Characterising exoplanetary atmospheres with ARIEL

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Abstract: Future instruments (e.g. JWST, ARIEL) will study the atmospheres of transiting exoplanets with an unprecedented level of detail. In this work, the retrievability of atmospheric parameters of exoplanets is studied for hot Jupiters, a warm Neptune and a cool sub-Neptune in the context of the ARIEL mission. Synthetic observations are generated using TauREx III for forward-modelling and retrieval. The results show that ARIEL is able to significantly detect main gaseous species in hot Jupiters and warm Neptunes with a single transit observation. The study of smaller and cooler planets will require several observations. For K2-18 b, I estimate a minimum of 50 observations to distinguish a primary atmosphere from a secondary one. This work outlines the scientific capabilities of ARIEL and provides estimates on the quality of observations for different types of exoplanets.

I. INTRODUCTION

In recent times our ability to study the properties of extrasolar planets, or exoplanets, has significantly increased. More than 4000 exoplanets have been discovered to date and now we aim to understand the nature of these worlds. Current and future instruments will allow us to characterise the physical and chemical properties of the atmosphere of exoplanets, or exoatmospheres. The first ones were detected with observations from the Hubble Space Telescope (HST) and the Spitzer Space Telescope (SST) [1]. The next generation of instruments, primarily the NASA/ESA James Webb Space Telescope (JWST) and the ESA **Atmospheric Remote-sensing Infrared Exoplanet Large-survey (ARIEL)** are designed, in part or entirely, to study the chemical composition and structure of exoatmospheres.

Transmission spectroscopy of transiting exoplanets (see II), combined with powerful retrieval tools allow us to detect gaseous species, constrain pressure-temperature profiles, study the presence of clouds and more. Unlike the JWST, ARIEL (see III) is in the early stages of development. Further investigations are required to assess the optimal observing strategies and the most promising targets for the mission.

Atmospheric retrieval is an inverse-method used to recover the properties of exoatmospheres from its transmission or emission spectrum. In the present work, retrievals from simulated spectra are analysed to determine the capabilities of ARIEL. Synthetic data sets are generated with state-of-the-art code to estimate the noise on ARIEL observations. Thence, I combine the data sets with forward models to perform the retrievals of the physical and chemical properties of the atmosphere. The results hereby presented (see V) illustrate ARIEL's performance to constrain the abundance of gaseous species, determine the isothermal temperature of exoatmospheres and detect the presence of clouds. In VI, I estimate the number of observations required to discern a primary from a secondary atmosphere in the sub-Neptune exoplanet K2-18 b. This project addresses current topics in the field and aims to highlight exoplanetary science in the ARIEL era.

II. TRANSMISSION SPECTROSCOPY

Transiting exoplanets are planets that cross our line of sight as they orbit their host star. While the exoplanet passes in front of the star (transit) the stellar brightness decreases, observing at different times during the event generates a light curve. The points of minimum flux on the light curve are observed as a dip with depth proportional to the square of the ratio between the planetary radius R_p and the stellar radius R_s. The depth is wavelength dependant (D_λ) for exoplanets with a substantial atmosphere:

$$D_\lambda = \frac{R_p^2 + a_\lambda}{R_s^2}. \tag{1}$$

The apparent radius of the exoplanet changes at each wavelength, instruments with an spectrograph are able to produce transmission spectra. When the exoplanet has no atmosphere the transmission spectrum is flat. The equivalent atmospheric depth a_λ represents the effective area contributing to the increase in the apparent radius of the exoplanet. All atmospheric absorption and dispersion mechanisms are included in the optical depth function τ_λ. Integrating along the vertical direction z from the surface $z = 0$ to the top of the atmosphere $z = z_{\max}$,

$$a_\lambda = 2\int_0^{z_{\max}} (R_p + z)(1 - \mathrm{e}^{-\tau_\lambda(z)})dz. \tag{2}$$

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III. ARIEL

The ARIEL medium-size ESA mission (scheduled to launch on 2028) will acquire photometry and spectroscopy of more than 1000 transiting exoplanets with the goal of studying their atmospheres. ARIEL is expected to reach a precision of 10-100 ppm in the atmospheric signal with a continuous wavelength coverage in the range of 0.5-7.8 μm [12]. The main goal of the mission is the characterisation of hot and warm exoplanets around bright stars (K$<$ 11).

IV. TauREx III

TauREx is a Bayesian 1D radiative transfer and retrieval code. In this framework, the atmosphere is modelled in a plane-parallel geometry with a discrete set of 100 layers ranging from the surface to the top of the atmosphere, hence substituting the integral at eq. (2) to a sum over all the layers. The optical depth τ_λ for each wavelength is computed using high-resolution ($R = 1500$) line-by-line cross sections [11]. Contributions for H_2-H_2 and H_2-He are added in the form of Collision Induced Absorption, CIA, [9] and Rayleigh scattering [5]. The atmospheric features of the models (see fig. 1) include scattering (e.g. Rayleigh, Mie), CIA, grey clouds and pure absorption. The constant-with-altitude relative mixing ratios of the gaseous species are set as free parameters in the retrievals. The mixing ratios have no chemical constraints (e.g. equilibrium). This is the common practice when the chemistry of the atmosphere is unknown. The pressure-temperature profile is approximated as isothermal. Transmission spectra is not extremely sensitive to the thermal structure of the atmosphere, other techniques like emission spectroscopy require more realistic temperature-pressure profiles. The presence of clouds is modelled by considering a uniform cloud with a pressure at the cloud deck, below which no radiation is transmitted. This simplistic approach is sufficient to predict cloud absorption at short wavelengths (1.1 - 1.7 μm). The presented models here assume some simplifications that are valid with current data sets but further work is needed to asses the validity of an isothermal profile and a constant-with-altitude composition on each of the considered exoplanets.
In this work, the Nested Sampling (NS) algorithm [7] is employed. This bayesian inference code is the current standard in the field and has proven faster and more powerful than other Monte Carlo methods like MCMC [14]. The signal noise is simulated with ArielRad [8], a dedicated tool to evaluate the capabilities of ARIEL observations. It estimates the noise for each instrument in their corresponding wavelength range. The data used in this project was specifically produced by courtesy of Lorenzo Mugnai to accurately estimate the uncertainties on the spectra (see fig. 1).
I would like to note that several retrievals are required to establish the main species first, retrievals thereafter only include the most abundant species to optimize the analysis. Retrievals with a greater number of free parameters are plausible, however, computing time increases significantly and parameter degeneracies will not allow to correctly retrieve all magnitudes at once.

V. RESULTS FROM THE RETRIEVALS

The targets selected (see table I) for the modelling and retrieval are of three different types: two hot Jupiters, a warm Neptune and a cool sub-Neptune. All four planets are in the list of potential targets for ARIEL [6], the first three have been studied extensively and represent the main class of planets ARIEL is designed for. K2-18 b is a unique target because it is the first and only exoplanet in the habitable zone known to have an atmosphere. Recent observations of K2-18 b [2] confirmed the presence of water vapour in its atmosphere. However, the limited wavelength and spectral resolution of the HST/WFC3 produces significant degeneracies in the retrievals. Previous studies ([2]; [4]) have determined that three different models are in agreement with the observed transmission spectrum. The three models, listed here as B(lue), O(range) and G(reen) are,

- Model B: Secondary atmosphere with a high content of water vapour and H/He.
- Model O: Secondary atmosphere with a high abundance of an inactive absorber N_2 and H/He. Water vapour is present as a trace gas.
- Model G: Primary atmosphere with clouds. High abundance of H/He and water vapour added as a trace gaseous species.

In this work, the retrievals are performed with 5 to 6 free parameters. The planetary radius R_p and the isothermal temperature T_{p} are explored in linear mode and the rest of parameters in logarithmic mode. For the radii at 10 bar R_{p}, the boundaries encompass a range of values corresponding to $\pm$ 25% of the input value. For the T_{p}, the range extends to $\pm$ 50% and the rest of parameters explore a parameter space of six order of magnitudes. The retrieved mixing ratios for K2-18 b (see fig. 2) are *relative* mixing ratios instead of *absolute* because the trace species make up a significant fraction of the atmosphere which could lead to non-physical situations where the sum of the mixing ratios is higher than 1. The computing time is about 10 hours for each retrieval [15].

The modelled atmospheres are dominated by H/He. The retrieval of high mean molecular weight (HMMW) $\mu > 5$ exoatmospheres is more challenging due to smaller scale heights $H \sim 1/\mu$. Water

TABLE I: Parameters of the star-planet systems considered. For the star, the effective temperature T_{eff}, the radius R_s in solar radii and the apparent magnitude in the K band. For the exoplanet, the equilibrium temperature T_{eq}, and the planetary radius R_p in units of Jupiter radius.

Planet type	Name	T_{eff}(K)	$R_s(R_\odot)$	K(mag)	T_{eq}(K)	$R_p(R_J)$	Source
Hot Jupiter	HD209458 b	6086	1.18	6.3	1487	1.35	[3]
Hot Jupiter	HD189733 b	4875	0.80	5.5	1182	1.11	[10]
Warm Neptune	GJ436 b	3684	0.46	6.1	726	0.37	[13]
Cool Sub-Neptune	K2-18 b	3457	0.44	8.9	255	0.23	[2]

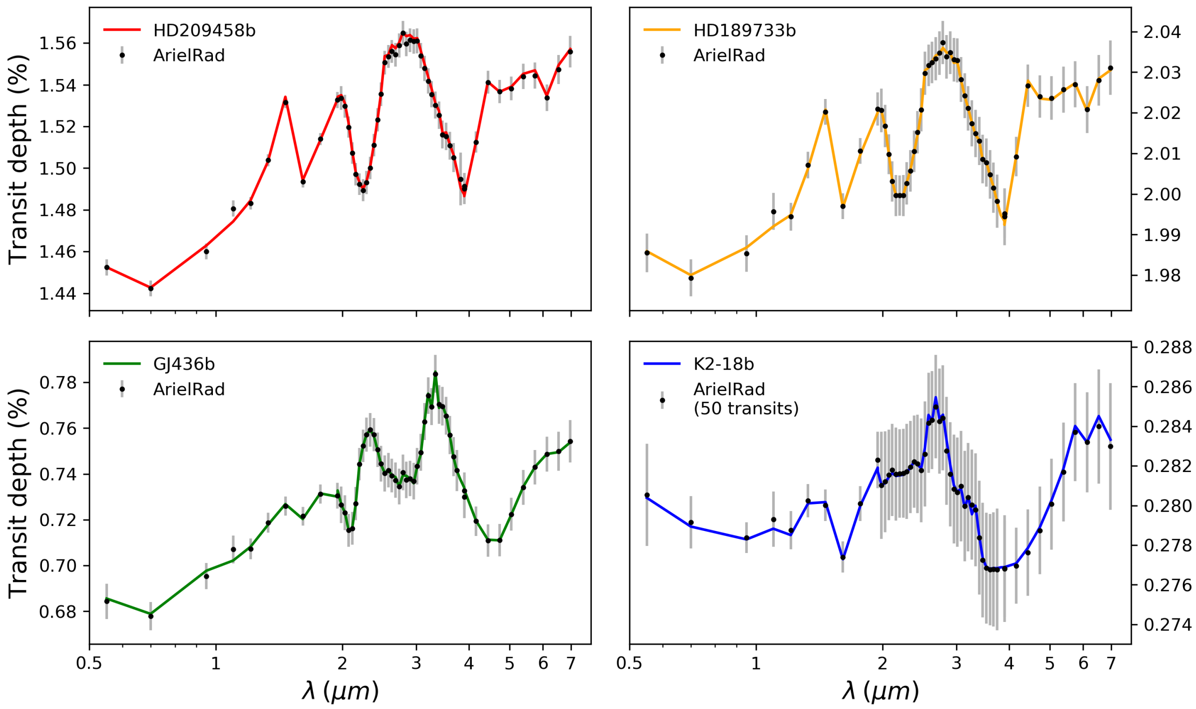

FIG. 1: Transmission spectra for the four selected exoplanets. The synthetic observed data (shaded regions) is generated for one transit for all exoplanets except K2-18 b which includes 50 transits. The solid lines show the best fits from the retrievals.

vapour is expected to be a common species in the atmosphere of most exoplanets, hence it is included in the four modelled exoatmospheres. In fig. 2, the equilibrium temperature of the planet is compared to the isothermal temperature of the atmosphere. This is just a reference value given that the isothermal temperature is a first-order approximation for the thermal structure of the atmosphere.

Hot Jupiters are expected to possess H_2O, CO and CO_2 as trace gases. The values for water and carbon dioxide are retrieved within 1σ uncertainties. The forward-model did not include high altitude clouds. In the retrieval the pressure of the cloud's top has a large uncertainty but the results are consistent with no clouds. This is a common issue in atmospheric retrieval and the main factor contributing to degeneracies of the posterior distributions among the chemical abundances and the cloud's top pressure (see fig. 3). The mixing ratio of water vapour is retrieved better than the other two gases.

The sub-Neptune exoplanet GJ436 b is modelled with H_2O, CH_4 and NH_3 as trace gaseous species. Unlike for the hot Jupiters, here the retrieved mixing ratios for CH_4 and NH_3 are better constrained than for H_2O. The retrieval statistically favours an atmosphere without clouds.

The posterior distribution of K2-18 b presents significant noise (see fig. 3). Degeneracies among several parameters are high, including the isothermal temperature, chemical mixing ratios and cloud top pressure. The retrieved mixing ratio of H_2O in model B is the least precise, showing the challenges of retrieving high mean molecular weight (HMMW) exoatmospheres. The models B and O are modelled as secondary atmospheres, however, the retrievals fail to significantly detect the main gaseous species, H_2O and NH_3, respectively. The presence of clouds is not correctly retrieved in any of the three models.

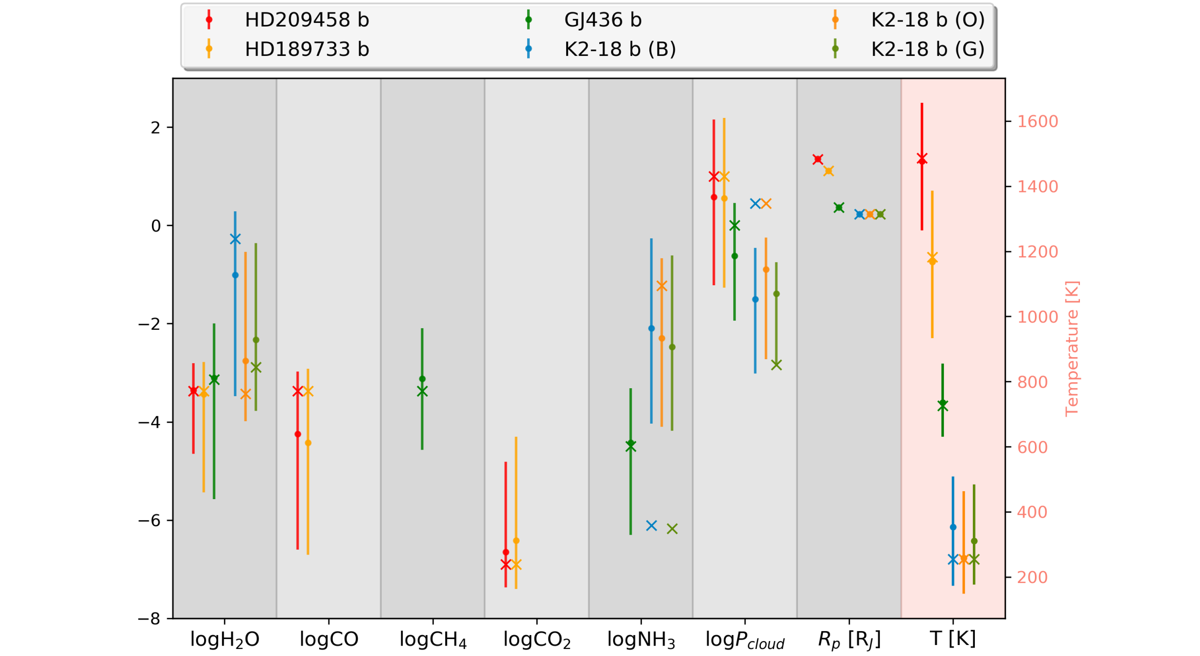

FIG. 2: Plot for the retrieved (●) and true (×) values of the atmospheric parameters. The error bars correspond to the uncertainties at 1σ. The temperature values correspond to the secondary y-axis (right). The radii error bars are within marker size.

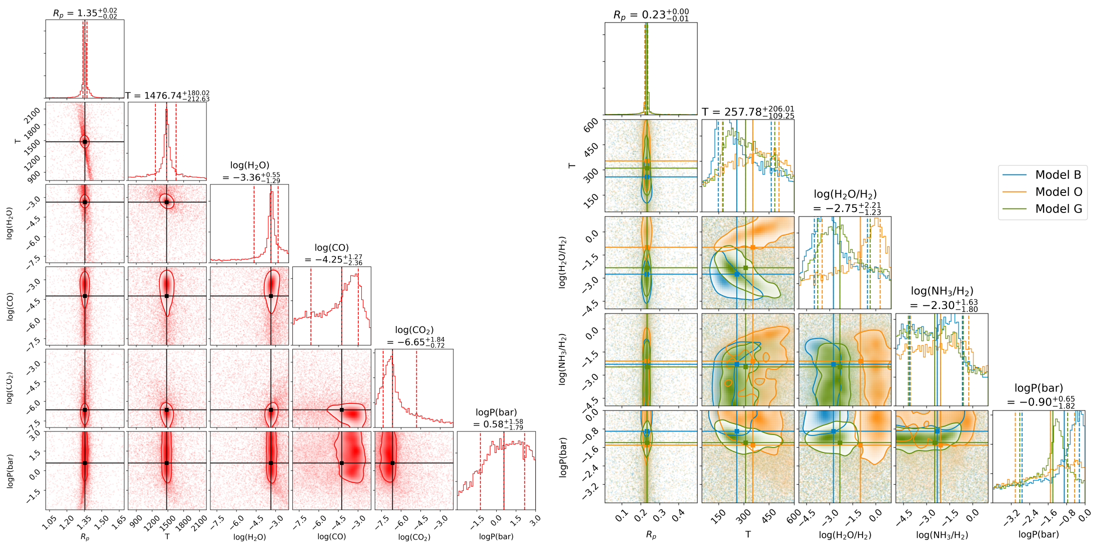

FIG. 3: Posterior distributions for the atmospheric retrievals. Hot Jupiter HD209458 b in red (left). For K2-18 b (right) three retrievals are superposed corresponding to the three atmospheric models B, O, G.

VI. SIGNAL AND NOISE ON K2-18 b

Different plausible models (see section V) for K2-18 b describe current observed data [2]. Increasing the number of observations improves our ability to discard models and constrain parameters. However, there is an upper limit to the number of observations an instrument can perform on a transiting exoplanet. The physical limit is imposed by the mission lifetime τ_{mission}(years) and the orbital period of the exoplanet P(days). The ARIEL mission is expected to last for 4 to 6 years [12]. Hence, an optimistic measure to the maximum number of transits is $n_{\max} = \frac{365\times\tau_{\text{ARIEL}}}{P}$ In the case of K2-18 b, the orbital period is $P = 32.94$ days, therefore the maximum number of ARIEL observations on this target is $n_{\max} = 66$ during its 6-year mission. As it is presented in fig. 4, the different atmospheric scenarios in K2-18 b will be difficult to disentangle for ARIEL, only with $n \geq 50$ observations, the G model and the BO models could potentially be separated. Thus, unveiling whether K2-18 b retains a primary atmosphere (model G) or possesses a secondary one.

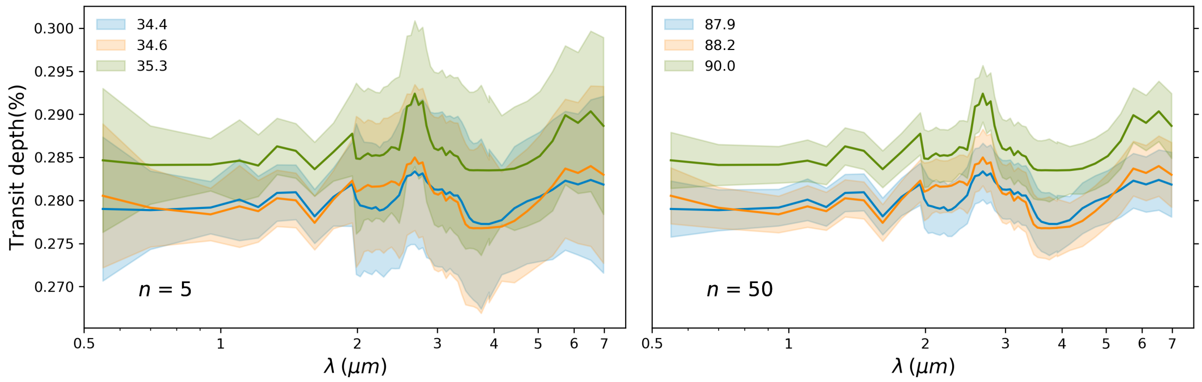

FIG. 4: Transmission spectra for K2-18 b for different number (n) of observations. The median signal-to-noise ratio (SNR) for each atmospheric model is presented in the corresponding legend.

VII. CONCLUSIONS

In the present work I have highlighted some of the scientific possibilities in atmospheric characterization with the upcoming ARIEL space mission. The simple models employed here illustrate that main gaseous species can be detected and their mixing ratios can be constrained within reasonable margins. A single transit is sufficient to acquire useful data for hot Jupiters and warm Neptunes but cooler and smaller exoplanets need a higher number of observations. I estimate that, at least, 50 ARIEL observations are required to discern a primary from a secondary atmosphere on K2-18 b. High mean molecular atmospheres are very challenging in general, and are probably beyond ARIEL's capabilities. The results show that studying smaller and cooler exoplanets like K2-18 b is a difficult task for ARIEL, however, it can be an excellent complement to other instruments like JWST or ground based telescopes.

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[14] MCMC: Markov chain Monte Carlo.
[15] In a Linux i7-3770 CPU @ 3.40 Hz.