters. The method is not sensitive to strong broadband variability of a host star and has been used to detect water vapor in exoplanet atmosphere from ground-based observatories (Crossfield, 2015; Birkby et al., 2017).

**1.2 Water**

One of the most anthropologically fascinating molecules is H$_2$O. Water is abundant on the surface of the Earth and can be found in all phases. Carbon compounds and liquid water form an ideal compound-solvent pair due to water’s high dipole moment (Encrenaz, 2008). Water as a medium is suspected to be essential for pre-biotic chemistry and the origin of life (Westall et al., 2018). As a result the detection of H$_2$O is considered a requirement in the search for extraterrestrial habitable environments (van Dishoeck et al., 2014).

Water’s elemental constituents, hydrogen and oxygen, are the first and third most abundant elements in nature respectively (Anders and Grevesse, 1989), yet H$_2$O was not initially predicted to be found in the interstellar medium. After the detection of several free radicals including OH, the general consensus was that gas densities were too low and ultraviolet radiation fields too intense in space to allow for the survival of other polyatomic molecules (Townes, 2006). The discovery of interstellar NH$_3$ altered this perception and led to a search for other interstellar molecules (Cheung et al., 1968). Shortly thereafter water was first detected beyond the Earth in the Orion Nebula (Cheung et al., 1969). However, it was discovered that this emission occurred via the maser process $6_{16} \rightarrow 5_{22}$ and thus required the special astrophysical circumstances to create a level population inversion, such that it could not be used to probe the bulk of interstellar water.

Water emission lines which are thermally excited have been detected since in minor bodies and planets of the solar system (Mumma et al., 1986) (Encrenaz, 2008), around other stars (Melnick et al.

\[\text{https://exoplanetarchive.ipac.caltech.edu/cgi-bin/TblView/nph-tblView?app=ExoTibs&config=planets}\]
protoplanetary disks (Hogerheijde et al., 2011), and star forming regions (van der Tak et al., 2006). How is it that water is transported to the planets? Protoplanetary disks consist of gas and dust at a canonical mass ratio of 100:1. While the disk surface is heavily irradiated by its star, it contains a warm sub-surface molecular layer and a cold midplane in which volatiles can condense. H$_2$O can form in the molecular layer of the disk where $T_{\text{gas}} > 100$ K (Glassgold et al., 2009). Gas phase reactions and surface processes form H$_2$O in the disk. The primary gas phase reactions are neutral-neutral at $T_{\text{gas}} > 300$ K via

$$O + H_2 \rightarrow O + OH$$
$$OH + H_2 \rightarrow H_2O + H$$

The radiation fields of protostars irradiate the protoplanetary disks, resulting in multiple sublimation radii for volatile species such as H$_2$O and NH$_3$. Within the ‘water ice snow line’, water ice sublimes. Gaseous H$_2$O is then photodissociated by UV stellar photons into atomic hydrogen and the hydroxyl radical OH. The inner several au of forming planetary systems are thus stripped of water. A combination of accretion prior to the loss of gaseous H$_2$O, delivery by planetesimals, comets, and the outgassing of a secondary atmosphere have in the case of the Earth resulted in the presence of abundant surface water (Morbidelli et al., 2000; Drake, 2005). The other solar system planets also are presently or were once enriched to varying degrees in water. Mars is believed to have once had sufficient water reservoirs to form a polar ocean (Baker et al., 1991; Clifford and Parker, 2001). Planets forming beyond the respective snow lines are comparatively enriched in volatiles. Based on a solar abundance of elements one could expect a water volume mixing ratio (vmr) of 0.0015 (Anders and Grevesse, 1989). Water vapor was first detected in the atmosphere of Jupiter at a relative abundance $N$(H$_2$O)/$N$(H$_2$) $\approx 4 \times 10^{-6}$ (Larson et al., 1975) now known to be $> 0.0005$ (Taylor et al., 2004) and Saturn (de Graauw et al., 1997), as well as Saturn’s moon Titan (Coustenis et al., 1998).

Water is the dominant source of opacity in the Earth’s atmosphere, particularly in the far-infrared and the (sub)millimeter. Despite this the observation of water in exoplanet atmospheres by transit spectroscopy may be challenged by the existence of so-called cold traps. When surface water evaporates it is transported vertically in the atmosphere by convection. As the temperature falls with increasing altitude the water condenses as it reaches the tropopause, preventing further mixing. Much of the condensed water then precipitates and returns to the surface. The stratosphere is thus left relatively dry (Pierrehumbert et al., 2007). Cold trap efficiency may be reduced strongly by a lack of non-condensing gas such as N$_2$ (Wordsworth and Pierrehumbert, 2014). Important water lines in the (sub)millimeter are included in Table 2 (Gordon et al., 2017).

<table>
<thead>
<tr>
<th>Frequency (GHz)</th>
<th>Transition</th>
<th>$S_{ij} \times 10^{22}$*</th>
<th>$E_i$ [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>22.3152</td>
<td>6$<em>{16}$ - 5$</em>{23}$</td>
<td>0.004454</td>
<td>642.4335</td>
</tr>
<tr>
<td>183.3100</td>
<td>3$<em>{13}$ - 2$</em>{20}$</td>
<td>0.7736</td>
<td>195.9108</td>
</tr>
<tr>
<td>325.1528</td>
<td>5$<em>{15}$ - 4$</em>{22}$</td>
<td>0.9077</td>
<td>454.3392</td>
</tr>
<tr>
<td>380.1975</td>
<td>4$<em>{14}$ - 3$</em>{21}$</td>
<td>8.262</td>
<td>305.2440</td>
</tr>
<tr>
<td>448.0013</td>
<td>4$<em>{23}$ - 3$</em>{30}$</td>
<td>8.633</td>
<td>410.6513</td>
</tr>
<tr>
<td>474.7012</td>
<td>5$<em>{33}$ - 4$</em>{40}$</td>
<td>1.090</td>
<td>702.3208</td>
</tr>
<tr>
<td>556.9361</td>
<td>1$<em>{10}$ - 1$</em>{41}$</td>
<td>523.8</td>
<td>34.2346</td>
</tr>
<tr>
<td>752.0519</td>
<td>2$<em>{11}$ - 2$</em>{22}$</td>
<td>345.4</td>
<td>100.8444</td>
</tr>
<tr>
<td>916.1945</td>
<td>4$<em>{02}$ - 3$</em>{31}$</td>
<td>14.26</td>
<td>410.3646</td>
</tr>
</tbody>
</table>

| 547.6902**     | 1$_{10}$ - 1$_{01}$ | 1.010                   | 34.1778  |

Table 2: Water Lines in the (Sub)millimeter

* $S_{ij}$ is the spectral line intensity [cm$^{-1}$ / (molecule cm$^{-2}$)] at T = 296 K
** $^{18}$H$_2$O
The 183, 325, 474, and 916 GHz transitions are known as a group of low-excitation lines (including 899 and 906 GHz not shown in Table 2). Another group: 96, 137, 209, 250, 263, 297, 488, 610 and 832 GHz, are some of the high-excitation water lines in the (sub)millimeter (Gray et al. 2016).

1.2.1 Detections

In Hot Jupiter atmospheres H$_2$O is expected in vapor form at all pressures which can be probed spectroscopically. Coupled with the large (> 100 km) atmospheric scale heights this results in strong infrared H$_2$O absorption seen in transmission and emission. For cooler giant planets (~300 K) H$_2$O condenses in deeper layers of the atmosphere (Atreya et al., 1999). Water has been successfully discovered on several Hot Jupiters. Water absorption features with a depth of 200 ppm at 1.3 μm were found by HST transmission spectroscopy of the Hot Jupiters HD 209458 b and XO-1 b (Deming et al. 2013), WASP-12b (Swain et al. 2013), WASP-17b (Mandell et al. 2013), WASP-19b (Huitson et al. 2013) and WASP-43b (Kreidberg et al. 2014). H$_2$O spectral features are in general found to be less prominent than expected. Clouds or hazes as continuum absorbers are suspected to obscure the H$_2$O features (Sing et al. 2016).

Water vapor has been detected in the cloud-free atmosphere of the Hot Neptune HAT-P-11b by simultaneous HST and Spitzer observations (Fraine et al. 2014). Strong water absorption was seen in the emission spectrum of the directly imaged HR 8799 b in the K band of the Keck OSIRIS instrument (Barman et al. 2015). Water vapor has also been detected to a depth of 525 ppm in the Hot Neptune HAT-P-26b with HST transmission spectroscopy (Wakeford et al. 2017). Importantly, ground based detections have been possible: high dispersion spectroscopy with CRIRES/VLT was used to detect water in the atmosphere of the non-transiting 51 Pegasi b (Birkby et al. 2017). Ground based high dispersion near infrared detection of H$_2$O has also been made in the atmosphere of HD 189733 b with $R > 20000$ (Brogi et al. 2018).

1.3 (Sub)millimeter Astronomy

The electromagnetic spectrum spanning ~200 μm - 10 mm wavelength range is known as the millimeter and sub-millimeter (together (sub)millimeter), lying between the microwave and far infrared wavelength ranges. Primary emission mechanisms which produce radiation in this regime are thermal (cold dust), rotational line-transitions (molecular gas), and to a lesser extent Bremsstrahlung (ionized gas), and Synchrotron emission (via the acceleration of relativistic charged particles). As early as 1954 the millimeter and submillimeter thermal emission of the Sun and Moon were studied in the USSR (Salomonovich et al. 1958; Salomonovich, 1958). The first specialized (sub)millimeter telescopes appeared in the 1960’s. In 1968 the 11-meter infrared telescope at Kitt Peak was converted for use in radio astronomy and became one of the most productive early instruments (Lequeux 2009). The submillimeter range remained difficult to observe due to the stringent atmospheric restrictions (Braithwaite et al. 1969) and observations above the Earth’s atmosphere were sought. The Submillimeter Wave Astronomy Satellite (SWAS) was launched in 1998 and could observe a band 487–557 GHz (538–616 μm). In 2009 the HIFI (Heterodyne Instrument for the Far-Infrared) was launched aboard the Herschel Space Observatory with a 3.5 meter primary mirror, covering a frequency range in 2 bands of 480-1250 GHz and 1410-1910 GHz.

1.3.1 Application

In the case of thermal radiation we can determine the temperature $T$ corresponding to the peak emission wavelength $\lambda_{\text{max}}$ by Wien’s displacement law

$$T = \frac{b}{\lambda_{\text{max}}}$$

where $b$ is Wien’s displacement constant $\sim 2.9 \times 10^{-3}$ m K. Over the (sub)millimeter range we find $T \sim 3 - 20$ K. Consequently the field of (sub)millimeter astronomy has excelled in the detection and characterization of cold interstellar and circumstellar dust and gas radiating thermally (Ricci et al. 2014; Ansdell et al. 2016). Many of the triumphs of (sub)millimeter astronomy have been in the study of star forming regions and protoplanetary disks (van der Tak et al. 2000; Stahler and Palla 2005).
The energy levels corresponding to rotational modes of several cosmically abundant molecules, when converted to electromagnetic radiation by the emission of a photon, fall within the submillimeter wavelength range (Wilson, 2009). This has allowed for the expansion of the field of molecular spectroscopy and interstellar chemistry to include the bulk of di- and tri-atomic light molecule’s rotational spectral lines.

Ground based submillimeter astronomy is challenged by the pressure-broadened absorption features in the Earth’s atmosphere caused by O2 and H2O which limit atmospheric transmission (Pardo et al., 2002). Earth’s atmospheric opacity necessitates that ground based observatories be built at high altitude, and locations such as the Chajnantor Plateau, Mauna Kea, or the South Pole (Radford, 2011).

1.3.2 ALMA

The most sensitive and capable instrument today is the Atacama Large Millimeter/Submillimeter Array (ALMA) which has been fully operational since 2013. ALMA is an aperture synthesis radio telescope with 66 antennae arranged in three configurations. The 12-m array consists of 50 widely spaced antennae, and the Atacama Compact Array (ACA) is composed of twelve closely spaced 7 m antennae and the Total Power (TP) Array; four 12 m antennae for single-dish observations. The ALMA bands will cover the wavelength range 0.32 to 10 mm (84 - 950 GHz), making it a powerful tool for high-resolution molecular spectroscopy (Wootten, 2008). Channel widths between 3.8 kHz and 15.6 MHz are possible, with a simultaneous bandwidth of 8 GHz. As an interferometer with baselines of up to 16 km, spatial resolutions of 0.025 arcseconds have been demonstrated in observations of the protoplanetary disk of HL Tau (ALMA Partnership et al., 2015). ALMA is located in the Chilean Andes on the Chajnantor plain at (lat:-23.02917°, lon:-67.754649°) at ∼5000 m altitude. The arid environment is required for observations at millimeter and submillimeter wavelengths, as atmospheric opacity both reduces signal strength by absorption and contributes to the noise via thermal emission from the atmosphere (Tremblin et al., 2013).

ALMA’s capabilities have yet to be applied to the direct detection of exoplanets or to the characterization of atmospheric absorption or emission features in exoplanets. Indirect detection may have occurred by the observation of non-Keplerian gas motion in a protoplanetary disk (Pinte et al., 2018). It has been suggested that a forming protoplanet could be detected by its heating of dust (Wolf and D’Angelo, 2005). Indirect detection of an exoplanet by the transit method has been suggested as feasible with ALMA, including the possibility of an enhanced transit signature caused by the occlusion of a radio-bright stellar surface feature (Selhorst et al., 2013). Sub-milliarcsecond astrometric detection of an exoplanet with ALMA via the displacement of thermal emission from a stellar photosphere has been studied (Lestrade, 2003). Over 400 nearby stars have been calculated to have thermal flux densities > 0.1 mJy and thus could be detected by ALMA with realistic integration times at the optimal frequency of 345 GHz (for a thermally radiating body where emission ∝ λ−2 as SNR ∝ ν2/ΔS , where ΔS is the noise at frequency ν), with at least 60 stars requiring less than an hour of observation to achieve a SNR = 30 (Lestrade, 2008).

Direct detection is also considered plausible given a sufficiently massive and nearby planet. The planetary flux in Jansky (1 Jy = 10⁻²⁶ W m⁻² Hz⁻¹) at 345 GHz is

\[ F_{345\text{GHz}} = 6 \times 10^{-8} T_p \frac{R_p}{R_J} \left( \frac{1}{d} \right)^2 \]  

(13)

where d is the distance to the system in parsec, T is the planetary temperature in K, and R_p is the planet radius and R_J is Jupiter’s radius (Butler et al., 2004; Perryman, 2014). Cooled Jupiters (a ≥ 0.1 au) are thus only detectable out to ~1 pc. The nearest star system is the triple α Cen which lies at 1.3 pc (van Leeuwen, 2007) and only one additional main-sequence star lies within 2 pc. Limits on the Msini of planets in the classical habitable zones of the α Cen system are 53 M⊕ for component A, 8.4 M⊕ for B, and 0.47 M⊕ or Proxima (Zhao et al., 2018). Furthermore for A planets with Msini > 2 M_J at a < 4 au are ruled out as are planets of Msini > 2.5 M_J at a < 4 au for B (Endl et al., 2001).

A population of free-floating planetary mass objects of 3-15 M_J is expected to be possibly twice as abundant as main sequence stars, given local stellar density (Perryman et al., 1997) we could expect...
∼0.28 planetary mass objects per cubic parsec. Within a spherical volume of radius 1 pc we could thus expect ∼1 such object. The $T_{\text{eff}} = 225-260$ K planetary mass object WISE J085510.83-071442.5 is 2 pc distant and may be a gas giant ejected from its star system (Luhman, 2014). A proto-Jupiter, with a much larger radius $R = 30R_J$ and temperature $T = 2500$ K could be detected out to tens of parsec (Butler et al., 2004).

Stellar (Sub)millimeter Emission

An exoplanet’s host star must be well characterized in order to make inferences regarding exoplanet properties. The stellar mass is required to derive a true mass for a planet detected via radial velocity measurements. The stellar radius must be known to derive a true exoplanet radius when observed in transit. The stellar spectrum must be understood in order to disentangle it from a planetary atmospheric spectrum observed in transit, as well as any variability. In the millimeter and submillimeter the primary sources for stellar opacity are two forms of free-free absorption; electron-ion and $\text{H}^-$ free-free absorption (Reid and Menten, 1997). At wavelengths far below a blackbody’s peak emission wavelength the Rayleigh-Jeans approximation is valid

$$B_\nu \approx \frac{2k_B}{c^2} T_\nu^2$$

These processes result in the continuum thermal emission (Wedemeyer et al., 2016). Several non-thermal mechanisms contribute transiently to the stellar spectrum. Gyrosynchrotron radiation is observed during flaring events as flares form loops filled with accelerated electrons. The gyrosynchrotron solar spectrum peaks at 5-20 GHz.

Stellar spectra which are distinctly non-thermal have been detected in the millimeter enhancing the stellar signal. In the case of the M8.5V ultracool dwarf TVLM 513-46 flux densities were measured to be $66 \pm 8\mu$Jy at 91.46 GHz and $31 \pm 18$ at 103.49 GHz implicating gyrosynchrotron radiation as the origin of non-flaring radio emission in ultracool stars (Williams et al., 2015) while millimeter flares of up to 400 mJy have been observed in T Tauri stars (Furuya et al., 2003; Bower et al., 2003).

Synthetic stellar spectra have been shown to exhibit CO absorption features in the (sub)millimeter originating from the lower chromosphere (Wedemeyer et al., 2016). The pure rotational transitions of CO are predicted such as the $\text{CO} J = 6 \rightarrow 5$ at 691 GHz and the $J = 7 \rightarrow 6$ transition at 806 GHz which fall within the ALMA bands and are expected to be significantly broadened. Water has also been detected where sunspot temperatures fall below 3000 K which could impose significant constraints on the interpretation of transmission spectra from fast-rotating stars (Wallace et al., 1995).

1.4 Aims

We aim to determine the detectability of various spectroscopic signatures of $\text{H}_2\text{O}$ in the (sub)millimeter considering current and future observatories as well as a range of atmospheres, and to determine the suitability of (sub)millimeter astronomy for the spectroscopic characterization of exoplanets.
2 Methods

To test whether ALMA or other (sub)millimeter telescopes could detect exoplanetary H$_2$O we will produce synthetic planetary spectra and compare them with documented or calculated instrumental sensitivities. Spectra will be produced for both transiting and non-transiting cases where the planets are spatially resolved from their host star. To provide a medium from which to produce spectra a general atmospheric model is constructed to simulate a variety of exoplanet atmospheres.

2.1 Ingredients of an Atmospheric Model

In this section we will review the elements of atmospheric physics which are incorporated into the model.

2.1.1 Pressure

Spectral line shapes are functions of pressure via collisional broadening. Consider a slab of a planet’s atmosphere of infinitesimal thickness $dz$, with area $A$ at some altitude $z$. The slab experiences pressure from the surrounding atmosphere. The bottom side of the slab experiences an upwards pressure $p(z)A$ and the top side experiences a downward pressure $p(z+dz)A$. The gravitational pull on the slab results in an additional downwards force of $\rho Agdz$ where $\rho$ is the slab density and $g$ the gravitational acceleration. To be in hydrostatic equilibrium the forces must be equal

$$\rho Agdz = (p(z) - p(z+dz))A$$

Recognizing $p(z+dz) - p(z)$ as the definition of $dp/dz$ and rearranging we find

$$\frac{dp}{dz} = -\rho g$$

Using the ideal gas approximation we can substitute $\rho = pM/RT$ where $p$ is the pressure, $M$ the slab mass, $R$ the gas constant, and $T$ the slab temperature. The ideal gas law is considered a valid approximation for planetary atmospheres [Seager 2010]. This allows us to write

$$\frac{1}{p} \frac{dp}{dz} = -\frac{Mg}{RT}dz$$

Now we can solve for pressure as a function of altitude. In the case of an isothermal atmosphere the expression can be integrated to obtain

$$p(z) = p(0) \exp\left(-\frac{Mg}{RT}z\right)$$

which can further be simplified by the inclusion of the atmospheric scale height. To consider a general atmosphere of arbitrary mean molecular weight we define $R/M = k/\mu$ where $k$ is the Boltzmann constant $1.38 \times 10^{-23}$ J K$^{-1}$ and $\mu$ is the mean molecular mass of an atmospheric particle and take an arbitrary acceleration due to gravity on another planet as $g_p$. The scale height is then defined as

$$H = \frac{kT}{\mu m_H g_p}$$

where $m_H$ is the mass of a Hydrogen atom. Finally we can write the pressure as a function of scale height and altitude in an isothermal atmosphere with a completely mixed (chemically homogeneous such that there is no altitude dependence of $\mu$) atmosphere.

$$p(z) = p(0) \exp(-z/H)$$

For an Earth-like atmospheric composition and surface pressure ($p(0) = 1.01325$ atm) we find a scale height $\sim 8$ km while heavily irradiated Hot Jupiters ($a < 0.1$ au) can have $H = 200 - 500$ km [Showman et al. 2008].
2.1.2 Vertical Temperature Structure

The lower boundary of an atmosphere’s vertical temperature structure is the surface. To determine a surface temperature we assume that all stellar radiation incident on the planet reaches its surface. We assume that the energy of absorbed stellar radiation is evenly distributed around the planet by atmospheric circulation and that the planet surface is entirely homogeneous. We can calculate a planet temperature given an equilibrium between incident radiation and re-emitted power. This is referred to as the equilibrium temperature \( T_{eq} \) seen in equation \( T_{eq} \). This equilibrium temperature formulation is valid only for cloud-free isothermal planets which have reached equilibrium with the stellar radiation field and have a negligible greenhouse effect. In reality rotating planets will have a periodic temperature fluctuations driven by the day-night cycle. A tidally locked planet which rotates once per orbital period will maintain orientation of a single face towards its host star and have a permanently asymmetrical longitudinal dependence of temperature. The planet flux will have an orbital phase dependence that peaks when the planet approaches full phase and reaches a minimum during transit. Denser planetary atmospheres act to more efficiently circulate heat across the terminator while tenuous atmospheres are less efficient at heat circulation (Turbet et al., 2016).

In order to derive a term for the surface temperature rather than the equilibrium temperature we consider a simple 1-layer atmosphere model. This case is known as the ‘leaky greenhouse’ model (Seager and Deming, 2010). Again we assume that all incident stellar radiation reaches the planet surface without scattering. The radiation is absorbed by the planet’s surface layer and re-emitted at longer wavelengths. This radiation then travels upwards and is partially absorbed by the single atmospheric layer. We define the temperature of this layer to be \( T_a \) and the surface temperature to be \( T_s \). We define a greenhouse variable \( \alpha \) ranging from 0-1 where \( \alpha=1 \) represents the case where the atmospheric layer absorbs all radiation which has been re-emitted by the planet surface. From the balance of energy we know that the energy emitted by the atmosphere and the surface must be equal to the absorbed radiation. From this we find

\[
\sigma_R T_{eq}^4 = \sigma_R T_a^4 + \sigma_R T_s^4(1 - \alpha) \tag{21}
\]

where \( \sigma_R \) is the radiation constant. When this equation is solved for the surface temperature \( T_s \) we see that

\[
T_s = \left(\frac{2}{2 - \alpha}\right)^{1/4} T_{eq} \tag{22}
\]

Note that in this model for all cases \( T_s \leq T_{eq} \leq T_a \) which follows from Kirchhoff’s law (Seager, 2010). Equipped with an estimate for the surface temperature we can now explore its evolution with altitude \( z \). In the non-inverted case temperature simply decreases with altitude. The rate at which temperature decreases as a function of altitude is known as the lapse rate. The lapse rate for an adiabatic atmosphere is defined as

\[
\frac{dT}{dz} = -\frac{g}{c_p} \tag{23}
\]

where \( g \) is the local gravitational acceleration [m s\(^{-2}\)] and \( c_p \) is the specific heat capacity of the atmosphere [J kg\(^{-1}\) s\(^{-1}\)] which is a measure of a material’s resistance to an increase in temperature with the absorption of heat per unit mass. Specifically it is the amount of energy that must be transferred to the gas in order to raise its temperature by 1 K. Convection dominates as the form of energy transport within the atmosphere when the lapse rate is small for a large heat capacity. A large lapse rate will be stable against convection (Seager, 2010). Earth like planets with solid surfaces below relatively thin atmospheres are expected to have a convective regime immediately above the surface. This arises from a sharp discontinuity in the temperature of the surface relative to that of the atmosphere directly above it. A large fraction of the incident radiation is absorbed by the surface while a much smaller fraction is absorbed by the atmosphere resulting in a steep temperature gradient. The adiabatic lapse rate is considered a valid approximation for a convection-driven troposphere.
Temperature Inversions

A temperature inversion is a phenomenon where the atmospheric lapse rate switches its sign. Temperature will begin to rise with rising altitude rather than drop and vice versa. A single atmosphere can contain multiple temperature inversions, as has been observed on the Earth. See Fig. 1.

![Temperature Profiles](image)

Figure 1: The vertical axis indicates atmospheric pressure which is used as a proxy for altitude. The horizontal axis displays temperature. The different P-T profiles are shifted arbitrarily for illustrative purposes. The four profiles are a) An isothermal atmosphere, b) A profile where temperature decreases monotonically within the troposphere (adiabatic lapse rate), c) A profile with two temperature inversions, d) A profile with a single temperature inversion.

All solar system planets with substantial atmospheres have temperature inversions at high altitudes, typically near an atmospheric pressure of 0.1 bar. A possible mechanism unifying the solar system thick atmosphere’s temperature inversions has been proposed. At pressure greater than 0.1 bar the atmosphere is relatively opaque to shortwave radiation (optical or UV), convection dominates and this region of the atmosphere contains weather. At pressures below 0.1 bar the atmospheric transparency to thermal radiation allows shortwave heating to dominate, creating a stratosphere. The tropopause is thus found to occur generally at 0.1 bar for the atmospheres of Earth, Jupiter, Saturn, Uranus and Neptune, while kinks appear on the pressure-temperature profile of both Mars and Venus at this pressure altitude (Robinson and Catling [2014]).

In our atmospheric model we will only physically motivate the surface temperature and tropospheric layer of the temperature-pressure profile via the adiabatic lapse rate while the layers above will be parametrized and adjustable.
2.1.3 Chemical Abundances

Today it is known that all of the classical planets host atmospheres of some kind. Mikhail Lomonosov hypothesized the presence of a Venusian atmosphere to explain his 1761 observations of an aureole around Venus during the transit ingress and egress, caused by the refraction of sunlight through the planet’s atmosphere \cite{Shiltsev2014}. Other planets such as Jupiter and Mars were speculated to have atmospheres due to temporarily varying features visible on their disks \cite{Challis1863}. The discovery of spectroscopy allowed for the remote sensing of planet atmosphere compositions. Early spectroscopic observations of the terrestrial planets indicated atmospheric composition different than that of the Earth, including both a lack of oxygen, water, and an overabundance of CO_2 \cite{Webster1927, Adel1937}.

Planetary atmospheres have temperatures below the coolest stars and so are dominated by molecules. Massive gaseous exoplanets are often expected to form with solar abundances initially \cite{Madhusudhan2014, Venot2015}. For gas giants the expected species are H_2, He, H_2O, CO, CH_4, H_2S, Na, K, NH_3 and PH_3 \cite{Burrows2014b}. Other metals are expected to be found at lower atmospheric depths due to differentiation and be spectroscopically unobservable. Terrestrial planet atmosphere abundant species are expected to be N_2, CO_2, HNO_3, with O_2, O_3 and N_2O are expected as possible bio-signatures \cite{Burrows2014b}.

Line lists for our model have been taken from the HITRAN database \cite{Rothman2013}. Absorption cross sections have been calculated for P = 1 bar and T = 300 K for the gases expected to be prevalent in Fig. 2 and for the isotopologues of water in Fig. 3.

\footnote{http://hitran.org/}
Self-consistent chemical models of planetary atmospheres rely on molecular mixing ratios calculated with the assumptions of chemical equilibrium and solar abundances. Hot Jupiter atmospheres are expected to exhibit non-equilibrium chemistry (Liang et al., 2003) demonstrating that chemical equilibrium should not always be assumed (Madhusudhan and Seager, 2009) and is not assumed in our atmospheric model.

2.1.4 Hazes and Clouds

Clouds and hazes are found throughout the atmospheres of the solar system. Clouds form when atmospheric volatile species condense from the gas to the liquid or solid phase. This takes place whenever the partial pressure of vapor $P_V$ exceeds the saturation vapor pressure $P_{cl}$. This occurs where $P_{cl} = P_V / X_c$ where $X_c$ is the molar mixing ratio of the gas (Sánchez-Lavega et al., 2004). The saturation vapor pressure curve of water can be described by the Clapeyron equation

$$\frac{dP_v}{dT} = \frac{L P_v}{R_v T^2}$$

where $L$ is the latent heat of phase transition ($J \, g^{-1}$), $R_v$ is the specific gas constant for the vapor, $P_v$ is the vapor pressure curve and $T$ is the temperature. Note that for water the specific latent heat of fusion is described empirically by $L_{water} = 2500.8 - 2.36 T + 0.0016 T^2 - 0.00006 T^3$ giving a typical value of 334 J g$^{-1}$). In general the latent heat is defined as

$$\left(\frac{\partial L}{\partial T}\right)_P = \Delta C_P$$

where $\Delta C_P$ is the specific heat change between the two phases. Expanding the specific heat at each phase we find the general form of the saturation vapor pressure curve is

$$\ln(P_v) = \ln(C) + \frac{1}{R_v} \left( - \frac{L_0}{T} + \Delta \alpha T + \frac{\Delta \beta}{2} T \right)$$

where $L_0$ is an integration constant, $\alpha$ and $\beta$ are empirical constants for each phase, and the $\Delta$ represents the change in the constants $\alpha$ and $\beta$ between the phase transitions. This equation must be now solved simultaneously with the vertical pressure profile. The points of intersection identify regions of cloud formation.
The pressures at which clouds can form are found by the simultaneous solving of the Claudio-Clapeyron equation and the formula representing the P-T profile of the atmosphere. The points of intersection represent altitudes at which clouds can form. The green curve represents a fiducial inverted P-T profile. The dashed blue line is the saturation vapor pressure of water. The horizontal bars are the sites of cloud formation. Thick cloud cover is not expected to form at the high altitude low-pressure intersections due to low water vapor abundances. In this example clouds are expected to form at approximately 2 km altitude where the pressure is $\sim 0.85$ bar.

Using the values of the empirical constants $\alpha$ and $\beta$ for H$_2$O in an Earth-like atmosphere we can observe multiple points of intersection, the lowest at $P = 0.85$ bar corresponding to an altitude of 1-2 km.

Water cloud induced attenuation in the (sub)millimeter has a strong frequency dependence. Attenuation of 0.06-0.12 dB km$^{-1}$ has been found at 10 GHz increasing to 6-12 dB km$^{-1}$ at 100 GHz (Sarkar and Kumar, 2002), and from the relation found by Chen (1975) up to $10^3$ dB km$^{-1}$ at 1 THz. Typical cloud thicknesses range from 0-12 km, with 6% of clouds of thickness 0-1 km, decreasing linearly to 1% of clouds having a thickness of 11-12 km with 90% of clouds being less than 8 km thick (Wang et al., 2000).

Given that in the transiting geometry the light rays are expected to pass through the cloud layer altitude at least twice (or once if the chord intersects the cloud layer at its maximum vertical extent), and that at 100 GHz a cloud layer 3-4 km thick could cause attenuation by a factor 500-4000, we take the clouds to be opaque. While a planet-encircling cloud cover is known to be possible, Earth-like atmospheres have only partial cloud coverage. In the case of the Earth $\sim 70\%$ of the surface is obscured by clouds at any given time (Stubenrauch et al., 2013). As the transmission signal is averaged over the entire annulus surrounding the planet we consider only the fractional cloud coverage of the entire planet to act on a single ray passing through. This way the fractional cloud coverage becomes an adjustable parameter for every modeled planet atmosphere.

2.1.5 Refraction

Refraction is an optical phenomenon which influences the trajectory of a light ray passing through a medium of variable density. When electromagnetic radiation crosses an interface of changing density at an oblique angle the phenomenon of refraction will act to alter the direction of the light ray. Given a light ray propagating through a medium with index of refraction $n_1$ crossing the interface at an incident angle from the interface normal $\theta_i$ the resulting transmitted exit angle $\theta_t$ is found via Snell’s law

$$n_1 \sin \theta_i = n_2 \sin \theta_t$$

(27)
where \( n_2 \) is the index of refraction of the medium beyond the interface. Refraction in atmospheres is of direct consequence to exoplanet atmospheric study. The denser regions of planet’s atmospheres also have the steepest gradients of temperature and density, so this is where the effect of refraction is expected to be the most pronounced. During a planet transit the light rays will be partially deflected. A sufficiently large deflection will bend a light ray out of the path to the observer on Earth. In effect the high pressure vertical extent of the atmospheres can be shielded from observation via transit spectroscopy. It has been determined that the lower 20 km of an Earth-like atmosphere of a planet orbiting a Sun-like star may be rendered opaque, reducing the depth of transit features by as much as 60\% (Misra et al., 2014).

The index of refraction of a medium is frequency dependent, which allows for the dispersion of light by its transmittance through a prism. In the submillimeter regime the index of refraction of air can be described by a function of pressure and temperature

\[
(n - 1) \times 10^6 = 105.65 \frac{P_{N_2}}{T} + \frac{86.26(5748 + T)}{T^2} P_{H_2O} + 1.5P_{H_2O}
\]  

(28)

where \( n \) is the index of refraction, \( P_{N_2} \) is the partial \( N_2 \) pressure, \( P_{H_2O} \) is the partial \( H_2O \) pressure, and \( T \) is the temperature (Chamberlain et al., 1965). Note that this formula was calculated at 889 GHz and variations in \( n \) occur due to contributions to the refractive index from rotational \( H_2O \) transitions and other contributions from dimeric water vapor molecules are also not considered. The relation can be considered accurate within \( \pm 3\% \) (Bradley and Gebbie, 1971).

I have constructed a ray tracing model to study the propagation of (sub)millimeter radiation through a planet’s atmosphere. Each ray is initialized with an orientation tangential to the planet terminator in transit. An observer at distances > 1 pc will only be able to observe the light rays which exit the planet atmosphere collimated along the star-planet axis. In order to determine which light rays could reach the observer the simulation is run in reverse. The “initial” ray orientation is taken to be the final orientation. Once the light rays are refracted through the atmosphere in reverse each entrance angle is recorded. Entrance angles which would be incident on the stellar disk thus represent light rays which could plausibly have been emitted by the star. The angular size of the host star as seen from the planet can be calculated by

\[
\theta = \arctan \left( \frac{0.5R_*}{a} \right)
\]

(29)

where \( \theta \) is the stellar angular target that the rays must intersect to be emitted, \( R_* \) is the stellar radius, and \( a \) is the planet orbital distance during the transit. The rays propagate over a distance \( H \) per time step. At each position their local temperature and pressure is calculated on the basis of a specified P-T profile. The local partial pressure of water vapor is also calculated and from this information the local index of refraction is calculated. At every time step the rays refract by the ratio of their previous and current indices of refraction. The initial ray \( n \) at atmospheric interface is set to 1. In Fig. it can be seen that the rays exiting the atmosphere (on the left) corresponding to the lowest altitudes probed cannot originate from the stellar disk, as they would need to originate on the planet surface - this corresponds to the low-altitude cutoff ‘refraction floor’.
Figure 5: A side-view of the transit geometry. The bending of light by refraction is apparent and where $\delta P$ is large. The dark curved region near the bottom is the planet surface boundary. Note the vertical exaggeration of the diagram. Light rays propagate from right to left although the simulation was run in reverse from left to right.

Several cases of stellar size and planetary orbit combinations are considered and are presented as the horizontal lines in Fig. 6 for a wavelength of 0.3 mm. Planets at wide orbital angular separation suffer restrictions on the altitudes which can be probed by transmission spectroscopy. For a planet orbiting a Sun-like star at 1 au we find a refraction floor of 25 km. For a planet orbiting in the classical habitable zone of an M-dwarf with $R = 0.12R_\odot$ the refraction floor is lower at 5 km, which would begin to intersect with large topographic surface features. The worst case scenario is a planet in a large orbit ($a > 5$ au) around a small star ($R < 0.2R_\odot$) as $\theta \to 0$ for ever wider orbits and smaller stars.

Figure 6: The vertical axis displays the entrance angle of light rays into the atmosphere. The horizontal lines indicate the cut-off for several arrangements of stellar radii and planetary orbits a) Earth orbit around Sun-like star, b) Jupiter orbit around Sun-like star c) Trappist-1 D orbit and star. The refraction floor can be found by the reading off the initial ray altitude value at the intersection of the blue line with the various horizontal lines. The red shaded region represents rays which have intersected the planetary surface. Small fluctuations in the relation are the result of numerical precision in the atmospheric spatial grid and discontinuities in the water vapor abundance profile.
From Fig. 6 we see that the lower kilometers of an Earth-like planet atmosphere are less accessible to transit spectroscopy. The resulting submillimeter index of refraction does not materially alter the conclusion of authors that have studied refraction during transit spectroscopy in the infrared and optical wavelength ranges (Alp and Demory, 2018). Only scattering will allow for some rays to have passed through the atmospheric regions highest pressure and also reach the observer, but is ignored in our model. The light which passes below the refraction floor reaches the observer out-of-transit. We have found that refraction will limit the possibility of water detection on terrestrial exoplanets given a heterogeneous vertical H2O distribution where condensation and weather keep the bulk of H2O near the planet surface. However this effect is far less pronounced in the case of planets orbiting very near their host star - such as temperate zone M dwarf orbiting planets.

2.1.6 Doppler Shift

Ground-based observation of water necessitates that the doppler shift of the lines is large enough to be distinguished from contaminating telluric lines (Encrenaz, 2008). A radial velocity of 30 km s\(^{-1}\) was sufficient for the detection of water in Halley’s comet at 2.65 \(\mu\)m (Mumma et al., 1986). Exoplanet motion relative to the Earth is two-component. Exoplanets are gravitationally bound to their host stars and the star’s motion through space is the constant systemic component. The varying component is the planet’s orbital motion around its host star. FGKM stars in the stellar neighborhood have a standard deviation in radial velocity of approximately 25 km s\(^{-1}\). The planetary radial velocity will oscillate around the stellar velocity. The amplitude of the induced radial velocity periodicity is proportional to the cosine of the system inclination. An orbit inclined at \(i = 90^\circ\) (face-on) will induce no radial velocity variations. A 0° inclined orbit (seen edge-on) will result in an a maximal observed radial velocity variation over an orbital half-period of \(\pm v_o\). Circular and elliptical orbits of planets in stable orbital configuration will to first order follow Keplerian motion. Keplerian instantaneous orbital velocity for an elliptical orbit can be calculated by

\[
v_o = \sqrt{\frac{GM}{a}} \left(\frac{2}{r} - \frac{1}{a}\right) \tag{30}\]

where \(G\) is the gravitational constant \(6.674 \times 10^{-11}\) m\(^3\) kg\(^{-1}\) s\(^{-2}\), \(M\) is the mass of the host star, \(r\) is the instantaneous planet-star separation, and \(a\) is the planet’s orbital semi-major axis. For a circular orbit where \(r = a\) we find \(v_o = \sqrt{GM/a}\). From this we can approximate the velocity of several known exoplanets. For the Earth we find a velocity of approximately 30 km s\(^{-1}\). The shorter period Mercury has an orbital velocity of 47.5 km s\(^{-1}\) and so would produce a radial velocity peak-to-peak amplitude of more than 90 km s\(^{-1}\). Jupiter orbits at a stately 13 km s\(^{-1}\). For the exoplanet TRAPPIST-1b with \(a = 0.011\) au we find \(v_o = 80\) km s\(^{-1}\). Hence in the case of short period exoplanets the planetary periodic radial velocity signal can be in excess of the stellar systemic radial velocity.

During a planetary transit the planetary radial velocity for a circular orbit is near zero. For an elliptical orbit it is possible that there will still be non-zero radial velocity during transit. Consider an extreme case of a planet with orbital eccentricity \(e = 0.9\) orbiting a \(M = 1\ M_\odot\) star. We orient the planet relative to Earth such that the angle between the Earth-star axis and the planet’s semi-major axis is 45° with the apoapsis on the near side of the star. In this case when a planet transits the true anomaly \(f\) will be 135°. With a semi-major axis of \(a = 1\) we find from the relation \(b = a(1 - e^2)^{0.5}\) that \(b = 0.43\) au. We can determine the planet’s instantaneous orbital radius with

\[
r = \frac{a(1 - e^2)}{1 + e \cos f} \tag{31}\]

The periapsis is then 0.1 au and the orbital distance \(r\) at the moment of transit is approximately 0.52 au. Then \(v_o = 53\) km s\(^{-1}\). At the moment of transit the angle between the Earth-star axis and the planet’s velocity vector is approximately 25°. The radial velocity is thus 53cos25° km s\(^{-1}\), or 48 km s\(^{-1}\). This is an increase by a factor 1.6 over a purely circular velocity. We consider this near the
limiting plausible case for an eccentric orbit velocity deviation from the circular approximation [Kane et al., 2012].

Even during a transit of a circularly orbiting planet the Doppler effect may contribute to the spectrum via rotational broadening. We consider the case of planetary rotation. Planet rotational velocity is thought to scale with planet mass with the relation \( v_{\text{rot}} \propto \sqrt{M} \) [Scholz et al., 2018]. The Earth’s rotational velocity is given by \( 460 \cos l \text{ m s}^{-1} \) where \( l \) is the angle of longitude as measured from the equator (±90°). Hence it is maximal at the equator (460 m s\(^{-1}\)) and minimal at the rotational poles. See Fig. 7 for a representation of the radial velocity field over the planet disk.

Figure 7: An illustrative representation of the radial velocity over a planet’s disk in the case of a where it is viewed stereographically along its equator. The planet’s rotational axis is vertical. The equatorial rotational velocity is 500 m s\(^{-1}\).

Jupiter experiences differential rotation as its latitudinal atmospheric bands rotate at differing velocities. Atmospheric winds can enhance the observed Doppler shift. Jupiter has been measured to rotate at \( \sim 12 \text{ km s}^{-1} \) [Higgins et al., 2011] and the exoplanet β Pic b has had its rotation rate measured to be greater than that of any solar system planet [Snellen et al., 2014] in line with the mass-rotational velocity relation. CO lines detected from β Pic b have a measured broadening of 25 ± 3 km s\(^{-1}\).

In summary we have found that planets will experience a typical systemic radial velocity on the order of 25 km s\(^{-1}\). Orbital velocities for short period planets may approach 80-100 km s\(^{-1}\), but not during transit except in the most extreme case of eccentric orbits with favorable alignments. Rotational velocity of planets will broaden emission due to the redshifted light emitting from the retrograde hemisphere and blueshifted light emitting from the prograde hemisphere, although this effect will be most pronounced at the equator and vanish at the poles for planets with their rotational axis normal to their orbital plane.

2.2 Radiative Transfer

Before introducing our spectral modeling tool we review the fundamentals of radiative transfer. SPAM uses HAPI in order to compute radiative transfer [Kochanov et al., 2016]. The intensity of electromagnetic radiation received \( I_\nu \) (W m\(^{-2}\) Hz\(^{-1}\) sr\(^{-1}\)) on an infinitesimal surface area d\( \sigma \) (m\(^2\)) is defined as

\[
dP = I_\nu \cos \theta \, d\Omega \, d\sigma \, d\nu \tag{32}
\]

where dP is the power (Watts), \( \theta \) is the angle between the direction to the emitting region d\( \Omega \) (steradian) and the normal to the surface d\( \sigma \), and d\( \nu \) is the frequency range (Hz). The equation of radiative transfer describes the absorption and emission processes that influence a ray of electromagnetic radiation as it
travels through a medium, such as a volume of gas over a distance \( s \). In a plane-parallel atmospheric approximation we define \( \mu = \cos \theta = dz / ds \). The time-independent plane-parallel form of the radiative transfer equation is then

\[ \mu \frac{dI_\nu}{ds} = -\kappa_\nu I_\nu + \epsilon_\nu \] (33)

where \( \kappa_\nu \) is the frequency dependent extinction coefficient, \( \epsilon_\nu \) is the emission coefficient (Seager and Deming [2010]). In the condition of local thermodynamic equilibrium Kirchhoff’s law applies. Kirchhoff’s law states that for any body emitting and absorbing thermal radiation at all frequencies in equilibrium, the ratio of the emissive power to the absorption coefficient is equal to a universal blackbody emissive power function of temperature.

\[ \frac{\epsilon_\nu}{\kappa_\nu} = B_\nu(T) \] (34)

We can now define the dimensionless optical depth \( \tau \), the logarithm of the ratio of incident to transmitted power

\[ d\tau_\nu = -\kappa_\nu ds \] (35)

substituting this definition into the equation radiative transfer we find

\[ -\frac{1}{\kappa_\nu} \frac{dI_\nu}{ds} = \frac{dI_\nu}{d\tau_\nu} = I_\nu - B_\nu(T) \] (36)

which, when solved and integrated results in the expression

\[ I_\nu = I_\nu(0)e^{-\tau} + B_\nu(1 - e^{-\tau}) \] (37)

Note that in the optically thick limit where \( \tau \to \infty \) the equation reduces to \( I_\nu = B_\nu \) and the resultant spectrum is purely thermal. This limit is valid for solid planetary surfaces although optical depth is dependent on wavelength and light will probe to different depths in the planet atmosphere at different wavelengths for a given opacity.

The function \( B_\nu \) describes the spectral distribution of thermally radiating blackbodies in equilibrium. It is given by the Planck law

\[ B_\nu = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1} \] (38)

The combination of equations (33) and (38) forms the core of the HAPI radiative transfer code.

2.3 SPAM, the Simple Planetary Atmospheric Model

The 2D atmospheric model dubbed ‘Simple Planetary Atmospheric Model’ (SPAM) is Python code we have written around the HITRAN Application Programming Interface (HAPI) radiative transfer code (Kochanov et al., 2016). SPAM allows for the flexible handling of multiple observation geometries, atmospheric chemical compositions, temperature-pressure profiles, planetary dimensions, surface gravities, and orbital parameters over the same range of frequencies and temperatures which HAPI is able to process. HITRAN (High Resolution Transmission) is a database with spectroscopic parameters for high resolution line transitions. HITRAN parameters are a mixture of experimentally determined values, theoretical calculations, and semi-empirical values. HITRAN includes data for 47 molecular species and their isotopologues.

SPAM computes the effects of refraction and cloud absorption on light passing through planet atmospheres. SPAM is limited in that it cannot yet allow a variable vertical abundance profile of more than two chemical species simultaneously, it does not compute self-consistent chemical abundances, it does

\[ \text{http://hitran.org/hapi/} \]
\[ \text{http://hitran.org/} \]
not physically motivate the vertical temperature structure by iteratively solving the radiative transfer,
hydrostatic and radiative equilibrium equations, and does not consider orbital phase-dependent observa-
tional effects. Further limitations involve the approximation of a plane-parallel emitting surface rather
than a spherical model, and no modeling of heat redistribution within the planet’s atmosphere is per-
formed. Planets surfaces are taken to be perfect black-bodies with isothermal surface conditions, with
no latitudinal dependence on temperature.

2.3.1 HAPI

The core of SPAM is the HITRAN Application Programming Interface (HAPI) (Kochanov et al., 2016).
HAPI is a set of Python routines which allow access to the HITRANNonline functionality. HAPI allows
for high-resolution spectral simulation as a function of temperature, pressure, and optical path length.
Absorption, transmission, and radiance spectra can be calculated with the implementation of conven-
tional line profiles such as the Gaussian, Lorentzian, or Voigt profiles. Furthermore HAPI allows for
the convolution of spectra with instrumental effects to simulate observations (Kochanov et al., 2016).
The temperature range which HAPI can consider is limited to 70-3000 K. Strongly irradiated exoplanets
such as the $T_{\text{eq}} = 7600$ K planet Kepler-70b can thus not be considered (Charpinet et al., 2011). An
additional limitation is that HAPI uses only lines which appear in the HITRAN database, where the
wavenumber range coverage of various isotopologues is not always complete over 0-50 cm$^{-1}$ such that
not all isotopologues of the atmospheric gases considered could be included in the model atmospheres.

2.3.2 Model Process

In this section we will describe the process by which the combined atmospheric-radiative transfer model
produces spectra.

Initialization

The model is initialized by loading a standard user-defined template parameter file described in Table
3. From the input parameters that define the various atmospheric gas abundances and their respective
molecular weights the model calculates the atmospheric mean molecular weight $\mu_m$. Combining $\mu_m$ with
the surface gravity $g$ and temperature $T$ input parameters the atmospheric scale height $H$ is calculated
by eq.19. Given that the overall physical dimensions of the planet’s atmosphere are dictated by the
atmospheric scale height, $H$ is used to define the vertical grid resolution for the transiting geometry
model. The user specifies what fraction or multiple of $H$ by which to subdivide the grid in the vertical
axis. There is no pressure gradient dependence of the grid dimensions; i.e. the steeper pressure gradients
near the planet surface do not result in a more finely subdivided sampling grid.

Given the input handles $t_0$, $t_1$, $t_2$, $t_3$ the log-interpolator module simpletemp generates a smooth,
continuous temperature-pressure profile. The four temperature parameters are each assigned to prede-
termined log-spaced pressure intervals. In the case of $t_0 = t_1 = t_2 = t_3$ the atmosphere is said to be
isothermal. In the case where $t_1, t_2$ or $t_3 > t_0$ the atmosphere is said to be inverted. Up to two inversions
can be specified in this manner. The reasoning for the first handle being placed at a pressure of 0.1 bar
follows from the results of Robinson and Catling (2014) however for input values of $p_0 < 1$ the handles
are shifted proportionately.

After the temperature-pressure profile has been calculated the raytracing module raytracer is called.
raytracer calculates the refraction floor $z_{\text{floor}}$, the altitude at which refraction prevents unscattered light
from reaching an observer on Earth. This value is passed back to SPAM which will then avoid computing
radiative transfer along chords which pass below $z_{\text{floor}}$.

The temperature-pressure profile is also passed to the cloudcover module which uses the Claudius-
Clapeyron equation to determine the pressures at which water clouds would be expected to form in the
atmosphere. These pressures are then converted back to altitudes and SPAM is then able to include the
absorption effect of the clouds on light rays which pass through these cloud layers as described in § 2.1.4.
Whether or not a particular atmosphere should include clouds can also be toggled by the user. Only
water clouds are included and cloud formation conditions for other volatiles such as NH$_3$ are not included.

Figure 8: Illustrated representation of the model geometry. (i) An isometric overview of the transit model geometry. The stellar light (a) passes through the planet atmosphere (b) and produces an annulus of partially absorbed light (c). (ii) the side view of the transit in detail viewed along the Y axis. The light rays (c) enters the atmosphere (b). The model splits the atmosphere into a grid of slabs (d) in which pressure, temperature, and chemical abundances are individually calculated. Absorption coefficients can then be calculated for the gas mixture within each cell.

Model Radiative Transfer

After the atmospheric model has been completely initialized the radiative transfer can begin. For a given atmospheric slab HAPI splits the spectral synthesis into distinct absorption and emission spectra. In the case of the transiting geometry, a light ray begins at the edge of the planet’s atmosphere and travels along a chord as seen in Fig.8(ii). The light ray is initialized as a stellar blackbody emission spectrum. The chord is split into slabs by the tangential resolution parameter. At every slab along the chord an absorption and emission spectra are separately calculated by HAPI. First the absorption
coefficients are determined by the HAPI function `absorptionCoefficient_Voigt` which requires as input the relative abundances of species in the gas as well as the environmental parameters of temperature and pressure. The Voigt line profile is a convolution of the Gaussian and Lorentzian line profiles, appearing more Gaussian near line center. In HAPI the Voigt profile is based on the Hartmann-Tran profile [Tran et al., 2013]. Line parameters for the relevant species are taken from the HITRAN database. The partition function is calculated by `PYTIPS` a C implementation of the Total Internal Partition Sums (TIPS) as a function of the species and temperature [Cubillos et al., 2016]. Doppler and collisional broadening terms are calculated with environmental dependence. The final absorption coefficients are calculated as a multiple of the relative abundances, the line intensity, and the line shape which are then summed for every line within the specified wavenumber range out to a specified maximum line wing size.

Within a single atmospheric slab conditions are homogeneous along the slab length $x$ such that we can say

$$\tau_{\text{slab}} = \int_0^x \kappa \, dx = x \kappa$$  \hspace{1cm} (39)

Given that the absorption coefficient $\kappa$ varies with $P$, $T$ and the abundances $X$ the subdivision of the atmosphere into slabs (by the tangential resolution $r_t=x$) allows us to take into account the varying conditions in the atmosphere through which the light ray propagates.

The initially un-attenuated stellar spectrum is partially absorbed by multiplying it by the dimensionless transmittance spectrum defined by $e^{-\kappa x}$ where $x$ is both the slab length and optical path. The radiance spectrum is multiplied by $(1-e^{-\kappa x})$ and then added to this attenuated stellar light resulting in a new spectrum which has taken into account absorption and emission processes within the slab. The resulting combined spectrum is then passed into the next slab along the chord where the process is repeated until the light ray eventually exits the atmosphere.

The atmosphere is sampled vertically by multiple chords being initialized at different altitudes (see Fig. 8 (ii) (a)). Each new chord begins at an altitude determined by the vertical resolution parameter. The vertical range begins at the refraction floor and extends up to an altitude of $10H$. Once a spectrum along a single chord has been fully computed it is stored. A single chord’s spectrum is taken to be representative of an annulus corresponding to the chord altitude and vertical height. The annulus for a chord calculated at altitude $z$ thus has an inner radius $z$ and outer radius $z+dz$ where $dz$ is the vertical resolution of the model. Once all annuli have a spectrum computed the annular spectra are combined and weighted by their relative areas. The contribution of the planet atmosphere $\delta$ to the stellar spectrum is calculated analytically and the absorption features are scaled proportionately in the final output spectrum based on the relative star-planet radii. For the transit geometry spectral normalization is calculated by dividing out the initial source stellar blackbody curve. Stellar spectra are always assumed to be purely thermal in the model. For the spatially resolved emission geometry the normalization is performed by dividing out the planetary blackbody.

In the emission geometry case radiative transfer is only calculated along a single chord normal to the planet surface. The atmosphere is plane-parallel. The atmosphere is vertically subdivided into multiple slabs where pressure, temperature and chemical abundances are input to HAPI’s absorption coefficient calculator and spectral synthesizer. Radiative transfer is performed from $z = 0$ to $z = 10H$. The extent of atmospheres is typically taken to lie somewhere between 5 and 10 scale heights [Seager et al., 2009] above which stellar ionizing radiation can lead to photodissociation of molecules and escape of the lighter dissociation products.

6https://github.com/pcubillos/pytips
2.3.3 Numerical Precision

The numerical precision of the model atmosphere and radiative transfer code rests primarily on two aspects; first, the spatial grid resolution of the atmosphere. Secondly, the wavenumber resolution of the HAPI code.

What happens when the atmosphere is spatially undersampled? The sampling of the various temperature-pressure regimes is then too sparse and no longer representative of the annulus. Most importantly the region of the atmosphere with the largest gradient in pressure and chemical abundances is the troposphere, i.e. the lower several kilometers near the surface. If this region is not sampled effectively the representativeness of the spectra will be compromised. The net absorption over the entire spectrum is calculated and used as a proxy for precision, given that increased precision tends to produce more continuum absorption (seen in Fig.10) but converges rapidly with increasing resolution. Generally an undersampled grid returns a lower net absorption, likely due to significantly broadened lines in the troposphere. This net absorption is calculated for a series of resolution values. SPAM has two spatial resolution parameters. The first is the vertical resolution and the second is the tangential resolution (relative to the planet’s surface at the terminator). The vertical spatial resolution is input as a multiple of the atmospheric scale height $H$ while the tangential resolution is set as a fraction of the planet radius. In this example the net absorption has been calculated for a terrestrial planet’s atmosphere with an $H$
∼ 10 km. Values are calculated over a range of vertical resolution from 1-10 km, and over a tangential resolution of 50-1000 km. Note that the tangential chord through which the light rays pass is typically 20× the vertical extent of the planet’s atmosphere.

A typical effect of altering the spatial sampling resolution is a net increase or decrease in absorption uniformly across the entire generated spectrum. This net absorption variation is quantified as a function of vertical and tangential spatial resolution in Fig.9 and displayed in Fig.10. This net absorption variation is also quantified as a function of wavenumber resolution in Fig.11. The wavenumber resolution of HAPI sets the channel width of a synthetic spectrum.

Figure 9: Results of varying the spatial sampling of an Earth-like atmosphere in units of H (scale height) for a simulation with wavenumber resolution \( r_\Omega = 0.01 \). The color signifies deviation from the net absorption calculated over the entire spectrum relative to the most finely sampled grid.

It is found that variations of up to ∼8% are found over the considered range of sampling resolutions in Fig.9. A strong dependence on tangential resolution is found to be absent. Vertical resolutions of < 10 km are found to be necessary for Earth-like vertical water abundance profiles which vary dramatically in the troposphere. A second consequence of an undersampled grid is that light rays which pass through clouds effectively skip across the cloud layer without triggering the “in cloud” condition which calculates additional absorption. In order to be guaranteed to strike a cloud layer in its path the light ray’s tangential resolution can be no more than the length of the chord intersecting the annulus representing the cloud layer.
Figure 10: The dependence of the spectral offset on the vertical and tangential spatial resolution. Note the much stronger dependence on the vertical sampling of the atmosphere.

Figure 11: The offset is defined as difference between the mean of the normalized planet transmission spectrum for an arbitrary wavenumber resolution and the default HAPI $R = 0.01$ cm$^{-1}$.

A low wavenumber resolution decreases the processing time required to generate a single spectrum but will in effect reduce the contrast of spectral features which are typically on the order of 0.5-1 GHz. Some balance must be found between the computation time of a single spectrum and the precision. In Fig. 13 it can be seen that wavenumber resolutions below the HAPI recommended 0.01 begin to lose substantial structure in the spectrum. From wavenumber resolution 0.1 $\rightarrow$ 0.01 line contrast increases. The depth of spectral features converges quickly after 0.005 and becomes difficult to distinguish for resolutions smaller than 0.001.
**Figure 12:** A very steep dependence of computer processing time on wavenumber resolution is found.

**Figure 13:** Influence of the wavenumber step resolution $r_\Omega$ [cm$^{-1}$] on the spectral line shapes. The wavelength ranges chosen are to illustrate the effect on both emission and absorption features.

### 2.3.4 Validation

In order to validate the use of HAPI we first construct a 1D model of the Earth’s atmosphere to compare with studies of submillimeter transmission [Pardo et al., 2001]. Molecular absorption coefficients are calculated by HAPI from the local temperature, pressure, and molecular abundance ratios.

**The Earth’s Atmosphere**

The Earth is surrounded by a thin ($P_0 = 1013.25$ mbar [Jacob, 1999]) gaseous envelope. Clouds cover 68% of the planet’s surface on average [Stubenrauch et al., 2013]. Approximately 85% of the mass of the Earth’s atmosphere is found in the lowest layer; the troposphere [Seager, 2010] which extends to an altitude $z \approx 5 – 20$ km. Within this layer gas temperature decreases with increasing altitude and most weather phenomena occur. In order to determine the atmospheric temperature and pressure at
each altitude, a toy P-T profile based upon the NASA Glenn Research Center Earth Atmosphere model has been created. The model includes relations for four regimes; the meso- to thermosphere (altitude \( z > 50 \) km), the upper stratosphere (50 km > \( z > 25 \) km) where temperature increases with altitude as a result of \( \text{O}_3 \) UV-photodissociation, the lower stratosphere (11 km < \( z < 25 \) km), and the troposphere (\( z < 11 \) km). The model can be seen in Fig.14.

Figure 14: Pressure and Temperature profile of a 1D Earth-like planet, with surface pressure \( P = 1 \) atm, surface temperature 288 K. Based on the NASA Glenn Research Center Earth atmospheric model. Note that 1 atm = 1.01325 bar.

This exact pressure-temperature (P-T) structure is most likely unique to the Earth’s gravitational field, its atmospheric total mass, chemical abundances and radiation field. However the presence of clouds, aerosols, and temperature inversions are now expected to be commonly occurring properties of planet atmospheres given their frequent occurrence in the atmospheres of the solar system [Madhusudhan et al. 2014]. The interpretation of spectroscopic observations of exoplanet atmospheres relies on an understanding of the local conditions in each layer of the planet’s atmosphere which are probed. The local pressure, temperature, and chemical abundances must be known in order to calculate a synthetic spectrum.

Abundance profiles of the most prevalent molecular constituents of the Earth’s atmosphere have also been included. While we include in these simulations gaseous \( \text{H}_2\text{O} \), \( \text{O}_2 \), \( \text{CO}_2 \), \( \text{N}_2 \), and \( \text{CH}_4 \), only \( \text{H}_2\text{O} \) and \( \text{O}_2 \) are expected to produce strong absorption features in the (sub)millimeter. In the Earth’s atmosphere, \( \text{O}_2 \), \( \text{CO}_2 \), and \( \text{N}_2 \) abundances have weak dependence on \( z \) while atmospheric water vapor does have a strong dependence on \( z \). Due to the sensitivity of (sub)millimeter transmission to \( \text{H}_2\text{O} \) gas and the strongly variable \( X_{\text{H}_2\text{O}}(z) \) we consider a more detailed abundance profile as a function of altitude. We construct a profile from the results of the Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment [Irion et al. 2002]. ATMOS measured the detailed composition of the Earth’s atmosphere from 20-120 km at 2-3 km vertical resolution over the 2-16 \( \mu \text{m} \) band from orbit. The ATMOS experiment spectra were generated by transmission of sunlight through the Earth’s atmosphere as seen from low Earth orbit. Atmospheric refraction and significant absorption prevented reliable abundance ratio determinations at \( z < 20 \) km although in-situ measurements at the surface level do exist.

7https://www.grc.nasa.gov/www/K-12/airplane/atmosmet.html
Each ATMOS spectrum is generated at a single latitude. H$_2$O abundance profiles derived from these spectra are then averaged over all sampled latitudes. The H$_2$O abundance is extrapolated beyond the low altitude limit of the ATMOS data with the relation $n_{\text{H}_2\text{O}} \propto e^{-0.5z}$, the result from which we find to be consistent with observed surface variability in water vapor. The resulting data is interpolated to allow for arbitrary vertical sampling of the profile. Results can be seen in Fig. 15.

On Earth the bulk of water is contained within the troposphere at $z < 20$ km. Volume mixing ratios are significantly variable and sensitive to local conditions, ranging from 0.01% at 230K to 4.24% at 300K (McElroy 2002). By calculating the transmission spectra starting from an altitude of 5000 m (the elevation of the ALMA at the Chajnantor plateau) we avoid some of the uncertainty introduced in near-surface water vapor abundance. Generating transmission spectra as would be seen by ALMA allowed us to compare the result with a relevant and well characterized range of atmospheric absorption features.
Figure 16: Earth atmospheric transmission as calculated with HAPI for pwv = 0.5 mm at altitude 5000 m using the gases H$_2$O, N$_2$, O$_2$, CH$_4$ and CO$_2$. Vertical abundances profiles for H$_2$O are derived from the ATMOS experiment. Almost all absorption is due to O$_2$ and H$_2$O; see Fig. 17.

Figure 17: Earth atmospheric absorption coefficients for H$_2$O and O$_2$ which cause the majority of (sub)millimeter absorption. Coefficients are weighted by the relative molecular abundances.

For the radiative transfer calculations the atmosphere has been divided into 100 linearly spaced slabs. Each slab has a single transmission spectrum calculated and these are multiplied in order to calculate the total transmission from the top of the atmosphere down to the observatory. For Earth with a mean molecular weight $\sim 30$ amu, we find $H = 8$ km. Each vertical slab of the atmosphere was then assigned a temperature, pressure, and a set of relative chemical abundances in order to calculate local absorption coefficients for Voigt profiles. The final product represents absorption or transmission from a light ray path normal to the surface extending from an altitude $10H$ down to the 5000 m ($\sim 0.6H$). These results can be seen in Fig. 16 and the features are can be identified in Fig. 17.
2.4 Sensitivity Calculations

In order to detect an astronomical source the brightness temperature of the source must be larger than the $T_{\text{rms}}$ of the integration (typically the detection threshold requires $T_{\text{source}}>3T_{\text{rms}}$). $T_{\text{rms}}$ can be reduced by increasing the number of samples of $T_{\text{sys}}$ by integrating the signal over time or increasing the bandwidth. The radiometer equation states

$$T_{\text{rms}} = \sqrt{\frac{2T_{\text{sys}}}{\Delta\nu t}}$$

where $T_{\text{sys}} = (1-e^{-\tau})T_{\text{sky}}+T_{\text{rx}}+T_{\text{ cmb}}+T_{\text{rsb}}$, $t$ is the integration time, $\Delta\nu$ is the bandwidth, and together the term $\Delta\nu t$ represents the number of independent samples. $T_{\text{sky}}$ is the sky temperature and $\tau$ is its optical depth, $T_{\text{rx}}$ is the receiver temperature, $T_{\text{ cmb}}$ is the cosmic microwave background temperature, and $T_{\text{rsb}}$ is the radio source background defined as

$$
\left(\frac{T_{\text{rsb}}}{0.1\text{K}}\right) = \left(\frac{\nu}{1.4\text{GHz}}\right)^{-2.7}
$$

The sensitivity of a telescope can be expressed in units of flux density as $\sigma_{\text{rms}}$ for which we use the expression

$$\sigma_{\text{rms}} = \frac{\rho T_{\text{sys}}}{\eta_p N (N-1) n_p \Delta\nu t^{\text{int}}}
$$

Comparing this sensitivity model with documented ALMA sensitivity we can validate its results

![Figure 18: Comparison of the documented ALMA sensitivity for a 60 s integration with $\Delta\nu = 8$ GHz over the instrumental wavelength coverage and the custom model. The residual is calculated as the ratio between the modeled and documented sensitivity in the ALMA technical handbook](https://www.iram.fr/IRAMFR/ARC/documents/cycle6/ALMA_Cycle6_Technical_Handbook.pdf)

The model can now be adjusted to simulate an arbitrary interferometric radio telescope where the parameters listed in Table 4 can be adjusted. Parameters for ALMA, estimated parameters for SKA, and theoretical parameters for a fictional "Next Generation Millimeter Array" are presented in Table 4.
Table 4: Radio Telescope Sensitivity Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>ALMA</th>
<th>SKA</th>
<th>NGMA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Antenna diameter</td>
<td>$D$</td>
<td>12</td>
<td>9-15</td>
</tr>
<tr>
<td>Aperture efficiency</td>
<td>$\rho$</td>
<td>0.75-0.45</td>
<td>1</td>
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<tr>
<td>System temperature</td>
<td>$T_{\text{sys}}$</td>
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<td>10 K</td>
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<td>Correlator efficiency</td>
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<td>0.95</td>
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<td>3000</td>
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<td>Number of polarizations</td>
<td>$N_p$</td>
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<td>2</td>
</tr>
<tr>
<td>Bandwidth</td>
<td>$\delta\nu$</td>
<td>8 GHz</td>
<td>350 MHz</td>
</tr>
<tr>
<td>Frequency Range</td>
<td></td>
<td>35-950 GHz</td>
<td>0.07-25 GHz</td>
</tr>
</tbody>
</table>

For the SKA the stated capability goal is $A_{\text{eff}}/T_{\text{sys}} = 12000$ m$^2$ K$^{-1}$. (Cordes, 2005) Following from

$$P_\nu = k_B T_{\text{sys}} = \frac{S_{\text{sys}} A_{\text{eff}}}{2}$$

we find $S_{\text{sys}} = 0.23$ Jy. From the radiometer equation $\sigma_{\text{rms}} = 0.23$ Jy / $\sqrt{2 \delta \nu t_{\text{int}}}$ for $\delta \nu = 350$ MHz and $t_{\text{int}} = 10^6$ s we find $\sigma_{\text{rms}} = 9$ nJy beam$^{-1}$

Figure 19: ALMA sensitivity for multiple integration times as a function of observing frequency. Note that $10^6$ s is approximately 12 days.

The sensitivity model can now be applied to the results of the atmospheric model and radiative transfer code to determine necessary exposure times or telescope parameters to detect arbitrary signals.
3 Results

3.1 Parameter Space

The basis of the parameter space exploration are the “archetypical planets” found in Table 5. These are a set of 5 planets and 1 moon constituting a mix of solar system and extrasolar objects (hereafter simply referred to as planets). The planets have been selected for their natural variety of dimensions, orbital parameters, atmospheric properties, host stars and insolation. Four terrestrial sized $R < 1.5 R_\oplus$ planets are included as well as 2 Jovian planets. Each planet will have spectra generated for a variety of planet parameters. The parameters of the archetype templates can be found in Table 5 and Table 6 and the parameter space which will be explored is found in Table.

Table 5: Archetypical Planet Parameters

<table>
<thead>
<tr>
<th>Name</th>
<th>Mass [M_\oplus]</th>
<th>Radius [R_\oplus]</th>
<th>T_{bb} [K]</th>
<th>P_0 [bar]</th>
<th>g [m s^{-2}]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Earth*</td>
<td>1.0</td>
<td>1.0</td>
<td>298</td>
<td>1.0</td>
<td>9.81</td>
</tr>
<tr>
<td>Mars*</td>
<td>0.1</td>
<td>0.53</td>
<td>210</td>
<td>0.006</td>
<td>3.71</td>
</tr>
<tr>
<td>TRAPPIST-1 d †</td>
<td>0.3</td>
<td>0.78</td>
<td>282</td>
<td>1.0?</td>
<td>4.70</td>
</tr>
<tr>
<td>Titan*</td>
<td>0.02</td>
<td>0.40</td>
<td>82</td>
<td>1.45</td>
<td>1.35</td>
</tr>
<tr>
<td>51 Pegasi b‡</td>
<td>317</td>
<td>11.2</td>
<td>109</td>
<td>$\geq$1000</td>
<td>24.79</td>
</tr>
</tbody>
</table>

* (Beatty and Chaikin 1990; Rauf et al. 2015)
† (Grimm et al. 2018)
‡ (Birkby et al. 2017)

- Earth represents the class of theoretically inhabited planets, its atmosphere is strongly out of chemical equilibrium and dominated by the spectrally muted N_2 and active O_2. Earth-like targets are of very high priority for future space-based spectrometers such as JWST’s Mid-Infrared Instrument (MIRI) however the known temperate exoplanets mostly orbit M-Dwarfs.
- Mars is used as an archetype to represent lighter, colder terrestrial planets with tenuous CO_2 dominated atmospheres.
- TRAPPIST-1 d has no constrained atmospheric composition beyond the exclusion of a cloud-free hydrogen dominated atmosphere (de Wit et al. 2018) but represents a roughly Earth-sized planet in orbit around an M-dwarf. TRAPPIST-1d’s density has been constrained to 3.39±0.35 g cm^{-3} (Grimm et al. 2018) compared to the Earth’s 5.513 g cm^{-3}. One possible explanation is that the planet formed with a relatively high fraction of light volatiles and later migrated inwards (Unterborn et al. 2018). The short-period orbit allows the refraction floor to be pushed to lower altitudes and a better sampling of the high-pressure region during transit spectroscopy. The atmosphere has been based on the comet-like composition speculated to be possible for volatile-rich temperate terrestrial planets (Kaltenegger et al. 2013) primarily (90%) H_2O dominated with 5% initial NH_3 which quickly photodissociates to N_2 and H_2 with an additional 5% CO_2.
- Jupiter is the archetypical cold gas giant. Its atmosphere is H_2 dominated and its surface gravity is high relative to its temperature, suppressing the atmospheric scale height. The presence of atmospheric PH_3 introduces additional features into the (sub)millimeter spectrum. Cold Jupiters are more likely to be observed in emission than in transmission given the bias of the transit technique to detecting short-period exoplanets.
- Titan is unique in the solar system. While not a planet, it is the only moon to have a thick atmosphere ($P_0 = 1.45$ bar). Titan’s atmosphere contains complex organic chemistry and is dominated
Titan-like exoplanets may occur where volatile-rich worlds orbit at large semi-major axes. Titan’s atmospheric scale height is large relative to its size, $H_{\text{titan}} \approx 40 \text{ km} \approx 5H_{\oplus}$.

- 51 Pegasi b is the archetypical Hot Jupiter. Compared to Jupiter it has a large atmospheric scale height and short orbital period. This makes it an ideal planet type for transmission spectroscopy. The majority of exoplanets that have been spectroscopically studied are Hot Jupiters.

There is a conspicuous absence of super-Earths in the list of archetypical planets. The terrestrial planets will instead be tested in the parameter space as both small and super-sized versions of themselves with appropriately scaled radii and surface gravity. In this way the Earth, Mars, Titan, and TRAPPIST-1d will be present in super-Earth form.

<table>
<thead>
<tr>
<th>Name</th>
<th>$H_2O$</th>
<th>$CO_2$</th>
<th>$O_2$</th>
<th>$CH_4$</th>
<th>$N_2$</th>
<th>$H_2$</th>
<th>$CO$</th>
<th>$PH_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Earth</td>
<td>600 ppm</td>
<td>400 ppm</td>
<td>0.2</td>
<td>1.8 ppm</td>
<td>0.8</td>
<td>-</td>
<td>10 ppb</td>
<td>-</td>
</tr>
<tr>
<td>Mars</td>
<td>210 ppm</td>
<td>0.953</td>
<td>0.0013</td>
<td>0.4 ppb</td>
<td>0.027</td>
<td>-</td>
<td>0.008</td>
<td>-</td>
</tr>
<tr>
<td>TRAPPIST-1 d</td>
<td>0.9?</td>
<td>0.05?</td>
<td>-</td>
<td>-</td>
<td>0.05?</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Titan</td>
<td>1-10 ppb</td>
<td>14 ppb</td>
<td>-</td>
<td>0.014</td>
<td>0.984</td>
<td>0.01</td>
<td>-</td>
<td>&lt; 1 ppb</td>
</tr>
<tr>
<td>Jupiter</td>
<td>4 ppm</td>
<td>20 ppb</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.898</td>
<td>1.6 ppb</td>
<td>1.1 ppm</td>
</tr>
<tr>
<td>51 Pegasi b</td>
<td>300 ppm</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>200 ppm</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

Table 6: Archetypical Planet atmospheric chemical composition. Major atmospheric constituents are listed as fractions of the total atmospheric composition. Trace gases are labelled either as parts-per-million (ppm) or parts-per-billion (ppb) or if listed without a unit, as a fraction of 1. A value of "-" represents zero or negligible abundance. Values with an appended "?" denote speculative assumed values. Parameters retrieved from [Brogi et al., 2013; Cottini et al., 2017](#).

Fig.20 contains the normalized emission spectra of the archetypical planets. The normalization process is performed by computing a blackbody spectrum for each planet given its surface temperature and area. The blackbody spectrum is then divided out of the atmospheric spectrum. A value of 1 represents regions of the atmospheric spectrum which are indistinguishable from blackbodies, and values below 1 represent absorption features caused by transmission through the atmosphere. Values above one are possible given $T_{\text{eff}} > T_{\text{bb}}$ for some inverted atmospheres, such as Fig.20 (d) as Titan experiences a reverse-greenhouse effect. From the initial results it is apparent that tenuous atmospheres produce very high contrast absorption features in emission while in thicker atmospheres there is a strong continuum absorption which pushes down the entire spectrum. The haze-free and water-free Titan-like atmosphere produces the highest contrast absorption features, but these are not due to water. In almost all cases the low excitation 916 GHz p-$H_2O$ line is prominent in absorption.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
<th>Step</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2O$ VMR</td>
<td>0 - $10^{-4}$</td>
<td>logarithmic</td>
<td>7</td>
</tr>
<tr>
<td>$a$ [au]</td>
<td>0.01 - 10</td>
<td>logarithmic</td>
<td>4</td>
</tr>
<tr>
<td>$P_0$ [bar]</td>
<td>0.1-100</td>
<td>logarithmic</td>
<td>7</td>
</tr>
<tr>
<td>$T_0$ [K]</td>
<td>75-2000</td>
<td>irregular</td>
<td>6</td>
</tr>
<tr>
<td>Chemistry</td>
<td>CO, PH$_3$, H$_2$</td>
<td>-</td>
<td>3</td>
</tr>
<tr>
<td>P-T Profile</td>
<td>a,b,c,d</td>
<td>-</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 7: Planet Parameter Space. The column range describes the minimum and maximum values (where applicable). The step column describes how the values within the range are spaced. The number column describes how many steps there are in the range. The P-T profiles correspond to a, b, c, and d from Fig.1.
Figure 20: Submillimeter emission spectra of the planet archetypes. Flux has been normalized to the planetary blackbody. A perfect blackbody emitter would thus have a flux of 1.0 across the entire wavelength range.
3.2 Emission

In the (sub)millimeter planets are expected to shine most brightly by their thermal radiation. Nearby planets with larger temperatures and surface areas will be the brightest emitters. We first review the known catalog of exoplanets and then extrapolate to undiscovered planets given planet occurrence rates.

3.2.1 Searching for the Brightest Emitters

In order to estimate the radiant power of an exoplanet we must determine likely planet temperatures and dimensions. Data for 3748 exoplanets and stars has been acquired by downloading the confirmed planets of the NASA exoplanet catalog, including the orbit semi-major axis, mass, radius, distance, stellar effective temperature, and stellar radius. Of these planets 777 have no measured radius which must be inferred.

Estimating Planetary Radii and Temperatures

Planetary radii have been inferred from the boundaries of the mass-radius relation of Chen and Kipping (2017). Planets which have a mass below $2 \ M_{\oplus}$ are designated as likely terrestrials with bulk densities similar to that of the Earth: $5500 \ \text{kg m}^{-3}$. Planets with masses above $2 \ M_{\oplus}$ but below $100 \ M_{\oplus}$ are assigned Neptunian densities: $1600 \ \text{kg m}^{-3}$. Planets with masses above $100 \ M_{\oplus}$ are assigned Jovian densities: $1300 \ \text{kg m}^{-3}$. Planet radii are then calculated. Results of applying this schema to the solar system planets given only their mass are presented in Fig. 21.

![Figure 21: Results of the planet radius inference on planets of the solar system. Mean errors are 7.5% and maximum error is 23%. The dashed line indicates an equality between the inferred and actual radius.](image)

Planets which have both an unknown mass and unknown radius are filtered out of the data set, leaving planets with known radii or masses only. Planets where the host star radius is entirely unconstrained are also filtered, due to the difficulty of inferring an accurate stellar radius without spectroscopically confirming the host star to be on the main sequence. After all filters are applied the original set of 3748 planets is reduced to 1611 planets. An equilibrium temperature is then calculated using eq. 5 for all planets given the "best observational case" scenario of an albedo of 0 - such that all planets are taken to...
be perfect blackbodies. A planet which absorbs light completely has a Bond albedo $A_B = 0$, and would have a larger equilibrium temperature than a planet with an albedo $> 0$. In reality, the solar system planets all have $A_B > 0$ (see table 1). The planet most closely resembling a black body is Mercury, with an $A_B$ of 0.068. The gas giants of the solar system have albedos $\sim 0.3-0.35$. Hot Jupiter albedos have been found to lie in the range $0.4 \pm 0.1$ (Schwartz and Cowan 2015).

The dependence of temperature on the albedo goes as $T_{eq} \propto (1 - A_B)^{1/4}$. Assuming an $A_B = 0$ gives us a greenhouse-free temperature upper limit, which could easily be several hundred K below the true surface temperature for a CO$_2$ dominated atmosphere. Assuming completely efficient heat redistribution within the planetary atmosphere $T_{eq}$ is taken to be the global temperature such that phase-dependent effects can be ignored. In reality the efficiency of temperature circulation is a function of the atmospheric density. Tenuous atmospheres result in large day-night side temperature variations, such as in the case of Earth’s moon where surface temperatures oscillate by $\pm 100$ K over a single lunar day despite having a temperate $T_{eq} = 270$ K. In short these estimates must be considered very rough approximations to inform the search for detectable exoplanets and are more likely to be lower limits.

At incident fluxes greater than $2 \times 10^5$ W m$^{-2}$ (\( \sim 800 \) S$_\oplus$) a large fraction of gas planets are known to become larger than predicted by traditional mass-radius relations, with the most inflated planets having mass in the range $0.37$-$0.98 M_J$ (Miller and Fortney 2011, Sestovic et al. 2018). One example is WASP-17 b with $M = 0.486 \pm 0.032 M_J$ but with a radius $1.991 \pm 0.081 R_J$ (Anderson et al., 2011). The results in the simple mass-radius relation breaking down for the most heavily irradiated planets. If radii are inflated by a factor 2-4 over the predicted radii then flux will be under-predicted by a factor 4-8 as it scales proportionally to the planet surface area.

The Brightest Planets

Given a radius and an equilibrium temperature the planet emitted power can be calculated by integrating over the Planck relation. It is also possible to use eq.13 to estimate the flux density of a giant planet at the optimal thermal blackbody observing frequency of 345 GHz where SNR is maximized (Butler et al. 2004).

![Figure 22: Planet-star angular separation and expected 345 GHz flux density from a subset of the NASA exoplanet catalog. The vertical blue line is the ALMA maximum spatial resolution at 345 GHz and 15 km baseline. The dashed horizontal line represents the $\sigma_{\text{rms}}$ of an ALMA observation with 43 of the 12 meter antennae over 27 days with bandwidth 7.5 GHz.](image)
Note the bulk of detected exoplanets in the lower-left of Fig. 22. These are predominantly the planets detected by the Kepler spacecraft which typically lie at distances of several hundred pc. The 1σ RMS noise for a $\Delta \nu = 7.5$ GHz integration at 345 GHz for 27 days is 1 $\mu$Jy. Only two of the planets found in the NASA Exoplanet Archive have $F_{345} \geq 1 \mu$Jy, one of which is due to a spurious distance value which was low by 200 pc. The angular separation in Fig. 22 is determined via $\arctan(a/d)$ where $a$ is the planet orbit semi-major axis and $d$ is the distance to the star. This value indicates the maximum possible angular separation for a circular orbit.

Figure 23: A close-up of the most promising candidates of mature giant exoplanets.

<table>
<thead>
<tr>
<th>Star Name</th>
<th>$T_{eq}$ [K]</th>
<th>D [pc]</th>
<th>$M \sin(i)$ [M$_J$]</th>
<th>$F_{345}$ [$\mu$Jy]</th>
<th>Dec [deg]</th>
<th>Resolved</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tau Boötis A</td>
<td>1684</td>
<td>15.6</td>
<td>6.00 ± 0.28</td>
<td>1.06</td>
<td>+17.5</td>
<td>N</td>
</tr>
<tr>
<td>Gj 86</td>
<td>661</td>
<td>10.91</td>
<td>3.90 ± 0.32</td>
<td>0.87</td>
<td>-50.8</td>
<td>Y</td>
</tr>
<tr>
<td>HD 29139</td>
<td>1086</td>
<td>20.43</td>
<td>5.8 ± 0.7</td>
<td>0.53</td>
<td>+16.5</td>
<td>Y</td>
</tr>
<tr>
<td>HD 62509</td>
<td>536</td>
<td>10.34</td>
<td>2.30 ± 0.45</td>
<td>0.50</td>
<td>+28.0</td>
<td>Y</td>
</tr>
<tr>
<td>70 Virginis</td>
<td>522</td>
<td>18.11</td>
<td>7.40 ± 0.02</td>
<td>0.35</td>
<td>+13.8</td>
<td>Y</td>
</tr>
</tbody>
</table>

Table 8: The five known exoplanets with the largest modeled 345 GHz flux. Note mass values are minimum mass derived from radial velocity. The ALMA limiting elevation is 47° although shadowing becomes > 5% for declinations > 25°.

*Quantities derived in this work

A summary of the brightest 345 GHz flux density candidates, both spatially resolved and unresolved is found in Table 8 and are shown in detail in Fig 23. For a typical solar system gas giant albedo of 0.35 we find calculated equilibrium temperatures reduced to a fraction $\sim 0.89$ of their listed value. The planets listed in Table 8 are all warm or Hot Jupiters ($T_{eq} > 500$ K). Hot Jupiters are expected to have much lower albedos due to TiO and VO absorption, although the geometric albedo of Kepler-7b has been found to be 0.32 ± 0.03, similar to the solar system gas giants (Demory et al., 2011).

The brightest (sub)millimeter exoplanet is Tau Boötis Ab ($\tau$ Boo Ab), which orbits the primary star of the $\tau$ Boo binary, the F6 IV variable Tau Boötis A (Mallik, 1999), at $a=0.0481 \pm 0.028$ au. The planet has a theoretical radius 1.06-1.2 $R_J$ and geometric albedo $A_G < 0.37$ (Lucas et al., 2009). The
secondary star $\tau$ Boo B is a M3V star at a separation of 240 au and so contributes negligibly to the planet irradiation (Roberts et al., 2011). Its spectrum has been based on the 51 Pegasi b parameter template, adjusting the values for $R_p$, $a$, $g$, $T_0$, $R_*$, $T_*$ and $d$ to match those of Tau Boötes Ab and can be seen in Fig. 24 where it is shown both before and after transmission through the Earth’s atmosphere.

Figure 24: The emission spectrum of Tau Bootis (isothermal atmosphere, $X_{H_2O} = 0.0015$ isochemical) at the top of the Earth’s atmosphere (green) and at 5000 m altitude (blue).
Figure 25: The Tau Bootis emission spectrum and the planet idealized blackbody after transmission through the Earth’s atmosphere.

Given that τ Boo represents an unresolved case where the stellar and planetary spectra would be combined for ALMA, in Fig. 24 and Fig. 25 the stellar spectrum has been divided out. Note that stellar variability of τ Boo A has been found to be periodic corresponding to the planet’s orbital period (Walker et al., 2008) possibly caused by magnetic interaction between the tidally locked planet and stellar chromosphere, resulting in fluctuations of 1000 ppm over a single orbit. Any observation of τ Boo Ab could require simultaneous high dispersion monitoring of Ca II H and K reversals in order to account for this variability. The planet signal relative to the stellar emission in this unresolved case is, given a stellar $T_{\text{eff}} = 6309$ K and $R_*=1.331 \pm 0.027\, R_\odot$, 1300 ppm which is similar in magnitude to the optical photometric variability at 420 to 900 nm (Nordström et al., 2004). Given the short planet orbital period 3.3 d (Wang and Ford, 2011) phase effects play a significant role for integrations of comparable duration to the planet orbital period for low system inclinations. However as stellar reflected light is taken as negligible only thermal planetary emission is observed, in which case the day-night phase contrast depends on the efficiency of heat redistribution within the planet atmosphere. Heat maps of Hot Jupiters have revealed evidence for efficient heat redistribution. In the case of the Hot Jupiter HD 189733b the minimum 8 $\mu$m brightness temperature of 973 $\pm$33 K and a maximum of 1212$\pm$11 K, for a day-night contrast of 239$\pm$35 K (Knutson et al., 2007). A similar day-night contrast for τ Boo would result in an emission flux modulation factor 0.1$\cos\,i$ over 1.5 d. The system inclination is 44.5$\pm$1.5° (Brogi et al., 2012) resulting in a phase dependent flux modulation of 0.06 $\mu$Jy resulting in $F_{345} = 1.06\pm0.06\, \mu$Jy.
<table>
<thead>
<tr>
<th>Isotopologue</th>
<th>$\nu$ [GHz]</th>
<th>$E_L$ [K]</th>
<th>$\mathcal{T}$ [%]</th>
<th>Band</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>96.259</td>
<td>3059.4078</td>
<td>97.2</td>
<td>3</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>139.614</td>
<td>4431.7191</td>
<td>94.6</td>
<td>4</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>209.118</td>
<td>3451.8440</td>
<td>94.2</td>
<td>5</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>232.686</td>
<td>3450.7158</td>
<td>93.9</td>
<td>6</td>
</tr>
<tr>
<td>HDO</td>
<td>263.832</td>
<td>1839.3765</td>
<td>93.2</td>
<td>6</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>293.664</td>
<td>3919.4462</td>
<td>92.0</td>
<td>7</td>
</tr>
<tr>
<td>HDO</td>
<td>317.151</td>
<td>675.7371</td>
<td>86.0</td>
<td>7</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>321.222</td>
<td>1845.8200</td>
<td>73.5</td>
<td>7</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>331.123</td>
<td>4865.5498</td>
<td>82.0</td>
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</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>336.227</td>
<td>2939.0496</td>
<td>86.0</td>
<td>7</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>339.044</td>
<td>5483.0566</td>
<td>87.3</td>
<td>7</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>354.809</td>
<td>5763.8100</td>
<td>84.9</td>
<td>7</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>402.914</td>
<td>5356.2144</td>
<td>78.6</td>
<td>8</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>435.169</td>
<td>6567.1481</td>
<td>59.5</td>
<td>8</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>437.347</td>
<td>1503.5973</td>
<td>59.2</td>
<td>8</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>463.170</td>
<td>2744.3814</td>
<td>61.9</td>
<td>8</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>498.500</td>
<td>3673.0033</td>
<td>45.0</td>
<td>8</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>637.292</td>
<td>8242.3184</td>
<td>54.0</td>
<td>9</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>645.766</td>
<td>2574.0504</td>
<td>56.6</td>
<td>9</td>
</tr>
</tbody>
</table>

Table 9: Water Lines in the (sub)millimeter seen in synthetic Hot Jupiter spectrum at frequencies where Earth’s transmission is > 40% from 80-650 GHz. $\nu$ is the line frequency, $E_L$ is the lower state energy, $\mathcal{T}$ is the transmittance of the Earth’s atmosphere at that frequency, and ‘Band’ is the ALMA band number. Isotopologues labelled in bold are the strongest lines. 24 additional lines in emission are found in the 800-900 GHz band.

In Table 9 the most prominent water lines which are not significantly absorbed by the Earth’s atmosphere but do appear in the emission spectra of several modeled Hot Jupiters are summarized.

### 3.2.2 The Contribution of Stellar Reflected Light

To what degree does reflected stellar light contribute to the planetary (sub)millimeter emission spectra? The relative contribution of the planetary thermal and reflected stellar thermal radiation is a function of the planet’s true anomaly $f$ and the resulting phase. A planet in primary transit will present a night-time face. For tidally locked planets with extreme day-night temperature disequilibria the corresponding thermal emission will be reduced below the calculated $T_{eq}$ without a significant greenhouse effect. Reflected stellar light will thereafter increase as the planet orbits towards the theoretical maximum immediately prior to the secondary eclipse. For a system viewed edge on this effect is maximal as the planet illumination moves from waxing/waning crescent to gibbous.

In Fig. 26 a two component spectrum of the Earth has been constructed. The planet’s intrinsic thermal emission and the reflected stellar light are the two components. The stellar reflected spectrum is at its peak frequency a factor $10^2$ weaker than the intrinsic planet thermal peak emission for $T_{\text{planet}} = 277$ K and $T_\ast = 5880$ K at an orbital distance of 1 au and $A_B = 0.306$. We conservatively take the planet to be at full phase. Note that for extremely high values of the Bond albedo ($\sim 0.99$) this ratio could at most be altered by a factor ~0.3.
Figure 26: The Earth as a blackbody with reflected stellar light. The blue line indicates the intrinsic blackbody thermal emission of the Earth for $T_{\text{eff}} = 273$ K. The orange line represents the solar reflected component of the spectrum, arising from a $T_{\text{eff}} = 5880$ K blackbody at a distance of 1 au. The green line is their combination. The red vertical band from 100-1000 GHz indicates the ALMA wavelength range.

The same calculation as in Fig. 26 has been performed for other solar system bodies in Fig. 27. Note Mercury’s relatively low reflected component, primarily due to its low albedo and high $T_{\text{eq}}$.

Figure 27: Calculated idealized blackbody planetary spectra. All spectra are combined intrinsic planetary thermal emission and reflected stellar light. The red vertical band from 100-1000 GHz indicates the ALMA wavelength range.
It can be seen that the planetary thermal emission dominates over reflected stellar emission for the solar system planets (minimum $a = 0.3$ au) in the (sub)millimeter regime. For Jupiter, Mars, Earth and Mercury the ratio of intrinsic-reflected (sub)millimeter flux is $\sim 10^5$, for Mercury it is for Hereafter we will neglect the stellar contribution to the planetary spectra.

3.2.3 Non-thermal planetary emission

Planetary radio flux originates from stellar wind impinging on the planet’s magnetosphere resulting in the acceleration of charged particles [Perryman 2014]. The expected planet radio observed power can be estimated by

$$P_{\text{radio}} \propto \dot{M}_{s}^{3/2} V_{w}^{5/3} \mu_{p}^{2/3} a^{-4/3} d^{-2}$$  (44)

where $\dot{M}_{s}^{3/2}$ is the stellar mass loss rate, $V_{w}$ is the speed of the stellar wind at the planet, $\mu_{p}$ is the planet’s magnetic moment, $a$ is the planet semi-major axis and $d$ is the distance to the star from the observer [George and Stevens 2007]. From Blackett’s law we can say $\mu_{p} \propto \omega M_{p}^{5/3}$ where $\omega$ is the angular rotation frequency of the planet [Blackett 1947] and given that there appears to be a mass-rotational velocity relation where more massive planets rotate faster, massive planets will generally have larger magnetic moments. A peak in non-thermal emission is expected at 8-48 MHz [Stevens, 2005]. While there is some overlap with the non-thermal emission mechanisms and the millimeter wave part of the spectrum we will consider non-thermal radiation as negligible in the model.

3.2.4 Limits on Detectability of Emission

In Fig.28 the archetypical planets are placed at a distance of 1 pc (similar to the nearest star system at 1.3 pc [van Altena et al. 1995]) in order to calculate comparative flux values. The blue, orange and green lines show the RMS noise sensitivity limits given integration times of $10^4$, $10^5$, $10^6$ s (2.7 h, 27 h and 11.5 d respectively) with ALMA. Only in the case of (d), the nearby inflated Hot Jupiter is quickly detected (ignoring atmospheric absorption) at $3\sigma$ in only 3 hours of observation with $\Delta \nu = 7.5$ GHz and the RMS noise level approaches that of the majority of the spectral features within a single day of observation while a minimum of 3 such integrations would be necessary for a single line. However several lines stand out as being significantly more absorbed than others. A blend of the 645.77 GHz $^9_{73} - ^8_{80}$ and 645.91 GHz $^9_{72} - ^8_{81}$ para- and ortho- water lines in ALMA band 9 are not present in the telluric spectrum and absorb 68% of the continuum level for $X_{H_{2}O}=1.5 \times 10^{-3}$. However the lines would likely require $\Delta \nu < 7.5$ GHz to resolve. Including Earth’s atmospheric absorption the integration time for the same detection significance increases by $\sim 30\%$ at 345 GHz.

In case (c), a Jupiter analog at 1 pc distance, the planet thermal emission could still be detected at $< 2\sigma$ with $10^6$ s integration time. None of the terrestrial sized planets are detectable in the considered range of integration times. Given that none of the considered terrestrials are short-period planets this is unsurprising, their low (0.1-1 $E_{\oplus}$) insolation results in comparatively small values of $T_{eq}$ and from the Stefan-Boltzmann law $L \propto T^4$. 

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(a) Earth \((X_{\text{H}_2\text{O}} = 6 \times 10^{-4})\)

(b) Mars \((X_{\text{H}_2\text{O}}=2 \times 10^{-4})\)

(c) Jupiter \((X_{\text{H}_2\text{O}} = 1.5 \times 10^{-3})\)

(d) Titan (haze-free) \((X_{\text{H}_2\text{O}} = 0)\)

(c) TRAPPIST-1 d \((X_{\text{H}_2\text{O}} = 2 \times 10^{-4})\)

(d) 51 Pegasi b \((X_{\text{H}_2\text{O}} = 1.5 \times 10^{-3})\)

Figure 28: Submillimeter emission spectra of the planet archetypes. Flux has been normalized to the planetary blackbody. A perfect blackbody emitter would thus have a flux of 1.0 across the entire wavelength range.

In Fig. 29 there is a study of several of the prominent water lines from Table 2 of the theoretical 51 Pegasi b Hot Jupiter type planet also placed at a distance of 1 pc presented without the intervening absorption by telluric lines. Integration time is set to \(10^6\) s. Note that every data point and associated error bar represents a single \(10^6\) s integration. We are able to recover the 183 GHz \(3_{13} - 2_{20}\) and 380
GHz $4_{14} - 3_{21}$ lines, while the 325 GHz line becomes blended with the 321 GHz $10_{29} \rightarrow 936$ o-H$_2$O line in ALMA band 7 to enhance the signal at the 7.5 GHz bandwidth continuum-mode measurements. The 448, 474, 556, 752, and 916 Ghz lines (last two not displayed in Fig. 29) are not unambiguously detected at a 1σ level in $10^6$ s integration.

Figure 29: Study of the major water lines of the theoretical Hot Jupiter at 1 pc, with $10^6$ s integration time. The blue line is the synthetic spectrum, and the green boxes show the 1σ uncertainties for a bandwidth of 7.5 GHz.
In Fig. 30 the TRAPPIST-1d archetype planet has been placed at a distance \( d = 0.01 \) pc, close enough to enable the detection of water lines at \( 1\sigma \) within \( 10^6 \) s integration time for a 7.5 GHz bandwidth. A distance of 0.01 pc is still firmly within the solar system so could only be of use for currently hypothetical trans-Neptunian planets (Brown and Batygin, 2016). In Fig. 30 (d) it can be seen that the 556 GHz line could be detected at 2-3 \( \sigma \) given an appropriate center frequency \( \nu_0 \) of the observing bandwidth. While many deep line-cores are found due to the P-T structure of the atmosphere, they are of generally too narrow width to allow detection with the maximum ALMA bandwidth (see Fig. 30 (c)) and integration time must be increased to detect the line at the lower bandwidth as \( \sigma_{\text{rms}} \propto (\Delta \nu)^{-0.5} \). The line width is 380 MHz, increasing \( t_{\text{int}} \) by a factor 4.5.

The primary difficulty in achieving a detection of interstellar H\(_2\)O with ground-based observatories is the presence of water vapor in the Earth’s atmosphere. Water lines are significantly broadened by the high pressures and temperatures of the troposphere where most water resides. SPAM has been used to reproduce the results of (Pardo et al., 2002). The transmission spectrum in Fig. 16 will be used to simulate the telluric absorption present during ALMA observations. The synthetic exoplanetary spectra are multiplied by Earth’s transmission spectrum. Unambiguous detection of exoplanetary water features will require significant Doppler shifted sources, sources with rapidly fluctuating radial velocity signals, or high excitation lines which are not present in telluric absorption features.

A prominent water line near the optimal 345 GHz observing frequency is the 325.152 GHz \(^{5}\!_{15} \rightarrow ^{4}\!_{22}\) transition. With a pwv = 0.5 mm it has a FWHM of 4 GHz in the Earth’s atmosphere. Transmission through the rest frame line center at 5000 m altitude is approximately 18\pm2\% . A radial velocity of 100 km s\(^{-1}\) results in a shift away from the rest frame by \( \sim 110 \) MHz, improving atmospheric transmission at the line center by approximately 3\%. A radial velocity of 1000 km s\(^{-1}\), still a plausible velocity given known hyper-velocity stars (Boubert et al., 2018) results in a line shift of 1.1 GHz improving atmospheric transmission to 36\%. Very few Milky Way stars with radial velocity \( > 1000 \) km s\(^{-1}\) are known and represent only limiting cases, the majority of stars with detectable planets have \( v_r < 100 \) km s\(^{-1}\).

Tau Boötis A radial velocity is -16 km s\(^{-1}\) (Nidever et al., 2002). The maximum circular orbital velocity for the planet is 150 km s\(^{-1}\). Given the system inclination of 44.5\(^\circ\) or 45\(^\circ\) (Lockwood et al., 2014) we find a maximum possible planetary radial velocity of 120 km s\(^{-1}\). We find at 345 GHz a maximum line shift of 140 MHz, which is generally insufficient to avoid telluric absorption features with FWHM \( \sim 4-5 \) GHz.

If we consider the capabilities of the theoretical NGMA telescope described in Table 4 we find that unambiguous detection of water features is possible for known exoplanets at their true distances. For the 15.6 pc distant \( \tau \) Boo see Fig. 31.
Figure 30: Study of the major water lines of the theoretical TRAPPIST-1d at 0.01 pc (\(\sim\)2000 au, nearly double the proposed aphelion of Planet 9 [Brown and Batygin, 2016]), with \(10^6\)s integration time. The blue line is the synthetic spectrum, and the green boxes show the 1\(\sigma\) uncertainties for a channel width of 7.5 GHz. Gaussian noise has been added to the spectrum at the level of the RMS noise.
The Effect of Surface Pressure on Emission

Only terrestrial planets with well defined surfaces are included in the surface pressure series of spectra. In Fig.32 the result of varying the surface pressures on several of the terrestrial planet models is shown. Pressures from 0.1-500 bar are shown for Earth \(X_{\text{H}_2\text{O}} = 6 \times 10^{-4}\) and a relatively wet Mars \(X_{\text{H}_2\text{O}} = 2 \times 10^{-4}\). Atmospheric temperature is identical to the archetypical cases. Notably several lines go from absorption to emission with increasing surface pressure including the 474.69 GHz \(5_{33} \rightarrow 4_{40}\) o-H\(_2\)O line seen in Fig.32(d) for the Mars-like planet or the 906.21 GHz \(9_{28} \rightarrow 8_{35}\) p-H\(_2\)O for the Earth-like planet in Fig.32(c).
Figure 32: The effect of varying surface pressure. All units are in bars. Frequencies displayed are to illustrate the most significant changes as a result of varying pressure. All spectra are normalized to the planet surface blackbody continuum emission.

The Effect of Water Abundance on Emission

In Fig.33 the result of varying the atmospheric water abundance $X_{H_2O}$ is shown for several planets both gaseous and terrestrial. $X_{H_2O}$ is taken to be constant over all pressures. The structure of the produced spectra has been found to be the most sensitive to water abundance over all other explored parameters; the level of the continuum, which lines are present, their strength as well as whether they appear in absorption or emission are all influenced. In Fig.33 (c) and (d) the planet atmosphere shown is that of Gliese 876 b, a relatively warm Jupiter of $2.2756 \pm 0.0045 \, M_J$ [Rivera et al. 2010] with $T_{eq} = 194 \, K$. It is found that for 51 Pegasi b the optimal water absorption line contrast with the continuum occurs in the millimeter regime at $X_{H_2O} = 10^{-4}$ but at $X_{H_2O} = 10^{-6}$ for the submillimeter regime. For Gliese 876 b lines are found in emission at $X_{H_2O} = 10^{-6}$ and exhibit absorption for greater abundances. The considered range of water abundances for the TRAPPIST-1 d case is different from the other considered planets given its initial very high water abundance ($X_{H_2O}=0.9$) and it is found that variations between 0.3-0.9 are not as dramatic as for the other planets all with $X_{H_2O}<0.1$ (see Fig.33 (e) and (d)).
Figure 33: The effect of varying water abundance. All spectra are normalized to the planet surface blackbody continuum emission.

The Effect of Alternative Chemistry on Emission

Various atmospheric compositions have been explored as described in table 10. Atmospheres which contain the same fraction of water vapor yet which are dominated by H$_2$, or contain significant fractions of CO and PH$_3$ are shown in Fig. 34. The presence of abundant PH$_3$ is observed to strongly reduce the
contrast of many water lines with the continuum while the influence of CO is generally less profound.

Table 10: Alternative Atmospheric Chemistry

<table>
<thead>
<tr>
<th>Name</th>
<th>(X_{\text{H}_2\text{O}})</th>
<th>(X_{\text{PH}_3})</th>
<th>(X_{\text{CO}})</th>
<th>(X_{\text{N}_2})</th>
<th>(X_{\text{CO}_2})</th>
<th>(X_{\text{H}_2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>0.0006</td>
<td>0</td>
<td>0.1</td>
<td>0.8</td>
<td>0.0004</td>
<td>0</td>
</tr>
<tr>
<td>(\text{H}_2)</td>
<td>0.0006</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.0004</td>
<td>0.8</td>
</tr>
<tr>
<td>(\text{PH}_3)</td>
<td>0.0006</td>
<td>0.1</td>
<td>0</td>
<td>0.8</td>
<td>0.0004</td>
<td>0</td>
</tr>
</tbody>
</table>

Figure 34: The effect of varying dominant atmospheric chemical abundances. All spectra are normalized to the planet surface blackbody continuum emission.

The Effect of various P-T Profiles on Emission

Multiple P-T profiles have been evaluated as described in Fig.1. The strongest dependence has been found on variations to the lower (\(z < 20 \text{ km}\)) atmosphere. A profile which at first lapses within the troposphere but becomes isothermal above the tropopause is found to have a great similarity to the profile which is inverted above the tropopause, but differs considerably from a completely isothermal atmosphere, as seen in Fig.35.
Figure 35: The effect of varying the P-T profile of the planet atmospheres. All spectra are normalized to the planet surface blackbody continuum emission.

The Effect of Surface Temperature on Emission

Results of varying the planet surface temperature in increments of 100 K can be found in Fig. 36. The results for the Earth archetype are complex. As temperature increases from the default 288 K many high excitation lines are seen to become excited. At $T + 500$K several of these lines are seen to go into absorption. A blend of up to 3 lines at 577-579 GHz possibly including D$_2$O goes into absorption above 300 K as do tens of other lines. The 509 GHz $J_{10} \rightarrow 1_{01}$ HDO line appears at $T + 150$ K and continues to deepen relative to the continuum. There are 29 lines between 900 and 920 GHz including a narrow $E_L = 381.6$ K HDO line at 912.6 GHz that goes into emission as does an $H_2^{18}O$ line at 909.5 GHz. The water rich TRAPPIST-1d atmosphere in Fig. 36 (c) and (d) only gains new high excitation lines with increasing temperature. Overall transit signal contribution increases with increasing scale height brought on by the higher surface temperature.
Figure 36: The effect of increasing the surface temperature for an Earth-like planet and for the water-rich TRAPPIST-1d seen in emission. All P-T profiles are case (b) from §2.1.2.
Figure 37: (Sub)millimeter transmission spectra of the planet archetypes with their default parameters. The ordinate displays the depth that the planet atmospheric absorption contributes to the overall stellar signal. Note the order of magnitude difference between the atmospheric contribution of the Hot Jupiter in (f) relative to all other cases.
3.3 Transmission

In the case of transmission we consider the geometry described in Fig[8], where the planet moves between its star and the observer and partially occludes the stellar emission. Spectral absorption features are imprinted on the light which passes through the annulus of the planet’s atmosphere. The 6 archetypical planet's transmission spectra are shown in Fig[37]. Notable differences with the emission spectra include the relatively narrow line widths and high contrast spectral features, caused by the low pressure and temperature conditions in the upper 80 – 90% of the planet atmosphere through which the majority of the light rays have passed.

![Transmission Spectra](image)

Figure 38: (Sub)millimeter normalized transmission spectra of Earth with varying degrees of atmospheric water vapor $X_{\text{H}_2\text{O}}$. The prominent non-water lines in (b) are due to oxygen.

In Fig[8] the influence of the presence of H$_2$O on an Earthlike planet’s ($R = R_{\oplus}$) transmission spectrum is shown for a $R = R_{\odot}$ star. Major features which are not due to the presence of water are primarily due to molecular oxygen. The 60 GHz band comprises ranges from 44.9-74.7 GHz and includes 58 lines, 13 of which have $E_{L}<300$ K centered on 56.36-62.48 GHz and is caused by magnetic-dipole transitions in the $^3\Sigma$ electronic ground state [Tretyakov et al., 2005]. Additionally there are the isolated rotational lines at 118.75, 368.50, 424.76, 487.24, 715.39, 773.84, and 834.15 GHz below 1 THz [Remijan et al., 2007]. Further investigation of the effect of water on the different archetypes will follow in this section.

3.3.1 Searching for the Deepest Transits

Which known exoplanets produce the largest transit signatures? Again we consult the NASA Exoplanet Archive[8]. Exoplanets with host stars of unknown radius are filtered from the catalog. Planet radii, stellar radii, and distance are used to calculate the expected transit depth per planet from eq[2] ranging from 25 ppm up to 6%. For each exoplanet host star we determine a likely thermal emission flux. Given that many known exoplanets are Kepler discoveries their distance is too great and stellar flux too low to allow (sub)millimeter detections, and we extend the catalog of host stars to brighter and relatively nearby stars of the TESS input catalog (TIC) which will be observed for transiting planets over the next several years. Detectability is a function of stellar luminosity in the (sub)millimeter and the ratio between the areas of the stellar and planetary disk. Known exoplanets are plotted in Fig[39] together with the brighter stars of the TIC. At 230 GHz a $3\sigma_{\text{rms}}$ of 10 $\mu$Jy requires 17 h of integration time, longer than a typical transit time of 1-2 h.

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[8] https://exoplanetarchive.ipac.caltech.edu/
Figure 39: Stellar flux at 230 GHz on the abscissa and depth of planet transit on the ordinate. A transit depth value of 1 signifies a 100% occlusion of the stellar light by the transiting planet. The solid and dashed black lines show the resulting flux differential caused by a planet transit. The green vertical lines show the stellar flux of the brightest TIC stars with unconstrained planet transit depths.

3.3.2 Limits on Detectability by Transmission

An RMS noise of 10µJy at 230 GHz corresponds to an integration time of approximately $10^{4.5}$ s or 8-9 h. In that case only a single of the known exoplanets (HD 189733 b) would be detectable at 1σ by the transit method in under 10 hours. HD 189733 b’s atmosphere is known to contain water vapor and be nearly isothermal (Timetti et al., 2007). HD 189733 b is a short period planet with a relatively short transit duration. The ingress and egress phase duration are each approximately 0.25 h, and the duration of the transit at maximum depth is approximately 1.2 h. Hence multiple planet transits would be necessary in order to detect the transit signature. Temporal sampling of the transit curve is essentially ruled out by the > 8 h integration time required. Multiple observations both pre- and post- transit would be needed in order to have a stellar baseline with which to compare the in-transit signature.

To what degree can the planet radius be constrained? As the planet itself could only be detected with a significance of 1σ in ~8 h we consider the integrated observation of 100 orbits resulting in 120 h of in-transit signal. One transit of HD 189733b occurs every ~53.25 h requiring a minimum of 220 d of observations to reach 100 transit events. After 120 h of in-transit observations at 230 GHz the RMS noise is now reduced to 1.5 µJy. The expected flux of the transit depth is 15.2 µJy as per Fig 39, resulting in a transit depth of 15.2±1.5µJy, constraining the planet radius to within 10%. Photometrically the radius has been constrained to within 2.3% of the true value (Boyajian et al., 2015).
Figure 40: Sensitivity to transit atmospheric signal for TRAPPIST-1d if the star TRAPPIST were only 1 pc distant.

Figure 41: Sensitivity to transit signal for the Hot Jupiter HD 189733 b for $T_*=5800$ K, $R_*=1$ $R_\odot$ at $d=1$ pc
In Figures 40 and 41 the telescope sensitivity to the transit atmospheric signal is shown. The 1 pc distant terrestrial planet goes undetected at $10^6$ s integration while the Hot Jupiter at 1 pc is detected at $3\sigma$ between 200-300 GHz. In Figure 42 the Hot Jupiter HD 189733 b's spectrum is shown in transmission with $1\sigma$ error bars for a $10^6$s integration.

Figure 43: Transit contribution of Hot Jupiter atmosphere ($T_*=5570$ K, $R_*=1.13 R_\odot$, $d=15.6$ pc) in blue after passage through the Earth’s atmosphere, relative to Earth’s transmission spectrum in orange.

In Fig.43 the transit spectrum of the Hot Jupiter is compared to the Earth’s atmospheric transmission in the (sub)millimeter. Many new lines appear in absorption in wavelength ranges of high transmittance, particularly from 200-300 GHz. These lines are identified in Fig.44.
Figure 42: Study of the major water lines of the Hot Jupiter HD 189733 seen in transmission by ALMA but placed nearby at a distance of 1 pc (actual distance 19.5 pc), with $10^6$ s integration time per data point. The blue line is the synthetic spectrum, and the green boxes show the 1σ uncertainties for a channel width of 7.5 GHz. Synthetic Gaussian noise has been added to the signal at the level of the RMS noise.
Figure 44: Hot Jupiter transmission spectrum absorption lines not significantly absorbed by the Earth’s atmosphere.
The Effect of Surface Pressure on Transmission

The surface pressure of the planets has been modeled over the range from 0.1-500 bar. Several of these results are presented in Fig. 45. Generally the effect results in enhanced pressure broadening of the water lines. Increased collisional broadening pushes down the continuum, but does begin to damp lines until $P > 50\text{bar}$ at which point the depth of the 183 GHz line for Earth-like planets reduces from 0.45-0.55 ppm to 0.2 ppm for $P = 500\text{ bar}$. This effect is also apparent in Fig.45 (a) and (b). The relation is found to be proportional by $\Delta C \propto e^{-0.025P}$ where $\Delta C$ is the reduction in the continuum in ppm.

![Figure 45](image1)

Figure 45: The effect of varying the surface pressure for several of the terrestrial worlds. Units of the displayed pressure quantities in the legend are in bar.

The Effect of Water Abundance on Transmission

A range of atmospheric water volume mixing ratios is considered. In these models the abundance of water does not vary with altitude. It is found that increasing water abundance does not necessarily imply a greater ease of detection. Greater water abundances in fact reduce overall the continuum and increase line width without increasing the line depth as can be seen in Fig.46. In Fig.46 (a) for the Hot Jupiter 51 Pegasi b the 752 GHz line has the greatest contrast with the continuum at abundances $X_{\text{H}_2\text{O}} \approx 10^{-6}$ (150 ppm) after which the continuum is damped at $X_{\text{H}_2\text{O}} > 10^{-4}$ (80 ppm and below). A similar effect is found at 380 GHz (177, 151, 100ppm for $X_{\text{H}_2\text{O}} = 10^{-6}$, $10^{-4}$, and $10^{-2}$ respectively). This indicates that extremely water rich, hot atmospheres may counter-intuitively be more challenging to detect than
Figure 46: The effect of varying the water abundance for a Hot Jupiter (a) and (b), and a temperate terrestrial (c).

Comparatively desiccated atmospheres. Conversely for the temperate terrestrial TRAPPIST-1d in Fig. 46 (c) the relative depth of the 448 GHz line does not appreciably change with varying $X_{\text{H}_2\text{O}}$; with depths of 39, 42 and 39 ppm for $X_{\text{H}_2\text{O}} = 10^{-6}$, $10^{-4}$, and $10^{-2}$ respectively while new lines begin to appear in Fig. 46 (d) which were not detectable such as the 658 GHz line.

**The Effect of Chemical Composition on Transmission**

Results can be seen in Fig. 47. As opposed to the case of emission, the transmission geometry is very sensitive to the atmospheric scale height. An H$_2$ dominated atmosphere has a lower mean molecular weight (8.04 amu) than the CO (28.80 amu), CO$_2$, or PH$_3$ heavy atmospheres, resulting in a larger $H$ (31 km and 8-9 km respectively) resulting in a larger contribution of the atmosphere to the transit signal.

**The Effect of P-T Profiles on Transmission**

The four variations of general P-T profiles from Fig. 1 are explored in Fig. 48. Case (a) represents an isothermal atmosphere, (b) represents an adiabatically lapsing atmosphere that becomes isothermal at the tropopause, (c) represents a doubly inverted profile, and case (d) represents a singly inverted atmosphere. The effect of temperature inversion is less pronounced on the transmission spectra than on the emission spectra. The primary effect is to increase or decrease the level of the continuum. Which profile results
Figure 47: The effect of varying the dominant chemical atmospheric species. The sensitivity of the transit signal depth to the atmospheric scale height is rendered clear.
in a net increase in the continuum is not the same for the different model planets, see Fig.48 (i) where the strongly inverted profile has the highest continuum level while for in (ii) it is the isothermal profile.

The Effect of Planet Mass and Radius on Transmission

Three different planet sizes of the terrestrial planets are considered. A “mini” version of the planets with approximately half the radius and surface gravity, and a “super” version with 1.5\times the radius and approximately double the default surface gravity are plotted against the archetypical templates. Results can be seen in Fig.49. Counter-intuitively the “super” Titan atmosphere produces a 400\% enhanced transit signal despite the increased surface gravity pushing the scale height down. The same process occurs for Mars. The annular area of the atmosphere does increase for the “super” planets by a factor 3, yet for the Earth the transit contribution actually drops for the “super” case. This result is difficult to explain.

The Effect of Surface Temperature on Transmission

The effect of varying the planet surface temperature on transmission spectra of the Earth archetype planet can be seen in Fig.50. The most profound effect is on the level of the continuum. The scale height is directly proportional to the surface temperature \( H \propto T \) so this explains the monotonic rise.
Figure 49: The effect of varying the mass and radius of the terrestrial worlds. (a), (c) and (d) show the full modelled spectrum for Earth, Mars and Titan while (b) shows a study of Earth’s 380 GHz line.
Figure 50: The effect of varying the surface temperature for an Earth-like planet seen in transit. (a) the 115-230 GHz gap (b) the 230-320 GHz gap (c) near the 345 GHz optimal observing frequency. Surface temperature legend is shown in (a). All P-T profiles are case (b) from §2.1.2.

of the atmospheric contribution to the transit signal with increasing temperature. At $T_0 \geq 500$ K lines with higher excitation temperatures such as the 336.23 GHz $5_{23} - 6_{16}$ ortho-water line begin to become prominent at the level of 0.75 ppm in the case of a Sun sized star, or 51 ppm for a TRAPPIST-1 sized star ($R = 0.121R_\odot$) or the 232.69 GHz $5_{50} - 6_{43}$ line at 1 and 68 ppm, respectively.

The Effect of Orbital Semi-Major Axis on Transmission

In §2.1.5 it was determined that for transiting planets the probe-able depths of the atmosphere are determined in part by the physical size of the star and the distance between the star and planet. In Fig.51 the results of placing the Earth at varying distances from the Sun is explored. It is clear that for closer-in orbital distances that the atmosphere is probed more closely to the planet surface. The water lines visible for the short-period planets are broader particularly in the wings, resulting again in a damping of the entire continuum and a reduction with contrast of the lines and continuum. Note that the depth of the core of the 380 GHz line does not appreciably alter in Fig.51 (a) or similarly the 556.9 GHz line in (b) while several lines which are excited only at higher temperatures do begin to appear in absorption, such as at 22 or 503 GHz. Also note that the temperature structure of the model Earth tested in Fig.51 was non-inverted, but lapsed adiabatically up until the tropopause.
3.3.3 Stellar Variability and Transit Enhancement

(Sub)millimeter Transit Characteristics

Stars exhibit a phenomenon in the optical known as limb-darkening. Limb-darkening describes the decreasing intensity of emission across a stellar disk when approaching the edge, or limb, of the disk. Limb darkening results from optical depth effects in the star’s atmosphere that limit emission at large angles off-normal to the stellar surface. In practice limb darkening smooths the transit light curve, where the most extreme case would result in a light curve where $t_F << t_T$ which becomes difficult to distinguish from a glancing transit where an exoplanet never fully overlaps the stellar disk. Observations in the (mid) infrared have determined that stellar disks are uniform in brightness and that the effect of limb-darkening on the transit curve is minimal, resulting in very steep-walled and flat-bottomed light curves. In the radio and submillimeter it is predicted that the opposite effect may occur, limb-brightening, which would result in dips within the light curve during ingress and egress [Selhorst et al., 2013]. This effect would arise due to the increasing temperature gradient in the stellar chromosphere where the emission is produced.

(Sub)millimeter Flares

A characteristic feature of transits in the radio regime is the possibility of the occlusion of active regions on the stellar surface with significantly higher brightness temperature than the surrounding areas. In the case of a very active surface region with $50 \times$ the brightness temperature of its surroundings, and a planetary radius $R_p = 0.02 R_*$, an enhancement of the transit signal by a factor 20 could be achieved [Selhorst et al., 2013]. Millimeter observations of the Proxima Centauri system with ALMA revealed a significant flare peaking at $10^3 \times$ the quiescent flux (peak $100 \pm 4$ mJy) for approximately 1 minute out of 19 hours of observation [MacGregor et al., 2018].

Naively we take a probability of the star being in a flaring state to be 0.1% based on this observation. The transit duration for a $P = 11$ d planet is $\sim 1$ h [Anglada-Escudé et al., 2016]. Assuming statistically independent flaring events we deduce the probability of the star entering a flaring state over 1 h of transit observation to be 6%, with 1 flare being observed 5% of the time, and in 1% of cases multiple flares occur during a single transit. Along its transit chord the planet sweeps out a fraction of the stellar disk’s area approximately $\leq R_p/R_*$. However, as the duration of the flare $t_{\text{flare}} << t_T$ the planet will not be able to sweep out the entire chord during an active flare, but will instead move a distance less than its own radius, resulting in a flare occultation probability per transit of $\sim (0.3 R_p)^2/R_*^2$. However, a flare which
begins and ends while completely occluded by the planet will not be detectable.

Given an M-dwarf which is known to host a transiting planet or planets, with a similar flaring probability and intensity as Proxima, we find for every transit a $\sim 0.02\%$ probability of flare occultation. The duration of the flare crossing transit $t_{fc}$ for a circular orbit is the time it takes the planet to move along its orbit a length equal to its own projected diameter and the apparent diameter of the emitting region.

$$t_{fc} = 2(R_p + R_e)\left(\frac{a}{GM*}\right)^{1/2} \quad (45)$$

where $R_p$ is the planetary radius, $G$ is the gravitational constant, $M*$ is the stellar mass, $a$ the planet’s semi-major axis, and $R_e$ the radius of the surface emitting region, which is assumed to be circular. The T Tauri star V773 Tau A at 130 pc distance was observed to flare at 90 GHz with an e-folding time of 2.31\pm0.19 h, enhancing the stellar signal up to 400 mJy (Massi et al., 2006; Torres et al., 2012). A massive transiting planet that could cause a 1% dip in flux would then produce a signal of 4 mJy which could be detected within only 30 ms by ALMA and would allow for high temporal sampling of the transit light curve to account for variability within the flare structure, however it would require the flaring region to be entirely occluded by the planet to produce a 4 mJy dip. The emission mechanism is proposed to be intra-binary interaction at periastron passage where the emitting region is a “helmet streamer”, a large elongated asymmetrical structure rooted to one member of the binary of length 15-20$R_*$. The proposed geometry makes it difficult for a hypothetical transiting planet to occlude a significant fraction of the streamer except at conjunction of the binary.

Millimeter flares from the object GMR-A, suspected to be a weak-line T Tauri, lasting up to 13 days have been observed to peak at 36.2\pm4.1 mJy at 3mm (10 GHz) (Furuya et al., 2003) and was also observed to flare at 86 GHz peaking at 160 mJy and remained above 100 mJy for a minimum of 4 h (Bower et al., 2003). Given a stellar flux density of 160 mJy, and an emitting region which is homogeneous over the stellar disk or equal in apparent area, ALMA could reach RMS noise levels equivalent to the depth of Hot Jupiter water lines in transit after only 30 minutes of integration at 96.26 GHz.
4 Discussion

The challenge of ground-based observations

The radial velocity distribution of stars in the local neighborhood precludes the detection of atmospheric water vapor in temperate Earth-identical exoplanets by emission. The stellar and planetary combined Doppler shift and broadening is not sufficient to move water line centers out of the heavily attenuated wavelengths of the Earth’s atmosphere, in the best possible case improving telluric atmosphere transmission by 1-10%, although at 325 GHz in ALMA band 7 the transmission can reach >20% for pwv = 0.5 mm. Given that the signals are already very weak (≤ 1µJy at 345 GHz for temperate terrestrial planets around the nearest star at 1.3 pc and up to 100µJy for Hot Jupiters) any further reduction of the signal by atmospheric attenuation is undesirable. In this regard Hot Jupiter and Hot Neptune atmospheres have an advantage. Multiple narrow water lines (∼90 absorption and 115 emission lines up to 1 THz for the Hot Jupiter case, such as FWHM 0.43 GHz at 96.26 4_{33} \rightarrow 5_{33} or FWHM 0.23 GHz at 147.51 GHz possible blend with HD^{18}O) appear in the emission and transmission spectra of the Hot Jupiters which correspond to wavelengths of low opacity (> 90% transmission) for ground based observations, several of which are identified in Fig.44. Cross-correlation of Doppler shifted lines with significant telluric contamination can be used to detect water in exoplanets from ground-based observations and can require many tens of strong absorption lines in the template spectra [Birkby et al., 2017]. The dozens of spectra produced in this work could function as templates for (sub)millimeter line cross-correlation. Because planetary peak emission strength lies in the mid-infrared for temperate planets and near infrared for hot planets (T > 700 K) limitations on detector sensitivity imply that the (sub)millimeter offers no particular advantage over near- to mid-infrared observations which are able to employ high dispersion (R = 100000) spectrometers which can make ground-based Hot Jupiter water line detections in ∼4 hours while ALMA observations must employ maximum bandwidth (for 7.5 GHz bandwidth R ≈ 40 at 345 GHz) to detect planetary - not atmospheric - signals over hours to days.

Water abundance and detectability

More water does not necessarily imply an easier detection of the water vapor. Large water abundances (X_{H2O} > 10^{-3}) in warm or hot atmospheres typically result in the 556.9 and 752 GHz line wings absorbing nearly all other features of the (sub)millimeter spectrum. The water dominated atmosphere proposed for TRAPPIST-1d proves to be one of the more challenging spectra in which to detect water in emission for continuum mode observations, given the broad but weak emission features with very narrow (FWHM< 5 GHz) cores in absorption. Water abundances below 10^{-5} produce negligible absorption in Hot Jupiters but dramatic features in Fig.33 (a) for X_{H2O} = 10^{-4} producing dozens of lines that absorb more than half of the planet continuum. For even greater water abundances X_{H2O} > 10^{-3} the entire continuum is suppressed and the spectral features are muted.

For the cooler (T = 194 K) Jupiters in emission, as the water abundance increases the spectrum goes from flat to displaying multiple emission features from 250-450 GHz at X_{H2O} = 10^{-6} to absorption of the same lines at X_{H2O} = 10^{-4}, broadening further at X_{H2O} = 10^{-2} demonstrated clearly in Fig.33 (c) and (d). For the water rich TRAPPIST-1d varying water abundance between X_{H2O} = 0.3-0.9 has a negligible effect as seen in Fig.33 (e) and (f).

Intermediate amounts of water (X_{H2O} = 10^{-5} - 10^{-6}) tend to produce the highest spectral contrast (100-150 ppm in transit for large H > 100 km Hot Jupiters) and ease of detection. Even small planets with very thin atmospheres (Mars) can produce lines at frequencies above 600 GHz which produce near maximum possible absorption (see Fig.37 (b)) when observed in transit with X_{H2O} = 2×10^{-4} but with widths too narrow to have their cores measured by a maximum ALMA 8 GHz bandwidth integration. The solution is to decrease bandwidth but integration times are already prohibitive. TRAPPIST-1d’s water lines have more contrast in transmission spectra than in emission as seen in Fig.46 producing the 183 GHz absorption line at nearly 70 ppm transit depth, as well as additional non-telluric lines from 70-130 GHz.
Limits on Detection

ALMA, the current state of the art (sub)millimeter detector, could possibly detect inflated Hot Jupiters by their unresolved excess emission (over the expected stellar flux) for distances below 4 pc although no such planets are known to exist. Beyond 4 pc the maximum possible thermal emission begins to fall below $10^9 \mu Jy$ at 345 GHz. Within 4 pc there are approximately 30 stellar and sub-stellar objects. A 2 R$_J$ Hot Jupiter in the Alpha Centauri system at $d=1.3$ pc with a flux density of 100 $\mu Jy$ could be detected within $10^3$ seconds at 1$\sigma$ and possibly at 3$\sigma$ within $10^4$ seconds. Hot Jupiter line strength is very sensitive to the vertical temperature profile of the atmosphere (see Fig.35(d)) where a strongly inverted atmosphere can cause dozens of strong lines to appear in emission at nearly double the level of the continuum, or they can be suppressed by a factor 5 in the case of an isothermal atmosphere. The line centers of temperate terrestrial atmospheres also tend to revert from absorption to emission when the atmosphere is singly inverted with a thermosphere at $P < 10^{-5}$ bar.

RMS noise levels of $\sim 1 \mu Jy$ at 345 GHz would be required to detect the brightest currently known exoplanet in emission, necessitating lengthy integration times ($\sim$1 month) and which ALMA could not spatially resolve. Only a hypothetical super-telescope such as the NGMA with 40,000 12 m antennae could detect water absorption features on the brightest known exoplanet $\tau$ Boo Ab within 10 h. Some integration times for a range of planet temperatures and distances is shown in Table 11.

<table>
<thead>
<tr>
<th>Planet</th>
<th>$T_{eq}$ [K]</th>
<th>$d$ [pc]</th>
<th>$t_{ALMA}$</th>
<th>$t_{NGMA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Earth</td>
<td>270</td>
<td>1</td>
<td>5556 d</td>
<td>12.25 m</td>
</tr>
<tr>
<td>Super-Earth</td>
<td>270</td>
<td>1</td>
<td>1097 d</td>
<td>2.42 m</td>
</tr>
<tr>
<td>Hot Super-Earth</td>
<td>1500</td>
<td>1</td>
<td>41.29 d</td>
<td>5.46 s</td>
</tr>
<tr>
<td>Jupiter</td>
<td>110</td>
<td>1</td>
<td>2.82 d</td>
<td>0.37 s</td>
</tr>
<tr>
<td>Hot Jupiter</td>
<td>1500</td>
<td>1</td>
<td>19.30 m</td>
<td>1.77 ms</td>
</tr>
<tr>
<td>Earth</td>
<td>270</td>
<td>10</td>
<td>$150 \times 10^4$ y</td>
<td>85.08 d</td>
</tr>
<tr>
<td>Super-Earth</td>
<td>270</td>
<td>10</td>
<td>$30 \times 10^3$ y</td>
<td>16.80 d</td>
</tr>
<tr>
<td>Hot Super-Earth</td>
<td>1500</td>
<td>10</td>
<td>1122 y</td>
<td>15.17 h</td>
</tr>
<tr>
<td>Jupiter</td>
<td>110</td>
<td>10</td>
<td>766 y</td>
<td>62.34 m</td>
</tr>
<tr>
<td>Hot Jupiter</td>
<td>1500</td>
<td>10</td>
<td>8.32 d</td>
<td>1.12 s</td>
</tr>
</tbody>
</table>

Table 11: Required integration times for 3$\sigma$ detections of planets in emission at 345 GHz with 7.5 GHz bandwidth, 50$\times$12 m antennae for ALMA and for 40,000 12 m antennae for the NGMA. Units of time are measured in years, days, hours, minutes, seconds, and milliseconds. Planets are taken to be ideal blackbodies. The Earth spectrum was found to emit at 80% of the ideal blackbody flux at 345 GHz which would result in a 56% increased integration time to achieve the same detection significance.

For transits the (sub)millimeter brightness of the host star largely determines whether or not a planet is detectable given that the planet SNR is a direct function of the stellar emission. Stellar (sub)millimeter thermal emission is weak. The nearest M dwarf produces emission at the 100 $\mu Jy$ level at 1.3 mm, and the nearest G and F type stars produce 26.06$\pm$0.19 mJy and 12.04$\pm$0.23 mJy at 343.5 GHz, respectively [Liseau et al., 2015]. Stellar emission could be enhanced above this level non-thermally (even non-transiently [Williams et al., 2015]), such as by the synchrotron emission of a T Tauri reaching peaks of 400 mJy at 90 GHz [Massi et al., 2006] which could not only allow for the millisecond-level integration time to detect a planet in transit with ALMA, but also $< 1 - 10$ h integration time to detect water absorption features in the planetary atmosphere in transit given water lines of depth 100-500 ppm seen in the synthetic (sub)millimeter spectra of Hot Jupiters around FGK stars or around even volatile dominated terrestrials orbiting M dwarfs. However the actual transit signature is contingent on the geometry of the emitting region and the planetary orbit and is not explored in this work. It is thus critical to identify stars with excess non-thermal emission. Integration times to detect several Hot Jupiter water lines in transit with varying stellar (sub)millimeter emission are listed in Table 12.
Table 12: Required integration times for ALMA $t_{ALMA}$ and the NGMA $t_{NGMA}$ for a 3 $\sigma$ detection of the line center in a typical Hot Jupiter atmosphere transiting an F or G type main sequence star of variable flux ($F_* = 100 \mu$Jy-500 mJy). Earth atmospheric transmission is not taken into account, and should increase integration time $\sim 60\%$ for a transmission of 80% to reach the same SNR. Note that actual line depths vary, reaching up to 300-500 ppm for completely ideal combinations of water vapor abundance and atmospheric scale height, stellar radius and $T_B$.

<table>
<thead>
<tr>
<th>Line [GHz]</th>
<th>Depth [ppm]</th>
<th>$F_*$</th>
<th>$t_{ALMA}$</th>
<th>$t_{NGMA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>209.12</td>
<td>150</td>
<td>100 $\mu$Jy</td>
<td>$25\times10^4$ y</td>
<td>13.8 d</td>
</tr>
<tr>
<td>232.69</td>
<td>130</td>
<td>100 $\mu$Jy</td>
<td>$22\times10^3$ y</td>
<td>12.3 d</td>
</tr>
<tr>
<td>336.23</td>
<td>140</td>
<td>100 $\mu$Jy</td>
<td>$77\times10^3$ y</td>
<td>43.0 d</td>
</tr>
<tr>
<td>209.12</td>
<td>150</td>
<td>1 mJy</td>
<td>247 y</td>
<td>3.3 h</td>
</tr>
<tr>
<td>232.69</td>
<td>130</td>
<td>1 mJy</td>
<td>222 y</td>
<td>3.0 h</td>
</tr>
<tr>
<td>336.23</td>
<td>140</td>
<td>1 mJy</td>
<td>771 y</td>
<td>10.3 h</td>
</tr>
<tr>
<td>209.12</td>
<td>150</td>
<td>10 mJy</td>
<td>903 d</td>
<td>2.0 m</td>
</tr>
<tr>
<td>232.69</td>
<td>130</td>
<td>10 mJy</td>
<td>810 d</td>
<td>1.7 m</td>
</tr>
<tr>
<td>336.23</td>
<td>140</td>
<td>10 mJy</td>
<td>2815 d</td>
<td>6.2 m</td>
</tr>
<tr>
<td>209.12</td>
<td>150</td>
<td>500 mJy</td>
<td>8.7 h</td>
<td>47.0 ms</td>
</tr>
<tr>
<td>232.69</td>
<td>130</td>
<td>500 mJy</td>
<td>7.8 h</td>
<td>42.8 ms</td>
</tr>
<tr>
<td>336.23</td>
<td>140</td>
<td>500 mJy</td>
<td>27 h</td>
<td>149 ms</td>
</tr>
</tbody>
</table>

Advantages and Disadvantages of the (Sub)millimeter

The (sub)millimeter wavelength range has several advantages for the detection of water. There are many water lines which can be excited within the temperature and pressure regimes of planetary atmospheres ($T = 50-7600$ K) (Beaulieu et al., 2006; Charpinet et al., 2011). Only very small amounts of water vapor ($X_{H_2O} = 10^{-8}$) are required to produce high contrast absorption features for cooler ($T < 500$ K) planets. Few universally abundant planetary gases (e.g. H$_2$, CO$_2$) are able to contaminate the water lines.

The (sub)millimeter, and particularly ground-based observations have several disadvantages. The Earth’s atmosphere makes it difficult to observe atmospheres which are very similar to the Earth’s. While transmission spectra of Earth-like planets do produce lines which do not appear prominently in the Earth’s (such as the 22 GHz line) the emission spectra would require higher altitude (>5000 m) or even space-based observatories to avoid reducing the SNR of already weak signals. In transit photometry the stability of the detector is the primary driver. The *Kepler* spacecraft attempted to achieve a 20 ppm level of stability which in practice was closer to 30 ppm. With a ground-based (sub)millimeter telescope similar levels of precision for stellar thermal emission requires exceedingly long integration times (> $10^7$ s) which for not only practical observational reasons renders detections challenging but also because of the timescales of stellar rotation, stellar variability, and variability in the Earth’s local weather conditions and pwv all producing variations that exceed or are of the same magnitude as planetary signals. Stellar variability in the (sub)millimeter is also poorly constrained, with new classes of flares from main sequence stars only recently being discovered serendipitously, possibly owing to the small (<100) number of stars that can have their continuum emission detected by ALMA within several hours. Stars which emit considerable non-thermal emitting stars have been detected with ALMA from their synchrotron emission even when not flaring (Williams et al., 2015).
5 Conclusion

The near- to mid-term future of (sub)millimeter water spectroscopy of Earth-like exoplanets will likely not be ground-based. The theoretical NGMA with 40,000 dishes of 12 m diameter, with incremental improvements over the ALMA $T_{\text{sys}}$, $\eta_c$, and aperture efficiency $\rho$ can detect atmospheric water around Hot Jupiters in the best case (large scale height, intermediate $\text{H}_2\text{O}$ abundances $\sim 10^{-4}$ with a strongly-inverted atmosphere and strong vertical mixing of water vapor) out to $20 - 30$ pc within several (< 10) hours given three 7.5 GHz bandwidth integrations of 3 hours each in order to measure the core and wings of a single line, where the RMS noise could be reduced to a level of 0.05 $\mu$Jy. The radio source background is not the limiting factor at lower frequencies; at 22 GHz we find $T_{\text{rsb}} = 0.058$ mK so its contribution to $T_{\text{sys}}$ is negligible even for the low frequencies considered for NGMA, while extragalactic background sources may present a challenge to spatially resolving planets at higher frequencies (MacGregor et al., 2018) but has not been investigated in this work. Excluding the possible interpretation of a planetary signal as a background galaxy would require multi-epoch observations to constrain the planet-star common proper motion.

Observing potentially habitable, temperate planets in the (sub)millimeter with similar conditions to the Earth thus requires space-based observatories. Space based interferometric arrays with dozens of antennae are currently only in very preliminary stages of design and planning and do not present a near-term solution although they have been considered (Harwit et al., 2006). While the tolerances on station keeping of an orbiting (sub)millimeter interferometer are not as stringent as for an optical interferometer, an even more ideal solution would be to place the array on a solid surface without an atmosphere - such as the lunar surface (Vilas, 1991). The lunar atmosphere is sufficiently tenuous and composed primarily of $^4\text{He}$, $^{20}\text{Ne}$, $\text{H}_2$, $^{40}\text{Ar}$ and $^{22}\text{Ne}$, such that transmission to the surface in the (sub)millimeter is essentially total, with no water vapor detected in-situ (Hoffman et al., 1973).

Highly irradiated exoplanets offer the best opportunity to study absorption features in emission and transmission spectra given the plethora of available water lines resulting from the high temperature environment and the inflated atmospheric scale height. High dispersion sub(millimeter) spectroscopy could serve as a technique to detect exoplanet water vapor with ground-based observatories but does not offer advantages over the near- and mid-infrared for hot and warm exoplanets which have peak thermal emission in these wavelengths.

Direct detection of nearby exoplanets will be practical given a 1-2 orders of magnitude improvement in telescope sensitivity over current designs. In that case the high angular resolving power of ground-based interferometers may be able to verify many radial-velocity planet candidates as real planets by spatially resolving them and remove the degeneracy with system inclination to constrain true mass.

Stellar variability in the (sub)millimeter is not fully understood but has been observed to boost (sub)millimeter emission by $> 3$ orders of magnitude. The timescale of the variability necessitates higher than currently achievable sensitivities in order to perform observations in sufficiently short windows to exclude stellar variability as the source of a planet-like signal. Further studies on the mechanisms of stellar (sub)millimeter non-thermal emission are needed as are ALMA millimeter observations of nearby (< 20 pc) main sequence stars. Pre-main sequence stars which flare for days at millimeter wavelengths offer the exciting possibility to perform atmospheric spectroscopy of transiting hot inflated (proto-)planetary atmospheres and the detection of (proto-)planets orbiting pre-main sequences stars, but is entirely contingent on the emitting geometry. Transit photometry with the K2 mission of the low mass star forming region $\rho$ Ophiuchus has revealed multiple dimming events (Hedges et al., 2018), some of which are possibly due to proto-planets and their dusty envelopes, such as the dimming events observed in V1334 Tau (Rodriguez et al., 2017). Remarkably the first 3 mm detection of a main sequence star occurred as recently as 2015 (Williams et al., 2015). There is thus much work left to be done in order to characterize main sequence stellar (sub)millimeter emission as a first step towards planet detection, beginning with a survey of nearby stars with ALMA in order to address the modern adage “Know thy star, know thy planet”.

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References


