The influence of atomic alignment on absorption and emission spectroscopy

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Abstract

Spectroscopic observations play essential roles in astrophysics. They are crucial for determining physical parameters in the universe, providing information about the chemistry of various astronomical environments. The proper execution of the spectroscopic analysis requires accounting for all the physical effects that are compatible to the signal-to-noise ratio. We find in this paper the influence on spectroscopy from the atomic/ground state alignment owing to anisotropic radiation and modulated by interstellar magnetic field, has significant impact on the study of interstellar gas. In different observational scenarios, we comprehensively demonstrate how atomic alignment influences the spectral analysis and provide the expressions for correcting the effect. The variations are even more pronounced for multiplets and line ratios. We show the variation of the deduced physical parameters caused by the atomic alignment effect, including alpha-to-iron ratio ([X/Fe]) and ionisation fraction. Synthetic observations are performed to illustrate the visibility of such effect with current facilities. A study of PDRs in ρ Ophiuchi cloud is presented to demonstrate how to account for atomic alignment in practice. Our work has shown that due to its potential impact, atomic alignment has to be included in an accurate spectroscopic analysis of the interstellar gas with current observational capability.

Key words: ISM: magnetic fields – turbulence – (galaxies:) quasars: absorption lines – (ISM:) HII regions – submillimetre: ISM – ultraviolet: ISM

1 INTRODUCTION

Spectroscopy plays a crucial role in studying the universe. Analysing atomic and ionic spectral line intensity is one of the most important part of spectroscopic study. Absorption and emission atomic lines have numerous applications in astronomy. They are the direct measurements of column density of lots of elements (e.g., Fox et al. 2013; Richter et al. 2013; D’Onghia & Fox 2016), and thus help the analysis of chemical evolution and composition of astronomical structures. Physical parameters derived from the spectral line ratio (e.g., ionisation rate, temperature) facilitate us to understand the astrophysical environments better (see, e.g., Draine 1978; Hogerheijde et al. 1995; Salgado et al. 2016). Progress has been made in modelling the physical processes, such as cloud extinction in Photodissociation regions (PDRs) and outflows of Active Galactic Nuclei (AGN), with atomic spectra (e.g., Kaufman et al. 1999; Coil et al. 2015; Youngblood et al. 2016).

The rapid development of spectroscopic observations requires an accurate measurement of the spectral lines that is compatible to the higher signal-to-noise (S/N) ratio. Therefore, all relevant physical effects that are capable to produce the spectral fluctuation larger than the noise amplitude have to be counted for the high precision observations. We will demonstrate in this paper the fluctuation of atomic/ionic lines from Interstellar Medium (ISM) induced by ground state alignment (GSA) effect can have significant impact on the physical parameter derivation. One may naively argue that the physical effect will be averaged out given the possible line-of-sight dispersion of the magnetic field line in the medium. Synthetic observations are performed accounting for the averaging and the results show that such argument does not hold. We shall demonstrate that the influence of GSA cannot be neglected for an accurate spectral line intensity analysis with current observational capability and provide analytical expressions for the correction.

This paper is organised as follows: The general physics for the modulation of spectral lines due to GSA is briefly discussed in §2. We then demonstrate in §3 the influence of radiative alignment on the spectrum, where the magnetic field does not exist/ vary. In §4, we further discuss the impact of magnetic realignment, where the radiative geometry is fixed and the fluctuation of the spectral lines originates from the change of magnetic field. In addition, the influences of GSA on various astrophysical properties derived from spectral line ratios, including alpha-to-iron ratio ([X/Fe]) and ion-...
We present below the expressions for the modulation of absorption and emission coefficients. The atomic density of different angular momentum is depicted by the density matrix tensor, e.g., for the lower level $J_l$ it is denoted as $ρ_{lj}^K$. Only unpolarized incoming light is considered and therefore $k = 0$, 2 here. The ratio between the density tensor and the total density of the level is defined as the alignment parameter $Ω_q^i ≡ ρ_q^i/ρ_{0q}$. In the regime of GSA, $q$ is always 0 for the levels on the ground state. It is most convenient to calculate the GSA in the theoretical frame $x'y'z'$-system (Fig. 1a), where the magnetic direction is $z'$-axis. The direction of the line of sight is denoted as $Ω$ and $J_Q^K(i,Ω)$ is the irreducible geometric tensor for the observed light. Due to GSA, the absorption coefficients of the atomic transitions are expressed by (Landi Degl’Innocenti 1984, see also Yan & Lazarian 2006):

$$\eta_i(ν,Ω) = \frac{hν_0}{4\pi} B_{lu} n(J_l) ψ(ν - ν_0) \sum K (-1)^{J_1} ω_{J_2}^K ρ_{0q}^K J_Q^K(i,Ω),$$

(1)

where $K = 0$, 2, $ω_{J_2}^K ≡ 1$, $ω_{J_1}^K ≡ \{1, 2; J_1, J_2\}/(1, 1; 0; J_1, J_2)$, in which the matrix with braces "[ ]" represent the $-j$ symbol. The quantity $B_{lu}$ is the Einstein coefficient for absorption. The total atomic population $n(J_l)$ on the lower level $J_l$ is defined as $n(J_l) = \sqrt{J_l(J_l + 1)}$, where $[j] = 2j + 1$. $ψ(ν - ν_0)$ is the line profile. As shown in Eq. (1), the radiative pumping and the magnetic direction will modulate the absorption coefficients $η_i$ and thus the absorption spectrum varies.

For resonance emission lines, the excited states are influenced by the differential occupation on the ground state through radiative excitation (see, e.g., Yan & Lazarian 2008). In diffuse ISM and IGM, the magnetic field is weak and the decay rate of atoms from the levels on the excited states is much higher than the magnetic precession rate ($A ≃ 2πν_Q$). Thus, $q$ can be non-zero for the density tensor of the atoms on the excited states. The emission coefficients $ε_i(i = 0 \sim 3)$ from the upper level $J_u$ are (see Yan & Lazarian 2007):

$$ε_i(ν,Ω) = \frac{hν_0}{4\pi} A_{ul} n(J_u) ψ(ν - ν_0) \sum K Q ω_{J_2}^K J_Q^K(i,Ω).$$

(2)

where $K = 0$, 2; $Q = 0, ±1, ±2$. The quantity $A_{ul}$ is the Einstein coefficient for emission. Similar to the case of absorption, the emissivity $ε_i$ is also influenced by the anisotropic radiative pumping and magnetic field, as demonstrated in Eq. (2). In the following, we will evaluate quantitatively the influence of GSA on absorption and emission spectral lines in the observational frame (see Fig. 1b).

3 INFLUENCE OF RADIAITIVE ALIGNMENT ON THE SPECTRUM INTENSITY

Spectral line intensity are modulated due to the GSA induced by the anisotropic radiation. We first consider the unmagnetized case, and study only the dependence modulation on the scattering...
angle $\theta_0$, the angle between line of sight and the incident radiation direction. It is worth noting that there is no alignment (i.e., the alignment parameter $\sigma_0^2 = 0$) at $\theta_0 = 54.7^\circ$ or $180^\circ - 54.7^\circ$ (Van Vleck angle, Van Vleck 1925; House 1974), the corresponding intensity $I_{\perp V}$ is used as the “standard” for comparison in this section.

The intensity fluctuations due to radiative alignment for several selected spectral lines are plotted in Fig. 2(a). We find that the intensity fluctuation ratio due to radiative alignment can be fitted with a simple analytical expression with $5\sigma$ confidence:

$$r_{\text{pump}}^{\text{em}}(\theta_0) \equiv \frac{r_{\text{pump}}}{I_{\perp V}} = p_1 + p_2 \cos 2\theta_0,$$

where $p_1, p_2$ vary with spectral lines. The fitting for Fe II 12600Å is presented as an example in Fig. 2(b). The comprehensive fitting parameters for various transitions are presented in Table 1.

The influence is more significant for multiplets and line ratios since it varies among different lines. We perform synthetic observation on a cloud that is illuminated by a star located at two different positions (case 1 and case 2, whose picture plane projections are marked in Fig. 3(a)). The resulting fluctuations of the line ratio of two components in the Si triplets $\lambda = 1474$Å are shown in Fig. 3(b) and Fig. 3(c), respectively. Moreover, the possible fluctuations will be further enhanced if magnetic field exists. Fig. 3(d) and Fig. 3(e) are the results of synthetic observations for case 1 and 2 with the same magnetic field. The fluctuation of the line ratio ranges from overestimation of $\gtrsim 30\%$ to underestimation of $\gtrsim 10\%$. By comparing Fig. 3(d) and Fig. 3(e), we further conclude that the influence of GSA on the same spectral line also varies according to radiation geometry even with the same underlying magnetic field.

We define $R_{th}$ to depict the possible intensity fluctuation range introduced by GSA:

$$R_{th} = \frac{\max(I_{\parallel V} + \Delta I)}{\min(I_{\perp V} - \Delta I)},$$

The comprehensive results for the $R_{th}$ are shown in Table 2. Owing to GSA, the same column density could produce an intensity variation by a factor of $\gtrsim 1.5$, which is far beyond the noise amplitude of current high S/N telescope.

### 4 Influence of Magnetic Realignment on Spectral Lines

In this section we investigate the fluctuation of spectral lines from the magnetic realignment. The variation ratio of the line in-

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**Table 1. Fitting Parameters for Radiative Alignment**

| Species | $\lambda$ (Å) | Emission | $p_1^{\text{em}}$ | $p_2^{\text{em}}$ |
|---------|--------------|----------|-----------------|-----------------|
| C I     | 1193.03      |          | 1.0307          | 0.0898          |
| C II    | 1334.53      |          | 1.0451          | 0.1320          |
| O I     | 1025.76      |          | 0.9984          | -0.0047         |
| S I     | 1474.75      |          | 1.0376          | 0.1099          |
| S II    | 1474.38      |          | 0.9625          | -0.1097         |
| Si II   | 1250.58      |          | 1.0107          | 0.0314          |
| S III   | 1012.50      |          | 1.0210          | 0.0613          |
| S IV    | 1062.66      |          | 1.0042          | 0.0123          |
| Fe II   | 1142.36      |          | 1.0097          | 0.0283          |
|         | 1143.22      |          | 0.9839          | -0.0411         |
|         | 1144.93      |          | 1.0053          | 0.0154          |

**Table 2. The Range of Fluctuation Arising from GSA**

| Species | $\lambda$ (Å) | Emission $R_{th}^{\text{em}}$ (%) | $R_{th}^{\text{em}}$ |
|---------|--------------|-----------------------------------|-------------------|
| C I     | 1193.03      | 1.3632                            |                   |
| C II    | 1334.53      | 1.1307                            |                   |
| O I     | 1025.76      | 1.1217                            |                   |
| S I     | 1474.75      | 1.1054                            | 1.3509            |
| S II    | 1250.58      | 1.1126                            | 1.1216            |
| S III   | 1012.50      | 1.1472                            |                   |
| S IV    | 1062.66      | 1.1590                            | 1.1359            |
| Fe II   | 1142.36      | 1.1150                            | 1.1216            |
|         | 1143.22      | 1.1034                            | 1.1359            |
|         | 1144.93      | 1.0361                            | 1.1904            |
Figure 2. (a) The modulation of several selected atomic lines owing to radiative alignment; (b) The fitting of the analytical expression for Fe II λ2600 Å emission line.

4.1 UV/optical spectra

As an example, we show in Fig.5 a typical scenario, in which the effect of magnetic realignment leads to the measurable variation in the observed line intensity. Consider a typical late-type galaxy with an extended neutral gas disk and an interstellar magnetic field. Star-formation is expected to take place in distinct regions in the disk (i.e., in spiral arms). Therefore, the interstellar radiation field is likely to be anisotropic at a given point in the disk. In the spectrum of the background point source (e.g., a Quasi-Stellar Object, hereafter QSO), the gas disk will leave its imprint through many absorption lines from neutral and ionised species, where most of the lines are located in the (rest frame) UV. Such disk absorbers are known to contribute to the population of the so-called DLA absorbers at redshifts z̃ < 2. The DLA absorbers adopted to illustrate the influence of magnetic fields on the spectroscopy are dominated by cold neutral hydrogen (see, e.g., Rao & Turnshek 2000). As long as the angle between the ambient magnetic field and the direction of the incident radiation at the place where the sightline pierces the disk is not Van Vleck angle, the GSA will cause changes in the central absorption depths of unsaturated absorption lines. The variation of the line intensity of S II λ1250.58 Å with respect to different magnetic field direction is presented in Fig.4(a) given the line of sight perpendicular to the direction of the incident radiation (θ0 = 90°).

As shown in Fig.4(a), the spectra observed change with the direction of magnetic field. In addition, the error of the observation for S II λ1250.58 Å due to photon noise is 2.5% in current observation (see Prochaska et al. 2007), which is smaller than the variations due to GSA in most of the areas top at 7% in Fig.4(a). The maximum enhancement and reduction caused by magnetic realignment for different absorption lines are presented in Table 3, in which the absorptions are from all the levels on the ground state that have much longer life time than magnetic precession period. The fluctuation of intensity ΔI/ I0 = r mag − 1. The influence of magnetic fields are different among the lines. For some of the lines, the variation is more than 20%. Thus, The measurable changes of absorption spectrum can be introduced due to magnetic realignment. The influence of GSA on the derived alpha-to-iron ratio of the DLA absorbers will be discussed in §5 with real observation analysis.

Simulations are performed in Fig. 6 to compare the spectrum profiles of the S II triplets for a synthetic absorption spectrum of a DLA with and without the magnetic alignment included. Fig. 6 was designed up to illustrate the effect in a realistic instrumental set up, with a given typical pixel size and S/N for an optical spectrum taken by an 8m-class telescope. The graphical use of steps instead of curves, which is common in absorption spectroscopy, is intended to visualize the pixel-by-pixel noise variations in the data. The three transitions of singly-ionised Sulfur (S II; upper ionisation potential 23.3 eV) at λλ 11250.58, 1253.81, 1259.52 represent important tracers for neutral and weakly ionised gas in the local interstellar and intergalactic medium and in distant galaxies (e.g., Kisielius et al. 2014a, 2014b; Welsh & Lallement 2012; Richter et al. 2001; Fox et al. 2014a). Being an α element, singly-ionised Sulfur only has a weak depletion into dust grains (e.g., Savage & Sembach 1996). Thus the interstellar Sulfur abundance is often used as a proxy for the α-abundance in the gas. In addition, Sulfur has a relatively low cosmic abundance (Asplund et al. 2009) and under typical interstellar conditions (in particular in low-metallicity environments) these lines are not saturated. The three lines are observed in the same wavelength region with identical S/N. The important parameters for simulations are presented in the caption, such as the assumption of S II column density, etc. The synthetic spectra were generated using the FITLYMAN routine (Fontana & Ballester 1995) implemented in the ESO-MIDAS software package. Atomic data were taken from Morton (2003). To show the effect clearly, we zoom in the spectrum to the radial velocity range [−10 km s−1, 10 km s−1]. The enhancement and reduction of the spectral line profile due to

5 These lines are detected at the places such as galactic halos (Richter et al. 2013; Fox et al. 2014b) and circumstellar medium in GRB (Fynbo et al. 2006).
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Figure 3. The influence of radiative alignment. Magnetic field is not accounted for. (a) The geometric illustration, the synthetic ISM is illuminated by the O-type star from different positions, the picture plane projection is on the right; (b,c) variations of the line ratio of two components in the S I triplets $\lambda \sim 1474$ Å ($1473.99, 1474.38$ Å) for case 1,2, respectively; (d,e) same as (b,c), but with constant magnetic field along $x$–axis included.

Figure 4. The variation ratio of the line intensity under the influence of magnetic fields for (a) S II $\lambda 1250$ Å absorption, (b) Fe II $\lambda 1143$ Å emission, and (c) C I $\lambda 610 \mu$m emission, respectively. The line of sight is vertical to the direction of the incident radiation ($\theta_0 = 90^\circ$), which corresponds to a face-on disk.

The maximum and minimum variations of intensity for different emission lines due to the magnetic realignment are presented in Table 4. The fluctuation of intensity $\Delta I/I_0 = r_{\text{mag}} - 1$. The variations are different among the lines, e.g., for $\theta_0 = 90^\circ$, S II $\lambda 1259.52$ Å is enhanced up to 21%; S I $\lambda 1473.99$ Å is reduced more than 25% whereas the line S II $\lambda 1253.81$ Å is enhanced up to 38%. Fe II emission spectra in UV and optical band are important for modelling

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Table 3. VARIATIONS OF UV/OPTICAL ABSORPTION LINES DUE TO GSA

| Species | \( \lambda \) (Å) | \( (\Delta I/I_0)_{\text{min}} \) % | \( (\Delta I/I_0)_{\text{max}} \) % | \( \theta_{\text{min}} \) ° | \( \theta_{\text{max}} \) ° |
|---------|------------------|------------------|------------------|------------------|------------------|
| O I     | 1025.76          | -6.37            | +0.81            | 0°               | 0°               |
| S I     | 1474.57          | -27.29           | +0.181           | 54.7°            |
| S II    | 1474.38          | -22.82           | +2.62            | 30°              |
| O II    | 1473.99          | -19.99           | +0.08            | 54.7°            |
| S II    | 1250.58          | -7.56            | +6.33            | 90°              |
| S II    | 1253.81          | -4.71            | +7.60            | 0°               |
| S II    | 1259.52          | -1.61            | +1.22            | 90°              |
| Ti II   | 3072.97          | -1.64            | +1.30            | 90°              |
| Ti II   | 3221.98          | -1.03            | +1.33            | 0°               |
| Ti II   | 3225.19          | -0.33            | +0.26            | 90°              |
| Fe II   | 1142.36          | -1.69            | +4.42            | 90°              |
| Fe II   | 1143.22          | -2.86            | +7.94            | 0°               |
| Fe II   | 1144.93          | -0.46            | 35.3°            | +5.21            | 90°              |

Absorption from metastable levels of the ground state

| Species | \( \lambda \) (Å) | \( (\Delta I/I_0)_{\text{min}} \) % | \( (\Delta I/I_0)_{\text{max}} \) % | \( \theta_{\text{min}} \) ° | \( \theta_{\text{max}} \) ° |
|---------|------------------|------------------|------------------|------------------|------------------|
| C I*    | 1260.93          | -24.20           | +1.54            | 54.7°            |
| C I*    | 1261.00          | -17.45           | +0.46            | 35.3°            |
| C I*    | 1261.72          | -15.76           | +0.00            | 0°               |
| C II*   | 1037.02          | -9.02            | +3.68            | 0°               |
| C II*   | 1335.66          | -10.34           | +1.29            | 54.7°            |
| O I*    | 1027.43          | -9.57            | +0.00            | 0°               |
| Si II*  | 1264.74          | -5.59            | +5.32            | 0°               |
| Si II*  | 1265.00          | -3.00            | +0.27            | 54.7°            |
| Si I*   | 1303.11          | -21.05           | +1.72            | 54.7°            |
| Si I*   | 1302.86          | -14.43           | +0.50            | 35.3°            |
| Si II*  | 1302.34          | -12.74           | +0.00            | 0°               |
| S III*  | 1015.50          | -24.67           | +1.53            | 54.7°            |
| S III*  | 1015.57          | -17.88           | +0.46            | 0°               |
| S III*  | 1015.78          | -16.19           | +0.00            | 0°               |
| S IV*   | 1072.97          | -1.20            | +2.20            | 0°               |
| S IV*   | 1073.52          | -0.20            | +0.56            | 90°              |
| C I**   | 1193.65          | -24.65           | +1.06            | 54.7°            |
| C I**   | 1193.39          | -20.93           | +1.51            | 35.3°            |
| S III** | 1193.24          | -18.74           | +0.00            | 0°               |
| S III** | 1202.12          | -24.20           | +0.95            | 54.7°            |
| S III** | 1201.73          | -20.62           | +1.37            | 35.3°            |
| S III** | 1200.97          | -18.33           | +0.00            | 0°               |

Note: The comparison is made by first considering a specific \( \theta_0 \) and changing the magnetic direction in the full space to find the maximum enhancement and reduction for the chosen \( \theta_0 \). Then we scan \( \theta_0 \) for all the possible angles and compare the maximum variation for different \( \theta_0 \). \( (\Delta I/I_0)_{\text{min}} \) means the maximum enhancement of the observed intensity due to magnetic realignment and \( (\Delta I/I_0)_{\text{max}} \) means the reduction. The corresponding geometry are denoted as \( \theta_{\text{min}} \) and \( \theta_{\text{max}} \), respectively.

Planetary Nebulae (PNe) (Dinerstein et al. 2006) and cloud near AGNs (Wills et al. 1985). The variation of Fe II 1144.93 emission line due to magnetic realignment are presented in Fig.4(b) as an example. In this geometric condition, the magnetic realignment enhances more than 10% of the spectrum when the magnetic field is perpendicular to both the line of sight and the direction of the incident radiation (\( \theta = 90°, \phi = 90° \)).

As demonstrated in Tables 3,4, the modulation due to magnetic realignment is more significant among all the measured multiplets for both absorption and emission spectra.

4.2 Submillimeter fine-structure lines

Submillimeter fine-structure spectra, which arise from magnetic dipole transitions within the ground state, have a broad applicability in astrophysics, such as, determining chemical properties of star-forming galaxies (Kobulnicky et al. 1999), predicting the star burst size (Diaz-Santos et al. 2013), etc. However, previous spectral analysis does not consider the anisotropic radiation and the magnetic realignment. In diffuse ISM and IGM, the influence of GSA on the submillimeter fine-structure absorption lines is exactly the same as that on the UV/optical resonance absorption lines. The atoms on all the levels in the ground state are magnetically aligned (i.e., only those matrix tensors \( B_{kq} \) with even \( k \) and \( q = 0 \) exist) since the life time of these atoms on all the levels of the ground state are much longer than the magnetic precession period in diffuse ISM and IGM (see Yan & Lazarian 2006). For example, the influence of magnetic realignment on C I 4610μm in a face-on disk is presented in Fig.4(c). The configuration of the ground state of C I has 3 levels 3P_{0,1,2}. C I 4610μm line represents the transition between the levels within the ground state 3P_{1} and 3P_{0}. Table 5 presents

Figure 5. Schematics for the typical environment where atomic lines are altered by magnetic fields. Presented is a DLA region on the spiral arm of a galaxy.

6 Thanks to such equivalence, the fine-structure absorption lines are not discussed to avoid repetition. Readers may refer to the results in §4.1.
the influence of magnetic fields for a list of submillimeter emission lines.

4.3 Observations from the medium with turbulent magnetic fields

In order to address the issue of how much modulation can be induced with the line-of-sight dispersion of magnetic field, we perform synthetic observation on ISM with turbulent magnetic field from numerical simulation. A three-Dimensional (3D) super-Alfvenic \((M_a = 1.43)\) MHD datacube \((512 \times 512 \times 16)\), which corresponds to a \(1pc(x) \times 1pc(y) \times 0.2pc(z)\) diffuse layer of a reflection nebula, is generated by the MHD-simulation with the PENCIL-code\(^7\). Note that the simulation is dimensionless and not sensitive to the choice of corresponding physical size. The line-of-sight dispersion is evaluated by the chosen total Alfvenic-Mach Number \(M_a\). A massive O-type star radiates UV-photons to illuminate the medium. Synthetic observations are performed on the medium for two emission lines in the S\(\text{I}\) triplets \(\lambda \sim 1474\)Å, which share the same S/N ratio. The intensity variation is integrated along the line of sight and the influence of GSA on these two lines are shown in Fig. 7. Magnetic alignment induces more than 10\% variation and for a sufficient amount of areas more than 20\% for both lines. In addition, the variations due to the GSA for the same environment (density, magnetic field, and radiation field) differ substantially for the two spectral lines. Since the injection scale of interstellar turbulence \(\sim 100pc\) is much larger than the adopted value here (see Armstrong et al. 1995; Chepurnov & Lazarian 2010), the line-of-sight dispersion of the magnetic field in real observations can only be less than that in the synthetic data (Fig. 7), and thus the intensity variation due to GSA can be more significant in real circumstances.

\(^7\) See https://code.google.com/archive/p/pencil-code/ for details.

Figure 6. Synthetic spectrum (in velocity scale) of a single-component S\(\text{II}\) \(\lambda\lambda 1250.58, 1253.81, 1259.52\) absorption system with a S\(\text{II}\) column density of \(N(S\text{II}) = 4 \times 10^{14} \text{cm}^{-2}\), a Doppler parameter of \(b = 5 \text{km s}^{-1}\), a spectral resolution of \(R = 45,000\), and a S/N of 100 per resolution element for the source-in-disk scenario. Such a S\(\text{II}\) column density would be expected for a DLA with \(\log N(\text{H}\text{I}) = 20.48\) and a sulfur abundance of 0.1 solar assuming solar reference abundances of Asplund et al. (2009). The geometric condition is \(\theta_0 = 90^\circ\). (a) The blue solid lines show the spectrum without the magnetic realignment, the red solid lines show the spectrum when \(\theta = 90^\circ, \phi = 90^\circ\). (b) The red-/blue-shaded areas indicate the excess/deficiency of the absorption due to the magnetic realignment.
Many important physical parameters in astronomy are derived from spectral line ratios. For example, the ratio of different transitions of C II (λ1036.34 and λ1334.53) is used to estimate the electron density in different astrophysical environments (see Lehner et al. 2004; Zech et al. 2008; Richter et al. 2013 for details). As illustrated in §3.4, the influence of the GSA varies for different spectral lines. Therefore, the variation of the resulting spectral line ratio is expected to be more significant, e.g., with one line reduced and the other enhanced. According to Eq. (1), the ratio of the intensity between two different absorption lines is given by

$$\rho_{\lambda_{1}, \lambda_{2}}(\theta_{0}, \theta_{r}, \theta) = \frac{r_{\lambda_{1}}(\lambda_{1}, \theta_{0}, \theta_{r}, \theta)}{r_{\lambda_{2}}(\lambda_{2}, \theta_{0}, \theta_{r}, \theta)} \rho_{\lambda_{2}}^{0}(J_{2}) \sqrt{\omega_{2}^{2} + \omega_{r}^{2}} \rho_{\lambda_{1}}^{0}(J_{1}) \left(1 - 1.5 \sin^{2} \theta\right).$$

Note: Same as Table 3, but for submillimeter fine-structure lines.

Table 4. VARIATIONS OF UV/OPTICAL EMISSION LINES FROM GSA

| Species | λ (Å) | (ΔI/Ip)_{min} | (ΔI/Ip)_{max} | θ_{min} | θ_{max} |
|---------|-------|---------------|---------------|---------|---------|
| C I     | 1193.03 | −20.85 | 0° | +21.00 | 90° |
| C II    | 1334.53 | −29.17 | 0° | +28.90 | 90° |
| O I     | 1025.76 | −14.30 | 0° | +10.44 | 90° |
| Si II   | 1190.42 | −27.20 | 0° | +31.49 | 90° |
| S I     | 1474.57 | −6.32  | 0° | +0.50  | 54.7°|
|         | 1474.38 | −19.62 | 90° | +7.49  | 0° |
|         | 1473.99 | −38.67 | 0° | +3.89  | 54.7°|
| Si III  | 1253.81 | −20.51 | 0° | +38.79 | 90° |
|         | 1259.52 | −23.04 | 0° | +21.27 | 90° |
| S IV    | 1012.50 | −32.02 | 0° | +6.01  | 110°|
| Fe II   | 1062.66 | −35.44 | 0° | +44.09 | 90° |
|         | 1142.36 | −2.90  | 65° | +12.10 | 0° |
|         | 1143.22 | −9.37  | 0° | +22.44 | 0° |
|         | 1144.93 | −14.38 | 0° | +13.64 | 90° |

Note: Same as Table 3, but for resonance emission lines in the UV/optical band.

Table 5. VARIATIONS OF SUBMILLIMETER LINES DUE TO GSA

| Species | λ (µm) | (ΔI/Ip)_{min} | (ΔI/Ip)_{max} | θ_{min} | θ_{max} |
|---------|--------|---------------|---------------|---------|---------|
| C I     | 610    | −24.2         | 90°           | +1.54  | 54.7°|
|         | 157.7  | −9.02         | 90°           | +3.68  | 0° |
| O I     | 63.2   | −10.77        | 0°            | +0     | 0° |
| Si II   | 34.8   | −8.76         | 0°            | +4.90  | 90° |
| S I     | 25.2   | −12.73        | 0°            | +0     | 0° |
| Si III  | 33.3   | −24.67        | 0°            | +1.53  | 54.7°|
| S IV    | 10.5   | −2.04         | 0°            | +2.00  | 90° |
| Fe II   | 26.0   | −0.39         | 35.3°         | +3.11  | 90° |

Note: Same as Table 3, but for submillimeter fine-structure lines.

5 INFLUENCE ON PHYSICAL PARAMETERS DERIVED FROM LINE RATIOS

Figure 7. Synthetic observations to super-Alfvenic ISM (M_a = 1.43) generated by PENCIL MHD code for S I emission lines (a) λ1473.99Å and (b) λ1474.38Å, respectively. The ISM corresponds to an 1 pc x 1 pc area on the picture plane and the optical depth is 0.2 pc. The radiation source, a massive O-type star, resides to the south of the medium 0.1 pc away. The color scale represents the intensity variation ratio with and without GSA. The percentage of enhancement and depletion are noted with color on the contour.
And the ratio of the intensities of two emission lines is obtained from Eq. (2):

\[
R_{\text{ab}}^{\text{rem}}(\theta_d, \theta_r, \theta) = r_{\text{rem}}(\lambda_1, \theta_d, \theta_r, \theta, \lambda_2, \theta_d, \theta_r, \theta) + 1.
\]

Thus, the inferred N(S)/N(Fe) is influenced by GSA, as shown in Eq. (5). The variation of the ratio N(O)/N(Fe) reduced by 9% in Eq. (5). The variation of the ratio N(S)/N(Fe) is inferred from O\ _{\text{II}} since in DLAs these elements are mostly singly-ionised. Thus, the ratio of all the possible geometric conditions (\[\theta_d, \theta_r, \theta\])\_0 for the \[\lambda_{\text{ab}}\text{Fe}\_\text{II}\] field is perpendicular to both the line of sight and the direction of the magnetic field, whereas the inferred N(O)/N(Fe) reduced by GSA are more significant than the error produced by photon noise. In addition, the depletion of iron in the dust is calculated by [S/Fe] (Noterdaeme et al. 2008). As demonstrated in Fig. 9, some of the variations due to GSA will even result in the changing sign of [S/Fe].

A few examples will be presented in the following subsections.

### 5.1 Nucleosynthetic studies in DLAs

The alpha-to-iron ratio is widely used in spectral analysis. It reflects the nucleosynthetic processes in SFRs (e.g., Prochaska et al. 2001). The \[\alpha\] elements include O, Si, S, Ti, etc. Iron refers to Fe elements such as Cr, Mn, Co, Fe, etc. \[\alpha\] elements in the medium of the galaxy with low metallicity ([Fe/H]<-1.0) are produced exclusively by Type-II supernovae (SNe II), but the \[\alpha/Fe\] ratio suffers a drop when the delayed contribution of Fe from Type-Ia supernovae (SNe Ia) is effective (McWilliam 1997; Cooke et al. 2011). The alpha-to-iron ratio [X/Fe] index (X represents the chemical elements for \[\alpha\] elements) is defined by the ratio of abundance observed from the medium in comparison with that from the sun:

\[
[X/Fe] = \log[N(X)/N(Fe)] - \log[N(X)/N(Fe)]_0
\]

The abundance of the elements is assumed to be equal to the column density of the element in the dominant ionisation state, e.g., Fe\ _{\text{II}} for the iron abundance and S\ _{\text{II}} for the \[\alpha\]-element abundance since in DLAs these elements are mostly singly-ionised. Thus, the ratio N(S)/N(Fe) is inferred from the line ratio S\ _{\text{II}}/Fe\ _{\text{II}}. Nevertheless, the inferred N(S)/N(Fe) is influenced by GSA, as shown in Eq. (5). The variation of the ratio \[R_{\text{ab}}^{\text{rem}}\] with respect to different direction of magnetic fields is presented in Fig. 8(a) for the geometric condition \[\theta_d = 90^\circ\]. Furthermore, taking into account of all the possible geometric conditions (\[\theta_d\])\_0, the maximum and minimum variations for the inferred N(S)/N(Fe) due to GSA is [-14%, +10%]; i.e., [-0.07,+0.04] for [S/Fe].

In comparison, another \[\alpha\] element, Oxygen, is presented as an example. Most oxygen in DLAs are neutral and therefore the ratio N(O)/N(Fe) is inferred from O\ _{\text{I}}/Fe\ _{\text{II}}. The influence of GSA on the ratio \[R_{\text{II}}^{\text{rem}}\] is presented in Fig. 8(b) when \[\theta_d = 90^\circ\]. Comparing Fig. 8(a) and Fig. 8(b), the inferred N(S)/N(Fe) is enhanced by 10% whereas the inferred N(O)/N(Fe) reduced by 9% when magnetic field is perpendicular to both the line of sight and the direction of the incidental radiation, i.e., [S/Fe] varied by +0.04 while [O/Fe] varied by 0.06.

Furthermore, Fig. 9 illustrates the influence of GSA on the [S/Fe] modelled in DLAs absorbers on QSO spectra observed by VLT/UVES (see Table 1 in Noterdaeme et al. 2008 with X=S). By applying the maximum variation of [S/Fe] obtained in this section to the observational data, the upper and lower variation thresholds due to GSA are obtained. As shown in Fig. 9, the variations due to GSA are more significant than the error produced by photon noise. In addition, the depletion of iron in the dust is calculated by [S/Fe] (Noterdaeme et al. 2008). As demonstrated in Fig. 9, some of the variations due to GSA will even result in the changing sign of [S/Fe].

### 5.2 Ionisation studies in diffuse gas

The line ratio of the same element from different ionisation states is often used to determine the ionisation fraction (see, e.g., Richter et al. 2016). For instance, (S\ _{\text{II}})/S\ _{\text{III}} ionisation line ratio is employed to determine the ionisation fraction in extragalactic H\ _{\text{II}} region (see, e.g., Vilchez et al. 1988), because higher ionised sulphur is insignificant in most of these H\ _{\text{II}} regions (Mathis 1982, 1985). The line ratio S\ _{\text{III}}/S\ _{\text{II}} is adopted to represent (S\ _{\text{III}})/(S\ _{\text{II}}). Fig. 10(a) demonstrates the influence of GSA with respect to different magnetic directions for \[\theta_d = 90^\circ\]. The influence of magnetic fields on inferred ionisation fraction varies with different geometric conditions. By taking into account all the possible geometric conditions (\[\theta_d\])\_0 in Fig. 10(b), the range of variation under the influence of GSA is [-27%, +12%], which means a variation of [-0.14,+0.05] in log index.

### 6 REMOVING THE GSA EFFECT FROM RAW DATA

In this section, we use the observational data of spectral lines from PDRs in \[\rho\ \text{Ophiuchi}\] cloud as an example to demonstrate how to account for GSA effect. The cloud, 150pc from the earth, is illuminated by the UV/optical radiation from the B\_\text{III}\ _{\text{V}} star HD4147889, which resides approximately 5.75pc behind the cloud (Liseau et al. 1999). Atomic and single-ionized Carbon traces the neutral gas of the PDRs in the cloud whereas molecular lines are also detected (e.g., C\ _{\text{II}}\ _{\text{O}} Kamegai et al. 2003). Two stripes in the cloud are used here as examples to perform the analysis. Dashed lines plotted in Fig. 11 are adopted from the observational analysis in Kamegai et al. (2003). We first consider only the radiative alignment. We adopt the fitting curves for [C\ _{\text{II}}] and [C\ _{\text{I}}] lines from Table 1 in §3:

\[
r_{\text{pump}}(\theta_d) = 1.0332 + 0.094 \cos 2\theta_d,
\]

\[
r_{\text{pump}}(\theta_d) = 0.9795 - 0.0599 \cos 2\theta_d,
\]

\[
\theta_d = - \arctan \frac{r_{\text{source}}}{d_{\text{source}}} = - \arctan \left[ 5.82 \times 10^{-2}(r_{\theta_d}/arcmin) \right],
\]

where \(r_{\theta_d}\) is the picture plane angular distance from the source to the analyzed medium in arcmin. The intensity (\(I_{\text{VV}}\)) after correcting the effect from radiative alignment is thus obtained from the observational intensity (\(I_{\theta_d}\)) by:

\[
I_{\text{VV}} = I_{\theta_d}/r_{\text{pump}}(\theta_d).
\]

The results are shown with solid lines in Fig. 11. The Van Vleck angle flipping is seen at \( \sim 24^\circ \). We further take into account the magnetic realignment. The picture plane magnetic field in \[\rho\ \text{Ophiuchi}\] cloud is obtained through star polarization in Kwon et al. (2015). The unknown component of magnetic field along the line of sight leads to some uncertainties in the correction, as marked by the error bars in Fig. 11. The potential neutral Carbon peak can be shifted from the original one in raw data (dashed lines). The intensity of atomic and single-ionized Carbon can be significantly modified by GSA. The real column density distribution of neutral Carbon may be synchronized with or largely deviated from that of C\ _{\text{II}}\ _{\text{O}}. Therefore, more accurate magnetic field analysis with compatible resolution to the spectral analysis has to be performed in such area for a proper study of the interstellar gas.
7 DISCUSSION

As illustrated in this paper, the variation of spectral line intensity induced by GSA varies among different spectral lines. Thus, such influence could be precisely analysed if multi-spectral lines for the same element is achievable. In addition, the alignment on the ground state is transferred to the levels of atoms on the excited states through absorption process, as illustrated in §3 and 4. The intensity of the ultraviolet-pumped fluorescence lines, which are derived from successive decays to different levels of atoms and applied to the modelling of reflection nebulae (Sellgren 1984, 1986), are dependent on the initial upper levels, and thus is influenced by GSA through the scattering process. The influence of collision is neglected in this paper, which applies to most diffuse ISM and IGM. Collisions reduce the alignment efficiency (see Hawkins 1955). The collision effect can become important in the case of higher density medium where the collision rate \( r_\star \) (either inelastic collision rate or Van der Waals collision rate) dominates over optical pumping rate \( B_{\text{ul}} \) (see Yan & Lazarian 2006 for details). The focus of our paper is on the GSA effect that is a saturated state. When the magnetic precession rate is comparable to the optical pumping from the ground state \((2\pi r_\star \sim B_{\text{ul}})\), the ground-level Hanle effect is applicable (see Landolfi & Landi Degl’Innocenti 1986), which means the magnetic field influence on the spectrum is not limited to the change of direction but also the magnetic field strength. As demonstrated in Yan & Lazarian (2008), the effect becomes saturated when \( 2\pi r_\star \sim 10B_{\text{ul}} \). Therefore, we set \( r_{\text{Hanle}} \leq 2\pi r_\star \sim 10B_{\text{ul}} \) as the boundary between the ground-level Hanle regime and the GSA regime (see Fig. 12(a)):

\[
r_{\text{Hanle}} = r_\star \sqrt{\frac{n_{\text{flu}}(J_\star)}{1.76(B/\mu G)(\exp(h\nu/(k_B T)) - 1)/J_\star}}
\]

(10)

We calculate the boundary \( r_{\text{Hanle}} \) for C II \( \lambda 1037\AA \) in the presence of stars with different effective temperature \( T_{\text{eff}} \) and radius \( r_\star \) for the magnetic field with the strength range from \( \mu G \) to \( mG \) in Fig. 12(b). The \( r_{\text{Hanle}} \) increases as the magnetic field becomes weaker and as the effective temperature \( T_{\text{eff}} \) and radius \( r_\star \) increase. Nevertheless, even in the most optimistic scenario with \( T_{\text{eff}} = 4 \times 10^4 K, r_\star = 10 r_\odot, B = 1 \mu G \) (though rarely applies), the boundary \( r_{\text{Hanle}} \approx 180 A_{\odot} r_\star = 8.5 \times 10^4 pc \) which is a thousand times smaller than the normal H II Region which is in pc scale. All the analysis with GSA and their observational implication in this paper is applicable to most of the ISM, except when performing very high resolution spectral analysis on regions very close to the very bright O-type star.

Indeed, many spectral lines we measured reside in multiplets. It is worth noting that the influence of GSA becomes more signif-
Influence of atomic alignment on spectroscopy

(a) $R_{1012,1250}^\text{em}$ variation, $\theta_0 = 90^\circ$

(b) $R_{1012,1250}^\text{em}$ max & min variations

Figure 10. Variation of the ionisation fraction due to GSA: line ratio of $\lambda 1012.49 \text{Å}$ and $\lambda 1250.58 \text{Å}$ emissions. (a) The variation of line ratio with respect to the direction of the magnetic field in the case of line of sight vertical to the direction of the incident radiation ($\theta_0 = 90^\circ$); (b) The maximum and minimum variations as a function of $\theta_0$.

Figure 11. Modifications of different atomic line intensity due to GSA, the influence of anisotropic pumping and magnetic realignment. Line colors represent: Blue for $[^{12}\text{C}][\lambda 610 \mu m]$, Orange for $[^{12}\text{C}][\lambda 157 \mu m]$, and Yellow for $[^{18}\text{O}][1-0]$. The raw observational data are in dashed lines from Kamegai et al. (2003). The solid lines are the modifications purely due to anisotropic radiative pumping. The error bars that depict the possible range of the original column density of the corresponding element are produced accounting for the magnetic realignment. Potential peaks for neutral Carbon for both stripes are noted with green dotted lines. The intensity peaks for atomic and single-ionized Carbon lines are marked on the corresponding $y$–axis.

8 CONCLUSIONS

We have demonstrated the influence of GSA effect on the spectroscopy. We emphasize that GSA is a general physical process that induces visible systematic variations to both absorption and emission spectral lines observed from diffuse medium, e.g., DLAs, H II Regions, PDRs, SFRs, Herbig Ae/Be disks, etc. Comprehensive results are provided to demonstrate the influence of the GSA effect –including radiative alignment and magnetic realignment– on resonance UV/optical absorption/emission lines and submillimeter fine-structure lines observed from different astrophysical environments. Synthetic observations are performed to present such influence on spectral line profile and to investigate the influence of GSA in turbulent magnetic fields. Variations of the physical parameters inferred from line ratios due to GSA are studied. We illustrate how to remove the GSA effect from raw data. Our main conclusions are:

- Measurable modulations are induced on the absorption and emission lines observed from diffuse ISM and IGM due to GSA.
The influence of GSA on the spectral line intensity is not diminished due to line-of-sight dispersion of turbulent magnetic fields such as in ISM and IGM.

The enhancement and reduction of the same spectrum line change in accordance with the direction of the magnetic field and the radiation geometry.

The variation of the line intensity changes from line to line. As a result, the influences on the multiplets and line ratios are even more distinct, affecting the inferred physical parameters.

The analytical model set up in this paper can be used for correcting the GSA effect from interstellar spectroscopy. Without such correction, the physical environment inferred cannot achieve the accuracy that current instruments promise.

GSA should be considered in the future spectral analysis.

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APPENDIX A: BASIC FORMULAE ON ATOMIC ALIGNMENT

In this Appendix, we illustrate the basic equations on atomic alignment. The calculations in this Appendix are all performed in the theoretical frame $xyz$-system in Fig.1(a).

Anisotropic radiation excites atoms through photo-excitation and consequently results in spontaneous emissions. Occupations of the atoms on different levels of the ground state will alter when there exists anisotropic radiation field. Magnetic realignment will redistribute the angular momenta of the atoms due to fast magnetic precession, which only happens on the ground state in general ISM and IGM (see Yan & Lazarian 2012, 2015 for details). The equations to describe the evolution on upper and lower levels are (see Landolfi & Landi Degl’Innocenti 1986; Landi Degl’Innocenti & Tielens 2004):

\[ \rho^k_{q}(J_0) + 2\pi i \nu L_{\text{Eu}} q q^k_{J_0}(J_0) = - \sum_{J_1} A(J_0 \rightarrow J_1) \rho^k_{q}(J_1) + \sum_{J_1}[J_1] \]

\[ \times \left[ \delta_{kk'} \rho^k_{q}(J_0) B_{lu} J_0^0 + \sum_{Qq'} \rho_{kk'}(J_0, J_1; Q, q') B_{lu} J_0^2 \right] \rho^{k'}_{q'}(J_1), \tag{A1} \]

\[ \rho_{q}^{k}(J_1) + 2\pi i \nu L_{\text{Eu}} q q_{J_1}(J_1) = - \sum_{J_0} \rho_{q}^{k}(J_0, J_1) A(J_0 \rightarrow J_1) \rho_{q}^{k}(J_0) \]

\[ - \sum_{J_1 k' q'} \left[ \delta_{kk'} B_{lu} J_1^0 + \sum_{Qq'} s_{kk'}(J_0, J_1; Q, q') B_{lu} J_1^2 \right] \rho^{k'}_{q'}(J_1). \tag{A2} \]

in which

\[ p_l(J_0, J_1) = (-1)^{J_0 + J_1 + 1} \left\{ \begin{array}{ccc} J_l & J_1 & k \\ J_u & J_u & 1 \end{array} \right\}, \]

\[ p_0(J_0, J_1) = \frac{1}{\sqrt{[J_u, J_1]}}, \]

\[ r_{kk'}(J_0, J_1, Q, q, q') = (3[k, k', 2])^{\frac{1}{2}} \left\{ \begin{array}{ccc} 1 & J_0 & J_1 \\ 1 & J_1 & J_1 \\ 2 & k & k' \end{array} \right\} \left\{ \begin{array}{ccc} q & q & K \\ q' & q' & Q \end{array} \right\}, \]

\[ s_{kk'}(J_0, J_1, Q, q, q') = (-1)^{J_0 + J_1 + 1} [J_l][3[k, k', K])^{\frac{1}{2}} \]

\[ \times \left\{ \begin{array}{ccc} k & k' & 2 \\ J_l & J_0 & J_1 \\ J_1 & J_1 & J_1 \end{array} \right\} \left\{ \begin{array}{ccc} 1 & 1 & 2 \\ J_0 & J_1 & J_1 \end{array} \right\} \left\{ \begin{array}{ccc} k & k' & 2 \\ J_l & J_0 & J_1 \end{array} \right\}. \tag{A3} \]

The quantities $J_0$ and $J_1$ are the total angular momentum quantum numbers for the upper and lower levels, respectively. The quantities $\rho^k_{q}$ and $\rho^k_{Q}$ are irreducible density matrices for the atoms and the incident radiation, respectively. 6–$j$ and 9–$j$ symbols are represented by the matrices with “$\text{ cycl}$”, whereas 3–$j$ symbols are indicated by the matrices with “$\text{ Mag}$” (see Zare & Harter 1989 for details). The second terms on the left side of Eq. (A1) and Eq. (A2) stand for the magnetic realignment. The two terms on the right side represent spontaneous emissions and the excitations from lower levels. Note that the symmetric processes of spontaneous emission and magnetic realignment conserve $k$ and $q$. Therefore, the steady state occupations of atoms on the ground state are obtained by setting the left side of Eq. (A1) and Eq. (A2) zero:

\[ 2\pi i \rho^k_{q}(J_1) q \| v L - \sum_{J_0} \rho^k_{q}(J_0, J_1) \frac{[J_n]}{\sum J_n} A'/A + i\Gamma' q \]

\[ \times \sum_{J_0} B_{lu}[J_0] \left[ \delta_{kk'} \rho^k_{q}(J_0, J_1) J_0^0 + \sum_{Qq'} r_{kk'}(J_0, J_1; Q, q') J_0^2 \right] \rho^{k'}_{q'}(J_1) \]

\[ - \delta_{J_0 J_1} \left[ \delta_{kk'} B_{lu} J_1^0 + \sum_{Qq'} B_{lu} s_{kk'}(J_0, J_1; Q, q') J_1^2 \right] \rho^{k'}_{q'}(J_1) = 0 \tag{A4} \]

where $\Gamma'$ equals $2\pi \nu L_{\text{Eu}} A'/A$. Magnetic realignment on the levels in excited states can be neglected because the spontaneous emission rate from the excited states is much higher than magnetic precession rate in diffuse ISM and IGM. As a result, $\Gamma' \simeq 0$. On the other hand, the magnetic precession rate is much higher than the photo-excitation rate of the atoms on the ground state in the diffuse media of ISM and IGM ($\nu L \gg B_{lu} J_0^0$). Thus, Eq. (A4) is making sense only when $q = 0$ so that the first term on the left equals 0. By solving the above equations, the atomic density tensors on different levels ($\rho^k_{q}(J_1), \rho^k_{Q}(J_0)$) under the influence of atomic alignment are obtained.

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\[ \text{Influence of atomic alignment on spectroscopy} \]