

Article

# Accuracy and Validity Range of a Simplified Lorentzian Approximation for Pressure-Broadened $^{87}\text{Rb}$ Hyperfine Spectra

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## Abstract

Reliable modeling of pressure-broadened spectra is essential for maintaining physical consistency in alkali vapor-cell diagnostics. In this work, we investigate the low-power absorption spectra of isotopically enriched  $^{87}\text{Rb}$  vapor cells at the  $D_1$  and  $D_2$  transitions, systematically comparing three fitting algorithms: single Lorentzian, hyperfine-resolved Voigt, and the doublet Lorentzian approximation. Experiments were performed across optical intensities from 40 nW to 10 mW, buffer-gas pressures from 200 Torr to 520 Torr, and temperatures between 370 K and 390 K. It is shown that when the pressure broadening dominates over Doppler broadening and the optical intensity remains below the saturation regime, the reduced doublet Lorentzian model achieves a fitting accuracy of  $R^2 > 0.996$ . Under the pressure conditions of 350 Torr, the fitting error for both the doublet and Voigt approximations remains below 0.3 % for the  $D_2$  line and below 0.1 % for the  $D_1$  line. At the pressures of 520 Torr and under elevated optical intensities, the spectrum evolves toward a single-peaked profile, rendering a single Lorentzian model sufficient. The quantitative applicability boundary of the doublet approximation in  $^{87}\text{Rb}$  vapor cells is established, defining the operational regime where hyperfine-resolved modeling can be reduced under collision-dominated conditions in NMRG systems.

**Keywords:** absorption spectroscopy; pressure broadening; doublet Lorentzian approximation;  $^{87}\text{Rb}$  vapor cell; nuclear magnetic resonance gyroscope (NMRG)

## 1. Introduction

Spin-polarized state preparation and readout of alkali–noble hybrid ensembles in micro-fabricated vapor cells are central to quantum inertial sensing [1,2]. By probing atomic-ensemble information, micro-quantum systems with navigation-grade performance can be realized [3,4]. Typical systems comprise a vapor cell, an optical pumping module, a spin manipulation unit, and a quantum-state detection module [5]. The core component is a heated alkali vapor cell (typically K or Rb) containing buffer or quench gases that confine noble gas nuclei ( $^3\text{He}$ ,  $^{129}\text{Xe}$ ,  $^{131}\text{Xe}$ ) [6–8]. The alkali–noble number–density ratio determines the optical depth, nuclear spin-relaxation time, and achievable polarization, thereby directly influencing sensor sensitivity [9]. As the central sensing element, the vapor cell defines both the number of polarized atoms and their spin coherence time  $T_2$  [10–12], ultimately limiting rotation-rate resolution in atomic gyroscopes [13–15].

Alkali-metal vapor cells also form the core of nuclear magnetic resonance gyroscopes (NMRG) [16,17], spin-exchange relaxation-free (SERF) gyroscopes [18,19], and MEMS-based magnetometers [3]. The internal temperature controls alkali vapor density, which is



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essential for efficient spin-exchange optical pumping [20]. Accurate density determination is therefore critical [21]. Previous studies have investigated alkali-density optimization [22], spin-exchange characterization [23], and the interdependence of optical power, atomic density, and gas pressure, which remain key operational parameters in quantum inertial sensing.

Several spectroscopic techniques have been employed to determine alkali density and gas pressure, including pressure-broadening spectroscopy, Faraday rotation, magnetic-resonance linewidth analysis, and absorption spectroscopy. Raghavan et al. demonstrated temperature-controlled miniaturized magnetometers [24], while other studies proposed theoretical and experimental models with varying levels of generality [25]. Shang et al. introduced an impact-asymmetry-based modification of near-wing Lorentzian profiles [26], and Peng et al. analyzed mixed-gas vapor cells considering multiple broadening mechanisms [27,28]. Recent experimental work has explored enhanced absorption features and frequency stabilization techniques in Rb vapor cells, including bright-state spectroscopy to improve laser frequency locking via narrow hyperfine absorption signals [29]. In 2024, R.C. Das et al. investigated the narrow-line Rb spectroscopy under varying temperature and beam parameters, revealing complex linewidth dependencies relevant to precision spectral modeling [30].

Although these works provide a comprehensive description of alkali absorption spectra under combined broadening mechanisms, many approaches rely on fully hyperfine-resolved Voigt-type models or system-specific assumptions, which increase computational complexity and limit practical applicability. In particular, the experimental conditions under which the combined broadening effects permit a reduction to a simplified hyperfine-structure doublet Lorentzian description remain insufficiently quantified. This motivates the present work, which systematically evaluates the validity range, accuracy, and computational efficiency of the doublet Lorentzian approximation.

## 2. Principle and Method

The absorption spectra of freely moving alkali atoms are governed by natural broadening, pressure broadening, and Doppler broadening [31]. In practical vapor cells, these mechanisms act simultaneously, leading to significant broadening and overlap of hyperfine components. As a result, the choice of spectral model must balance physical fidelity against computational complexity. Transitions between hyperfine levels form the fundamental basis for atomic number-density determination and non-contact temperature measurement [32–34]. In this section, three spectral fitting strategies employed in this work are introduced, and their respective applicability and validity regimes are defined.

In the experiments, the laser is tuned near the  $^{87}\text{Rb}$   $D_2$  resonance (and similarly for the  $D_1$  line) and scanned across several tens of gigahertz while the transmitted optical power is recorded. The vapor cell is filled with  $\text{N}_2$  as a quenching and buffer gas to suppress radiation trapping and to reduce diffusion-induced relaxation.

The optical depth ( $OD$ ) is defined as

$$OD = n\sigma(\nu)l, \quad (1)$$

where  $n$  is the  $^{87}\text{Rb}$  number density and  $l$  is the optical path length. The absorption cross section satisfies the frequency-integral relation

$$\int_0^{+\infty} \sigma(\nu) d\nu = \pi r_{ef}, \quad (2)$$

where  $r_e$  is the classical electron radius and  $f$  is the oscillator strength (for the D<sub>2</sub> line,  $f \approx 2/3$ ).

### 2.1. Method I: Single Lorentzian Model

When pressure broadening dominates and the hyperfine structure is completely unresolved, the absorption profile can be approximated by a single Lorentzian function,

$$\sigma_L(\nu) = \pi r_e c f \frac{\Gamma_L/2\pi}{(\nu - \nu_0)^2 + (\Gamma_L/2)^2}, \quad (3)$$

where  $\Gamma_L$  denotes the full width at half maximum (FWHM). The optical depth is obtained from the measured transmission according to

$$OD = -\ln\left(\frac{I_{\text{out}}}{I_{\text{in}}}\right) = n\sigma_L(\nu)l. \quad (4)$$

This model provides the simplest physically consistent description and is applicable when the measured spectrum collapses into an effectively single-peaked profile.

### 2.2. Method II: Hyperfine-Resolved Voigt Convolution Model

OD characterizes the attenuation of light propagating through an alkali-metal vapor cell [26]. When Doppler broadening becomes non-negligible, each hyperfine component must be described by a convolution of the Lorentzian and Gaussian contributions.

Figure 1 illustrates the hyperfine structures of the D<sub>1</sub> and D<sub>2</sub> transitions, and Table 1 summarizes the corresponding relative transition strengths. The hyperfine-resolved absorption cross section can then be written as a Voigt sum,

$$\sigma_{\text{HF}}(\nu) = \pi r_e c f \sum_{F,F'} A_{F,F'} V(\nu - \nu_{F,F'}; \Gamma_L, \Gamma_G), \quad (5)$$

where  $A_{F,F'}$  and  $\nu_{F,F'}$  denote the relative strength and resonance frequency of each hyperfine transition, respectively, and  $V(\cdot)$  represents the Voigt profile obtained by convolving a Lorentzian of width  $\Gamma_L$  with a Gaussian of Doppler width  $\Gamma_G$ . Six hyperfine transitions are included for the D<sub>2</sub> line and four for the D<sub>1</sub> line. This method provides the highest physical completeness but requires increased computational effort due to convolution and the larger number of fitting parameters.

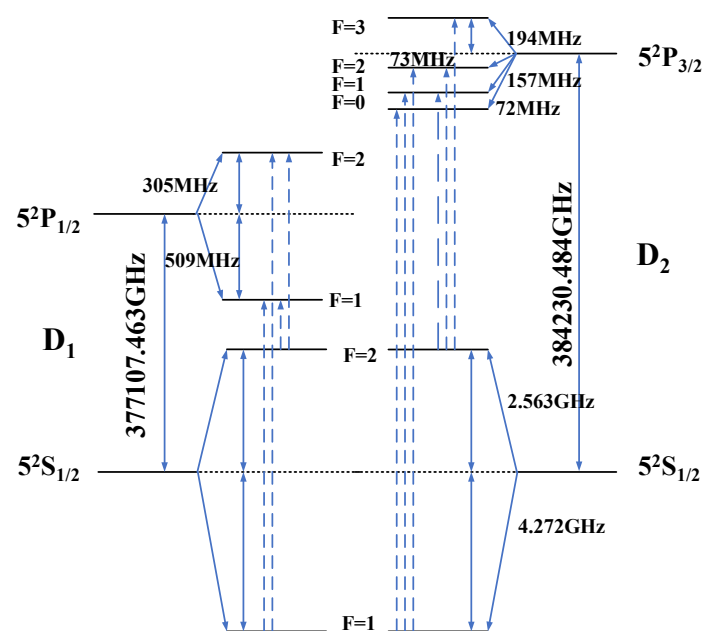
**Table 1.** Relative transition strengths of the hyperfine components of the <sup>87</sup>Rb D<sub>1</sub> and D<sub>2</sub> lines [14].

| Line           | Transition Number | Relative Strengths |
|----------------|-------------------|--------------------|
| D <sub>1</sub> | A <sub>11</sub>   | 0.0625             |
|                | A <sub>12</sub>   | 0.3125             |
|                | A <sub>21</sub>   | 0.3125             |
|                | A <sub>22</sub>   | 0.3125             |
| D <sub>2</sub> | B <sub>10</sub>   | 0.1667             |
|                | B <sub>11</sub>   | 0.4167             |
|                | B <sub>12</sub>   | 0.4167             |
|                | B <sub>21</sub>   | 0.0500             |
|                | B <sub>22</sub>   | 0.2500             |
|                | B <sub>23</sub>   | 0.7000             |

### 2.3. Method III: Doublet Lorentzian Approximation

As shown in Figure 1, the ground-state hyperfine splitting of <sup>87</sup>Rb between  $F = 1$  and  $F = 2$  is 6.835 GHz, whereas the excited-state hyperfine splittings are on the order of

several hundred MHz. In vapor-cell experiments where collisional broadening dominates and the linewidth approaches the GHz level, the excited-state hyperfine components are not spectrally resolved, and transitions originating from the same ground-state level strongly overlap. In this regime, the transitions sharing the same ground-state  $F$  can be grouped into an effective composite resonance, with line strengths obtained by summing the corresponding transition strengths in Table 1 (noting that saturation may modify these weights at higher optical powers). Accordingly, the full hyperfine-resolved Voigt model (Equation (5)) can be reduced to a two-frequency Lorentzian doublet approximation (Equation (6)) representing the  $F = 1$  and  $F = 2$  manifolds. This reduction preserves the dominant spectral structure while lowering computational cost and improving fitting stability. The approximation is generally more effective for the  $D_2$  line due to its relatively smaller excited-state splittings, whereas for the  $D_1$  line, it is mainly validated in the low-power regime to maintain accuracy.



**Figure 1.** Hyperfine structures of the  $^{87}\text{Rb}$  energy level transitions. Four and six hyperfine transitions are labeled according to the selection rules in  $D_1$  and  $D_2$  lines, respectively.

The absorption spectrum can be approximated by a reduced doublet Lorentzian model,

$$OD(\nu) = H \left[ A_\alpha \frac{\Gamma_L/2\pi}{(\nu - \nu_\alpha - \delta)^2 + (\Gamma_L/2)^2} + A_\beta \frac{\Gamma_L/2\pi}{(\nu - \nu_\beta - \delta)^2 + (\Gamma_L/2)^2} \right] + \Delta, \quad (6)$$

where  $A_\alpha$  and  $A_\beta$  represent the aggregated contributions of the unresolved hyperfine transitions within each ground-state manifold.  $A_\alpha + A_\beta = 1$ ,  $\nu_\alpha$  and  $\nu_\beta$  are effective resonance frequencies,  $\Gamma_L$  denotes the collisional linewidth,  $\delta$  is the pressure-induced frequency shift treated as a global fitting parameter common to both components, and  $\Delta$  accounts for a background offset. The fitting parameters  $(H, \Gamma_L, \delta)$  are obtained through nonlinear least-squares fitting.

From Equations (1) and (2), the amplitude coefficient  $H$  is directly proportional to the alkali-metal number density,

$$H = n\pi l r_{ef}, \quad (7)$$

which enables extraction of  $n$  from the fitted spectrum. The parameters  $\Gamma_L$  and  $\delta$  provide physically meaningful descriptors of collisional broadening and pressure-induced fre-

quency shifts. Under the impact approximation, these quantities are commonly expressed as additive contributions from individual buffer-gas species,

$$\Gamma_L(T) = \sum_i \gamma_i(T) p_i, \quad \delta(T) = \sum_i \kappa_i(T) p_i, \quad (8)$$

where  $p_i$  is the partial pressure of species  $i$ , and  $\gamma_i(T)$  and  $\kappa_i(T)$  denote the corresponding pressure-broadening and pressure-shift coefficients [20]. In the present work, these relations are used to ensure physical consistency of the fitted linewidths and shifts across operating conditions, rather than to perform an independent absolute calibration of  $p_i$ .

Finally, once the number density  $n$  is determined, the vapor temperature can be inferred from the saturated vapor-pressure relation,

$$\log_{10} \left( 5.1135148 \times 10^{-16} n T \right) = 4.321 - \frac{4040}{T}. \quad (9)$$

The fitting accuracy is evaluated using the coefficient of determination  $R^2$ , defined as

$$R^2 = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}, \quad (10)$$

where  $y_i$  are the measured data,  $\hat{y}_i$  are the fitted values, and  $\bar{y}$  is the mean of the measured data.

In summary, Method I is applicable when the spectrum reduces to a single pressure-broadened peak, Method II offers the most physically complete description when Doppler or saturation-related effects become significant, and Method III provides a computationally efficient approximation with explicitly defined validity limits.

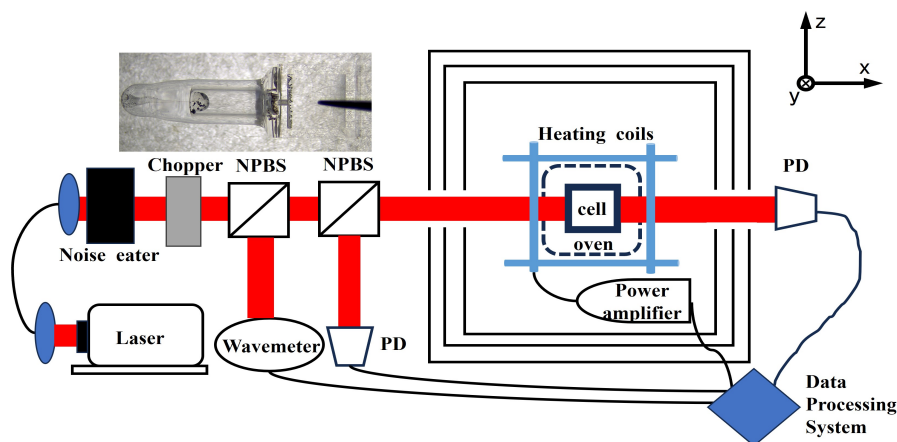
### 3. Experimental Setup

The experimental setup is shown in Figure 2. A distributed-feedback (DFB) laser operating at 780 nm is used to probe the  $^{87}\text{Rb}$  D<sub>2</sub> transition, with a tuning range of  $\pm 0.5$  nm controlled by the injection current and laser temperature [35]. A second laser source at 795 nm is employed for measurements on the D<sub>1</sub> transition. The output optical power is actively stabilized using a commercial noise eater. The laser linewidth is approximately 20 MHz, which is sufficiently narrow compared with the pressure-broadened linewidths investigated in this work and therefore does not limit spectral resolution.

The output beam is expanded to form a circular beam with a diameter of approximately 2.5 mm. It is then split by a non-polarizing beam splitter (NPBS). One fiber-coupled arm is directed to a wavemeter for real-time frequency monitoring, while the other arm passes through an additional beam splitter for incident optical power monitoring before entering the  $^{87}\text{Rb}$  vapor cell. The transmitted optical power is detected using a photodetector. By scanning the laser frequency and recording the transmitted optical power, absorption spectra are obtained. The optical depth is subsequently calculated from the ratio of transmitted to incident optical power and used for spectral fitting. As shown in the inset of Figure 2, the alkali vapor cell is cubic with an inner length of 3 mm and includes a stem, which has been shown to influence the nuclear spin coherence and the NMRG performance [19].

Each vapor cell contains isotopically enriched  $^{87}\text{Rb}$ , together with fixed noble-gas fillings of 2 Torr  $^{129}\text{Xe}$  and 8 Torr  $^{131}\text{Xe}$ . Additional buffer gas is introduced with the gas pressures of 200, 350, and 520 Torr. When the laser frequency is tuned near the Rb resonance, alkali-metal electrons absorb incident photons, resulting in optical transitions and spin polarization. Increasing the cell temperature enhances the saturated vapor density of Rb atoms and consequently increases the optical absorption. The above configuration enables systematic investigation of pressure- and power-dependent spectral broadening

under well-defined gas compositions and operating conditions. The extracted optical-depth spectra serve as the basis for applying the three fitting strategies described in Section 2, allowing quantitative comparison of their validity regimes.



**Figure 2.** Schematic diagram of the experimental setup. A photograph of the alkali-metal vapor cell is shown in the upper-left corner.

#### 4. Results and Discussions

Based on the experimental configuration described above, the transmitted absorption spectra of  $^{87}\text{Rb}$  vapor cells are analyzed using the three fitting strategies introduced in Section 2. Focusing on the  $D_2$  line near 780 nm and the  $D_1$  line near 795 nm, the hyperfine structures are considered to determine the number density of  $^{87}\text{Rb}$  and to evaluate collisional effects associated with buffer gases.

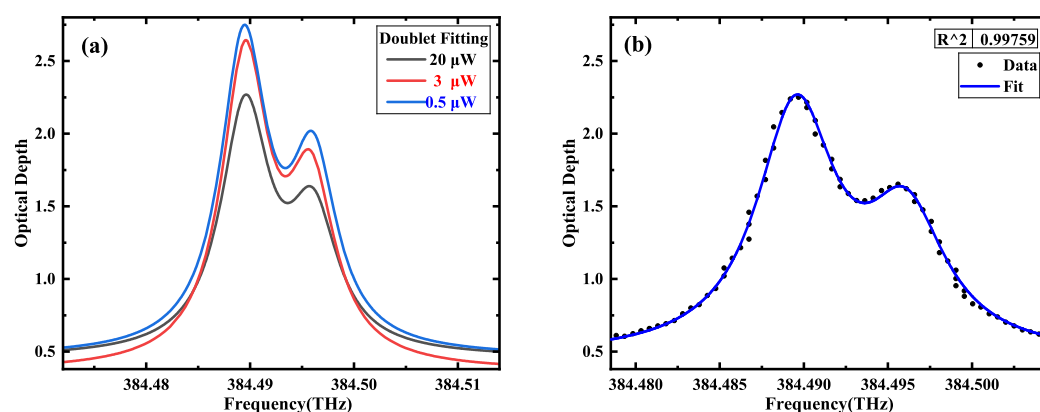
From the systematic comparison of spectra acquired under different pressures and optical powers, our investigation indicates that the doublet approximation is valid when pressure broadening clearly dominates over Doppler broadening, which is typical with buffer-gas pressures above approximately 200 Torr within the temperature range of 370–390 K. Under saturated vapor-pressure conditions typical of alkali vapor cells, multiple broadening mechanisms coexist.

The influences of optical power and gas pressure on hyperfine resolvability and fitting accuracy cannot be neglected. Under typical NMRG operation, the gas pressure (300 Torr) and the optical power (approximately 1 mW), computational complexity can be significantly reduced while maintaining high-fidelity fitting results. This approach is applicable to both  $D_1$  and  $D_2$  transitions. The alkali vapor cell was heated to approximately 373 K, allowing saturated vapor to accumulate inside the cubic millimeter-scale cell. The measured optical depth was plotted as a function of the output frequency  $\nu$  of the wavelength meter. Linearly polarized light and circularly polarized light were applied for comparison. When measured under microwatt-level optical power, distinct double peaks with resolvable maxima and overlapping lower parts are observed. In contrast, measurements under milliwatt-level optical power yield more asymmetric profiles that gradually evolve toward an effectively single-peaked structure. This behavior is consistent with the combined influence of power broadening and collisional broadening, which reduces hyperfine resolvability.

Figure 3a presents the doublet Lorentzian approximation fitting results of the  $D_2$  absorption spectra measured at different optical powers. Figure 3b shows the corresponding experimental data together with the fitted curve at 20  $\mu\text{W}$ , highlighting the fitting accuracy as well as the detailed agreement in both the peak and wing regions. The simplified model remains valid up to approximately 7 mW, with  $R^2$  values consistently above 0.996. This

indicates that, within this regime, saturation and Doppler contributions remain sufficiently weak for the doublet approximation to provide accurate fitting.

It is important to emphasize the practical trade-off between fitting fidelity and measurement noise. At very low probe powers (below the milliwatt level), the optical density (OD) signal becomes increasingly sensitive to ambient light fluctuations and electronic noise, which may result in scattered data points and irregular deviations in the spectral wings. As shown in Figure 3a, the red curve measured at 3  $\mu\text{W}$  deviates slightly from the other two fitting curves in the near-wing region. The off-resonant baseline variation can be attributed to several experimental factors, including mechanical vibrations of the optical platform, temperature fluctuations, variations in ambient light, and slight misalignment of the optical path. At lower optical powers, the signal amplitude decreases while the noise level remains comparable, leading to a reduced signal-to-noise ratio. As a result, the off-resonant baseline becomes more sensitive to environmental and electronic fluctuations, which can cause apparent distortions in the spectral wings. Similarly, the random fitting deviations observed in Figure 3b are also associated with these practical disturbances.



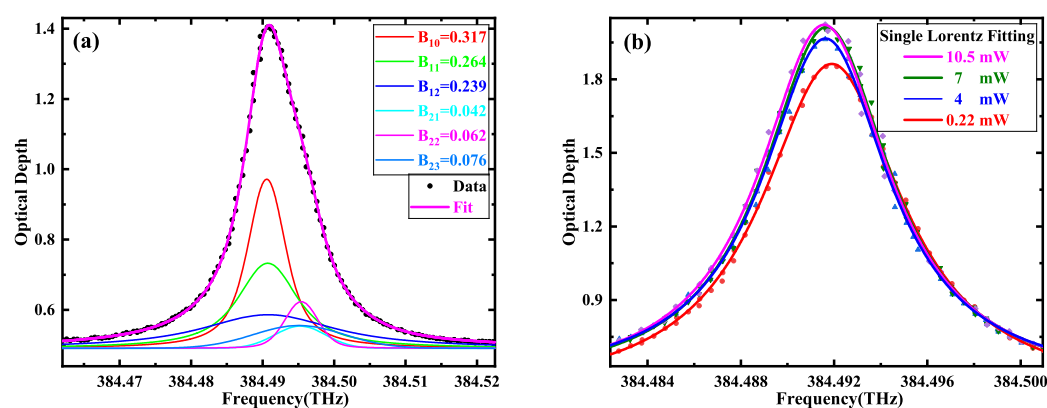
**Figure 3.** Doublet Lorentzian fitting of the D<sub>2</sub> absorption spectra acquired at 350 Torr and 383 K: (a) fitted spectra under different optical powers; (b) experimental data at 20  $\mu\text{W}$  together with the corresponding fitting curve, which is identical to the black curve shown in (a).

This behavior does not indicate the presence of additional physical resonances or a breakdown of the fitting model; rather, it reflects the reduced signal-to-noise ratio under ultra-low optical power conditions. In such cases, advanced modulation and lock-in detection can improve data quality, but the baseline configuration used here intentionally remains simple to demonstrate that the fitting strategy retains robustness under minimal experimental complexity. As shown by the consistently high  $R^2$  values in the low-power regime, the doublet Lorentzian fitting can still provide stable parameter extraction even when small local fluctuations are present.

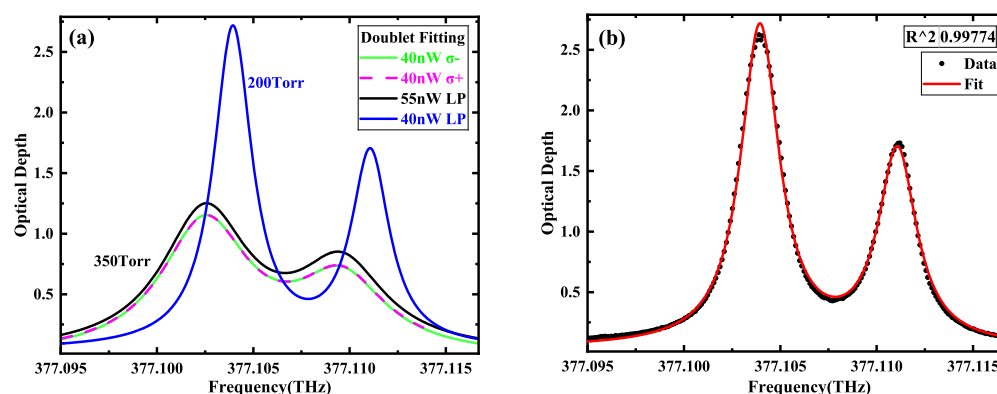
As the optical power increases toward the 10 mW level, the doublet fitting accuracy decreases to approximately 0.994. In this regime, power broadening and partial saturation modify the relative transition strengths of hyperfine components, and Voigt fitting becomes more appropriate, as shown in Figure 4a. The hyperfine components shown in Figure 1 correspond to the transition strengths listed in Table 1 under unsaturated conditions. At higher powers, deviations from these theoretical ratios are observed experimentally. With increasing gas pressure, collisional broadening dominates over Doppler broadening, and hyperfine components merge into a single broadened peak. Saturation effects simultaneously modify the relative intensity ratios of hyperfine transitions, rendering the fixed ratios in Table 1 strictly valid only in the low-power regime.

The laser source was replaced with a 795 nm laser, while the remaining optical configuration was kept unchanged. The laser beam was coupled into the original optical path

through an optical fiber. Vapor cells filled with buffer-gas pressures of 200 Torr and 350 Torr were used, and the  $D_1$  absorption spectra were measured at a temperature of 373 K. The experimental results are shown in Figure 4. Figure 4a shows the  $D_1$  absorption spectra obtained using right-handed circularly polarized light, left-handed circularly polarized light, and linearly polarized light at different optical powers. The corresponding doublet Lorentzian fitting curves are plotted in the same figure. At an optical power of 40 nW, the absorption spectra measured with left- and right-handed circular polarization nearly overlap. This observation indicates good repeatability of the optical alignment and suggests that the polarization handedness has a negligible influence on the  $D_1$  absorption spectra under the present experimental conditions. For linearly polarized light, increasing the optical power from 40 nW to 55 nW does not lead to a noticeable change in the overall spectral profile. The spectral wings remain highly consistent, and the central frequencies show only minor variations, indicating that the spectral shape is weakly dependent on optical power within this range. Figure 5b presents the raw experimental data points of the  $D_1$  absorption line measured at a buffer-gas pressure of 200 Torr and an optical power of 40 nW, together with the corresponding doublet Lorentzian fitting results.



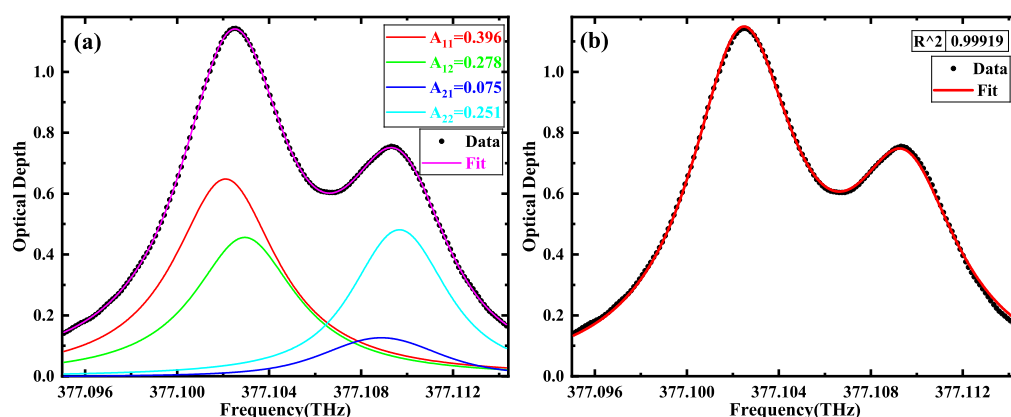
**Figure 4.** Voigt and single Lorentzian fitting of the  $^{87}\text{Rb}$   $D_2$  absorption spectra acquired using the same vapor cell at 520 Torr and 373 K. (a) Voigt fitting of the experimental data (black points) measured at an optical power of 0.5 mW, where the magenta curve represents the overall Voigt fit and the additional six curves illustrate the individual contributions of the  $D_2$  hyperfine transitions shown in Figure 1. (b) Single Lorentzian fitting of absorption spectra measured at optical powers of 0.22 mW, 4 mW, 7 mW, and 10.5 mW. The transition labels ( $B_{10}$ ,  $B_{11}$ , etc.) correspond to those listed in Figure 1 and Table 1, with effective relative strengths adjusted from the tabulated values to account for experimental conditions.



**Figure 5.** Doublet fitting of the  $D_1$  absorption spectra acquired at 373 K: (a) fitted spectra under different buffer-gas pressures and laser polarizations, as indicated in the panel; (b) experimental data acquired under linear polarization at 40 nW and 200 Torr together with the corresponding fitting curve, which is identical to the blue curve shown in (a).

Overall, the fitting curves agree well with the experimental data. Small deviations at the spectral wings and peak positions are observed, which can be attributed to environmental light interference and the stability of optical components. These deviations are within the experimentally acceptable uncertainty. The coefficient of determination of the fit satisfies  $R^2 > 0.997$ .

Figure 6 compares Voigt and Lorentzian fitting for the  $D_1$  line under low-power conditions. The extracted relative transition strengths are shown in the inset table of Figure 6a. The influence of polarization on the absorption profile remains marginal under the present operating conditions. To further clarify the practical meaning of the fitting results, we summarize the parameter trends extracted from the doublet Lorentzian model across the tested operating conditions. In Method III, the fitting parameters ( $H, \Gamma_L, \delta$ ) are obtained simultaneously from Equation (6). As discussed in Equation (7), the amplitude coefficient  $H$  scales with the  $^{87}\text{Rb}$  number density for a fixed optical path length, so that the fitted amplitude provides a direct indicator of vapor-density variation with temperature. In our measurements, increasing cell temperature generally increases the overall OD level (thus increasing  $H$ ), consistent with the expected enhancement of saturated vapor density. Meanwhile, the fitted linewidth  $\Gamma_L$  primarily reflects the dominant collisional broadening contribution under 200–520 Torr buffer-gas pressures, and the fitted shift  $\delta$  provides a compact descriptor of pressure-induced line displacement. Although the present work does not aim to provide an independent absolute calibration of buffer-gas partial pressures, these parameters remain useful for cross-checking the physical consistency of the spectra across different cells and operating points.



**Figure 6.** Doublet- and hyperfine-resolved fitting of the  $D_1$  absorption spectra at 373 K. (a) Fit using Method III: the measured data (black points) and the total fit (magenta), with additional curves showing the individual  $D_1$  hyperfine-transition contributions; the coefficients  $A_{11}$ ,  $A_{12}$ , etc., corresponding to the transitions in Figure 1 and Table 1 (relative strengths adjusted for experimental conditions). (b) Fit using Method II: the same measured data (black points) and the total fit (red) obtained with an alternative fitting strategy.

A key observation is that the applicability of the doublet approximation is jointly governed by buffer-gas pressure and optical power. At 520 Torr pressures, the line shape becomes increasingly collision-dominated and the hyperfine components within each manifold merge more strongly, which stabilizes the effective two-peak structure and improves the robustness of Method III over a wider range of optical powers. In contrast, at lower pressures and lower optical powers, the hyperfine-related structure becomes more pronounced and the spectrum can approach a more explicitly hyperfine-resolved form; in this regime, Method II can provide higher physical completeness at the expense of increased computational cost. Conversely, when optical power increases into the milliwatt regime, saturation and power broadening reduce the resolvability of the two-peak structure and

can introduce systematic deviations from the fixed relative-strength assumptions listed in Table 2. Therefore, the same spectrum can evolve from a clearly resolvable doublet at low power to a partially merged profile at higher power, even when the cell temperature and buffer-gas pressure remain unchanged.

Finally, from an application perspective, the purpose of introducing the  $R^2$  threshold is to provide an operational guideline for selecting the fitting strategy. In this work, we adopt  $R^2 = 0.995$  as a practical cut-off to delineate when Method III remains sufficiently accurate for rapid vapor-cell characterization. When the fitted  $R^2$  falls below this criterion, Method II (Voigt, hyperfine-resolved) becomes preferable for improved physical completeness. This criterion enables a straightforward workflow: Method III is used as the default fast-fitting approach under typical NMRG operating conditions (350–520 Torr buffer-gas pressure and low-to-moderate probe power), while Method II is invoked only when the spectral structure indicates that Gaussian or saturation-related effects are no longer negligible.

**Table 2.** Comparison of Voigt and doublet Lorentzian fitting of the  $D_1$  and  $D_2$  absorption spectra under different optical powers and gas pressures (200, 350, and 520 Torr).

| Line  | Gas Pressure (Torr) | Optical Power (mW)    | $R^2$ Lorentzian (Voigt) |
|-------|---------------------|-----------------------|--------------------------|
| $D_1$ | 200                 | $4 \times 10^{-5}$    | 0.99774                  |
|       | 350                 | $4 \times 10^{-5}$    | 0.99919 (0.99994)        |
|       | 350                 | $5.5 \times 10^{-5}$  | 0.99971                  |
| $D_2$ | 350                 | $5 \times 10^{-4}$    | 0.99773                  |
|       | 350                 | $3 \times 10^{-3}$    | 0.99837                  |
|       | 350                 | $1.36 \times 10^{-2}$ | 0.99706                  |
|       | 350                 | $2 \times 10^{-2}$    | 0.99759                  |
|       | 350                 | 0.5                   | 0.99698 (0.99868)        |
|       | 350                 | 3                     | 0.99672                  |
|       | 350                 | 7                     | 0.99884                  |
|       | 520                 | $4 \times 10^{-3}$    | 0.99629 (0.99833)        |
|       | 520                 | 0.22                  | 0.99761                  |
|       | 520                 | 4                     | 0.99697                  |
|       | 520                 | 7                     | 0.99682                  |
|       | 520                 | 10.5                  | 0.99448 (0.99999)        |

## 5. Conclusions

A practical applicability boundary is identified for using a reduced doublet Lorentzian model to fit pressure-broadened hyperfine spectra in  $^{87}\text{Rb}$  vapor cells under collision-dominated conditions. Experiments conducted over optical intensities from 40 nW to 10 mW, buffer-gas pressures from 200 to 520 Torr, and temperatures between 370 K and 390 K indicate that once collisional broadening reaches the GHz level and the optical intensity remains below the saturation regime, transitions sharing the same ground-state manifold merge spectrally and can be captured by a doublet Lorentzian description. With  $R^2 = 0.995$  adopted as an acceptance criterion, sub-percent fitting deviation is achieved throughout the validated parameter space. At the pressure of 350 Torr, the fitting error remains below 0.3 % for  $D_2$  transition and below 0.1 % for  $D_1$  transition, with  $R^2$  values exceeding 0.996 and 0.997, respectively. The model remains effective up to 520 Torr and into the mW optical power regime without invoking a fully hyperfine-resolved Voigt profile, whereas increasing Gaussian–Voigt contributions and saturation effects outside this regime constrain the simplified representation. These findings offer a physically grounded and computationally efficient, non-contact approach for vapor-cell parameter extraction in nuclear magnetic resonance gyroscope systems.

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