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NON-LTE EFFECTS OF Na I IN THE ATMOSPHERE OF HD 209458b

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ABSTRACT

The recent announcement that sodium absorption has been observed in the atmosphere of HD 209458b, the only extrasolar giant planet (EGP) observed to transit its parent star, is the first direct detection of an EGP atmosphere. We explore the possibility that neutral sodium is *not* in local thermodynamic equilibrium (LTE) in the outer atmosphere of irradiated EGPs and that the sodium concentration may be underestimated by models that make the LTE assumption. Our results indicate that it may not be necessary to invoke excessive photoionization, low metallicity, or even high-altitude clouds to explain the observations.

Subject headings: planetary systems — radiative transfer

1. INTRODUCTION

HD 209458b is the first extrasolar giant planet (EGP) observed to transit its parent star (Charbonneau et al. 2000; Henry et al. 2000), and, consequently, its mass (0.69 M_J) and radius (1.35 R_J) are known to a high degree of accuracy. These results leave little doubt that HD 209458b is a gas giant. and its special orbital inclination has drawn a great deal of attention from observers and theorists over the past year. Recently, an increase in the sodium absorption (relative to the continuum) at 5893 Å was observed with the *Hubble Space Telescope* (*HST*) during several transits of HD 2094598 (Charbonneau et al. 2002). The additional sodium absorption is believed to be due to Na D absorption in the EGP's atmosphere as stellar light passes through the planetary limb. This observation marks a major turning point in the study of EGPs, for now we have direct evidence of an atmosphere around HD 209458b and a measurement of one chemical species (Na). According to Charbonneau et al. (2002), the *HST* observations suggest either that the EGP atmosphere has a low concentration of neutral atomic Na (due to photoionization, molecular formation, or an overall low metallicity) or that high-altitude clouds exist and reduce the amount of stellar flux transmitted though the EGP limb.

In this Letter, we offer an alternate explanation for the observed Na absorption and explore the possibility that the Na D feature is altered by nonlocal thermodynamic equilibrium (NLTE) effects brought on by the impinging stellar radiation field and insufficient collisional thermalization. If true, NLTE effects would offer a natural explanation for the apparently low sodium absorption observed in HD 209458b without the need for excessive ionization, a reduced metallicity, or extremely high altitude clouds. Below we will present theoretical predictions for NLTE Na D doublet line profiles for the transmitted spectrum of an irradiated EGP atmosphere and will provide stringent limits on the non-LTE effects.

2. MODEL CONSTRUCTION

The construction of the model atmospheres presented below follows the procedure outlined in Barman, Hauschildt, & Allard (2001, hereafter BHA). In order to make a direct comparison with HD 209458b, we have adopted the best-fit values for the radius, mass, and orbital separation of HD 209458b and its parent star published by Brown et al. (2001) and Mazeh et al. (2000) (see Table 1). We have also assumed that the total flux received by the planet has been uniformly distributed over the planet's dayside. Therefore, the incident flux has been weighted by 0.5, whereas in the BHA models, no redistribution was assumed. The intrinsic effective temperature of the model (i.e., the effective temperature of the planet in the absence of irradiation) is 500 K. However, this intrinsic temperature has little effect on the structure of the outer atmosphere that is completely determined by the incident flux. With this redistribution, our models represent an upper limit to the equilibrium effective temperature that is about 1800 K. We further assume that the planet has a solar composition with an opacity setup identical to the "AMES-cond" models of BHA and Allard et al. (2001). In this situation, dust grains form in the atmosphere at locations determined by the chemical equilibrium equations, but their opacity contribution is ignored, mimicking a complete removal of the grains by efficient gravitational settling. Therefore, the models in this study represent cloud-free atmospheres.

We model the flux transmitted through the limb of the planet's atmosphere by solving the spherically symmetric radiative transfer equation (SSRTE) suitably adjusted to account for the incident radiation. The incident flux is taken from a separate calculation that reproduces the observed spectrum of HD 209458. The SSRTE has a significant advantage over the plane-parallel solution because a geometry more appropriate (and more accurate) for the upper atmosphere is already incorporated. When solving the SSRTE, the atmosphere is modeled as a discrete number of concentric shells surrounding the interior (or "core"). The solution along characteristic rays that pass through the outermost shells is all that is needed to calculate the transmitted intensities and automatically accounts for the curvature of the limb. The total transmitted flux is obtained by integrating over the planet limb:

$$F_{\mathrm{trans},\lambda} = \int_{R_{\min}}^{R_{\max}} I_\lambda(r) 2\pi r \, dr, \quad (1)$$

TABLE 1
Model Parameters

Parameters	HD 209458b	HD 209458
Radius	1.35 R_J	1.146 $R_\odot$
Mass	0.63 M_J	1.05 $M_\odot$
$T_{\rm eff}$ (K)	1800	6000
[Fe/H]	0.00	0.00
Semimajor axis (AU)	0.045	0.045

where r is the perpendicular distance from the planet center to a tangential characteristic ray. $R_{\rm max}$ is the planet radius at $\tau_{\rm std} = 0$, and $\tau_{\rm std}$ is the optical depth at 1.2 μm. $R_{\rm min}$ is chosen such that for $r \geq R_{\rm min}$ and $\lambda = 5880$ Å, $I(r) \geq 0.1 I^\star(r)$, where $I^\star$ is the incident stellar intensity. This lower limit ensures that the transmitted intensities are well sampled and that light from the core region is excluded. Note that both $R_{\rm max}$ and $R_{\rm min}$ are determined by the simulation and depend on the resulting structure of the model atmosphere. The only prescribed radius is $R_p = r\,(\tau_{\rm std} = 1)$, which is equal to the planet radius given in Table 1. With these definitions, the thickness of the limb ($H = R_{\rm max} - R_{\rm min}$) is roughly $0.07R_p$.

2.1. Na *in Non-LTE*

When a gas is assumed to be in LTE, the level populations for each species depend entirely on the gas temperature and electron pressure and are given by the Saha-Boltzmann distribution. In general, the LTE assumption is a matter of computational convenience and is not expected to be valid in most cases, especially in the optically thin regions of an atmosphere. However, it is often assumed that LTE is achieved in very late type stars (even brown dwarfs), despite the fact that this assumption has not been thoroughly tested. Departures from LTE have previously been investigated for Ti I (Hauschildt et al. 1997) and CO (Schweitzer, Hauschildt, & Baron 2000) for cool M dwarfs and for CH_4 in the Jovian planets (Appleby 1990). These earlier works found that for these particular species, NLTE effects were small.

Due to the close proximity of HD 209458b to its parent star, the planet's atmosphere is subjected to intense stellar radiation. This inherently *nonlocal* source of radiation dramatically alters the conditions of the outer atmosphere compared with an isolated EGP. In addition, the cool atmospheres of EGPs are dominated by strong opacity sources like H_2O and CH_4 and, therefore, have intensities that differ greatly from those of a blackbody. When combined with the relatively low pressures of the outer atmosphere, these conditions very likely will lead to departures from LTE that may play an important role in determining the atmospheric structure and resulting spectrum. If LTE is to be achieved in EGP atmospheres, then the collisional rates must be large enough to compensate for the deviations of the radiative rates from their LTE values. Unfortunately, a limitation of all NLTE models is a lack of well-determined collisional cross sections for interactions with important species like H_2, He, and H. However, it is unlikely, given the low thermal velocities, that these particles could restore LTE completely. In fact, the effects of collisions with hydrogen on the Na D profiles in M dwarfs with chromospheres are fairly small, and electron collisions dominate despite the fact that $N_{\rm H}/N_e \sim 10^6$ (Andretta, Doyle, & Byrne 1997).

The Na I model atom used in this work includes 53 levels, and 142 primary transitions (all bound-bound transitions with $\log gf > -3.0$) were included in the solution of the statistical equilibrium equations. For details of the method used to solve the rate equations, see Hauschildt & Baron (1999). As in Hauschildt et al. (1997) for Ti I, electron-impact bound-free collisional rates are approximated by the formula of Drawin (1961), and bound-bound collisional rates are based on the semiempirical formula of Allen (1973) with permitted transitions determined from Van Regemorter's (1962) formula. For the ground-state photoionization cross sections, we have used the Opacity Project data of Bautista, Romano, & Pradhan (1998). We have also assumed complete redistribution.

We have constructed four model atmospheres and resulting transmitted spectra for HD 209458b. The first irradiated model (A) only includes collisions with electrons, in which the source of free electrons is primarily the ionization of potassium. Even in an irradiated EGP atmosphere, the number density of electrons is very small ($N_e/N_{H_2} \sim 10^{-8}$), and the temperatures are too low for electronic collisions to be important. Model A, therefore, can be considered a lower limit for the collisional rates. The second irradiated model (B) has the same parameters as model A, except that collisions with H_2 are also included. In order to place a secure upper limit on the effects of collisions with H_2, we have treated H_2 as if it had the same rate coefficients as an electron. Assuming identical cross sections implies that the rate coefficients scale with $(\mu)^{-1/2}$, where μ is the reduced mass of the collision partners. Therefore, we are overestimating the H_2 collisional rates by more than an order of magnitude. The remaining two models (C and D) represent *nonirradiated* atmospheres with the same effective temperature as the irradiated models (∼1800 K) and include the same lower (model C) and upper (model D) limits for the collision rates. Each of these model atmospheres was produced from a self-consistent solution of the SSRTE, chemical equilibrium equations, and the NLTE rate equations. We did not prescribe the temperature structure or mixing ratios for any of the species.

3. RESULTS

The temperature-pressure profiles for models A and C are shown in Figure 1. Note that the profile for model B is identical to that of model A and that model D has the same profile as model C. The gas pressures in the limb are very low, ranging from 0.004 to 0.2 mbar. As is to be expected, the nonirradiated models look nothing like the irradiated models, which have temperatures nearly 1000 K higher in the outer atmosphere (BHA; Goukenleuque et al. 2000; Seager & Sasselov 1998). There were no significant changes to the temperature-pressure profiles in the four NLTE models compared with the LTE structures.

Departures of the level populations from LTE, for a particular species, are usually described by the departure coefficients, $b_i = n_i^\star/n_i$, where $n_i^\star$ is the NLTE population density for level i and n_i is the LTE value (Mihalas 1970). In Figure 2, we show the b_i's for the ground state (3s) and the first excited states ($3p^{1/2}$, $3p^{3/2}$) of the neutral sodium atom for several different physical conditions within an EGP atmosphere. The largest departures are seen in model A, where the 3s (ground state) and 3p levels are both underpopulated by many orders of magnitude, especially in the limb region. The main reason for such large departures is that we have only included collisions with electrons, and in such a cool atmosphere, the number density of electrons is ∼8 orders of magnitude below that of the dominant species, H_2. Consequently, there are essentially no collisions in model A to thermalize the level populations in the Na atom, thus allowing the radiative rates to dominate and drive the system out of LTE. Also, since the upper atmosphere

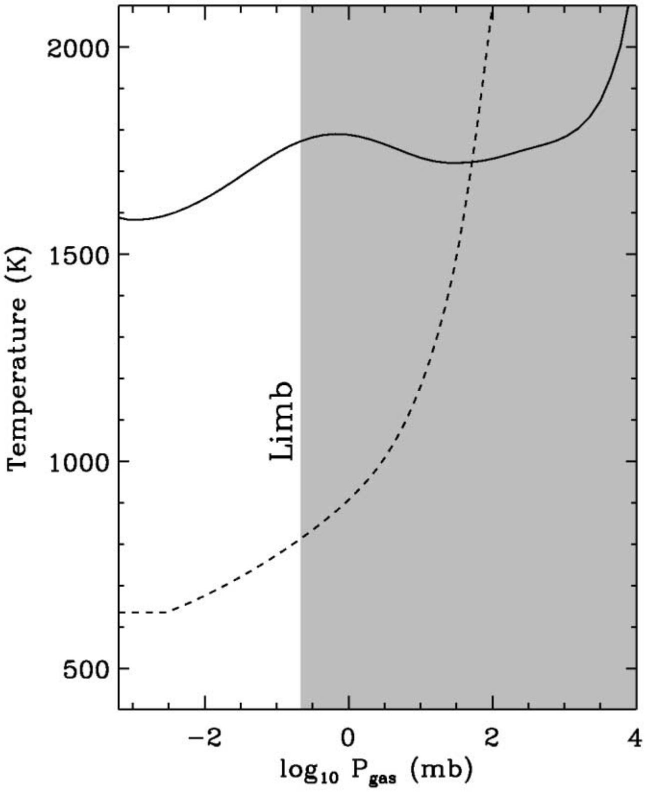

FIG. 1.—Temperature-pressure profiles for the irradiated (*solid line*) and nonirradiated (*dashed line*) models. The unshaded area indicates the limb region for the irradiated models.

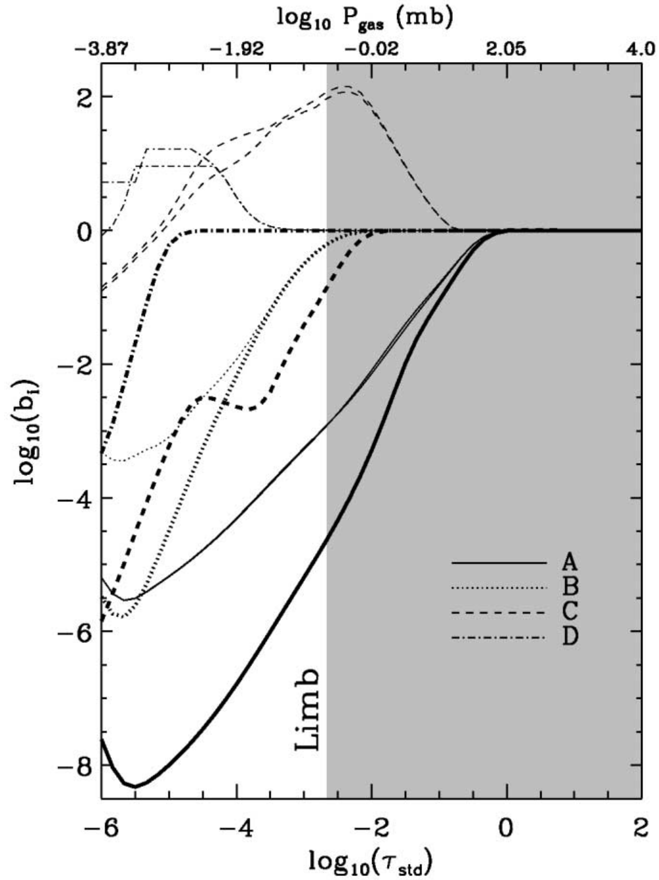

FIG. 2.—Departure coefficients for neutral sodium in the atmosphere of HD 209458b as a function of the radial optical depth at 1.2 μm (τ_{std}) and pressure (*top axis*). Model A demonstrates departures for an irradiated atmosphere including only collisions with free electrons. Model B is the same as A but includes collisions with H_2, assuming that H_2 has the same rate coefficients as an electron. Model C shows the departures in a nonirradiated atmosphere (where $T_{eq} = T_{eff}$) with collisions treated as in model A. Model D is the same as C, but with collisions treated as in model B. The thick lines refer to the 3*s* level (ground state), and the thin lines indicate the 3*p* levels (for $J = 1/2$ and $J = 3/2$). The unshaded region is the portion of the atmosphere where stellar flux is transmitted ("Limb") in the irradiated case.

is dominated by a large external radiation source (which happens to peak near the Na D doublet, ~5000 Å), the mean intensity of the line is much larger than the thermal source function, which implies a strong decoupling of the radiation field from the local conditions. Furthermore, the ratio of the line source function to a blackbody is roughly given by the ratio of the departure coefficients of the upper (3*p*) and lower (3*s*) levels for the transition (Bruls, Rutten, & Shchukina 1992). From Figure 2, we see that the line source function is far from a blackbody for the majority of the upper atmosphere (since $b_{3p}/b_{3s} \gg 1$).

An obvious question to ask is whether the system will return to LTE if collisions with the dominant species (H_2) are included. Model B, which has the same parameters and temperature profile as model A, includes collisions with both electrons *and* H_2 (but assuming that H_2 has the same rate coefficients as an electron). In effect, we have increased the importance of electronic collisions by more than 8 orders of magnitude. As is expected, the departure coefficients are closer to one, but the level populations in the limb are still far from the LTE values. However, since $b_{3p}/b_{3s} \sim 1$ for most of the atmosphere, NLTE effects will only be important in model B for $\tau_{std} < 10^{-4}$. The real situation is likely to be somewhere between models A and B.

We also show departure coefficients for nonirradiated models (C and D) with T_{eff} equal to the equilibrium effective temperature of the irradiated atmospheres (1800 K) for both collisional rate limits. Despite the absence of any extrinsic radiation and much lower temperatures in the upper layers, the nonirradiated atmospheres still have departures from LTE, although generally less significant than those found in the irradiated atmospheres. Model C (the near collision-free limit) has departures from LTE similar to those of the collision-dominated irradiated model (B) for the ground state, but with an overpopulated 3*p* level. With increased collisional rates, Na I has nearly returned to LTE for most of the atmosphere in model D, with departures still present in the topmost layers, whereas in the irradiated case, both levels were greatly underpopulated even in the collision-dominated model (B).

The effects on the Na D line profiles are quite dramatic for model A (see Fig. 3). In this case, the lack of thermalization reduces the line transfer to nearly a pure scattering case. As a result, the doublet appears completely in emission. However, in model B, as the collisional rates are increased, the line wings return to their LTE shape while the line cores are reversed. The data analysis of Charbonneau et al. (2002) does not directly reveal the Na line profile produced by the planet atmosphere. Instead, their work shows that a deeper transit is observed in the Na band, implying additional Na absorption by the planet limb. Given the current sensitivity of the observations, a core reversal feature like the one shown in our model B would be buried in the noise and would manifest itself as simply a smaller equivalent width. The Na absorption in model B would result in a transit deeper than in the continuum bands but not as deep as implied by the LTE model. The fact that Na D absorption

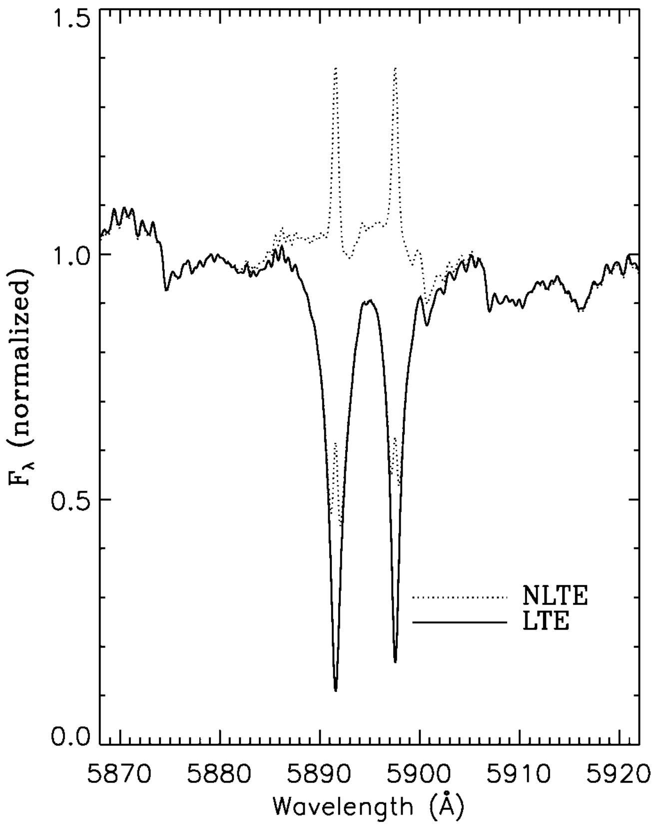

FIG. 3.—Na D doublet for model A (*top dotted line*), model B (*bottom dotted line*), and when assuming LTE (*solid line*). The flux has been normalized to one at 5880 Å.

(and not emission) has been observed in the transmitted spectrum of HD 209458b rules out our model A, indicating that some thermalization does occur in the limb region. However, it is unlikely that the collisional rates are as large as those in our model B, suggesting that the equivalent width of the Na D doublet will be substantially reduced by NLTE effects.

The reduced equivalent width predicted by our model is *not* due to photoionization of Na. In the majority of the limb, only 3% is ionized, and the neutral Na concentration is nearly constant with $N_{Na}/N_{H_2} \sim 10^{-5.5}$. Na is only significantly ionized ($\gg$5%) at the very top of the atmosphere, where $P_{gas} <$ 1 μbar. The shallow ionization depth of Na is due to the strong UV opacity provided by metals (e.g., atomic Mg, Al, Ca, Fe, and Ni) that effectively shield Na from the incident ionizing photons. The ionization predicted by our models (even 3%) is far greater than what is obtained from an LTE calculation but does not significantly affect the line profile. However, if the planet's atmosphere is substantially cooler than in our model, then additional condensation and settling could further deplete the atmosphere of metals and allow greater ionization of Na to occur. We also find that only a very small amount of Na is in molecular form and that neutral Na is nearly 3 orders of magnitude more abundant than NaCl (the most abundant Na-bearing molecule). Furthermore, condensation of Na via NaCl grains is unlikely. The reduced equivalent width and central core emission is purely a radiative transfer effect.

4. CONCLUSIONS

The recent *HST* observations provided the first direct measurement of the conditions inside the atmosphere of HD 209458b. However, even under the best circumstances, determining the concentration of any species based solely on one absorption feature is problematic, especially if this feature forms in the upper regions of an atmosphere where pressures are low and NLTE effects are greatest. Our models clearly show that Na is far from being in LTE in the upper atmosphere of HD 209458b and that the observed Na absorption can be explained with a solar metallicity atmosphere that is cloud-free or has only very low lying clouds. It is likely that other important species (e.g., CO and CH_4) are in NLTE, and we plan to test the LTE assumption for a wide variety of atomic and molecular species in a future work. Hopefully, the Na D doublets and other alkali metal lines will be useful diagnostics in the study of EGP atmospheres. However, only with detailed NLTE calculations, including well-determined collisional rates, will we have a chance at constraining the physical conditions in the atmosphere of HD 209458b.

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