Alkaline Exospheres of Exoplanet Systems: Evaporative Transmission Spectra

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ABSTRACT
Hydrostatic equilibrium is an excellent approximation for the dense layers of planetary atmospheres where it has been canonically used to interpret transmission spectra of exoplanets. Here we exploit the ability of high-resolution spectrographs to probe tenuous layers of sodium and potassium gas due to their formidable absorption cross-sections. We present an atmosphere-exosphere degeneracy between optically thick and optically thin mediums, raising the question of whether hydrostatic equilibrium is appropriate for Na I lines observed at exoplanets. To this end we simulate three non-hydrostatic, evaporative, density profiles: (i) escaping, (ii) exomoon, and (iii) torus to examine their imprint on an alkaline exosphere in transmission. By analyzing an evaporative curve of growth we find that equivalent widths of $W_{\text{Na D2}} \sim 1 - 10 \text{ mÅ}$ are naturally driven by evaporation rates $\sim 10^3 - 10^5 \text{ kg/s}$ of pure atomic Na. To break the degeneracy between atmospheric and exospheric absorption, we suggest that if the line ratio is $D2/D1 > 1.2$ the gas is optically thin on average and roughly indicating a non-hydrostatic structure of the atmosphere/exosphere. We show this is the case for Na I observations at hot Jupiters WASP-49b and HD189733b and also simulate their K I spectra. Lastly, motivated by the slew of metal detections at ultra-hot Jupiters, we suggest a toroidal atmosphere at WASP-76b and WASP-121b is consistent with the Na I data at present.

Key words: planets and satellites: atmospheres ; radiative transfer ; line: profiles ; techniques: spectroscopic

1 INTRODUCTION
The alkali metals, sodium (Na I) and potassium (K I), have long been predicted to be observable spectroscopically during an exoplanet transit (Seager & Sasselov 2000; Hubbard et al. 2001). While this launched the study of extrasolar atmospheres we remark here that alkaline observations are also consistent with extrasolar exospheres of diverse geometries in terms of the required source rates (Johnson & Huggins 2006; Oza et al. 2019b). This subtle degeneracy between collisional atmospheres and collisionless exospheres is due to the large absorption cross-sections of the Na & K atoms, enabling small column densities of gas to illuminate optically thin gas.

While transmission spectra can be simulated analytically (Lecavelier Des Etangs et al. 2008; de Wit & Seager 2013; Bétrémieux & Swain 2017; Heng & Kitzmann 2017; Jordán & Espinoza 2018; Fisher & Heng 2019), these approaches rely on the assumption of an atmosphere being in local hydrostatic equilibrium, an assumption which generally holds in dense atmospheric layers as gravity and pressure gradients are the dominant forces. Hydrostatic equilibrium becomes less accurate in more tenuous atmospheric layers, and can break down in certain circumstances such as in an escaping atmospheric wind. In fact, soon after the first detection of an exoplanetary atmosphere at HD209458b (Charbonneau et al. 2002), Vidal-Madjar et al. 2003 detected neutral hydrogen beyond the Hill sphere and interpreted this as an evaporating component of the atmosphere. Close-in exoplanet atmospheres were hence observed to be nonhydrostatic, and shown to be hydrodynamically evaporating $\sim 10^7 \text{ kg/s}$ of gas due to XUV-driven escape (Murray-Clay et al. 2009). Considerable endogenic modeling of evaporative transmission spectra is indeed underway, largely aiming at signatures of atomic hydrogen (Bourrier & Lecavelier des Etangs 2013; Christie et al. 2016; Allan & Vidotto 2019; Murray-Clay & Dijkstra 2019; Wyttenbach et al. 2020), but also by atomic helium (Oklopčić & Hirata 2018;
Lampón et al. 2020), atomic magnesium Bourrier et al. 2015 and ionized magnesium (Dwivedi et al. 2019). However, the retrieval of atmospheric parameters from observations using various techniques such as $\chi^2$-minimization, Bayesian analysis, or advanced machine-learning methods (Márquez-Neila et al. 2018; Hayes et al. 2020) is largely based on the assumption of hydrostatic equilibrium (e.g. Ehrenreich et al. 2006; NEMESIS Irwin et al. 2008; CHIMERA Line et al. 2013; TAU-REX1 Waldmann et al. 2015; BART Bleie et al. 2017; EXO-Transmit Kempton et al. 2017; ATMO Goyal et al. 2018; $\eta$ Pino et al. 2018; Aura Pinhas et al. 2018; HELIUS-T Fisher & Heng 2018; PLATON Zhang et al. 2019; MERC Seidel et al. 2020; among others). The problem is further amplified and fundamentally different if the gas were to be detached from the planet. Such an exogenic alkaline source, such as an outgassing satellite or a thermally desorbing torus, would not be in hydrostatic equilibrium. The impact of exogenic sources on transmission spectra has not yet been investigated until present. In the following we shall use evaporative and non-hydrostatic interchangeably.

In the present study, we examine evaporative transmission spectra of the Na I doublet ($\lambda_2 = 5899.95$ Å, $\lambda_1 = 5895.92$ Å) and the K I doublet ($\lambda_2 = 7664.90$ Å, $\lambda_1 = 7698.96$ Å). The lines when viewed in absorption are extremely bright due to resonance scattering (Brown & Yung 1976; Draine 2011) off the sodium atoms. The resonant scattering cross section is large, producing considerable absorption in highly tenuous columns of gas at pressures where one expects large deviations from hydrostatic equilibrium. Fortunately astronomers have had decades of fundamental understanding of the physics of the Na and K alkaline resonance lines by directly observing comets and moons in-situ from within our solar system (Oza et al. 2019b Table 1 and references therein). The most spectrally conspicuous aforementioned evaporative sources are Jupiter’s and Saturn’s moons Io & Enceladus, motivating the mass loss model of an evaporating exomoon shown to be roughly consistent with several extrasolar gas giant planets today (Oza et al. 2019b). Coupling an atmospheric escape model (termed DISHDOM) to a radiative transfer code capable of treating nonhydrostatic profiles (termed Prometheus) is the crux of our present study on evaporative transmission spectra. This coupling permits a holistic approach to transit spectra, capable of breaking endogenic-exogenic degeneracies in alkaline exospheres today.

We use a custom-built radiative transfer code to simulate high-resolution transit spectra in the sodium doublet for four scenarios, seeking the precise imprint of an evaporative transmission spectrum of an alkaline exosphere in regards to a canonical hydrostatic atmosphere. We present this code in Section 2.1. The mass loss model is laid out in Section 2.2. Our four examined scenarios, corresponding to a particular geometry and spatial distribution of the sodium atoms, are presented in detail in Sections:

- 2.3 Hydrostatic: A spherically-symmetric hydrostatic atmosphere.
- 2.4 Escaping: A spherically-symmetric hydrogen/helium envelope undergoing atmospheric escape.
- 2.5 Exomoon: A spherically-symmetric cloud sourced by an outgassing satellite.
- 2.6 Torus: An azimuthally-symmetric torus sourced by a satellite or debris.

We describe each of these scenarios with a particular number density profile $n(r)$ (since an exospheric collisionless gas cannot be described with a pressure profile) and two free parameters. These three components fully determine our simulated transit spectra. Of course, an exhaustive description of metals at a close-in gas giant system would involve a careful treatment of atmospheric collisional processes (e.g. Huang et al. 2017), exospheric physical processes (Leblanc et al. 2017), an atmospheric escape treatment in 3-D (e.g. Debretsch et al. 2019) and also the ability to track ions in the presence of a magnetic field (e.g. Carnielli et al. 2020). Since we reduce every scenario to a number density profile with two free parameters, our model is heuristic at present. Hence, this study isn’t targeted at providing an exhaustive model of hot Jupiter exospheres with the corresponding transit spectra, but rather encourages a novel approach by elucidating fundamental differences between hydrostatic and non-hydrostatic assumptions.

We use the synergy of our two distinct approaches (radiative transfer & mass loss) to gain a physical intuition on the four density scenarios described above, starting in Section 3. We find that evaporative sodium profiles naturally allow vastly more extended yet tenuous distributions of the absorbing atoms than hydrostatic profiles. This property of evaporative sodium can lead to absorption in a primarily optically thin regime, resulting in high-resolution transit spectra differing from spectra computed within a hydrostatic framework. In Section 3.4 we provide a simple diagnostic gathered from physics of the interstellar medium (e.g. Draine 2011), to determine if an alkaline gas is optically thin or thick at a transiting exoplanet. Given that several hot Jupiters observed in high-resolution appear to reveal an optically thin regime, we simulate the spectral imprint for each evaporative scenario at HD189733b in Section 4. The forward model in this section serves to demonstrate the differences between hydrostatic and evaporative transmission spectra by coupling mass loss $a$ priori.

For those more acquainted with inverse modeling, we use the observed transit spectra of the hot Jupiters WASP-49b and HD189733b to portray the behavior of evaporating alkalis in parameter space (Section 5). In our observational analysis, best-fit parameters are found within the radiative transfer code using a free $\chi^2$-minimization. We then check the plausibility of these retrieved parameters by comparing to the calculated values from the alkali mass loss model. We choose to comparatively analyze these two planets as they were observed by the same spectrograph (HARPS) and reduced by the same author (Wyttenbach et al. 2015; Wyttenbach et al. 2017) enabling a consistent comparison to the data of both hot Jupiters. These planets represent the first

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1 The TAU-REX code represents a notable exception to strict assumptions on hydrostatic envelopes, as it processes input files with arbitrary, user-defined pressure profiles.

2 Exogenic refers to an external source whereas endogenic refers to a planetary source.

3 No constraint on priors.
high-resolution Na I detections and therefore have been extensively studied by independent groups (Louden & Wheatley 2015; Cubillos et al. 2017; Huang et al. 2017; Fisher & Heng 2019) compared in Section 6.1. Furthermore, these planets were shown to be able to host exogenic sources of alkali metals i.e. satellites in terms of tidal stability and average column densities (Oza et al. 2019b). For our study of alkaline exospheres, we focus on the physics of evaporating Na I acknowledging the behavior of evaporating K I is nearly identical, simulated in Section 6.2. We discuss the imminence of metal detections at ultra-hot Jupiters (WASP-76b & WASP-121b) in the context of toroidal atmospheres in Section 6.3 and conclude in Section 7.

2 METHODS

2.1 Prometheus: Alkaline Transmission Spectra of Atmospheres and Exospheres

We simulate transit spectra using a simple and flexible custom-built Python code: Prometheus. Our code computes absorption either in the Na I or K I doublet for an exoplanet system in transit geometry. For a spherically-symmetric system (our first three scenarios), we divide the atmosphere using a linear grid in $x$- and a logarithmic one in $z$-direction with adjustable spatial resolutions to adapt to each scenario (see Figure 1). For the torus scenario exhibiting azimuthal geometry we also linearly discretize the $y$-axis which affects the computation of the transit spectra (Eqns. 1 and 3), see Section 2.6 for details. The transit spectrum is computed in the following two steps. First, we calculate the optical depth along the chord at a certain altitude $z$ and wavelength $\lambda$

$$\tau(z, \lambda) = 2 \int_0^\infty n(r) \sigma(\lambda, T(\lambda)) \cdot \chi_i(\lambda) \, dx,$$

(1)

given that $r = \sqrt{x^2 + z^2}$ and where $\chi_i(\lambda)$ is the volume mixing ratio$^4$ of the neutral absorber (either Na I or K I). Our code can be coupled to a chemistry code such as FastCHEM (Stock et al. 2018) to calculate these mixing ratio profiles, but we only examine constant mixing ratio profiles in the scope of this paper. Since (using Na as placeholder for the absorber) $\chi_{Na}(r) = \chi_{Na}(r) \cdot (1 - f_{ion}(r))$, the assumption of a constant mixing ratio of the absorber translates into the assumption of a constant ionization fraction $f_{ion}(r)$ for the absorbing species, given that the total (neutral plus ionized) mixing ratio of the absorber isn’t expected to vary significantly. At present we focus solely on the absorption of alkali metals as they dominate the absorption in the narrow wavelength regions around the doublets. We also included Rayleigh scattering from the background H$_2$ atmosphere in an earlier version of our code, but find this to be negligible.

We compute the absorption cross section $\sigma(\lambda, T)$ as the sum of the individual D2 and D1 absorption lines. These lines are modeled as Voigt profiles using scipy.special.wofz. Line broadening is included in our work either by temperature $T(r)$ (Doppler broadening) or pressure, although the latter is not relevant in high-resolution observations of the tenuous regime of the gas. Consequently we neglect pressure broadening throughout this work. Since the absorbing atoms reach velocities significantly above thermal speeds for our three evaporative, non-hydrostatic scenarios, we must also consider this non-thermal Doppler broadening. We incorporate this broadening by treating the average velocity $\bar{v}_i$ of the absorbing atoms as an effective line temperature:

$$T(r) = \frac{m_i}{8k_B} \bar{v}_i^2$$

(2)

where $m_i$ is the atomic mass of the absorber. The line is then broadened using Voigt profiles, with a Doppler broadening parameter given by this line temperature for the three evaporative scenarios. See Table 3 and Section 3.4 for a more extensive discussion on the temperatures and broadening.

This scheme is a general prescription for the computation of transmission spectra. To compare our calculations to observations WASP-49b (Wytenbach et al. 2017) and HD189733b (Wytenbach et al. 2015) we use a convolution, binning and normalization routine for all simulated transit spectra as in Pino et al. (2018) (see Section 2.7 for details). While our code is comparatively simple in terms of atmospheric chemistry, wavelength coverage, line broadening and absorbing species, it has the stark advantage that the number density profile can be arbitrarily defined without relying on the assumption of the atmosphere being in local hydrostatic equilibrium. This allows the simulation of transit spectra in two endogenic (hydrostatic & escaping) and two exogenic scenarios (exomoon & torms).

2.2 DISHOOM: Alkaline Mass Loss to Atmospheres and Exospheres

We couple a semi-analytic metal mass loss model DISHOOM (Destroying Interiors via Satellite Heating to Observing Outgassing Model) described comprehensively in Oza et al. (2019b) Sections 3 (Jupiter’s Atmospheric Sodium) and 4 (Jupiter’s Exospheric Sodium) to Prometheus in order to

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Table 1. System parameters of WASP-49b (Wytenbach et al. 2017) and HD189733b (Wytenbach et al. 2015), lifetimes of neutral sodium ($T_{Na}$) are estimated from Huebner & Mukherjee (2015). $v$ denotes the systemic velocity of the exoplanetary system, which is important for the comparison of the observational data to our simulated spectra.

| Parameter | WASP-49b | HD189733b |
|-----------|----------|-----------|
| $R_\ast$ | [R$_\odot$] | 1.038 | 0.756 |
| $R_0$ | [R$_J$] | 1.198 | 1.138 |
| $M_p$ | [M$_J$] | 0.399 | 1.138 |
| $T_{Na}$ | [K] | 1400 | 1140 |
| $\gamma$ | [km/s] | 41.7 | -2.28 |
| $ts$ | [s] | 241 | 1010 |

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$^4$ Relative abundance by number. We denote mass mixing ratios by $x$. 

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et al. 2015), as well as water-products H\textsubscript{2}O, CH\textsubscript{4}, and CO is included (see Johnson et al. 2015), as well as water-products H\textsubscript{2}O, O\textsubscript{2} (see Oza et al. 2019a) where the mechanisms leading to outgassing and eventual escape include solar heating, magnetospheric ion sputtering, and general space weathering. For close-in systems, like the ones studied here, nearly molten temperatures lead to volcanic and magma-products due to tidal heating or direct sublimation of grains (i.e. Section 2.6).

simulate evaporative transmission spectra for the Na I and K I lines.

2.2.1 Observing Outgassing During a Planetary Transit

An outgassing source undergoing mass loss can produce a prodigious quantity of foreground gas capable of generating a spectral signature during transit. Our escape model generalizes outgassing of planetary surfaces to include a wide-range of phenomena capable of producing spectral signatures as observed in the solar system. Escape of the so-called supervolatiles N\textsubscript{2}, CH\textsubscript{4}, and CO is included (see Johnson et al. 2015), as well as water-products H\textsubscript{2}O, O\textsubscript{2} (see Oza et al. 2019a) where the mechanisms leading to outgassing and eventual escape include solar heating, magnetospheric ion sputtering, and general space weathering. For close-in systems, like the ones studied here, nearly molten temperatures lead to volcanic and magma-products due to tidal heating or direct sublimation of grains (see Section 2.2.2 below). For a volcanically-active system Na & K are products of the parent molecules NaCl and KCl as observed at Io. The close-in systems are jeopardous in that the atomic lifetimes are strongly limited by photoionization. Following Huebner & Mukherjee (2013) we can estimate the atomic lifetime for a species i as \( t_i \approx \frac{1}{k_i} \) where \( k_i \) is the photoionization rate coefficient in s\(^{-1}\):

\[
k_{i,\lambda} = \int_\Delta \sigma_\lambda(\lambda')\Phi(\lambda') \, d\lambda.
\] (4)

in the wavelength of interest \( \lambda + \Delta \lambda \), a photoionization cross section \( \sigma_\lambda(\lambda) \) and the spectral photon flux:

\[
\Phi(\lambda) = \frac{2\pi e}{4\lambda^4[\exp(hc/\lambda k_B T) - 1]},
\] (5)

for a Blackbody of temperature T (e.g. Rybicki & Lightman 1979). As we describe in Section 2.2.2, photoionization timescales provide a critical lower limit to the atomic lifetime, as recombination processes due to the ambient plasma could boost these lifetimes. Independent of the mass loss mechanism, we can write the general mass loss rate for a source venting a species i depending on the number of atoms \( N_i \):

\[
M_i = \dot{m}_i k_i N_i = \dot{m}_i t_i^{-1} N_i.
\] (6)

The number of evaporating atoms is then fed into the number density profiles for each evaporative mechanism, enabling a straightforward computation of an evaporative transmission spectrum.

2.2.2 Metallic Mass Loss

In addition to the evaporation of NaI and KI, the code is equipped to estimate the destruction of rocky bodies of arbitrary composition (e.g. MgSiO\textsubscript{3}; Fe\textsubscript{2}SiO\textsubscript{4}). This description of atmospheric loss holds observational relevance given the recent explosion of heavy metal detections at gas giants (Hoeijmakers et al. 2018, Hoeijmakers et al. 2019; Sing et al. 2019; Cabot et al. 2020; Gibson et al. 2020). In our study of the alkali metals, we shall use chondritic ratios constrained by Fegley & Zolotov (2000) for Na and K, when estimating the mass loss rates due to thermal evaporation of silicate grains (i.e. Section 2.6).

In practice, the metal evaporation code computes different regimes of escape (e.g. thermal, nonthermal) due to several heating mechanisms (e.g. XUV, tidal heating) for a close-in irradiated body. The dominant mass loss rate is then either supplied to Prometheus to generate a forward-model transit spectrum, or compared to retrieved mass loss rates and velocities in the inverse modeling as a plausibility check if the different evaporative scenarios can indeed provide the required absorber source rates. The dominant mass loss mechanism varies between the different evaporative scenarios. We show the equations we use to estimate \( M_i \) in the respective subsection of the scenario (Sections 2.4 to 2.6). Generally, as data regarding the chemistry and plasma conditions are largely unknown at an exoplanetary system at present, we will find it useful to use scaling relations to solar system bodies observed in-situ (see Gronoff et al. 2020 and references therein for a full review on escape from solar system and exoplanet bodies).

In our heuristic model, we provide upper limits to the required mass loss rate based on the assumption that photoionization is the dominant process regulating the alkali lifetime. While to first order this is valid, two of our evaporative scenarios (Exomoon: 2.5 & Torus: 2.6 described below) are analogous to the radiation environment of a gas giant magnetosphere. As observed and simulated in the Jupiter- Io plasma torus system, recombination and charge exchange could considerably extend the net lifetime of the alkali atoms (see Wilson et al. 2002 and references therein). Radiative recombination is additionally important for a close-in magne-
Table 2. Sodium plasma processes.

| Plasma Process         | Reaction                        |
|------------------------|---------------------------------|
| Photoionization        | Na + γ → Na⁺ + e⁻               |
| Recombination          | Na⁺ + e⁻ → Na + γ               |
| Charge Exchange        | Na⁺ + Na → Na⁺ + Na              |
| Dissociative Recombination | NaX⁺ + e⁻ → Na⁺ + X⁺          |

tosphere as ions have the ability to accumulate in the magnetosphere so long as advection is small. We find, similar to Vidal-Madjar et al. (2013) for Mg at HD209458b, that \( n_e \sim 10^8 \text{ cm}^{-3} \) are required for electronic recombination of Na. In a toroidal B-field, we remark that ion-recombination and charge exchange can be effective to source the extended alkali clouds we describe here. In the absence of a toroidal B-field, a conservative ion density assuming charge neutrality based on the simulations by Dwivedi et al. (2019), ion densities of \( 10^3 - 10^5 \text{ cm}^{-3} \) were simulated up to \( \approx 3 \text{R}_0 \) validating a viable recombination mechanism at distances corresponding to our exogenic evaporating scenarios (Section 2.5, 2.6).

Furthermore, we find that for the alkali atoms studied here, loss rates due to radiation pressure are small mostly due to the dominating ionization rates discussed above. Balancing the radiation pressure force with that of gravitation (e.g. Vidal-Madjar et al. 2003; Murray-Clay et al. 2009), upper limits to the loss rate \( \sim 10^{-10} \text{ kg/s} \) are found for the range of sodium column densities studied in Section 3. In Tables 2 and 3 we qualitatively present the plasma processes regulating our evaporative scenarios and the average speeds of the alkali atoms \( \bar{v} \).

The simple coupling via mass loss rate and equation 6 we perform is to demonstrate the dramatic influence of mass loss and number densities on an alkaline transmission spectrum. We remark that more robust hydrodynamic codes focusing on individual planets are especially suited for this problem, as has been shown in Ly a at HD189733b (Bourrier & Lecavelier des Etangs 2013; Christie et al. 2016), Ha, Hβ, and Hy at KELT-9b (Wytenbach et al. 2020), Mg I at HD209458b (Bourrier et al. 2015), Mg II at WASP-12b (Dwivedi et al. 2019) and He I at HD209458b (Oklopcic & Hirata 2018; Lampón et al. 2020).

2.3 Hydrostatic scenario

This is the canonical scenario for transmission spectra. The number density profile is straightforward to derive by using the definition of the pressure scale height: \( H(r) = \frac{\text{d}P(r)}{\text{d}r} \frac{T(r)}{\mu(r) g(r)} \), where \( \mu(r) \) is the mean molecular weight and \( g(r) \) the local acceleration. Solving the equation of hydrostatic equilibrium \( \text{d}P(r)/\text{d}r = -\mu(n(r))g(r) \) for number density, \( n(r) \), yields the hydrostatic number density profile:

\[
n_{\text{hyd}}(r) = n_0 \cdot \frac{T_0}{T(r)} \cdot \exp \left[ -\int_{R_0}^{r} \frac{\text{d}r'}{T(r')} \right],
\]

where \( R_0 \) is a fixed reference radius, and quantities with subscript zero are evaluated at this reference radius. Although our code can process arbitrary temperature and mixing ratio profiles, we restrict ourselves to isothermal and vertically-mixed (i.e. with constant mixing ratios of the neutral absorber throughout the atmosphere) models, as we want to isolate the effect of varying the number density profiles within our different scenarios. Therefore, \( T(r) \) and \( \mu(r) \) are constant and the number density profile in Equation 7 can be integrated:

\[
n_{\text{hyd}}(r) = n_0 \cdot \exp(A(r) - A_0),
\]

where \( A(r) \) is the Jeans parameter given by \( A(r) = \frac{G M_p}{2 \pi T r} \). We use the canonical value of \( \mu = 2.3 \text{amu} \) (corresponding to a mass mixing ratio \( \chi_{\text{He}} = 0.25 \)) for our hydrostatic model. Using the number density profile of Equation 8 with constant temperature and mixing ratios throughout the atmosphere leads to three free parameters in this scenario: temperature \( T \), pressure at reference radius \( P_0 \) and absorber mixing ratio \( \chi_1 \). However, \( P_0 \) and \( \chi_1 \) are mutually degenerate in our model since we neglect pressure broadening, collision-induced absorption and other absorbers (see Heng & Kitzmann 2017 and Welbanks & Madhusudhan 2019 for a detailed discussion on this degeneracy). Therefore, we have the partial pressure of the absorber at the reference radius \( P_{\chi_i} = P_0 \cdot \chi_i \) as a second free parameter. We show how these two parameters, \( T \) and \( P_{\chi_i} \), affect the transmission spectrum for a hot Jupiter with planetary parameters of WASP-49b in Figures 2 and 3. We will find it useful to define auxiliary parameters which are easier to interpret than the free parameters, but don’t fundamentally affect the transmission spectrum. For the hydrostatic scenario we use \( P_0 \) as an auxiliary parameter (e.g. in Figure 2), calculated from \( P_{\chi_i} \) under the assumption of a specific absorber mixing ratio. A summary of free, auxiliary and fixed parameters for all scenarios can be found in Table 4.

2.4 Escaping scenario

Hot Jupiters are observed to have escaping planetary winds (Vidal-Madjar et al. 2003). Currently, there are significant modeling efforts to simulate escaping atmospheres by either

| Physical Process               | Nominal velocity distribution (Analog) | \( \bar{v} \) |
|-------------------------------|----------------------------------------|-------------|
| Atmospheric Sputtering\(^{a,b}\) | (Atmospheric Escape at Io)              | 10 km/s     |
| Charge Exchange\(^b\)         | (Sodium Exosphere at Jupiter)          | 60 km/s     |
| Pickup Ions\(^b\)             | (Io plasma torus)                       | 74 km/s     |
| Resonant Orbit\(^c\)          | (Io motion)                             | 17 km/s     |
| Thermal                       | (Volcano temperature)                  | 1.4 km/s    |

\(^a\) Smyth (1988); \(^b\) Wilson et al. (2002); \(^c\) Cassidy et al. (2009).
solving the Navier-Stokes equations or more computationally expensive yet robust, directly solving the Boltzmann equation on a particle to particle basis (see Gronoff et al. 2020 for both approaches to atmospheric escape). While atmospheric escape is not the prime focus of the current study, we emphasize that the latter kinetic model is sorely needed at present for a full description of an exoplanet exosphere. Nevertheless, the hydrodynamical approach of escaping atmospheres has been applied to different hot Jupiters, computing pressure, temperature and velocity profiles of the wind. Murray-Clay et al. (2009) found that at pressures $P > 1$ mbar, the atmosphere can still be treated as hydrostatic, while at lower pressures the atmospheric structure strongly deviates from a hydrostatic profile. As a first-order approximation for the number density profile we use a power law with $q_{\text{esc}} = 6$ for our analysis, which is roughly in line with the profiles found for WASP-49b (Cubillos et al. 2017) and HD209458b (Murray-Clay et al. 2009).

\begin{equation}
N_i = \int_{R_0}^{\infty} r^2 n_{\text{esc}}(r) \, dr = \frac{4\pi}{q_{\text{esc}} - 3} n_{0,\text{Na}} R_0^3.
\end{equation}

The escape index $q_{\text{esc}} = 6$ is indicative of ion-neutral scattering for an escaping neutral gas interacting with a plasma (Johnson 1990; Johnson et al. 2006b). The reference radius $R_0$ corresponds to the base of the wind in this scenario. As we want to isolate the different scenarios we neglect the hydrostatic layer below the base of the wind for the computation of the transit spectra. Since the hydrodynamical simulations generally just incorporate hydrogen and helium we don’t know the mixing ratio profile of the absorber, $\chi_i(r)$. As in the hydrostatic scenario we set this profile to a constant value, meaning that we encounter a similar degeneracy between $n_0$ and $\chi_i$ as in the hydrostatic scenario. Hence we have the number density of the absorber at the base of the wind, $n_{0,i}$, as a free parameter. We can convert this quantity into the total number of absorbing atoms as the volume integral of Equation 9:

\begin{equation}
N_i = \int_{0}^{R_0} n_{\text{esc}}(r) \, dV = 4\pi R_0 \int_{0}^{R_0} r^2 n_{\text{esc}}(r) \, dr = \frac{4\pi}{q_{\text{esc}} - 3} n_{0,\text{Na}} R_0^3.
\end{equation}

Given that $R_0$ and $q_{\text{esc}}$ are fixed we can use $N_i$ and $n_{0,i}$ interchangeably as free parameters. Since we use $N_i$ to compute the required source rate, comprising the coupling between our codes (Equation 6), we choose the total number of absorbing atoms in the systems as a free parameter. Since this quantity is difficult to interpret physically, we use the pressure at the base of the wind as auxiliary parameter. Assuming a certain absorbing mixing ratio and temperature, we calculate this pressure as $P_0 = n_{0,i}/\chi_i \cdot k_B T$. We expect photoionization of the alkali metals to be significant in the escaping scenario. We remark here that while photoionization probably affects $\chi_i(r)$, it doesn’t change the validity of setting $\chi_i(r) = \text{const}$. as long as the ionized fraction is constant in the escaping wind. However, the retrieved value of $N_i$ can’t be accurately converted into $P_0$ as we don’t know the mixing ratio of the neutral absorber, $\chi_i$. We show how $P_0$ affects the transmission spectrum for a hot Jupiter with planetary parameters of WASP-49b in Figure 4. Apparently, the transit spectrum depends strongly on the value of $P_0$ compared to Figure 2. We elucidate this behaviour in Section 4.

The speeds of the absorbing atoms in escaping winds greatly exceed the thermal speeds. As described in Section 5 we encountered this degeneracy in the hydrostatic setting between $P_0$ and $\chi_i$, as our knowledge of the temperature allowed for a direct conversion between pressures and number densities. As we don’t know the temperature in the escaping wind we formulate the degeneracy in this scenario as one between $n_0$ and $\chi_i$. 

\begin{figure}
\centering
\includegraphics[width=0.9\textwidth]{figure2}
\caption{Simulation of high-resolution transit spectra in the sodium doublet, for different reference pressures in the hydrostatic scenario. The shape of the transit spectra isn’t determined by $P_0$ but by the partial pressure of sodium at the reference radius, $P_{\text{Na}}$. For better readability we fix $P_{\text{Na}}$ and vary $P_0$. We set $\chi_{\text{Na}} = 1.7$ ppm (the solar mixing ratio) and $T = 3000$ K. The planetary parameters and data points are for WASP-49b, taken from Wyttenbach et al. (2017).}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=0.9\textwidth]{figure3}
\caption{Simulation of high-resolution transit spectra in the sodium doublet, for different temperatures in the hydrostatic scenario. We set $\chi_{\text{Na}} = 1.7$ ppm (the solar mixing ratio) and $T = 3000$ K. The planetary parameters and data points are for WASP-49b, taken from Wyttenbach et al. (2017).}
\end{figure}
2.1, we use the wind speed to calculate a line temperature, which is then treated as thermal Doppler broadening of the line. We simplify the velocity profile of the escaping wind to a constant value (as in the hydrostatic model with vertical winds of Seidel et al. 2020). We have therefore the mean speed of the absorbing atoms in the escaping wind, \( v_i \), as second free parameter. The impact of this parameter on a transmission spectrum for a hot Jupiter with planetary parameters of WASP-49b is shown in Figure 5.

We estimate the mass loss rate in this evaporative scenario using DISHOM. Hydrodynamically escaping atmospheres have two escape regimes: radiation-recombination limited (Murray-Clay et al. 2009) and energy-limited escape (Johnson et al. 2013): escaping absorber using the energy-limited approximation. Here we choose to crudely estimate the mass loss rate of the \( \text{DISHOOM} \) scenario using parameters of WASP-49b is shown in Figure 5.

Upper limits we use here are to examine the extremeties of the evaporative wind scenario. We note that the upper limits we use here are to examine the extremeties of the evaporative wind scenario. As the escaping atmosphere passes the exobase, the energy-limited approximation used here will overestimate the source rate (Johnson et al. 2013). Furthermore, as hot Jupiters are expected to have strong magnetic fields (Yadav & Thorngren 2017), the mass loss rates may be far less as pointed out by Christie et al. (2016) based on the MHD simulations of Trammell et al. (2011); Trammell et al. (2014); Tremblin & Chiang (2013) and Owen & Adams (2014).

\[
M_{\text{esc,1}} \sim x_i m_i \frac{Q}{U}, \tag{11}
\]

where \( Q \) is the XUV-heating rate of the upper atmosphere given a heating efficiency between 0.1 - 0.4, \( U \) is the binding energy of the atmosphere, \( x_i \) the mixing ratio by mass for the atom \( m_i \). For sodium, we use \( \chi_{Na} = 1.7 \times 10^{-5} \), which corresponds to the solar volumetric mixing ratio of sodium of \( 1.7 \pm 0.3 \times 10^{-5} \), multiplied by \( m_{Na} / \mu \) (with \( \mu = 21 \text{amu} \)). This mass loss rate, together with the required source rate estimated from equation 6, comprises the coupling between DISHOM and Prometheus for the escaping scenario. We note that the shape of the transit spectra is determined by \( \chi_{Na} \), but for better readability we show the auxiliary parameter \( P_0 \). We use the planetary equilibrium temperature (table 1) and a solar mixing ratio of \( \chi_{Na} = 1.7 \pm 0.3 \times 10^{-5} \) to calculate the reference pressures. We fix \( \chi_{Na} = 10 \text{km/s} \) in this Figure. The planetary parameters and data points are for WASP-49b, taken from Wyttenbach et al. (2017).

Figure 4. Simulation of high-resolution transit spectra in the sodium doublet, for different reference pressures in the escaping scenario. The shape of the transit spectra is determined by \( \chi_{Na} \), but for better readability we show the auxiliary parameter \( P_0 \). We use the planetary equilibrium temperature (table 1) and a solar mixing ratio of \( \chi_{Na} = 1.7 \pm 0.3 \times 10^{-5} \) to calculate the reference pressures. We fix \( \chi_{Na} = 10 \text{km/s} \) in this Figure. The planetary parameters and data points are for WASP-49b, taken from Wyttenbach et al. (2017).

2.5 Exomoon scenario

As observed in the Jupiter-Io system, a tidally-heated satellite can outgas significant amounts of particles, especially neutral sodium, via volcanism. For an exo-Io orbiting a hot Jupiter, the outgassing is further enhanced by sublimating the silicate surface (see Eqn. 19). At Io the observed volcanic escape is not due to outgassing however, but sublimation coupled with plasma-driven escape to space. We shall therefore refer to the observed gas near the satellite as atmospheric sputtering (Johnson 2004), although outgassing is often used interchangeably to describe the satellite itself.

To first order, we approximate the number density profile of the absorber by scaling \( n_i(r) = n(r) \chi_i(r) \) to the sputtered Na I number density profile observed at Io (Burger et al. 2001) with a power law exponent of \( q_{\text{moon}} = 3.34 \):

\[
n_{\text{moon},i}(r) = n_{\text{Io}} \cdot \left( \frac{R_M}{r} \right)^{q_{\text{moon}}} \tag{12}
\]

Figure 5. Simulation of high-resolution transit spectra in the sodium doublet, for different velocities in the evaporative wind scenario. We set \( \chi_{Na} = 2.16 \times 10^{-5} \), corresponding to a pressure at the base of the wind of \( P_0 = 0.1 \text{nbars} \) (using the planetary equilibrium temperature from Table 1 and \( \chi_{Na} \)). The planetary parameters and data points are for WASP-49b, taken from Wyttenbach et al. (2017).

where \( R_M \), the radius of the satellite, is set to Io’s radius. Since we directly calculate the number density of the absorber in this scenario we can drop the mixing ratio profile \( \chi_i(r) \) for the computation of the optical depth along the chord in Equation 1. As in the escaping scenario we use the total number of the absorbing atoms in the system as a free
parameter. We compute this quantity analogously to Equation 9 in the escaping scenario:

\[
N_i = \int n_i(r) dV = \frac{4\pi}{q_{\text{moon}}} - \frac{\pi}{2} R_0^3 M_i.
\]

Note that the gas in such a sputtered cloud isn’t in local thermodynamic equilibrium, therefore we don’t use pressure as an auxiliary parameter. Instead, we convert \(N_i\) into a source rate using Equation 6. Transit spectra for different values of this mass loss rate are shown in Figure 6. As we want to isolate the different scenarios we neglect the planetary atmosphere in this scenario, and consider only the sputtered cloud from the satellite for the computation of the transit spectrum. For computational convenience, we place the satellite in the center of our coordinate system (Figure 1) to exploit the spherical symmetry of the system. The reference radius in this scenario corresponds to the surface of the satellite, \(R_0 = R_M = R_o\).

We will again refer to the speeds of atoms instead of temperatures in this scenario as \(T\) isn’t well-defined, moreover irrelevant for an exosphere/collisionless gas. Similar to the escaping scenario, we describe the particles with a Maxwell-Boltzmann velocity distribution with a line temperature calculated from the mean velocity of the absorbing atoms (which we assume to be constant throughout the system). Therefore, we have the mean velocity of the absorbing atoms in the system, \(\bar{v}_i\), as our second free parameter.

We calculate the mass loss rate of the absorber within DISHOOM by using the scaling parameters \(\mathcal{P} = \frac{P_x}{T_\text{in}}, \mathcal{U} = \frac{U_x}{T_\text{in}}\), \(\mathcal{R}_x = \frac{R_x}{R_\text{in}}\), describing the total plasma pressure, binding energy, and exobase altitude respectively:

\[
M_{\text{moon},i} \sim \frac{P_x}{\mathcal{U}} x_i^2 M_0,
\]

\[
\sim \frac{\bar{v}_i}{\mathcal{U}} \left( \frac{B_i^2}{2 \mu_0} + n_i m_i \bar{v}_i^2 \right) \mathcal{R}_x^2 M_0.
\]

The dominant components of the total plasma pressure are the magnetic pressure, dependent on the magnetic field strength at the satellite radius \(B_x\) and \(\mu_0\) the permeability of space. The ram pressure is also critical, where \(n_i, m_i, \) and \(\bar{v}_i\) are the ion number density, mass, and velocity respectively. We adopt a value of \(x_{\text{Na}} = 0.1\) corresponding to the that used for an exo-Io; for a full description see Section 4.2.1 in Oza et al. 2019b. As DISHOOM does not explicitly track the ions that drive escape we use the velocity distributions modeled explicitly for Io by Smyth & Combi (1988); Smyth (1992) to constrain the velocities of the sodium gas sputtered from our satellite. The velocities range between 2-30 km/s, whereas speeds approaching 100 km/s are possible due to charge exchange. A summary of the plasma processes and mean velocities associated with various processes are presented in Tables 2 and 3 respectively.

### 2.6 Torus scenario

As observed at Saturn, a moon or debris around a planet can source a circumplanetary torus with neutrals (in our study

![Figure 6. Simulation of high-resolution transit spectra in the sodium doublet, for different mass loss rates of the sodium atoms in the exomoon scenario. We set \(v_{\text{Na}} = 10 \text{km/s}\). The planetary parameters and data points are for WASP-49b, taken from Wyttenbach et al. (2017).](image)

![Figure 7. Simulation of high-resolution transit spectra in the sodium doublet, for different mean velocities of the sodium atoms (corresponding to different effective temperatures) in the exomoon scenario. We set \(M_{\text{Na}} = 4 \cdot 10^8 \text{g/s}\), which corresponds to \(N_{\text{Na}} = 2.5 \cdot 10^{13}\) neutral sodium atoms in the system. The planetary parameters and data points are for WASP-49b, taken from Wyttenbach et al. (2017).](image)

Na & K) in two ways. (1) Direct outgassing from an active satellite: Enceladus outgasses water-products generating an OH torus along its orbital path (Johnson et al. 2006a). (2) Desorption of grains: UV photo-ionization of ice grains generates a close-in O2 torus at Saturn (Johnson et al. 2006b). We can model both sources of an exoplanet torus via the number density of the absorber as:

\[
m_{\text{tor},i}(a, z) = n_{0i} \cdot \exp\left[-\frac{z}{H_t}\right] \cdot \exp\left[-\frac{a - a_i}{4H_t}\right],
\]

which depends on the torus scale height \(H_t\) and the
satellite semimajor axis $a_t$, which approximates the distance between the planet and the circumplanetary torus. $a$ denotes the radial distance in the orbital $x − y$-plane (see Figure 1), $a = \sqrt{x^2 + y^2}$. We set $a_t = 2R_0$ for our analysis as in Oza et al. (2019b) based on Domingos et al. (2006) and Cassidy et al. (2009). The torus scale height can be expressed as $H_t = a_t \sqrt{\frac{\nu_o}{2G\nu}},$ where $v_o = \sqrt{\frac{GM_p}{a_t}}$ is the orbital velocity of the debris or venting moon and $v_d$ denotes the ejection velocity of the atoms, which we fix to 2 km/s based on Johnson & Huggins (2006). As in the exomoon scenario we can drop the mixing ratio profile of the absorber $\chi(r)$ for the computation as it is already incorporated into the number density profile.

The geometry for the computation of the transit spectra is more complex in this scenario due to the number density profile being azimuthally symmetric instead of spherically symmetric. Hence we also need to (linearly) discretize our coordinate grid along the y-axis. Equation 1 then needs to be adjusted to the new geometry:

$$\tau(y, z, \lambda) = \int_0^n \eta_{\text{tor},i}(a, z) \cdot \sigma(\lambda, T(a, z)) \, dz \, d\lambda.$$  

To obtain the flux decrease at a certain wavelength, the optical depth has to be averaged both over the y- and z-coordinates. Equation 3 changes to

$$\mathcal{R} = \frac{4}{\pi(R_e^2 - R_i^2)} \int_0^{R_e} \int_{R_i}^{\sqrt{R_e^2 - z^2}} \frac{R \, dz}{R_e^2 - z^2} \, dy \left[ 1 - e^{-\tau(y, z, \lambda)} \right].$$  

As in the exomoon scenario we have $\eta_i$ and $N_i$ as our free parameters. Transit spectra for some choices of these parameters are shown in Figures 8 and 9. There is again the following conversion between $N_i$ and $\eta_{\text{tor},i}$ which has to be solved numerically: $N_i = \int \eta_{\text{tor},i}(a, z) \, dV$. Since the circumplanetary torus isn’t in thermodynamical equilibrium, we again use the absorber mass loss rate $\dot{M}_i$ as an auxiliary parameter for an easier interpretation of $N_i$ and to couple the radiative transfer code to calculations within DISHROOM.

While the dominant escape mechanism which sources a cloud uniquely due to a satellite is atmospheric sputtering, a plasma torus can be fueled by several of the plasma processes described in Tables 2 and 3. For simplicity we focus on a Na I torus due to the desorption of particles similar to Saturn’s ring atmosphere (Johnson et al. 2006a) of O$_2$. These so-called toroidal atmospheres (Johnson & Huggins 2006) can be then approximated by thermal desorption of grains via $M_{\text{tor},i}$ (see Equations 10–12 in Oza et al. (2019b) and Table 5). If the desorption of grains can be described by experiments constraining the vapor pressure of rocky minerals $P_{\text{vap}}$ (see Table 3, Eqn. 13 van Lieshout et al. 2014) the source rate due to thermal evaporation of a torus fueled by an outgassing body of size $R_k$ can be written as:

$$M_{\text{tor},i} \sim M_{\text{levap}} \mathcal{R}(1 + \lambda_0) \exp(-\lambda_0) \sim x_i 4\pi R_k^2 P_{\text{vap}}(T_d) \left( \frac{m_i}{2\pi k_b T_d} \right)^{1/2} \mathcal{R}(1 + \lambda_0) \exp(-\lambda_0)$$

where the conduction prefactor $\mathcal{R}$ is relevant for Jeans parameters $10 < \lambda_0 < 100$ (see Johnson et al. 2015; Oza et al. 2019b), where $\lambda_0 = \frac{GM_p m_i}{R_k k_b T_d}$. $x_i$ is the mass fraction of the absorbing atom outgassing off of grains of exo-Io composition (Oza et al. 2019b), and $m_i$ the mass. For Na I we use $x_{\text{Na}} = 0.05$ as in Fegley & Zolotov (2000) for the chondritic composition of Io. We comment that due to the magmatic nature of these grains, more recent geophysical modeling of high-temperature rocky bodies is warranted to better predict $x_{\text{Na}}$ (e.g. Noack et al. 2017; Bower et al. 2019).

2.7 Comparison to observations

We compare simulated spectra for all four scenarios to high-resolution observations of the sodium D doublet at WASP-
Beer’s law or Lambert’s law (Rybicki & Lightman 1979):

\[ \text{as a slab the observed intensity can be written according to number of data points and the number of free parameters} \]

\[ \sigma \text{ deviation of this distribution is given by} \]

Consider a foreground gas of atomic species \( i \), illuminated \( B \) of the model given by

\[ \text{spectrum with the LSF of the instrument we use a Gaussian} \]

\[ \text{to the raw simulated spectra. Both observed transit spectra} \]

\[ \text{spread function (LSF), normalization and binning routine} \]

\[ \text{in the same way. For the convolution of the raw} \]

\[ \text{lines, which maximizes the signal-to-noise ratio according to} \]

\[ \text{to 0.2} \, \text{Å wide bins centered on the D2 and D1 absorption} \]

\[ \text{spread function of wavelength (which holds for our scenarios as we} \]

\[ \text{don’t vary the Doppler broadening parameter and neglect} \]

\[ \text{pressure broadening), the slant optical depth for the slab} \]

\[ \text{can be written as:} \]

\[ \tau(x) = N_i \sigma(x), \]

\[ \text{with the line-of-sight column density of species} \ i: \]

\[ N_i = \int_{-\infty}^{+\infty} n_i(x) \, dx. \]

For the setting of transmission spectroscopy, Eqn. 21 needs to be averaged over infinitely many line-of-sights. In the context of a hydrostatic atmosphere, this can be done analytically. We briefly review this formalism in the next section.

3.1 Canonical Hydrostatic Gas: an Effective Column Density at \( \tau \sim 1 \)

For a hydrostatic planetary atmosphere with constant pressure scale height \( H \), the line-of-sight column is given by (Fortney 2005):

\[ N_i(z) = n_i(z) \sqrt{2 \pi R_0 H}. \]

We have assumed that the mixing ratio of atomic species \( i \) doesn’t change throughout the line-of-sight. Combining Eqns. 22 and 24, one can define a reference optical depth:

\[ \tau(R_0, \lambda) \equiv \sigma_0(\lambda) \sqrt{2 \pi R_0 H}, \]

which can also be written in terms of a reference pressure. Continuing with a hydrostatic profile decaying over an altitude \( z \):

\[ \tau(z, \lambda) = \sigma_0(\lambda) e^{-z/H}. \]

Equation 26 is an analytical expression for the general optical depth profile (Eqn. 1) needed for the calculation of transmission spectra. Integrating over all lines of sight (Eqn. 3) using an identity (Chandrasekhar 1960), a closed form expression for the atmospheric transit radius \( R_t \) can be obtained (de Wit & Seager 2013; Bétrimieux & Swain 2017; Heng & Kitzmann 2017; Jordán & Espinoza 2018) given reasonable assumptions for an isothermal atmosphere and \( \sigma_0(\lambda) \rightarrow \infty \). The transit radius and transit depth are related via (c.f. Eqn. 3)

\[ 1 - \mathcal{R}(\lambda) = \frac{R_t^2 - R_e^2}{R_e^2}. \]

Remarkably, by assuming an optically thick reference pressure (\( \sigma_0(\lambda) \rightarrow \infty \)), it turns out that the optical depth at the transit radius \( \tau(R_t, \lambda) \equiv \tau_{\text{eff}}(\lambda) \) (termed effective optical depth) is \( \approx 0.56 \), independent of wavelength. This analytical result is elegant in that the notion of an atmospheric transit radius can be interpreted as an approximate boundary between opaque and tenuous layers. In this sense, it is appropriate for a single line-of-sight.

Table 4. Summary of free, auxiliary and fixed parameters. The free parameters fundamentally define the transmission spectrum in our setting. We derive auxiliary parameters from them to improve the physical interpretability. For instance, we calculate the reference pressure \( P_0 \) in the hydrostatic scenario as auxiliary parameter from the free parameter \( P_{0,i} \) assuming a specific mixing ratio of the absorber.

| Scenario       | Free   | Auxiliary | Fixed     |
|----------------|--------|-----------|-----------|
| Hydrostatic    | \( P_{0,i}, T \) | \( P_0 \) | \( R_0, \mu \) |
| Escaping       | \( N_i, \tilde{v}_i \) | \( M_i \) | \( R_0, q_{\text{osc}} \) |
| Exomoon        | \( N_i, \tilde{v}_i \) | \( M_i \) | \( R_M, q_{\text{moon}} \) |
| Torus          | \( N_i, \tilde{v}_i \) | \( M_i \) | \( R_0, a_i, v_{ej} \) |

49b and HD189733b. We restrict our retrieval analysis to the data points within the wavelength interval [5888, 5898] Å. We note that the Na I detections at these two planets were reduced and analyzed by the same algorithm, using the same instrument (HARPS) thereby validating a 1 to 1 comparison. We retrieve the two free parameters in every scenario using the reduced chi-squared statistic (Ocvirk et al. 2006; Andrae et al. 2010):

\[ \chi^2 = \frac{1}{v} \sum \left( \frac{O_i - C_i}{\sigma_i} \right)^2, \]

(20)

where \( O_i \) are observations with the corresponding errors \( \sigma_i \), \( C_i \) are computed values and \( v \) are the degrees of freedom of the model given by \( v = N_P - N_F \), the difference between the number of data points and the number of free parameters (in our analysis, \( N_P = 2 \) for all scenarios). The standard deviation of this distribution is given by \( \sigma = \sqrt{\frac{2}{v}} \). Lower values of \( \chi^2 \) indicate that the model is a better fit to data. If \( \chi^2 < 1 \) the model overfits the data.

To compare our simulated transit spectra to the observations we apply a convolution with the instrumental line-spread function (LSF), normalization and binning routine to the raw simulated spectra. Both observed transit spectra have been obtained with the HARPS spectrograph and have been reduced in the same way. For the convolution of the raw spectrum with the LSF of the instrument we use we a Gaussian with FWHM of 0.048 Å. We then bin the convolved spectrum to 0.2 Å wide bins centered on the D2 and D1 absorption lines, which maximizes the signal-to-noise ratio according to Wytenbach et al. (2017). Finally, we normalize the spectrum by the average transit spectrum \( \mathcal{R} \) in two reference bands, \( B = [5874.94; 5886.94] \) Å and \( R = [5898.94; 5910.94] \) Å.

3 OPTICALLY THIN GAS IN HIGH-RESOLUTION TRANSMISSION SPECTRA OF EXOPLANETS

Consider a foreground gas of atomic species \( i \), illuminated by a background radiation field \( F_{\text{out},\lambda} \). If we treat the gas as a slab the observed intensity can be written according to Beer’s law or Lambert’s law (Rybicki & Lightman 1979):

\[ F_{\text{in},\lambda} = F_{\text{out},\lambda} e^{-\tau(\lambda)}, \]

(21)
the (wavelength-dependent) location \( z \) at which \( \tau_T(z) \approx 0.56 \), which determines the transit radius and simultaneously the transit depth. This formalism implies that the effective atmospheric column density, at the atmospheric transit radius \( R_T \), converges for all wavelengths as \( N(R_T) \approx \frac{0.56}{\sigma(z)} \). At \( T = 10^7 \) K, the atmospheric column density probed at Na D2 line center is \( N(NaD2) \approx 5 \times 10^{11} - 1.5 \times 10^{12} \) cm\(^{-2}\).

### 3.2 Non-hydrostatic Gas: Evaporative Column Densities at \( \tau < 1 \)

In solving the same problem for a collisionless exosphere of arbitrary number density profile \( n(r) \), one cannot pinpoint the location of such a boundary, rendering the concept of an atmospheric transit radius inappropriate. On the other hand, as \( \tau < 1 \), the transit depth reveals the total number of absorbing atoms \( N_i \) spread over the stellar disk. The remarkable ability to constrain the total number of absorbing atoms \( N_i \) is a fundamental property of foreground gas well known from studies of the interstellar medium (Spitzer 1978; Draine 2011) using measurements of equivalent widths \( W_i \) (in units of Å):

\[
W_i = \int_{\lambda-\Delta \lambda}^{\lambda+\Delta \lambda} (1 - R_i(\lambda)) \, d\lambda.
\]

We can then give a lower bound to the column density of the absorbing species \( i \) (Eqn. 23) using the approximation of the curve of growth in an optically thin regime (Draine 2011):

\[
N_{\text{min},i} = 1.13 \times 10^{-12} \text{ cm}^{-1} \frac{W_i}{f_{ik}A_{ik}},
\]

where \( f_{ik} \) is the oscillator strength of the line and \( A_{ik} \) the wavelength of the transition. Unlike the interstellar medium where a single line-of-sight is considered, the background radiation field (star) is far larger than the foreground gas (the planetary atmosphere/exosphere). Therefore, a transmission spectrum requires averaging an arbitrary number density distribution \( n(r) \) over infinitely many line-of-sights (or chords) since the gas is not necessarily homogeneous\(^6\). In order to apply Equation 29, we reduce the various line-of-sight column densities in an exosphere to a disk-averaged column:

\[
\langle N_i \rangle = \frac{N_i}{\pi R^2}.
\]

Provided that that an outgassing or evaporative source is present, \( N_i \), the number of evaporating atoms, can be described by an arbitrary mass loss rate (e.g. Eqns. 11, 14, 19). The mass loss rates then directly supply the above disk-averaged column density. In other words, an evaporative column density \( N_i \) is equivalent to the observed column density \( N_{\text{min},i} \) (Johnson & Huggins 2006; Oza et al. 2019b), given

\(^6\) For an analogous derivation of optically-thin gas please see Appendix B of Hoeljmakers et al. 2020 in prep for a derivation of a homogenous, optically thin slab of gas. Here we present a heterogeneous, dynamic gas.

### 3.3 Evaporative Curve of Growth for Sodium at an Exoplanet

Using our radiative transfer code, we calculate equivalent widths at Na D2 line center for our three evaporative scenarios (Figure 10). The equivalent width depends on the free parameters \( \dot{M}_{Na} \) and \( N_{Na} \) (or, instead of \( N_{Na} \), \( N_{Na}^\prime \) or \( \dot{M}_{Na}^\prime \)). The dependence of the equivalent width on a (disk-averaged) column density is reminiscent of the classical curve of growth for a single line-of-sight. If the equivalent width is known to high precision, one can constrain an evaporative column density of occulting atoms depending on the scenario in Figure 10. These values coincide with the values from Oza et al. (2019b) (their Table 5) and indicate how effective each evaporative scenario is in generating the observed absorption.

To produce typical observed equivalent widths of \( W_{NaD2} \sim 1 - 10 \) mA at hot Jupiters, the required evaporative column densities range from \( \sim 10^{10} \) to \( \sim 10^{14} \) Na cm\(^{-2}\). For a torus, which is more similar to a Gaussian distribution, the column densities can be far larger. We note that absorption along a single line-of-sight (or, equivalently, in a homogeneous cloud as in Hoeljmakers et al. 2020 prep.) is always absorbing more efficiently than our evaporative sodium distributions.

Independent of the source driving mass loss, we confirm that extreme mass loss rates are required for observation of extrasolar evaporating sodium. To observe an equivalent width of \( 10 \) mA, for instance, roughly \( \sim 10^5 \) kg/s of sodium gas at 10 km/s is required for an escaping atmosphere or exo-Io as estimated by Oza et al. (2019b). In comparison, Io’s volcanism outgasses \( \sim 7 \times 10^6 \) kg/s of SO\(_2\) (Lellouch et al. 2015). A thermally desorbing torus, however, requires \( \dot{M}_{Na} \sim 5 \times 10^7 \) kg/s based on the scenario described. We note, based on the discussion in section 6.3, that this rate could be achieved if the grains are trapped in a toroidal magnetic field. This analysis provides an evaporative curve of growth for atomic sodium viewed at an exoplanet. The quantity of evaporating gas \( \sim 10^{11} - 10^{13} \) Na atoms, is able to govern the detection and non-detection of optically-thin absorption during transit. The evaporative curve of growth is drastically

---

**Table 5. Sodium source rates computed within DISHOOM.** The minimally required source rate \( \dot{M}_{\text{min},Na} \) is calculated using equation 29 with the observed equivalent widths at the Na D2 line (Wyttenbach et al. 2015; Wyttenbach et al. 2017) for the respective planet.

| Source rate | WASP-49b | HD189733b |
|-------------|----------|-----------|
| \( \dot{M}_{\text{esc},Na} \) [kg/s] | \( 1.3 \times 10^{2.4} \) | \( 10^{2.3} \) |
| \( \dot{M}_{\text{moon},Na} \) [kg/s] | \( 10^{4.3} \times 1.5 \) | \( 10^{7} \) |
| \( \dot{M}_{\text{tor},Na} \) [kg/s] | \( 10^{4.3} \times 1.3 \) | \( 10^{2.2} \times 1.5 \) |
| \( \dot{M}_{\text{min},Na} \) [kg/s] | \( 10^{4.7} \times 0.5 \) | \( 10^{3.8} \times 0.5 \) |

---

\[ W_{NaD2} \sim 1 - 10 \text{ mA} \]
influenced by the spatial distribution of the Na atoms across the star during transit.

3.4 The D2-to-D1 line ratio

At the Jupiter-Io system, the D2/D1 ratio is able to provide information on the velocity of the Na I atoms, which is observed to be variable over decades of observations. Therefore in our application to extrasolar systems, the ratio may be able to inform predictions on the average velocity distributions of the Na atoms and their ongoing behavior. However, the ratio first and foremost provides a very simple result.

Fortuitously, the oscillator strength of the Na D2 transition is twice as large as the D1 transition, meaning that the ratio first and foremost provides a very simple result.

\[ \sigma_{NaD2} = \sigma_{NaD1}/2 \]

This relation, together with the measured line ratios for HD189733b and WASP-49b, is shown in Figure 11. Throughout this paper, we calculate line ratios by using the transit depths averaged over bandwidths of 0.2 Å, centered on the absorption lines. We note that the exact value of the line ratio depends on the choice of the bandwidth, a negligible effect for modeled transmission spectra but not for the observations. For small bandwidths, the measurement error associated with the binned transit depth is large, while for large bandwidths, the observations at wavelengths which are more than ~ 0.5 Å away from the line center mostly contain noise. Hence, we choose an intermediate bandwidth of 0.2 Å (which maximizes the signal-to-noise ratio according to Wytenbach et al. 2017) for the calculation of the line ratios. While chords with NaD2 > 10 lead to a line ratio of one, NaD2/D1 transitions over two orders of magnitude of NaD2 to NaD1 = 2 for NaD2 < 0.1.

Unfortunately, for the setting of transmission spectroscopy, this relation isn’t applicable in a straightforward way since one observes a flux decrease averaged over infinitely many chords. For example, a line ratio of 1.5 can be achieved in different ways: By having a constant line-of-sight column density throughout the stellar disk with NaD2 ≈ 0, or by having ten percent of the area of the stellar disk blocked with NaD2 = 10 and the remaining ninety percent having NaD2 ≈ 0.1. Both of these models (and infinitely many other spatial distributions of the absorber) would lead to NaD2/D1 ≈ 1.5. For NaD2/D1 ≈ 1.5, given that the column density is a smooth function of impact parameter, we can therefore only state that the majority of the absorption occurs along chords with NaD2 roughly around 0.5, but chords with vastly different values of NaD2 are probably also present in the system. Hence, the D2-to-D1 ratio tells us in which regime (optically thin/thick) the majority of the absorption occurs.

In the following, we shall test how the predicted quantities of evaporating gas fare against canonical hydrostatic assumptions for high-resolution Na I spectra at hot Jupiters.

4 FORWARD MODELING AND SCENARIO COMPARISON

We elucidate the general features of evaporative transmission spectra in this section by constructing a forward model for the hot Jupiter HD189733b, using DISHOOM to calculate sodium source rates for the evaporative scenarios (listed in Table 5). These rates are converted into Nₙa (using Eqn. 6), a parameter which is then fed into Prometheus to compute the transmission spectra. We emphasize that these values of Nₙa should be regarded as lower limits, since we use a
lower limit to the lifetime of neutral sodium in Equation 6. We uniformly set \( \bar{\tau}_{Na} = 10 \text{ km/s} \) for the three evaporative scenarios in this forward model, a simplification which doesn’t affect the following analysis as the dominant effect of \( \bar{\tau}_{Na} \) is only the broadening of the lines. We also examine two hydrostatic scenarios: Our first hydrostatic model has \( T = T_{eq} = 1140 \text{ K} \) and \( P_0 = 1 \text{ bar} \), the second model\(^7\) has \( T = 10T_{eq} = 11400 \text{ K} \) and \( P_0 = 0.1 \mu \text{bar} \) (for the conversion of the reference pressures into \( P_{Na} \), we assume \( \bar{\tau}_{Na} = 1.7 \text{ ppm} \) for both scenarios). This choice of parameters for the hydrostatic scenario is arbitrary, and intentionally spans a large range within the free parameters. The forward-model transmission spectra are shown in Figure 12.

The three evaporative transmission spectra in figure 12 share some features such as negligible absorption between the lines and a D2-to-D1 line ratio significantly larger than one. The transit depth on the line cores is much larger for the exomoon scenario than compared to the two other evaporative scenarios (escaping & torus), stemming from the almost two orders of magnitude larger sodium source rate for an exomoon (Table 5). The two hydrostatic scenarios have, in contrast to the evaporative scenarios, a D2-to-D1 line ratio only slightly larger than one. Furthermore, the hydrostatic scenario with \( T = T_{eq} \) exhibits significant absorption between the line cores, due to the reference pressure of \( P_0 = 1 \text{ bar} \) leading to a very thick atmosphere.

The origin of the variety of transit spectra becomes apparent when examining the spatial structures of the different forward models. We show the corresponding sodium number density profiles in Figure 13. While the sodium number density in the hydrostatic scenarios drops fast (especially in the lower-temperature case), the three evaporative scenarios lead to more extended and tenuous exospheres. The sodium number density of the torus scenario peaks at \( r = 2 \cdot R_0 \) due to the fixed orbital separation of the torus of \( a_t = 2 \cdot R_0 \) (see Section 2.6). These number density profiles can be converted into optical depth profiles at a fixed wavelength using Equation 1. We fix the wavelength to the Na D2 line center and show \( \tau_{Na}\text{D2}(\nu) \) in Figure 14. Since the optical depth profiles\(^8\) are equivalent to the line-of-sight integrals of the sodium number density profiles times a constant depending on the Doppler broadening (Eqs. 22 and 23), the curves are similar in Figures 13 and 14, but decay slower in the latter plot (note that both plots cover approximately sixteen orders of magnitude). From the optical depth profiles we can derive the properties of the different transmission spectra in Figure 12.

- **Hydrostatic:** The hydrostatic scenario with \( T = T_{eq} \) exhibits an optical depth which drops very fast with increasing altitude. This behaviour leads to a small and very optically thick layer, which absorbs all incoming starlight nearly uniformly up to a certain altitude, followed by negligible absorption. This leads to \( f_{D2/D1} \) being very close to one in this model. We have a large reference pressure of \( P_0 = 1 \text{ bar} \) in this scenario, which leads to the slant optical depth at the reference radius \( \tau_{Na}\text{D2} \) being of the order \( 10^7 \) for the Na D2 line center. Since the absorption cross section does not drop by ten orders of magnitude between the line centers, we have significant absorption also between the lines.

- **Hydrostatic 10T_{eq}:** At a larger temperature the hydrostatic scenario has a more puffed up atmosphere. However, the optical depth still drops very fast, leading again to \( f_{D2/D1} \approx 1.1 \). Since the slant optical depth at the reference radius is only of the order \( 10^3 \), the atmosphere does not produce significant absorption between the lines.

- **Evaporative:** On the other hand, the three evaporative scenarios have extended and optically thin exospheres. Both the escaping and the exomoon scenario have long tails in their optical depth profiles. Since \( \tau_{Na}\text{D2} \) is lower than unity in these two scenarios for the largest part of the exosphere, the resulting transmission spectrum is optically thin. For optically thin chords, the proportion of absorbed light is directly proportional to the optical depth, leading to \( f_{D2/D1} \approx 2 \). Since the optical depth profile in the escaping scenario is offset by two orders of magnitude due to the lower sodium source rate, the flux decrease in this scenario is accordingly lower. The torus scenario has a plateau with \( \tau_{Na}\text{D2} \) slightly larger than one percent, extending over multiple radii, before the optical depth drops. Hence, the exosphere of the torus in this forward model doesn’t produce significant absorption as seen in Figure 12.

We conclude from this analysis that the three evaporative scenarios generally produce optically thin, extended exospheres, while hydrostatic models lead to a small, optically thick atmosphere. We find here that despite an atmosphere with a temperature ten times larger than the planetary equilibrium temperature, effectively enhancing the atmospheric scale height by a factor of ten, the hydrostatic atmosphere still drops very fast in number density and optical depth, such that the optically thin layer is negligibly small. This confirms our analysis in Section 3.2, in that the evaporative column densities are optically thin.

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\(^7\) The purpose of this model is to demonstrate the spectral imprint of extreme thermospheric heating.

\(^8\) If not specified otherwise, by optical depth we mean the optical depth at sodium D2 line center for the following discussion.
high-resolution observations of the sodium doublet. We de-

Figure 13. Sodium number density profiles of each scenario studied. The number density profiles correspond to our forward models for the hot Jupiter HD189733b. The exomoon profile starts in our model already at $r = R_{\text{Io}}$, we shift the curve to the planetary radius in this plot to enhance readability. For the torus scenario we show the number density profile through the orbital plane, $n_{\text{tot},Na}(r,0)$.


Figure 14. Optical depth (at NaD2 line center) profiles of each scenario studied. The optical depth profiles correspond to our forward models for the hot Jupiter HD189733b. The exomoon profile starts in our model already at $r = R_{\text{Io}}$, we shift the curve to the planetary radius in this plot to enhance readability. For the torus scenario we show the optical depth profile through the orbital plane, $\tau(r,0,NaD2)$. The line-of-sight column density is shown for a temperature Doppler broadening parameter corresponding to $T = 10T_{\text{eq}}$.

5 OBSERVATIONAL ANALYSIS OF EVAPORATIVE SODIUM TRANSIT SPECTRA

In the following we will perform a simple retrieval on two hot Jupiters (WASP-49b and HD189733b) applying the $\chi^2$ statistics to determine best fits for all four scenarios, using high-resolution observations of the sodium doublet. We de-

termine the two free parameters in all scenarios without any prior constraint. Next, we scrutinize the physical validity of the freely retrieved parameters based on our sodium source rate calculations from DISHOOM (Table 5), which comprises the coupling between our codes in this inverse modeling.

5.1 Inverse Modeling of WASP-49b

Wyttenbach et al. (2017) obtained a high-resolution spectrum of the hot Jupiter WASP-49b, observing significant absorption in the sodium doublet (more than two percent of the D2 line center). The spectrum shows negligible absorption between the line cores and a D2-to-D1-line ratio which is $f_{D2/D1} = 1.28 \pm 0.62$ (calculated in bands of 0.2 Å centered on the sodium D lines). The observation and the best-fitting models for each scenario are shown in Figure 15, we summarize the corresponding parameters in Table 6. Given the large uncertainty in $f_{D2/D1}$, all four scenarios have line ratios within the observational error bars. We remark that for the case of WASP-49b, this ratio converges to two for larger bandwidths since the D2 line is broader than the D1 line (Wyttenbach et al. 2017). If this line ratio was confirmed in a more precise measurement, the hydrostatic and the torus scenario would significantly underestimate $f_{D2/D1}$. The achieved goodness-of-fit is very similar in all four scenarios (between 1.44 and 1.49), with slightly lower $\chi^2$-values for the evaporative scenarios. The lowest $\chi^2$-values we achieve are still significantly larger than 1, leading to our best-fitting regions lying already two or more standard deviations away from the theoretically best-fitting model to the data. Since it is barely possible to get a better fit to the data by looking at Figure 15 we interpret this as an underestimation of the error bars in the observations.

We observe in the $\chi^2$-maps for all four scenarios that the shapes of the best-fitting regions are irregular and extend very far in a particular direction (Figure 16). In the hydrostatic scenario, the parameters are driven to values such that the resulting atmosphere is more optically thin.
We retrieve a large temperature of $T = 6100_{-3400}^{+6100}$ K, significantly above the planetary equilibrium temperature of WASP-49b of 1400 K (Wyttenbach et al. 2017). We retrieve similar velocities and source rates in the three evaporative scenarios, with the most prominent difference being the line ratio in the torus scenario of $f_{D2/D1} \approx 1.1$ (indicating absorption mostly in an optically thick regime). Although the torus scenario is evaporative, we see in Figure 14 that the optical depth profile is constant over a large range of radii and in the transition region between optically thick and optically thin chords. Since our best-fitting torus scenario requires a sodium mass loss rate more than three orders of magnitude larger than the model shown in Figure 14 (which is the forward model for HD189733b), the optical depth of the torus scenario approaches the optically thick regime for the best-fitting model of WASP-49b.

The comparison of the retrieved mass loss rates from Prometheus with the calculated rates within DISHoom is shown in Table 7. Since Prometheus doesn’t directly retrieve $M_Na$ but rather $N_{Na}$, we use Equation 6 to obtain an upper limit to the mass loss rate from the retrieved $N_{Na}$. The retrieved source rate in the escaping scenario is nearly three

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**Table 6.** Retrieval results for WASP-49b and HD189733b. We also evaluate the D2-D1 line ratio $f_{D2/D1}$ for our models. From the measurements, we estimate $f_{D2/D1,W49} = 1.28 \pm 0.62$ (Wyttenbach et al. 2017) and $f_{D2/D1,HD19} = 1.74 \pm 0.45$ (Wyttenbach et al. 2015).

| Scenario   | Parameter | Retrieved $f_{D2/D1}$ | $\chi^2$ Retrieved | HD189733b $f_{D2/D1}$ | $\chi^2$ |
|------------|-----------|------------------------|---------------------|------------------------|----------|
| Hydrostatic | $P_{r_{Na}}$ [bar] $T$ [K] | $10^{12.2 \pm 1.4}$ $6100_{-3400}^{+6100}$ | 1.1 | 1.94 | 10$^{-10.7} \pm 0.5$ $5200 \pm 1500$ | 1.1 | 1.49 |
| Escaping   | $N_{Na}$ [Na atoms] $v_{Na}$ [km/s] | $10^{31.1 \pm 1}$ $9_{-13}^{+13}$ | 1.6 | 1.44 | $10^{32.5 \pm 0.2}$ $19 \pm 9$ | 2 | 1.51 |
| Exomoon    | $N_{Na}$ [Na atoms] $v_{Na}$ [km/s] | $10^{33.4 \pm 0.6}$ $9_{-13}^{+13}$ | 1.6 | 1.45 | $10^{32.7 \pm 0.2}$ $18 \pm 8$ | 1.7 | 1.50 |
| Torus      | $N_{Na}$ [Na atoms] $v_{Na}$ [km/s] | $10^{33.5 \pm 0.8}$ $7_{-14}^{+14}$ | 1.1 | 1.45 | $10^{32.6 \pm 0.2}$ $18 \pm 9$ | 1.6 | 1.53 |
orders of magnitude larger than the one we calculate using DISHOOM, indicating that an escaping wind can probably not provide enough sodium to generate the observed transit depth. The retrieved source rates in the exogenic scenarios are also larger than the ones we calculate from DISHOOM, but still within the error bars.

### 5.2 Inverse Modeling of HD189733b

Wyttenbach et al. (2015) detected sodium at HD189733b in the Na I doublet. Compared to WASP-49b, this transit spectrum has weaker absorption features (less than one percent absorption at D2 line center), but a larger D2-to-D1 line ratio of $f_{D2/D1} = 1.74 \pm 0.45$ (again calculated in bands of 0.2 Å centered on the sodium D lines). The line cores for the transit spectrum of HD189733b are broader than the ones of WASP-49b, which leads to more data points lying on the line cores and enabling a more precise retrieval. Therefore, and due to the comparatively smaller error bars for this observation, the best-fitting regions are more regular and significantly smaller for HD189733b (note that we adjusted the color map scale for the parameter retrievals of HD189733b).

The observation and the best-fitting models for each scenario are shown in Figure 17. The retrieved parameters are summarized in Table 6, and due to the comparatively smaller error bars for this observation, the best-fitting regions are more regular and significantly smaller for HD189733b (note that we adjusted the color map scale for the parameter retrievals of HD189733b). Although the data points lie on the line cores and enable a more precise retrieval. Therefore, and due to the comparatively smaller error bars for this observation, the best-fitting regions are more regular and significantly smaller for HD189733b (note that we adjusted the color map scale for the parameter retrievals of HD189733b).

We compare the retrieved mass loss rates of Prometheus to the rates computed within DISHOOM in Table 7. Again, the escaping wind doesn’t produce enough sodium (by two orders of magnitude) to reproduce the observed transit depth. While the retrieved source rate in the exomoon scenario is very comparable to the calculated one using DISHOOM, the torus mass loss rate underestimates the retrieved source rate by nearly two orders of magnitude.

### 6 DISCUSSION

#### 6.1 Comparison to other Retrievals

##### 6.1.1 WASP-49b Studies

Different authors conducted a parameter retrieval using the same data from Wyttenbach et al. (2017) as we used. In the following we compare our findings to these studies. Wyttenbach et al. (2017) could fit the line cores and the line wings of the spectrum separately with hydrostatic, isothermal and vertically mixed models (equivalent to our hydrostatic scenario), but these authors couldn’t reproduce the entire spectrum with a hydrostatic model. Their best-fitting model for the line cores has $T \approx 2950^{+400}_{-500}$ K. Cubillos et al. (2017) attempted to fit the spectrum with a more sophisticated (but still hydrostatic) model (with a $T$-$P$ profile from a hydrodynamic simulation and variable mixing ratios computed with equilibrium chemistry). However, they run into the same difficulty as Wyttenbach et al. (2017): The observed spectrum at WASP-49b has large absorption on the line cores (approximately two percent on the D2 line), but very little absorption between the line cores. As seen in Section 4, this property along with $f_{D2/D1} > 1$ indicates that absorption occurs mainly in an extended, optically thin region. Since the hydrostatic models of Wyttenbach et al. (2017) and Pino et al. (2018) both retrieve temperatures smaller than 3000 K, they model a small and dense atmosphere leading to absorption
Figure 18. Parameter retrieval for HD189733b.

6.1.2 HD189733b Studies

As in the case of WASP-49b, different authors conducted a parameter retrieval using the same data from Wyttenbach et al. (2015) as we used. Wyttenbach et al. (2015) could fit different parts of the transit spectrum of HD189733b with isothermal, vertically-mixed, hydrostatic models and interpreted this as a temperature gradient in the atmosphere. Their hottest model to fit the D2 line core has a temperature of 3270 K. Huang et al. (2017) performed a very sophisticated hydrostatic simulation of HD189733b’s atmosphere incorporating many different forms of atmospheric chemistry and NLTE-effects. They find that the temperature rises steeply from 2000 K at 10 µbar to 12 000 K at 0.1 nbar (their Figure 3). These authors furthermore find that at pressures below 1 µbar most of the sodium atoms are ionized (their Figure 5). Huang et al. (2017) used very different parameters (namely LyC boost and atomic layer base pressure) to fit the full observed spectrum, making a comparison to our scenarios difficult. However, we note that the found atomic layer base pressure of 10 µbar compares well to our retrieved reference pressure ($P_0 = 11$ µbar assuming $\chi_{Na} = 1.7$ ppm) in the hydrostatic scenario, and our temperatures ($T = 5200 \pm 1500$ K), which are significantly larger than the ones retrieved by Wyttenbach et al. (2015), are in line with the atmospheric model from Huang et al. (2017). We also remark that these authors bin the observations in a slightly different way, using 0.05-Å-bins. For this particular choice of the bin size, the D2-to-D1 line ratio of HD189733b is approximately 1.1, in line with the hydrostatic models.

6.2 Potassium in the Atmosphere/Exosphere of Hot Jupiters

We have so far focused on the analysis of the Na I doublet. Our codes and the analysis of the D2/D1 line ratio can be readily applied to the K I doublet at 7667 Å and 7701 Å. Here, we don’t compare our models to observational data and refrain from a normalization and binning routine applied to the spectra as at Na I. We employ a HARPS-like instrumental LSF convolution procedure for our model spectrum. The model serves as a prediction for expected high-
resolution K I detections beginning by ESPRESSO (Chen et al. 2020) and PEPSI (e.g. Keles et al. 2019).

Identical to the forward model presented in Section 4, we use DISHOOM to calculate K I mass loss rates (Table 8), which are then converted into \( N_K \) (the number of neutral K I atoms in the system) using equation 6. The average lifetime of neutral K I is larger by a factor of 3.75 compared to that of Na I as determined by photoionization (Huebner & Mukherjee 2015). We set the velocities of the K I atoms in the evaporative scenarios uniformly to that of Na I as determined by photoionization (Huebner & Mukherjee 2015). We set the velocities of the K I atoms in the evaporative scenarios uniformly to that of sputtered atoms ~ 10 km/s. For the hydrostatic scenarios we use the retrieved temperature and reference pressure (Table 6). For the endogenic, planetary scenarios we use a volumetric the retrieved temperature and reference pressure (Table 6).

For the endogenic, planetary scenarios we use a volumetric sodium-to-potassium ratio of Na/K = 15.9 corresponding to the solar value (Asplund et al. 2009). For the exogenic, exomoon & torus scenarios we use lunar Na/K = 6 (Potter & Morgan 1988) which also corresponds to the maximum Na/K ratios for chondrites as studied by Fegley & Zolotov (2000). We note that the evaporative scenarios are strongly dependent on the Na/K ratios due to their optically thin nature. In comparison with the 0.18% K D1 absorption depth detection by Keles et al. 2019 for HD189733b, we find for the same 0.8 Å bandpass a K D1 absorption depth of ~ 0.15% for the hydrostatic scenario and ~ 0.06% for a exomoon scenario. At present we believe more observations are needed to make interpretations of the Na/K at exoplanets.

6.3 Toroidal Atmospheres/Exospheres at Ultra-Hot Jupiters

Ultra-hot Jupiters \( (T > 2000 \text{ K}) \) have recently been under spectral scrutiny after a remarkable detection of atomic iron at an exoplanet system (Hoeijmakers et al. 2018). Since then, several authors have detected not only Fe I but also Ti, V, and other heavy metals not normally present in gas giant atmospheres (Hoeijmakers et al. 2018; Hoeijmakers et al. 2019; Sing et al. 2019; Cabot et al. 2020; Gibson et al. 2020). However, the detection diaspora are vastly different at these bodies and the ‘ultra-hotness’ of the hot Jupiters does not appear to be a sufficient criterion for Fe I detections. For instance, Caubey et al. (2020) was unable to detect metals at WASP-189 using PEPSI (\( R > 50,000 \)) on the Large Binocular Telescope despite a planetary equilibrium temperature exceeding \( 2640 \text{ K} \). Therefore atmospheric heating, leading to heavy atom escape as proposed by Cubillos et al. (2020), should also lead to a Fe I signature at WASP-189. To better understand the temperature-independent metallic detections, we directly compare the latest Na I detections at two ultra-hot Jupiters by the HARPS spectrograph: WASP-121b (Hoeijmakers et al. 2020) and WASP-76b (Seidel et al. 2019). Average sodium lifetimes against photoionization are estimated from Huebner & Mukherjee (2015).

Table 8. Potassium source rates computed within DISHOOM.

| System  | \( M_{\text{esc,K}} \) [kg/s] | \( M_{\text{moon,K}} \) [kg/s] | \( M_{\text{tor,K}} \) [kg/s] |
|---------|-----------------------------|-----------------------------|-----------------------------|
| WASP-49 | \( 10^{1.4 \pm 0.3} \)     | \( 10^{3.2 \pm 1.6} \)     | \( 10^{8.1 \pm 1.3} \)     |
| HD189733 | \( 10^{1.3 \pm 0.3} \)     | \( 10^{2.9 \pm 1.3} \)     | \( 10^{9.8 \pm 1.5} \)     |

Table 9. System parameters for the ultra-hot Jupiters orbiting F stars: WASP-121b (Hoeijmakers et al. 2020) and WASP-76b (Seidel et al. 2019). Average sodium lifetimes against photoionization are estimated from Huebner & Mukherjee (2015).

| Parameter | WASP-121b | WASP-76b |
|-----------|-----------|-----------|
| \( R_1 \) [\( R_\oplus \)] | 1.46      | 1.3       |
| \( R_0 \) [\( R_\oplus \)] | 1.87      | 1.83      |
| \( M_P \) [\( M_J \)] | 1.18      | 0.92      |
| \( T_{\text{eq}} \) [K] | 2360      | 2190      |
| \( \gamma \) [km/s] | 38        | -1.07     |
| \( r_{\text{esc}} \) [\( R_\oplus \)] | 50        | 85        |
| \( f_{D2/D1} \) | 2         | 1         |

Note the break in the x-axis.
6.3.1 Toroidal Atmospheres

In light of the stark detection of $f_{D2/D1} \approx 2$ at WASP-121b in a companion paper by Hoeijmakers et al. 2020, we decide to model an identical exogenic, toroidal geometry to WASP-76b to better understand the physical mechanism fueling the (presumably temperature-independent) metal detections at ultra-hot Jupiters.

So far, the Na I and Fe I signatures at WASP-76b have been interpreted as endogenic atmospheric winds (Seidel et al. 2019; Ehrenreich et al. 2020). The scenario of day-night migration coupled with rotation leading to an evening/night or dusk/dawn asymmetry has surprisingly also been observed in an exospheric regime on other tidally-locked bodies (Ganymede: Leblanc et al. 2017; Europa: Oza et al. 2019a). In Oza et al. (2018) it was shown that the phenomena of asymmetric ‘atmospheric bulges’ is degenerate with a collisionless gas on a tidally-locked body. Therefore, while we find an asymmetric Fe I atmospheric wind quite reasonable, we test the degeneracy by simulating Na I rotating in a toroidal atmosphere (red line: WASP-76b $f_{D2/D1} \approx 1$) or exosphere (green line: WASP-121b $f_{D2/D1} \approx 2$) in Figure 21.

We find the WASP-121b observations (green) are roughly reproduced by fixing a Na source orbiting at $\sim 28$ km/s ejecting $\sim 10^9$ g/s extending to $\sim 1.9$ $R_p$, equivalent to the planet’s Hill radius. This corresponds to a toroidal scale height of $H_t (\text{W}12) \approx R/4$. In stark contrast, WASP-76b (red) is twice as thick with $H_t (\text{W}76) \approx R/2$. At WASP-76b, the torus is confined close to the planetary atmosphere with a much slower orbital speed of $\nu_{\text{orb}} \approx 7$ km/s at 1.125 $R_p$. For grain densities $\sim 3$ g cm$^{-3}$, the Roche radius for WASP-76b is roughly $\sim 0.97$ $R_p$. On the other hand, the required Na rate here is alarmingly large $\sim 10^9$ kg/s of pure atomic Na. This rate is $20 \times$ as large as the total energy-limited escape rate of the H/He envelope, assuming an XUV-efficiency of $\eta_{\text{XUV}} = 0.3$ (c.f. Section 2.4). To our knowledge, the only physical process capable of generating such a high quantity of Na I in a toroidal distribution is the thermal desorption of silicate grains as shown in Table 5 of Oza et al. (2019b).

As indicated, an exo-Io at WASP-76b would be catastrophically destroyed due to the mass loss as also implied by the radiative hydrodynamic simulations of Perez-Becker & Chiang (2013). The evaporation of such a body would imply a large quantity of metallic gas, as observed.

7 CONCLUSIONS

The advent of high-resolution transmission spectroscopy of transiting exoplanets has enabled a closer look at the environment immediately surrounding the exoplanet. By modeling the sodium D doublet, whose resonance lines are exceptionally bright given even meager column densities $\gtrsim 10^{10}$ cm$^{-2}$, we investigate three non-hydrostatic, evaporative scenarios in addition to the canonically used hydrostatic model atmosphere. To this end we use a custom-built radiative transfer code (Prometheus), coupled via sodium mass loss rates from a metal evaporation model (DISHOOM) to perform both forward and inverse modeling of high-resolution transmission spectra in the sodium doublet.

The three additional scenarios describe (i) an endogenically escaping medium (Equation 9), (ii) an exogenic outgassed cloud sourced by an exomoon (Equation 12), and (iii) an exogenic torus representing circumplanetary material (Equation 16). Profile (i) of an escaping atmosphere has been simulated in detail and observed across several species over the past decade. Should the exoplanet be close-in, it is highly likely that it is experiencing extreme atmospheric escape on the order of $\sim 10^7 \text{ to } 10^{10}$ kg/s (Wyttenbach et al. 2020) corresponding to $\sim 10 \text{ to } 10^4$ kg/s of pure sodium escape given solar abundance. The exogenic profiles are based on recent exomoon study by Oza et al. (2019b) as well as comparative solar system studies of Jupiter and Saturn’s (cryo-)volcanically active moons Io and Enceladus Johnson et al. 2006b, Johnson & Huggins 2006). We find that both hydrostatic and non-hydrostatic scenarios can fit HARPS transit spectra of WASP-49b and HD189733b.

In mitigating the apparent sodium degeneracy, we find that first determining whether the absorption occurs in a primarily optically thick or optically thin regime is critical (Section 3). A diagnostic based on the ratio of transit depths at the D2 and D1 line centers, $f_{D2/D1}$, is shown to be indicative of an optically thin or optically thick regime in Section 3.4. Hydrostatic models we find, despite arbitrary heating at $T = 10^4$K, cannot achieve line ratios larger than $\approx 1.2$. This is a consequence of the exponentially decaying number density profile prescribed by hydrostatic equilibrium in contrast to the tenuous and extended profiles of the non-hydrostatic scenarios primarily leading to $f_{D2/D1} \gg 1$. Given multiple observations with line ratios greater than one (WASP-121b, HD189733b, WASP-49b) an inclusion of evaporative sources of the sodium absorption seems warranted. We find that an evaporative scenario is nevertheless able to fit planets with $f_{D2/D1} \sim 1$ (e.g. WASP-76b) in Section 6.3.1. Upon analyzing the Na I source rates required to fit toroidal atmospheres to ultra-hot Jupiter spectra, we remark that a common source for Fe I and Na I due to the evaporation of a rocky body may be reasonable.

For observed transmission spectra, we find that all four
scenarios can be fit to the data, from a statistical point of view. From a physical point of view, however, we remark that the escaping scenario (for HD189733b and WASP-49b) and the torus scenario (for HD189733b only) are not able to supply the retrieved source rates, according to our mass loss calculations. Caution should be used in adjusting the solar abundance here in that an atmospheric metal enrichment enhancement $\gtrsim 100 \chi_i(r)$ is unlikely (Thorngren & Fortney 2019). Furthermore, we note that while the hydrostatic scenario can fit the high-resolution observations as well as the evaporative scenarios in terms of $\chi_i$, the models have $f_{\text{D2}}/f_{\text{D1}} \leq 1.1$, thereby unable to reproduce the observed line ratio at HD189733b and to a lesser extent WASP-49b.

At present, acknowledging that hydrostatic profiles have been excellent approximations to low-resolution transmission spectra, we suggest that radiative transfer and atmospheric escape models would benefit from the non-hydrostatic framework we have outlined in this paper for high-resolution transmission spectra. Further transmission spectra observations, at higher SNR, could validate non-hydrostatic line ratios in significant excess of $\approx 1.2$. Time-resolved observations such as phase curves could provide insight regarding the spatial distribution of alkali atoms.

Looking forward, the recent identification of heavy metals beyond the Hill sphere of gas giant exoplanets by high-resolution transmission spectroscopy (Hoeijmakers et al. 2019; Cubillos et al. 2020) is reminiscent of the remarkable identification of exocomets or falling evaporating bodies at the $\beta$ Pictoris system (e.g. Roberge et al. 2000; Lecavelier des Etangs et al. 2001). In this light, based on the evaporative transmission spectra modeling for gas giant exoplanets carried out here, we specifically suggest further modeling of escaping metals subject to ambient plasma fields, along with the likelihood of satellites and tori as at Jupiter and Saturn.

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