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## METHOD

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### Key Points:

- Common approaches to estimating the severity of nonlinear scattering processes (i.e., saturation) are invalid for many modern lidar systems
- Underestimation of saturation effects leads to lidar system designs subject to biases on inferred winds, temperatures and number densities
- We present a detailed approach and publicly available calculator for calculating saturation effects for sodium, iron, and helium lidars

### Supporting Information:

Supporting Information may be found in the online version of this article.

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## Saturation Effects in Narrowband Resonance Lidar Measurements, Part 1: Theoretical Consideration of Sodium, Iron, and Helium Lidar Systems

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**Abstract** Atmospheric resonance lidars targeting metallic species in the mesosphere and lower thermosphere have yielded insights into the dynamics of the middle and upper atmosphere for over 50 years. Recently, the technique has been extended to the metastable helium layer, which reaches up to 1,000 km or above. It has long been recognized that high energy concentrations in the laser beam can lead to nonlinear behavior during the scattering process, a phenomenon known as saturation. Nonetheless, commonly used approaches to calculating the severity of saturation effects are not accurate for modern resonance lidar systems. Here, we present an approach to calculating saturation for sodium, iron, and helium resonance lidars and discuss the biases in wind and temperature that arise from neglecting saturation. The saturation calculators presented here are publicly available and can be adapted to estimate saturation for current or future resonance lidar systems.

**Plain Language Summary** Atmospheric resonance lidars rely on powerful, pulsed lasers tuned to the resonance lines of different atmospheric constituents to make measurements of winds and temperatures in the middle and upper atmosphere. Modern lidar systems have achieved precise measurements of these parameters, but the high energy concentrations produced by these systems can lead to a situation in which the target constituent is “saturated”, that is, the back-scattered signal is no longer proportional to the laser power. This results in a reduced signal and can lead to biases in the measured winds and temperatures. Here, we present a detailed approach to determining whether a system is in this saturated regime and estimate the impact of this effect for lidar systems targeting sodium, iron, and helium.

## 1. Introduction

Over the last 50+ years, atmospheric resonance lidars have been widely used to address a range of scientific questions. The first demonstration of the technique by Bowman et al. (1969) resulted in density measurements of the sodium layer between 80 and 100 km; since then, the technique has been expanded to a range of atmospheric constituents, including potassium, iron, calcium, and helium. Gibson et al. (1979) used a narrow-band laser to scan the Doppler-broadened sodium spectrum, thereby retrieving temperature estimates. This approach is now widely used, with modern systems typically applying a 3-frequency approach to retrieve line-of-sight winds, temperatures, and number densities of the target species.

As atmospheric resonance lidars achieved higher pulse energies, nonlinear effects began to play an increasing role. This phenomenon, known as saturation, was first analyzed by Megie et al. (1978) for the case of a broadband laser (i.e., a laser with a linewidth larger than the Doppler-broadened width of the target resonance line). This work was extended by Welsh and Gardner (1989), but closed-form solutions were only found for the extreme cases: for lasers with bandwidths much broader than the Doppler-broadened linewidth of the resonance line, and for narrow-band lasers approximated by delta functions. A detailed treatment of saturation effects for sodium in the case of a narrow-band laser was provided by von der Gathen (1991) (referred to hereafter as “VDG”), who accounted for beam profile and pulse shape and determined the temperature biases that would arise from neglecting saturation effects. However, due to the choice of laser bandwidth and target species, along with minor errors in the analysis, the degrees of saturation predicted by VDG were not significantly higher than those obtained using the approach by Megie et al. (1978) for the same lidar system parameters (see Figure S1 in Supporting Information S1); this may have led to the misperception that VDG's work represented only an incremental improvement to the previous work, giving more precise but generally similar results. The most widely cited

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source on the subject, Chu and Papen (2005), follows the derivation by Megie et al. (1978) exactly but notes that the approach is “more suitable for broadband lidars.” This is an understatement, as we will show: the Megie approach is *only* suitable for lidar systems with broadband lasers and can lead to substantial underestimation of the magnitude of saturation effects for lidar systems employing narrow-band lasers. Given this mild formulation, it is perhaps unsurprising that subsequent authors did not heed the warning and applied the Megie approach in the case of narrow-band systems (Smith & Chu, 2015; Li et al., 2022; Zhao et al., 2024). Part of the confusion may have arisen from an imprecise definition of what constitutes a broadband laser: as will be shown, the condition for applicability of the Megie approach is not that the linewidth of the laser be broad compared to the natural linewidth of the target absorption line (on the order of 10 MHz, depending on the target species), as stated by Smith and Chu (2015), but that it be broad compared to the Doppler-broadened width of the absorption line (typically 100's of MHz or more, depending on the target species and atmospheric temperature).

In this paper, we will discuss previous attempts at estimating saturation; we will present an improved and extended version of the approach pioneered by VDG, generalized to resonance lidars of all types; and we will discuss the significance of this improved saturation calculator for sodium, iron, and helium resonance lidar systems. Potassium resonance lidars present a special case: severe saturation has been observed for measurements over many years (Höffner & Lübken, 2007; Lautenbach et al., 2017). Analysis of saturation effects for potassium lidars, and experimental validation for the saturation model discussed here, are discussed in a companion manuscript (Geach et al., 2026).

## 2. Estimation of Saturation Effects

Atmospheric resonance lidars stimulate resonance fluorescence in their targeted atmospheric constituent. The resonance scattering cross-sections of common resonance lidar targets are a factor of  $\sim 10^{16}$  higher than the Rayleigh scattering cross-section, allowing lidar retrievals at altitudes far above those typically probed by Rayleigh lidar systems. However, the finite lifetime of the fluorescent excited state gives rise to nonlinear effects in the scattering process: for each photon that is absorbed, the likelihood that subsequent photons be absorbed is temporarily reduced. Furthermore, later-arriving photons can also produce stimulated emission from the excited state, resulting in a non-detectable photon that propagates farther along the line-of-sight of the instrument. Finally, for transitions with fine structure, excited particles can relax into any of multiple ground states; this is a case of optical pumping, whereby specific ground states can be steadily depleted while others are enriched.

Each of these effects represents a departure from linear behavior of the scattering process. The issue intensifies with larger energy concentrations (whether this concentration is spatial, temporal, or spectral). As laser pulse energies increase, reducing statistical measurement uncertainties, accounting for these effects takes on increasing importance. Furthermore, the degree of saturation varies with laser output frequency, so neglecting the saturation effect leads to a spectrally varying bias to the return signal. While the largest induced bias is in the retrieved densities, significant biases in the retrieved winds and temperatures can also arise.

### 2.1. Megie Approximation

The common approach to calculating saturation was pioneered by Megie et al. (1978), who set up a differential equation for  $n_e$ , the number density of target atoms in the excited state. The likelihood of scattering is quantified via the effective scattering cross-section, defined as

$$\sigma_{\text{eff}}(\nu_L) = \int N_L(\nu_L, \nu) \alpha(\nu) d\nu \quad (1)$$

where  $N_L(\nu_L, \nu)$  is the normalized laser line shape (i.e.,  $\int N_L(\nu_L, \nu) d\nu = 1$ ) and  $\alpha(\nu)$  is the natural line shape of the resonance line, with:

$$\alpha(\nu) = \frac{\sigma_0}{\pi} \frac{\Delta\nu_n/2}{(\nu - \nu_0)^2 + (\Delta\nu_n/2)^2} \quad (2)$$

where  $\nu_0$  is the central frequency and  $\Delta\nu_n$  is the natural linewidth of the resonance line, and  $\sigma_0$  is the peak scattering cross-section, given by:

$$\sigma_0 = \frac{e^2}{4\epsilon_0 m_e c^2 f_o} \quad (3)$$

with  $e$  the charge of an electron,  $\epsilon_0$  the permittivity of free space,  $m_e$  the mass of an electron,  $c$  the speed of light, and  $f_o$  the oscillator strength of the resonance line. A differential equation for  $n_e$  can then be written, assuming a vertically oriented lidar:

$$\frac{dn_e}{dt} = -\frac{n_e}{\tau} + (n_t - n_e) \frac{\sigma_{\text{eff}} N(t) \mathcal{T}_a}{z^2 \Omega} - n_e \frac{\sigma_{\text{eff}} N(t) \mathcal{T}_a}{z^2 \Omega} \quad (4)$$

where  $\tau$  is the lifetime of the excited state,  $n_t$  is the total number density of the target species (including atoms in the ground and excited states),  $N(t)$  is the number of photons emitted by the laser per unit time,  $\mathcal{T}_a$  is the one-way transmission of the atmosphere at the laser frequency,  $z$  is the altitude of the observed layer, and  $\Omega$  is the solid angle illuminated by the laser beam, given by  $\Omega = \pi \alpha_L^2$ , with  $\alpha_L$  the full-angle divergence of the laser beam. We define further the average photon density  $u_0$  at altitude  $z$ , with

$$u_0 = \frac{\mathcal{T}_a N_t}{z^2 \Omega} \quad (5)$$

where  $N_t = \frac{E_L}{h\nu_0} = \int N(t) dt$  is the total number of photons per pulse emitted by the laser, with a pulse energy  $E_L$  and Planck's constant  $h$ , and we define the normalized pulse shape  $\tilde{N}(t) = \frac{1}{N_t} N(t)$ , so that Equation 4 becomes:

$$\frac{dn_e}{dt} = -\frac{n_e}{\tau} + (n_t - 2n_e) u_0 \sigma_{\text{eff}} \tilde{N}(t) \quad (6)$$

The first term on the right hand side of Equation 4 represents the loss of excited atoms through spontaneous emission; the second term represents the replenishment of the excited state through excitation of ground state atoms; and the third term represents the loss of excited atoms through stimulated emission. By assuming a top hat function for the laser pulse, Equation 4 can be solved to find  $n_e$  as a function of time, from which the expected number of re-emitted photons,  $N_R$ , can be derived in terms of  $N_R^0$ , the number of photons that would be emitted without saturation effects (see Equation 9 in Megie et al. (1978)):

$$N_R = \frac{t_s}{\tau + t_s} \left[ 1 - \frac{\tau}{t_L \tau + t_s} \left( \exp \left[ -\frac{t_L}{\tau} \left( 1 + \frac{\tau}{t_s} \right) \right] - 1 \right) \right] N_R^0 \quad (7)$$

where  $t_L$  is the length of the laser pulse, and  $t_s$  is the “saturation time”, defined as:

$$t_s = \frac{t_L}{2u_0 \sigma_{\text{eff}}} \quad (8)$$

We can then define the degree of saturation expected by this approach as:

$$S_M = 1 - \frac{N_R}{N_R^0} \quad (9)$$

The definition of  $\sigma_{\text{eff}}(\nu)$  given in Equation 1 represents our interpretation of the work by Megie et al. (1978); we make this interpretation because the authors give no indication that this quantity is temperature-dependent. However, many authors have interpreted the so-called “absorption coefficient” (symbolized by  $k_\nu$  in the Megie et al. (1978) paper and by  $\alpha(\nu)$  here) to be the Doppler-broadened resonance line shape (Chu & Papen, 2005; Smith & Chu, 2015; Li et al., 2022; Zhao et al., 2024) instead of the natural line shape, perhaps because the symbol  $\sigma_{\text{eff}}$  is often used in the context of resonance lidars to quantify the total likelihood of scattering when

accounting for the Doppler-broadened velocity distribution, which is the relevant parameter when estimating the expected signal of a lidar system. This quantity, which we will refer to as the total scattering cross-section, or  $\sigma_t$ , can be expressed in terms of the laser line shape and the Doppler-broadened resonance line  $\sigma_D(\nu)$ :

$$\sigma_t(\nu_L) = \int N_L(\nu_L, \nu) \sigma_D(\nu) d\nu \quad (10)$$

where  $\sigma_D(\nu)$  is given by:

$$\sigma_D(\nu) = \int D(\nu - \nu_0) \alpha(\nu) d\nu \quad (11)$$

with the normalized Doppler-broadened distribution  $D(\nu)$

$$D(\nu) = \frac{1}{\sqrt{2\pi}\Delta\nu_D} \exp\left(-\frac{\nu^2}{2\Delta\nu_D^2}\right) \quad (12)$$

where  $\Delta\nu_D$  is the rms linewidth of the Doppler-broadened spectrum and is given by.

$$\Delta\nu_D = \sqrt{\frac{k_B T}{Mc^2}} \nu_0 \quad (13)$$

with  $k_B$  the Boltzmann constant,  $T$  the temperature of the scattering layer, and  $M$  the mass of the scattering atom.

For the instrument described in Megie et al. (1978), for which the laser bandwidth was appreciably larger than the Doppler-broadened width of the resonance line, the difference between  $\sigma_{\text{eff}}$  and  $\sigma_t$  was negligible (hence the ambiguity as to which of those quantities was used), but for modern resonance lidars with laser bandwidths narrower than the Doppler-broadened width, the difference can be substantial. However, as will be shown, neither interpretation results in an accurate approximation of saturation for lidar systems with laser bandwidths on the order of or narrower than the Doppler-broadened linewidth of their targeted resonance line.

## 2.2. Improved Saturation Calculation

There are two main problems with the above approach (referred to hereafter as the “Megie approach”), both identified by VDG. The first problem lies in recognizing that a narrow-band laser cannot interact with the entire population of atoms, but rather only those atoms with velocity components along the laser line-of-sight such that the laser frequency matches the resonance line frequency due to the apparent Doppler shift. For that sub-population, however, the likelihood of scattering does not depend on either the total or the effective scattering cross-section but on the natural resonance line strength. The second problem is that for realistic laser line shapes, a non-negligible amount of power is emitted at frequencies other than the central frequency, at intensities significantly lower than the peak intensity. At these frequencies, saturation is less severe. Properly accounting for saturation across the entire spectrum requires taking a spectral average of the saturation, weighted by the emission at each frequency.

A more sophisticated approach to calculating the severity of saturation effects was introduced by VDG for the case of the sodium  $D_2$  line. Instead of analyzing the total number densities of the target atoms and of the atoms in the excited state as in Megie et al. (1978), he considered the relative densities of the target atoms in the ground and excited states,  $\tilde{n}_s(\nu_v, t)$  and  $\tilde{n}_{e,s}(\nu_v, t)$  respectively, as a function of their velocity-dependent Doppler shift  $\nu_v$ , imparted by their vertical velocity  $v_z$ , with  $\nu_v = \frac{v_z}{c} \nu_0$ . The subscript  $s$  is used to denote that saturation effects are being accounted for when calculating these quantities.

To demonstrate this approach, we consider a fictitious resonance line, consisting of a single transition from a non-degenerate ground state to a non-degenerate excited state. The associated excitation rate for a vertically oriented lidar will therefore be given by:

$$f_e(\nu_L, \nu_v, u_0, t) = u_0 \tilde{N}(t) L(\nu_L, \nu_v) \quad (14)$$

where  $L(\nu_L, \nu_v) = \int \alpha(\nu, \nu_v) N_L(\nu_L, \nu) d\nu$  represents the convolution of the laser line shape and the natural resonance line shape and we have assumed that the laser line shape is time independent. We can now set up a differential equation system (DES), analogous to the approach by Megie et al. (1978), but in terms of  $\tilde{n}_s$  and  $\tilde{n}_{e,s}$ :

$$\frac{d\tilde{n}_{e,s}}{dt} = -\frac{\tilde{n}_{e,s}}{\tau} + (\tilde{n}_s - \tilde{n}_{e,s})f_e \quad (15)$$

$$\frac{d\tilde{n}_s}{dt} = \frac{\tilde{n}_{e,s}}{\tau} - (\tilde{n}_s - \tilde{n}_{e,s})f_e \quad (16)$$

Given the added complexity of this approach, it is no longer feasible to find a closed form solution. Instead, we solve the DES numerically, initializing at  $t = 0$  when the laser pulse arrives at the target atoms with all atoms in the ground state (i.e.,  $\tilde{n}_s(\nu_v, 0) = 1$  and  $\tilde{n}_{e,s}(\nu_v, 0) = 0$ ). We then step forward in time, solving for the evolution of  $\tilde{n}_s$  and  $\tilde{n}_{e,s}$ , until a negligible number of atoms are still in the excited state—in practice, the necessary number and size of the time steps depend on the laser pulse length and natural lifetime of the target species. We keep the time step small enough that the maximum of  $f_e(\nu_L, \nu_v, u_0, t)$  remains below 0.1 to avoid numerical errors. To minimize computational time, once 99.99% of the laser pulse has been accounted for, the second term on the right-hand sides of Equations 15 and 16 are approximated as zero, and the DES are solved analytically.

Similarly, we set up a second DES to simulate the interaction without saturation:

$$\frac{d\tilde{n}_{e,ns}}{dt} = -\frac{\tilde{n}_{e,ns}}{\tau} + \tilde{n}_{ns}f_e \quad (17)$$

$$\tilde{n}_{ns} = 1 \quad (18)$$

where the *ns* subscript denotes “no saturation”. As before, we initialize the DES at  $t = 0$  with  $\tilde{n}_{e,ns}(\nu_v, 0) = 0$  and solve for the evolution of  $\tilde{n}_{e,ns}$  in time.

In each case (with and without saturation), the lidar signal is proportional to the number of spontaneously emitted photons. First, we integrate the  $\tilde{n}_{e,i}$  in time to find the relative density of spontaneous emission:

$$P_i(\nu_L, \nu_v) = \int_0^\infty \frac{\tilde{n}_{e,i}(\nu_v, t)}{\tau} dt \quad (19)$$

where *i* stands for *s* or *ns*. The  $P_i$  can be interpreted as the density of spontaneously emitted photons per laser pulse per target atom with a given Doppler shift. We then integrate the  $P_i$  weighted by the Doppler-broadened velocity distribution:

$$B_i(\nu_L) = \int D(\nu_v) P_i(\nu_L, \nu_v) d\nu_v \quad (20)$$

Thus defined, the  $B_i$  represent the total number of spontaneously emitted photons per laser pulse per target atom and are therefore proportional to the detected signal. The total saturation is just one minus the ratio between the number of spontaneously emitted photons when considering saturation to the number of spontaneously emitted photons in the case without saturation:

$$S(\nu_L) = 1 - \frac{B_s}{B_{ns}} \quad (21)$$

To illustrate the importance of this more detailed approach, we computed the expected saturation with this method and compared it to the solution based on the Megie approach, using both  $\sigma_{\text{eff}}$  as defined in Megie et al. (1978) and  $\sigma_t$  as assumed by later authors. To enable quantitative calculations, we used values for the various parameters

**Table 1**  
Relevant Parameters for Resonance Lines Targeted by Sodium, Iron, and Helium Lidars

| Species | Vac. Wavelength (nm) | Oscillator strength | Einstein a coefficient (MHz) |
|---------|----------------------|---------------------|------------------------------|
| Na      | 589.1583             | 0.641               | 61.6                         |
| Fe      | 372.0993             | 0.0411              | 16.2                         |
| Fe      | 373.8194             | 0.0381              | 14.1                         |
| Fe      | 386.1006             | 0.0217              | 9.69                         |
| He      | 1,083.3306           | 0.539               | 10.22                        |

Note. Values are taken from the NIST database (Kramida et al., 2024).

taken from the sodium  $D_2$  line (given in Table 1), keeping in mind that the calculation here represents a substantial simplification: the hyperfine structure of the  $D_2$  line is as yet missing from our calculation, as is any discussion of a non-uniform beam profile or of the Hanle effect. These effects will be incorporated in the next section, but this simplified representation is sufficient to show the substantial discrepancy between the different approaches. We assume further a layer with  $z = 90$  km,  $T = 200$  K, and  $\mathcal{T}_a = 0.7$ , and a lidar with  $E_L = 20$  mJ,  $t_L = 10$  ns, and  $\alpha_L = 1$  mrad. We assume a top-hat profile for  $\tilde{N}(t)$ , that is,

$$\tilde{N}(t) = \begin{cases} 1/t_L & \text{for } t \leq t_L \\ 0 & \text{for } t > t_L \end{cases} \quad (22)$$

to make the comparison between the two approaches more accurate. Note that the inclusion of more realistic laser pulse shapes adds no complexity to the simulation, since the DES are solved numerically in any case; this is a further advantage of the VDG approach. First, we assume a laser with a Gaussian beam profile, tuned to  $\nu_0$ , and let the full-width at half maximum (FWHM) linewidth vary from 20 MHz to 2 GHz. As shown in Figure 1a, the degrees of saturation calculated by all three approaches agree quite closely at large laser linewidths but diverge increasingly at smaller linewidths; the Megie approach using  $\sigma_i$  significantly underestimates the severity of saturation, while using  $\sigma_{\text{eff}}$  results in an overestimate.

Next, we fix the laser linewidth at 150 MHz and calculate the saturation as a function of the laser wavelength; the results are shown in Figure 1b. The von der Gathen approach shows a broad spectrum of saturation, demonstrating that saturation can be severe even at laser wavelengths far from the resonance line. Thus, for systems with narrow-band lasers, the Megie approach mischaracterizes not only the severity of saturation but also its spectral form. For

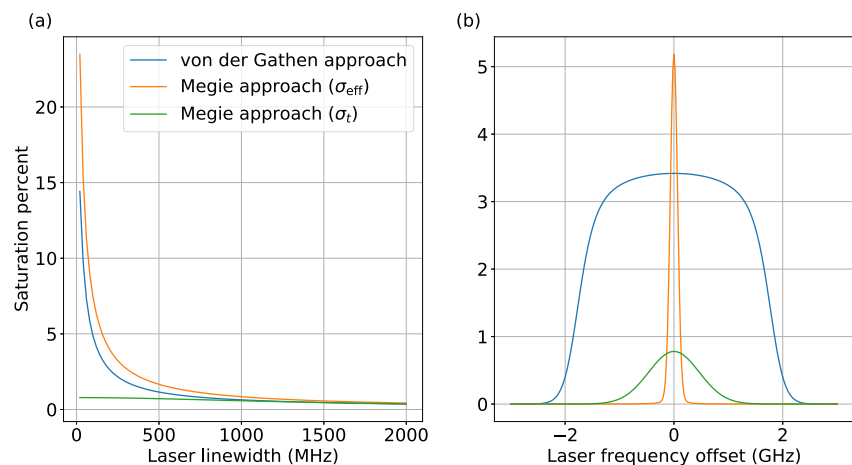


**Figure 1.** (a) Theoretical saturation percentages plotted as a function of laser linewidth for a fictitious resonance line using the approximate Megie approach or the more detailed VDG approach. (b) Same as (a), but plotted as a function of laser frequency offset relative to the line center, assuming a narrow-band (150 MHz) laser.

**Table 2**

Frequency Offsets and Relative Line Strengths  $g_j^k$  for the Sodium  $D_2$  Line (Fricke & von Zahn, 1985; Steck, 2000)

| $S_{1/2}$ | $P_{3/2}$ | $\Delta\nu_j^k$ (GHz) | $g_j^k$ |
|-----------|-----------|-----------------------|---------|
| $j = 1$   | $k = 0$   | 1.0408                | 2       |
|           | $k = 1$   | 1.0566                | 5       |
|           | $k = 2$   | 1.0911                | 5       |
| $j = 2$   | $k = 1$   | −0.7150               | 1       |
|           | $k = 2$   | −0.6805               | 5       |
|           | $k = 3$   | −0.6216               | 14      |

the rest of this work, we will refer only to the Megie approach using  $\sigma_t$  as the “Megie approach”, since we are unaware of any modern authors who have employed the Megie approach using  $\sigma_{\text{eff}}$ .

### 2.3. Fine and Hyperfine Structure

In contrast to the simple model described above, the sodium  $D_2$  line consists of 6 transitions between 2 ground states and 4 excited states, with three allowed transitions from each ground state. This requires several modifications to the DES: the relative densities of each ground and excited state must be tracked individually, the relative statistical weights and resonance frequencies for each transition must be accounted for, and the degeneracies of the ground and excited states must be factored in when

computing the likelihood of stimulated emission. These are all discussed in VDG and reproduced here, albeit with a correction to the calculation of the individual line strengths. The details that follow are specific to the sodium  $D_2$  line, but can be easily adapted to the hyperfine structure of the potassium  $D_1$  line (two ground states and two excited states) or the fine structure of the helium line at 1,083 nm (one ground state and three excited states).

Each transition has a unique resonance frequency  $\nu_j^k$  and line strength  $g_j^k$ , representing the transition between the  $j$ th ground state and the  $k$ th excited state, with  $j = 1$  or 2 and  $k = 0, 1, 2$ , or 3, with  $j$  and  $k$  representing the total angular momentum of the ground and excited states, respectively (see Table 2). Thus, Equation 2 must be replaced with:

$$\alpha_j^k(\nu, \nu_v) = \frac{\sigma_0}{\pi} \frac{g_j^k}{\sum_l g_j^l} \frac{\Delta\nu_n/2}{(\nu - \nu_v - \nu_j^k)^2 + (\Delta\nu_n/2)^2} \quad (23)$$

This formulation, which mirrors the detailed treatment of the sodium  $D_2$  line in She et al. (2015) (who, however, did not address saturation effects), represents a subtle but important departure from VDG, who normalized the individual transitions by dividing by the sum of the  $g_k^j$  over all 6 transitions rather than the sum over the transitions from a given ground state (i.e.,  $\sum_{l,m} g_m^l$  rather than  $\sum_l g_j^l$ ). The difference between these approaches lies in how the differing populations of the two ground states (arising from their respective degeneracies) are accounted for. The  $j = 1$  and  $j = 2$  states have degeneracies of 3 and 5, respectively, leading to relative populations  $n_j$  of 3/8 and 5/8, respectively, ignoring the correction due to the different energy levels, which is negligible at atmospheric temperatures. The formulation in VDG, which is widely used by for example Fricke and von Zahn (1985) and Chu and Papen (2005), incorporates these differing relative populations into the line strengths. That is, the total probability of scattering per atom would, following VDG, be given by:

$$\tilde{\alpha}_t(\nu, \nu_v) = \sum_{j,k} \frac{g_j^k}{\sum_{l,m} g_m^l} \frac{\Delta\nu_n/2}{(\nu - \nu_v - \nu_j^k)^2 + (\Delta\nu_n/2)^2} \quad (24)$$

where we have considered only homogeneous broadening of the resonance lines (i.e., Doppler broadening has been neglected). Though the formulation in Equation 24 leads to the correct spectrum of the total scattering cross-section, the individual line strengths are not correctly represented for the purposes of calculating saturation. This is because the degree of saturation relies not on the likelihood that a photon with a given wavelength will be absorbed but on the likelihood that an atom in a given ground state with a given line-of-sight velocity component will be excited; the relative populations of the respective ground states, like the absolute number density of the atoms, has no impact on the likelihood that a particular atom will be excited. This is an important point, with significant impact on the spectrum and severity of saturation for atoms with hyperfine structure. We write the total probability of scattering per atom as:

$$\alpha_i(\nu, \nu_v) = \sum_{j,k} \tilde{n}_j \frac{g_j^k}{\sum_l g_j^l} \frac{\Delta\nu_n/2}{(\nu - \nu_v - \nu_j^k)^2 + (\Delta\nu_n/2)^2} \quad (25)$$

The two formulations are mathematically equivalent—that is,  $\alpha_i(\nu, \nu_v) = \tilde{\alpha}_i(\nu, \nu_v)$ —but our formulation uses the correct expression for the individual resonance line strengths given in Equation 23. The individual transitions therefore have relative strengths given by 1/6, 5/12, 5/12, 1/20, 1/4, and 7/10, respectively (as given by Steck (2000) and She et al. (2015)), rather than 1/16, 5/32, 5/32, 1/32, 5/32, and 7/16 as given by VDG. The net effect is that all of the line strengths increase, and the line strengths for the transitions from the  $j = 1$  state experience a larger increase than the transitions from the  $j = 2$  state. Thus, the total line strength for atoms in each ground state sums to  $\sigma_0$  as required (Axner et al., 2004), which is not the case for the formulation in VDG.

Given these  $\alpha_j^k(\nu, \nu_v)$ , each transition line will have its own excitation rate  $f_{j,e}^k(\nu_L, \nu_v, t)$ , defined analogously to Equation 14:

$$f_{j,e}^k(\nu_L, \nu_v, t) = \frac{\tau_{am} N(t)}{z^2 \Omega} L_j^k(\nu_L, \nu_v) \quad (26)$$

with  $L_j^k(\nu_L, \nu_v) = \int \alpha_j^k(\nu, \nu_v) N_L(\nu_L, \nu) d\nu$ . Finally, each of the ground states  $\tilde{n}_{j,s}$  and excited states  $\tilde{n}_{e,s}^k$  must be kept track of separately:

$$\frac{d\tilde{n}_{e,s}^k}{dt} = -\frac{\tilde{n}_{e,s}^k}{\tau} + \sum_{j=1}^2 \left( \tilde{n}_{j,s} - \frac{2j+1}{2k+1} \tilde{n}_{e,s}^k \right) f_{j,e}^k \quad (27)$$

$$\frac{d\tilde{n}_{j,s}}{dt} = \sum_{k=0}^3 \left[ \frac{g_j^k}{g_1^k + g_2^k} \frac{\tilde{n}_{e,s}^k}{\tau} - \left( \tilde{n}_{j,s} - \frac{2j+1}{2k+1} \tilde{n}_{e,s}^k \right) f_{j,e}^k \right] \quad (28)$$

where the factor of  $\frac{g_j^k}{g_1^k + g_2^k}$  has been added to account for the relative probabilities of the excited state relaxing into each of the ground states and the factor  $\frac{2j+1}{2k+1}$  accounts for the degeneracies of the ground and excited states. The DES is initialized as before with  $\tilde{n}_{e,s}^k(\nu_v, 0) = 0$ , but in the ground state we must account for the differing populations of the two states due to their differing degeneracies as discussed above. Thus, we have  $\tilde{n}_{1,s}(\nu_v, 0) = 0.375$  and  $\tilde{n}_{2,s}(\nu_v, 0) = 0.625$ . This represents a further departure from VDG, who initialized both ground states with relative populations of 0.5.

For the “no saturation” case, we have:

$$\frac{d\tilde{n}_{e,ns}^k}{dt} = -\frac{\tilde{n}_{e,ns}^k}{\tau} + \sum_{j=1}^2 \tilde{n}_{j,ns} f_{j,e}^k \quad (29)$$

$$\tilde{n}_{1,ns} = 0.375, \quad \tilde{n}_{2,ns} = 0.625 \quad (30)$$

The DES are then solved as before to find the temporal evolution of each of the  $\tilde{n}_{j,i}$  and  $\tilde{n}_{e,i}^k$ . The relative densities of spontaneous emission can therefore be defined:

$$P_{j,i}^k(\nu_L, \nu_v) = \frac{q_j^k}{4\pi} \frac{g_j^k}{g_1^k + g_2^k} \int_0^\infty \frac{\tilde{n}_{e,i}^k(\nu_L, \nu_v, t)}{\tau} dt \quad (31)$$

where  $q_j^k$  are the Hanle factors for each transition. The total number of spontaneously emitted photons (again, per laser pulse and per target atom) is therefore:

$$B_i(\nu_L) = \int_{-\nu_0}^{\nu_0} D(\nu_v) \sum_{j,k} P_{j,i}^k(\nu_L, \nu_v) d\nu_v \quad (32)$$

and the saturation can be defined as in Equation 21. Note that the Hanle factors depend on the geographic location of the instrument, as well as the polarization and orientation of the laser beam. Since the degree of saturation is relatively insensitive to the strength of the Hanle effect, we assume  $q_j^k = 1$  for the calculations presented here.

## 2.4. Multiple Isotopes

There is only one stable isotope for sodium,  $^{23}\text{Na}$ , but other resonance lidar targets have multiple stable isotopes with non-negligible natural abundances. For each isotope, the resonance frequency (or frequencies, in the case of transitions with hyperfine structure) is slightly shifted. In contrast to the case with hyperfine structure, the individual resonance lines cannot interact, so the saturation for each isotope can be calculated independently. If we define the natural abundance fractions as  $p_n$  for each isotope  $n$  and calculate the total number of spontaneously emitted photons for each isotope individually, with and without saturation, as  $B_{n,s}(\nu_L)$  and  $B_{n,ns}(\nu_L)$ , respectively, then, the effective saturation for the line will be given by:

$$S_e(\nu_L) = 1 - \frac{\sum_n p_n B_{n,s}(\nu_L)}{\sum_n p_n B_{n,ns}(\nu_L)} \quad (33)$$

## 2.5. Realistic Beam Profiles

The above treatment assumes a spatially uniform laser beam intensity, that is, a top-hat profile. In order to simulate more realistic profiles, a spatial average of the total backscattered photons  $B_i$  can be calculated, weighted by the beam profile. As yet, we have calculated saturation as a function of the average density of photons at the scattering layer  $u_0$ . Now, assuming an azimuthally symmetric beam profile, that is, a beam profile that depends only on  $\beta$ , the angle to the optical axis of the beam, we define the photon number density for an arbitrary beam profile as  $u(\beta)$ . We define  $\tilde{B}_i(\nu_L, u) \equiv B_i(\nu_L)$ , where the dependence on  $u$  comes from the excitation rates calculated in Equation 14. We can then calculate the total number of backscattered photons from the entire beam:

$$\bar{B}_i(\nu_L) = \frac{2\pi}{\Omega} \int_0^{\alpha_r/2} \tilde{B}_i(\nu_L, u(\beta)) \beta d\beta \quad (34)$$

where  $\alpha_r$  is the full-angle field-of-view of the instrument. Finally, we can calculate the beam-averaged saturation:

$$\bar{S}(\nu_L) = 1 - \frac{\bar{B}_s(\nu_L)}{\bar{B}_{ns}(\nu_L)} \quad (35)$$

We will assume a Gaussian-distribution for the photon density:

$$u(\beta) = u_0 e^{-(4/\alpha_L^2)\beta^2} \quad (36)$$

where as before  $\alpha_L$  is the full-angle divergence of the laser beam. We will further assume a coupling efficiency that is constant across the field-of-view.

## 2.6. Narrow-Band Receivers

In the case of transitions with multiple isotopes or hyperfine structure, the return signal from each transition will result in an emitted photon with a specific frequency. The above formulation assumes a broadband receiver capable of detecting all received photons with equal efficiency (and atmospheric transmission that is frequency-independent). If this is not the case, for example, in systems with narrow-band filters to enable daytime measurements, then the effective saturation will depend on the differing transmission of the backscattered photons. If

we define  $\eta(\nu)$  to be the frequency-dependent detection efficiency (including potentially differing atmospheric transmission for backscattered photons), then Equation 32 becomes:

$$B_i(\nu_L) = \int_{-\nu_0}^{\nu_0} D(\nu_v) \sum_{j,k} \eta(\nu_b) P_{j,i}^k(\nu_L, \nu_v) d\nu_v \quad (37)$$

where the backscattered photons have frequencies given by  $\nu_b = \nu_j^k - \nu_v$  (Chu & Papen, 2005) and the subscript  $i$  again stands for either  $s$  or  $ns$  (note that this is an approximation: in fact, the backscattered photons have a spectrum determined by the natural linewidth of the resonance line centered at  $\nu_b$ . Thus,  $\eta(\nu_b)$  should be replaced by  $\eta_{\text{eff}}(\nu_b)$ , with  $\eta_{\text{eff}}(\nu_b) = \int \eta(\nu) \alpha_b(\nu, \nu_b) d\nu$ , where  $\alpha_b(\nu, \nu_b) = \frac{1}{\pi} \frac{\Delta\nu/2}{(\nu - \nu_b)^2 + (\Delta\nu/2)^2}$  is the normalized backscatter spectrum. Given that in general the frequency response of an instrument will vary very little over the natural linewidth of its targeted resonance line,  $\eta(\nu_b)$  is in general a good approximation). The effect of a narrow-band receiver depends on the receiver efficiency spectrum, and as such will vary considerably from instrument to instrument. In the calculations presented here, therefore, we do not include this effect.

## 2.7. Other Effects

Saturation of the sodium  $D_2$  line has also been studied extensively in the context of laser guide stars for astronomical telescopes. Here, either continuous wave (CW) lasers or lasers with long pulse lengths ( $>10 \mu\text{s}$ ) are typically used, generally at higher power and with smaller beam divergences relative to resonance lidars, all of which lead to further complications. These complications do not play a role for modern resonance lidars, but are included here for completeness.

First, a laser beam exerts a radiation pressure on its target atoms, which (using the sodium  $D_2$  line as an example) imparts on average a vertical velocity of 0.03 m/s per photon scattering event, corresponding to a Doppler shift of 50 kHz (Kibblewhite, 2009). For long laser pulses (or in the case of a CW laser), this can lead to a steady depletion of the population of target atoms at Doppler shifts that can interact with a given laser frequency. However, for all lidar systems that the authors are aware of, this plays a negligible role: given that typical laser linewidths are orders of magnitude larger than the imparted Doppler shift, many interactions per atom would be required for this effect to have a significant impact on the observed saturation.

The second effect that must be considered in the context of laser guide stars is the optical pumping of magnetic substates (Holzlöhner et al., 2010; Jeys et al., 1992). By employing a circularly polarized laser, which always results in a transition with a  $\pm 1$  shift in the magnetic quantum number  $m$ , sodium atoms can be optically pumped into for example, the  $j = 2, m = 2$  substate in order to exploit the relatively large line strength between that substate and the  $k = 3, m = 3$  excited state, resulting in enhanced brightness of the guide star. This phenomenon only becomes important for CW lasers or for lasers with pulse lengths much longer than the lifetime of the resonance line they excite; for all known lidar systems, its effect is negligible.

Finally, for iron lidars targeting the 374 nm line (see Section 3.2), atoms are excited from the  $j = 3$  ground state to the  $k = 4$  excited state, after which they have a non-negligible probability of relaxing into the  $j = 4$  ground state. This is another example of optical pumping, whereby the  $j = 3$  ground state is steadily depleted. In this case, the branching ratio,  $R_B$ , of the targeted relaxation pathway must be considered. Note that  $R_B = 0.9114$  for the  $k = 4$  to  $j = 3$  relaxation pathway (Chu et al., 2002). Then, Equation 16 becomes:

$$\frac{d\tilde{n}_s}{dt} = R_B \frac{\tilde{n}_{e,s}}{\tau} - (\tilde{n}_s - \tilde{n}_{e,s})f_e \quad (38)$$

and Equation 19 becomes:

$$P_i(\nu_L, \nu_v) = R_B \int_0^\infty \frac{\tilde{n}_{e,i}(\nu_v, t)}{\tau} dt \quad (39)$$

This could in principle lead to a rapid depletion of the  $j = 3$  ground state and a significant loss of signal. However, the impact of this effect on saturation would only become significant for a lidar system targeting the 374 nm line

with pulse lengths on the order of or longer than the natural lifetime of the transition. We are not aware of any such instrument.

### 3. Relevance of Saturation Effects for Modern Resonance Lidar Systems

As seen above, the severity of saturation effects depends on a wide variety of parameters: some of these are intrinsic to the target species (e.g., the natural resonance linewidth and lifetime of the excited state, the oscillator strength of the transition, the presence of fine/hyperfine structure and/or multiple naturally occurring isotopes, etc.); others are specific to each instrument (i.e., the laser frequency, pulse energy, linewidth, pulse shape, pulse length, and beam divergence); and some vary with atmospheric conditions (i.e., the height, temperature, and line-of-sight velocity of the layer and the atmospheric transmission at the laser frequency). As will be seen, for some target species, saturation effects play a relatively small role, whereas for others, saturation represents a significant challenge in instrument design. For each of the resonance lidar types below, an open-source saturation calculator has been made available at Geach (2026). This calculator can be freely adapted to incorporate instrumental effects, include the appropriate Hanle factors, or calculate saturation for a different resonance lidar target. Relevant parameters for the resonance lidar systems analyzed here are given in Table 1 (note that we only show results for the 386 nm resonance line of iron; however, calculators for the other two iron resonance lines have also been developed and can be found at Geach (2026)). The lifetime and natural linewidth of the resonance lines can be recovered from their respective Einstein coefficients  $A$  via  $\tau = \frac{1}{A}$  and  $\Delta\nu_n = \frac{A}{2\pi}$ .

To assess the impact of saturation effects on wind and temperature measurements, we define a scan pattern in frequency and perform a noiseless simulation to find  $B_s$  and  $B_{ns}$  at each of the simulated measurement frequencies. We define a fit function  $F(\nu_L, \rho, T, v_{av})$  as:

$$F(\nu_L, \rho, T, v_{av}) = \rho \int N_L(\nu_L, \nu) \sum_n p_n \sum_{j,k} \eta(\nu_b) q_j^k \sigma_{D,j}^k(\nu + \delta\nu_{av}) d\nu \quad (40)$$

where  $\delta\nu_{av} = \frac{v_{av}}{c}\nu_0$  is the Doppler shift due to the average vertical wind  $v_{av}$  and  $\rho$  is an overall amplitude (proportional to the number density of the target atoms). In analogy to Equations 11 and 23 the cross-sections  $\sigma_{D,j}^k(\nu)$  are defined as:

$$\sigma_{D,j}^k(\nu) = \int D(\nu_v) \alpha_j^k(\nu, \nu_v) d\nu_v \quad (41)$$

Note that the dependence of  $F$  on temperature is through  $\Delta\nu_D$ , which determines the width of the  $D(\nu)$  profile. We have defined Equation 40 as generally as possible, accounting for the possibility of multiple stable isotopes, fine or hyperfine structure, spectrally varying detection efficiency, and the Hanle effect. As previously stated, we assume in what follows that  $\eta(\nu) = 1$  and  $q_j^k = 1$ .

We then perform a fit of  $F(\nu_L, \rho, T, v_{av})$  to the  $B_i(\nu_L)$  obtained from our simulation, thereby obtaining estimates of  $\rho_i$ ,  $T_i$ , and  $v_{av,i}$ . We then infer biases on these fit parameters through:

$$\Delta\rho = \frac{\rho_s - \rho_{ns}}{\rho_{ns}} \quad (42)$$

$$\Delta T = T_s - T_{ns} \quad (43)$$

$$\Delta v_{av} = v_{av,s} - v_{av,ns} \quad (44)$$

The temperature and wind estimates obtained in the “no saturation” case reliably retrieve the input values of those parameters and thus can be used to quantify the bias arising from saturation. Note that the  $\rho_i$  are not estimates of the number density of the target atoms directly but are proportional to the number density, hence the fractional bias defined here is valid.

These bias estimates are based on the assumption that the laser parameters, the transmission of the atmosphere, and the effective divergence of the laser beam are constant across all measurement frequencies. If this is not the

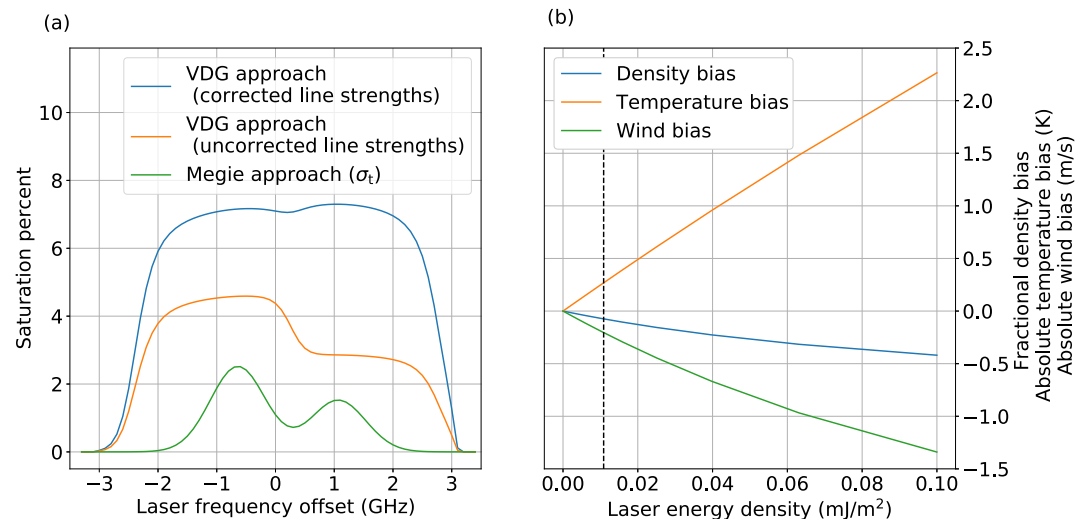


**Figure 2.** (a) Theoretical saturation percentages plotted as a function of laser frequency for the sodium  $D_2$  resonance line using the VDG approach, with both the corrected line strengths (blue curve) and uncorrected line strengths (orange curve), and using the Megie approach (green curve). Lidar system parameters are modeled after the Weber sodium lidar; see text for details. (b) Fractional density, absolute temperature, and absolute wind biases as a function of laser energy density at the sodium layer, assuming a retrieval of those parameters that neglects saturation effects. Laser bandwidth, pulse length, and the ratio between beam divergence and telescope field-of-view are the same as in (a). The dashed black line indicates the laser energy density corresponding to simulation parameters in (a).

case, for example, if the laser pulse energy is frequency dependent or the resonance line is near an absorption line of some constituent of the lower atmosphere, then the resulting biases can be substantially larger than those reported here. Even if the spectral effect itself is corrected for, it can lead to differential saturation that significantly increases the saturation-related biases. Furthermore, the bias estimates presented below assume perfect knowledge of the system parameters, which in practice is seldom realized. Uncertainties in these parameters (e.g., uncertainties about the far-field beam profile, uncertainties in the laser line shape, or unknown atmospheric seeing leading to larger effective beam divergence) lead to biases in the simulated degree of saturation that are difficult to avoid - the safest strategy is an instrumental design that avoids the saturated regime.

### 3.1. Sodium Resonance Lidars

Saturation of the sodium  $D_2$  line at 589 nm was discussed at length by VDG; the chief differences in the work presented here are (1) the correct normalization of the relative line strengths as discussed in Section 2.3, and (2) an updated method for estimating temperatures based on a three-frequency measurement technique, instead of the two-frequency technique assumed by VDG.

To assess the severity of saturation for the sodium  $D_2$  line, we calculated the spectrum of saturation using the laser parameters of the Weber sodium lidar at ALOMAR (Dunker et al., 2013), namely a pulse energy of 20 mJ, a FWHM pulse length of 6.7 ns, a FWHM laser linewidth of 130 MHz, a beam divergence of 450  $\mu$ rad, and a field-of-view of 600  $\mu$ rad. We assumed a Gaussian beam profile and (following VDG) a laser pulse shape given by:

$$N(t) = N_t t^2 e^{-at} \frac{a^3}{2} \quad (45)$$

where  $a = 3.4/t_L$ , with  $t_L$  the FWHM pulse length, and the factor of  $\frac{a^3}{2}$  is used for normalization. Finally, we assumed a sodium layer at 90 km altitude with a temperature of 200 K, and an atmospheric transmission of 70%.

The resulting saturation spectrum is shown in Figure 2a, using the corrected line strengths presented here (blue curve) and the uncorrected line strengths used in VDG (orange curve). (Note that VDG assumed a Lorentz profile for the laser beam shape, resulting in a slightly different spectrum of saturation—see Figure S1 in Supporting Information S1). The spectrum yielded by the Megie approach is shown in green. Though the degree of saturation

**Table 3**

*Isotopes (Berglund & Wieser, 2011) and Frequency Offsets for the Iron Line at 386 nm (Kaletta, 1969)*

| Isotope          | Relative abundance | Frequency shift (MHz) |
|------------------|--------------------|-----------------------|
| <sup>54</sup> Fe | 0.05854            | −743                  |
| <sup>56</sup> Fe | 0.91754            | 0                     |
| <sup>57</sup> Fe | 0.02119            | 375                   |
| <sup>58</sup> Fe | 0.00282            | 714                   |

is greater by a factor of  $\sim 1.5$  when using the corrected line strengths as compared to the uncorrected line strengths when evaluated at the peak of the sodium  $D_2$  spectrum, the degree of saturation is relatively constant for typical laser frequency offsets; thus, the resulting temperature and wind biases are small. To quantify this, we performed a three-frequency simulation at frequencies  $-1,270$  MHz,  $-640$  MHz, and  $-10$  MHz relative to the center of the sodium  $D_2$  line ( $589.1583$  nm in vacuum) as in Dunker et al. (2013) for a range of laser energy density values up to  $0.1$  mJ/m<sup>2</sup> (corresponding to a pulse energy of roughly  $130$  mJ at  $450$   $\mu$ rad beam divergence and  $90$  km altitude, neglecting atmospheric losses), otherwise keeping the same parameters as in Figure 2a. The results are shown in Figure 2b. Though the density biases

approach 30%, the temperature and wind biases remain below  $1.3$  K and  $0.9$  m/s, respectively; however, for the laser energy densities achieved by the Weber sodium lidar (dashed black line in Figure 2b, assuming an atmospheric transmission of 70%), we approximate the density, temperature, and wind biases to be less than 7%,  $0.25$  K, and  $0.2$  m/s, respectively.

Thus, though saturation effects have presumably led to a slight underestimation of sodium densities, the impacts on wind and temperature have probably not been significant (except perhaps in the case of vertical winds). This is due primarily to the relative insensitivity of the degree of saturation to chosen measurement frequencies. Additionally, many modern sodium lidar systems were designed conservatively to avoid saturation effects (Li et al., 2012; Smith & Chu, 2015), chiefly by maintaining a minimum beam divergence. Nevertheless, saturation-induced biases could become significant for future sodium lidar systems, if the trend toward larger pulse energies and smaller beam divergences continues.

### 3.2. Iron Resonance Lidars

Iron lidars have been employed since the late 1980's (Alpers et al., 1990; Granier et al., 1989), initially targeting a resonance line at  $372$  nm. In 1994, the Boltzmann lidar technique was proposed, whereby atmospheric temperature measurements are made by probing two resonance lines of iron, at  $372$  and  $374$  nm (Gelbwachs, 1994); this technique was subsequently implemented in 1999 (Chu et al., 2002). In 2004, the first Doppler measurements by an iron resonance lidar were made (Lautenbach & Höffner, 2004), this time at  $386$  nm, using a narrow-band frequency-doubled alexandrite laser. Later, this design was further refined to enable daylight measurements via a reduction in the instrument's field of view (and a corresponding reduction in the laser beam divergence) (Höffner & Lautenbach, 2009). Iron was identified as a suitable target for daylight measurements on the basis of its apparent insensitivity to saturation effects.

Naturally occurring iron is made up of 4 stable isotopes, with the abundances and associated frequency shifts given in Table 3 (note that the listed frequency shifts are valid only for the resonance line at  $386$  nm; the resonance lines at  $372$  and  $374$  nm have their own set of isotope frequency shifts). The other relevant resonance line parameters are given in Table 1.

We calculated the spectrum of saturation for an instrument modeled after the one described in Lautenbach and Höffner (2004), with a laser pulse energy of  $85$  mJ, a FWHM laser linewidth of  $12$  MHz, a beam divergence of  $130$   $\mu$ rad, and a field-of-view of  $200$   $\mu$ rad. We assumed a pulse length of  $250$  ns, an iron layer at an altitude of  $90$  km and a temperature of  $200$  K, and an atmospheric transmission of 50%. We calculated the expected saturation in the case of a laser with a line shape represented by a Lorentz profile (orange curve in Figure 3a) or by a Gaussian profile (blue curve), and compare both of these to the result expected from the Megie approach (green curve). Note that this resonance line has no hyperfine structure, so there is no question of "corrected" or "uncorrected" line strengths. Regardless of the laser line shape, the expected degree of saturation is significantly larger than the Megie approach suggests. The maximum saturation is approximately 70% more severe in the case of a Gaussian profile, due to the fact that there is more power in the "wings" of a Lorentz profile compared to a Gaussian profile, resulting in a lower energy concentration in frequency space. This highlights the importance of an accurate characterization of the laser line shape, as simplified metrics such as the FWHM linewidth do not describe the line shape with sufficient precision for the purposes of estimating saturation. Note that a similar sensitivity to the laser line shape exists for sodium and helium lidars; see Figures S1 and S2 in Supporting Information S1, respectively.

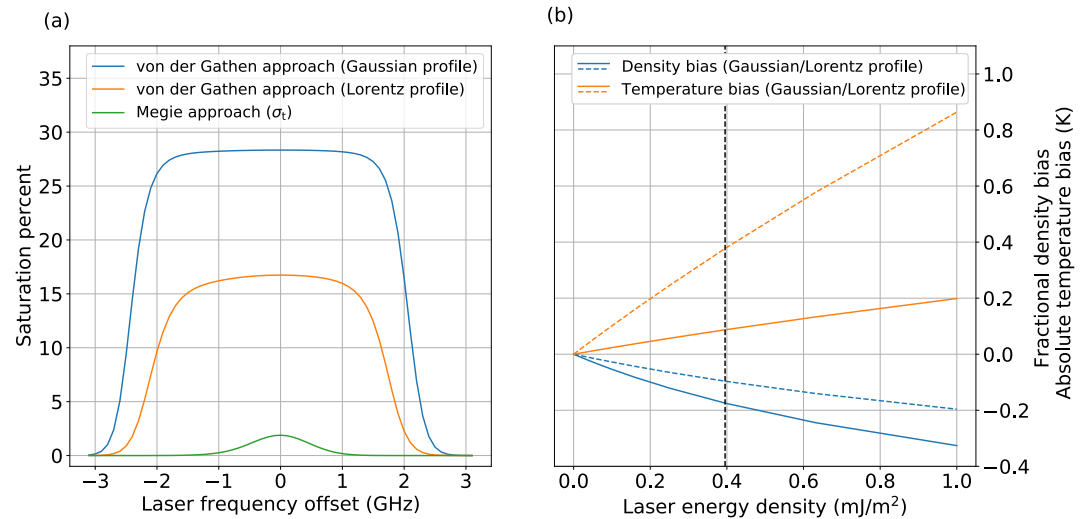


**Figure 3.** (a) Theoretical saturation percentages plotted as a function of laser frequency for the 386 nm resonance line of iron using the Megie approach (green curve) and the von der Gathen approach, assuming for the latter either a Lorentz profile for the laser line shape (orange curve) or a Gaussian profile (blue curve). Lidar system parameters are modeled after the iron lidar described in Lautenbach and Höffner (2004); see text for details. (b) Fractional density and absolute temperature biases as a function of laser energy density at the iron layer, assuming a retrieval of those parameters that neglects saturation effects. Lidar system parameters other than laser pulse energy are the same as in (a). The dashed black line indicates the laser energy density corresponding to simulation parameters in (a).

Despite the expected severity of saturation effects in this case, the resulting biases on wind and temperature are small. We simulated a scan of 16 measurement frequencies across a range of  $\pm 320$  MHz around the central frequency of the 386 nm resonance line, using the parameters outlined above, but for a range of laser energy densities up to  $1 \text{ mJ/m}^2$  (corresponding to a pulse energy of roughly 110 mJ at  $130 \text{ } \mu\text{rad}$  at 90 km, neglecting atmospheric losses), otherwise keeping the same parameters as in Figure 3a. The resulting temperature biases (orange curves) and density biases (blue curves) are shown in Figure 3b, again assuming both a Lorentz profile (dashed lines) and a Gaussian profile (solid lines), with the dashed black line showing the energy density used in the simulation in Figure 3a. Though a Gaussian line shape results in a greater degree of saturation than a Lorentzian line shape for a given FWHM laser linewidth, the associated temperature biases are appreciably smaller, since the spectrum of saturation for a Gaussian line shape is flatter across the range of probed frequencies. In all cases, the temperature biases are less than 1 K, and the wind biases (not shown) were less than  $0.0002 \text{ m/s}$ .

### 3.3. Helium Resonance Lidars

The resonance lidar technique was recently extended to metastable helium (Kaifler et al., 2022), which exists in a broad layer between altitudes of 250 and 1,000+ km. Since then, the first Doppler measurements of the metastable helium spectrum have been made (Kaifler & Geach, 2024) and the density measurements have been extended to an altitude of 1,000 km (Geach & Kaifler, 2025; Zhao et al., 2024). The question of saturation of the helium layer was addressed by Zhao et al. (2024), but the Megie approach was used.

Helium resonance lidars to date have targeted the 1,083 nm resonance line between the  $2^3\text{S}$  and  $2^3\text{P}$  states (there are additional transitions to the  $3^3\text{P}$  and  $4^3\text{P}$  states, but the associated cross-sections are appreciably weaker). The

resonance line at 1,083 nm is a triplet, but the strongest two lines of the triplet overlap at atmospheric temperatures; the third line is separated by almost 32 GHz and so can be ignored. The frequency offsets and multiplet strengths for the resonance line are given in Table 4; the other relevant parameters are given in Table 1.

We calculated the spectrum of saturation for an instrument modeled after the one presented in Kaifler and Geach (2024). We assume a pulse energy of 4.7 mJ, a pulse length of 200 ns, and a field-of-view of  $61 \text{ } \mu\text{rad}$ . The laser

**Table 4**  
Frequency Offsets and Line Strengths  $g_j^k$  for the Helium Line at 1,083 nm

| $2^3\text{S}$ | $2^3\text{P}$ | $\Delta\nu_j^k$ (GHz) | $g_j^k$ |
|---------------|---------------|-----------------------|---------|
| $j = 1$       | $k = 0$       | 31.9045               | 1       |
|               | $k = 1$       | 2.2911                | 3       |
|               | $k = 2$       | 0                     | 5       |

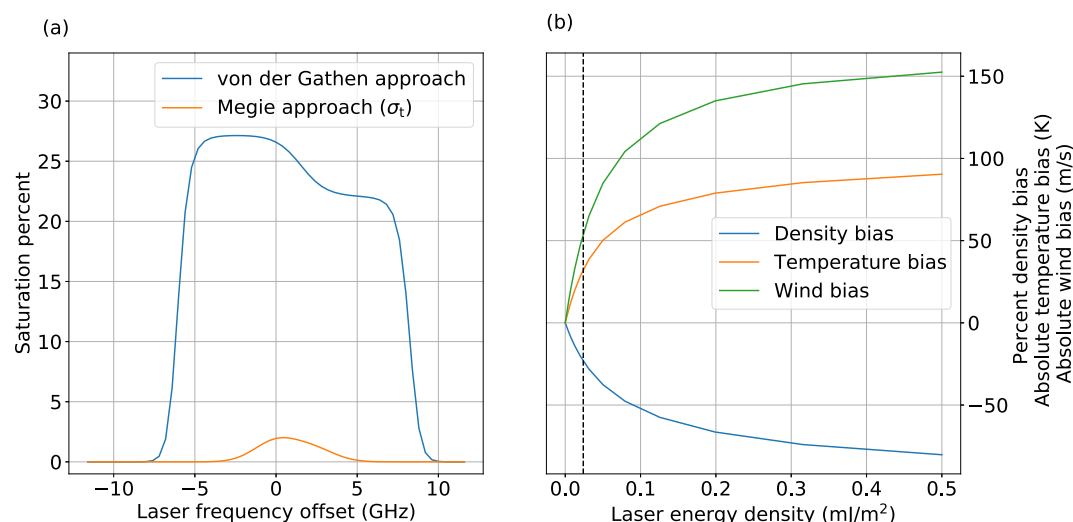


**Figure 4.** (a) Theoretical saturation percentages plotted as a function of laser frequency for the 1,083 nm resonance line of helium using the Megie approach (orange curve) and the von der Gathen approach (blue curve). Lidar system parameters are modeled after the helium lidar described in Kaifler and Geach (2024); see text for details. (b) Density, temperature, and wind biases as a function of laser energy density at the helium layer, assuming a retrieval of those parameters that neglects saturation effects. Lidar system parameters other than laser pulse energy are the same as in (a). Note that the density biases are plotted as percentages, in contrast to Figures 2 and 3. The dashed black line indicates the laser energy density corresponding to simulation parameters in (a).

linewidth was estimated in Kaifler et al. (2022) to be less than 500 MHz; this estimate was conservative, and we assume a value of 20 MHz here. The divergence of the laser beam was assumed to be 30  $\mu$ rad. We assume a Gaussian profile for the laser line shape, a helium layer at 500 km with a temperature of 1,000 K, and an atmospheric transmission of 90%. The resulting spectra of saturation are shown in Figure 4a, with the results following the VDG approach in blue and the results of the Megie approach in orange. The helium resonance line has no hyperfine structure, so no comparison of “corrected” and “uncorrected” line strengths can be made. Again, substantial differences are apparent, with the results of the VDG approach suggesting that the densities reported in Geach and Kaifler (2025) may have been underestimated by 30% or more.

Furthermore, the saturation spectrum shows significant frequency dependence, implying a substantial saturation-related bias on inferred winds and temperatures. We performed a four-frequency simulation at the measurement frequencies used in Kaifler and Geach (2024) (−3.58 GHz, 0 GHz, 2.04 GHz, and 3.32 GHz relative to the  $k = 2$  transition frequency) using the parameters outlined above, but for a range of laser energy densities up to 0.5 mJ (corresponding to a pulse energy of roughly 90 mJ at 30  $\mu$ rad beam divergence and 500 km altitude, neglecting atmospheric losses), otherwise keeping the same parameters as in Figure 4a. The resulting density biases (blue curve), temperature biases (orange curve) and wind biases (green curve) are shown in Figure 4b. In this case, substantial temperature and wind biases are expected: even for the relative modest pulse energy of 4.7 mJ used in Kaifler and Geach (2024) (dashed black line in Figure 4b, assuming an atmospheric transmission of 70%), biases of 35 K and 60 m/s in the measured temperature and wind, respectively, are possible.

Note that the instrument presented in Zhao et al. (2024) employed pulse energies of 70 mJ, appreciably higher than those used in Kaifler et al. (2022) and Geach and Kaifler (2025). This presumably led to significantly more severe saturation effects for those measurements and could account for the lower metastable helium densities measured in that work.

#### 4. Discussion

As has been demonstrated, it is likely that many modern resonance lidar systems have been affected by saturation effects to a larger degree than previously thought, though the degree to which each instrument has been affected depends strongly on the respective instrument parameters and target. For sodium and iron resonance lidar systems, the impact of these saturation effects on wind and temperature measurements is probably not significant for

typical instrument parameters; nevertheless, making measurements in the saturated regime opens the door for potential systematic biases if the performance of the instrument or the conditions of the atmosphere are not stable for the entirety of a measurement scan.

For helium resonance lidars, the necessity of this approach is more acute. Not only does saturation set in at relatively low energy densities, but the impact on wind and temperature measurements is substantially larger for a given degree of saturation than for sodium or iron systems. This is due in part to the small laser beam divergences used and in part to the peculiarities of the helium transition: the long lifetime of the excited state and correspondingly narrow bandwidth of the absorption line. Meaningful restraints on wind and temperature will require further increases to the laser pulse energies used; these increases must be offset by increases in the laser linewidth, pulse length, or beam divergence in order to avoid saturation.

Although care has been taken here to incorporate all relevant effects and to produce the most accurate prediction possible for the expected degree of saturation, relying on such calculations to account for the effects of saturation to correct the resulting wind and temperature biases is not advisable. The calculations depend sensitively on parameters that are typically only imprecisely characterized, such as the pulse-to-pulse line shape of the laser or the beam divergence. Changing atmospheric conditions, either through variable atmospheric transmission or variable atmospheric seeing (which changes the effective divergence of the laser beam) can also have a significant impact on the degree of saturation. Therefore, correcting for the effects of saturation will bring its own set of potentially large uncertainties. A safer approach would be to design lidar systems to avoid entering the saturated regime.

## 5. Summary and Conclusion

Since the introduction of the atmospheric resonance lidar technique, there has been a trend toward higher laser pulse energies, narrower laser linewidths, and smaller beam divergences. Together, these factors have enabled measurements of atmospheric parameters with increasing precision and provided a wealth of insight into the dynamics of the middle and upper atmosphere. However, this evolution has also lead to increasing spatial, spectral, and temporal energy concentrations, resulting in nonlinear behavior during the scattering process.

In order to design lidar systems for which saturation effects are minimal, these effects must be accurately simulated. Though a sophisticated approach to calculating the expected degree of saturation for sodium resonance lidar systems was published over 30 years ago by VDG, this approach has not been extended to other resonance lidar targets (furthermore, as discussed in Section 2.3, VDG contains a miscalculation of the individual line strengths of the hyperfine structure of the sodium D<sub>2</sub> resonance line). As a result, the overly simplified approach by Megie et al. (1978) continues to be used, resulting in significant underestimations of the severity of saturation effects. The approach presented here, which extends the work of VDG, can be applied to analyze the performance of current resonance lidar systems or to the design of future systems to minimize saturation-related biases on the resulting measurements. The code for each of the saturation calculators discussed here is available at Geach (2026) and may be freely used or adapted.

## Conflict of Interest

The authors declare no conflicts of interest relevant to this study.

## Availability Statement

The code for the saturation calculators used here have been made publicly available (Geach, 2026).

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