Study Turbulence and Probe Magnetic Fields Using the Gradient Technique: Application to H\textsubscript{1}-to-H\textsubscript{2} Transition Regions

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Abstract

The atomic-to-molecular (H\textsubscript{1}-to-H\textsubscript{2}) transition in photodissociation regions (PDRs) has been investigated over the past several decades through analytic and numerical modeling. However, classical PDR models typically assume a uniform-density gas, ignoring the turbulent nature of the interstellar medium. Recently, Bialy et al. have presented a theoretical framework for studying the H\textsubscript{1}-to-H\textsubscript{2} transition in a realistic turbulent medium with a nonhomogeneous density structure. Here we extend these turbulent-chemical models to explore the possibility of tracing the magnetic field direction in turbulent PDRs using the gradient technique. We utilize both subsonic and supersonic magnetohydrodynamic numerical simulations for chemical H\textsubscript{1}/H\textsubscript{2} balance calculations. We confirm that the density fluctuations induced by turbulence can disperse the distribution of the H\textsubscript{2} and H\textsubscript{1} fractions. We find that the energy spectrum of moment maps gets shallower when the sonic Mach number \(M_s\) increases. We explore the ability in magnetic field tracing of gradients of higher-order velocity centroids and compare their performance with that of traditional velocity centroid gradients (VCGs) and with intensity gradients (IGs). We find that the velocity gradients of the second-order centroids (VC\textsubscript{2}Gs) are more accurate than VCGs and IGs in probing the magnetic field orientation.

Unified Astronomy Thesaurus concepts: Interstellar medium (847); Interstellar magnetic fields (845); Interstellar dynamics (839)

1. Introduction

Photodissociation regions (PDRs) are regions in the interstellar space, typically at the boundaries of molecular clouds, where the far-ultraviolet (FUV) radiation plays a dominant role in photodissociating molecules and heating the gas (Hollenbach & Tielens 1999). Owing to dust absorption and H\textsubscript{2} self-shielding, the FUV is attenuated with increasing depth into a PDR and the gas undergoes a transition from atomic to molecular (H\textsubscript{1} to H\textsubscript{2}) form (e.g., Goldsmith et al. 2007; Krumholz et al. 2008; Hollenbach et al. 2009; Sternberg et al. 2014; Bialy et al. 2015, 2017a; Balashev & Kosenko 2020). The conversion to molecular form is critical for the formation of other molecules that are used as important observational tracers of the ISM (Herbst & Klemperer 1973; Sternberg & Dalgarno 1995; Tielens 2013; van Dishoeck 2015; Bialy & Sternberg 2015). The PDRs in the interstellar medium (ISM) are threaded by both magnetic field and turbulence (Larson 1981; Elmegreen & Scalo 2004; Ballesteros-Paredes et al. 2007; McKee & Ostriker 2007; Chepurnov & Lazarian 2010). There, magnetic field and turbulence play crucial roles in regulating molecules’ formation, controlling the heat transfer, and constraining star formation (Parker 1965; Jokipii 1966; Parker 1979; Li & Henning 2011; Hull et al. 2013; Capiroli & Spitkovsky 2014). For instance, the high-density contrast and filaments created by supersonic turbulence serve as the nurseries for new stars (Mac Low & Klessen 2004; McKee & Ostriker 2007; Federrath et al. 2010; Hu et al. 2020b).

In addition to turbulence, observational measurement of the magnetic field presents a big challenge. The primary ways to probe the magnetic fields in ISM include the measurements of polarized dust emission (Andersson et al. 2015; Fissel et al. 2016), stellar light polarization (Heiles 2000; Panopoulou et al. 2015), the molecular-line splitting Zeeman effect (Crutcher et al. 2010; Crutcher 2012), and the Faraday rotation (Oppermann et al. 2012). There are, however, difficulties when studying the magnetic field through dust polarimetry. For one, the stellar light polarization can only sample the magnetic fields in the direction toward stars producing discrete magnetic field morphology (Mathewson & Ford 1970; Goodman et al. 1990; Panopoulou et al. 2019). Also, the measurement of dust polarimetry is generally difficult, since the grain alignment efficiency drops significantly in the case of high optical depth, limiting the reliability of tracing the magnetic field in optically thick regions (Lazarian & Hoang 2007; Andersson et al. 2015). The Zeeman measurement only gives the signed magnetic field strength along the line of sight (LOS) and requires exceptionally high sensitivity and long integration times. As for Faraday rotation, it measures the electron-density-weighted magnetic field strength along the LOS and, therefore, generally does not probe the magnetic field in primarily neutral regions such as molecular clouds.

Nevertheless, the gradient technique (GT) has been developed as a promising way for studying the magnetic fields across multiple scales in the ISM (González-Casanova & Lazarian 2017; Yuen & Lazarian 2017a; Lazarian & Yuen 2018a; Hu et al. 2018). GT utilizes the advancements of MHD turbulence theory and turbulent reconnection (Goldreich & Sridhar 1995; Lazarian & Vishniac 1999), in particular, the prediction that turbulent eddies are elongated in the direction of the magnetic field surrounding the eddy, i.e., the local magnetic field. This theoretical prediction is reliably supported by numerical simulations (Cho & Vishniac 2000; Maron & Goldreich 2001). Cho et al. (2002) offer the conclusion that both gradients of density and velocity amplitude are perpendicular to the local
direction of the magnetic field. Therefore, the magnetic fields can be probed by rotating the gradients by 90° using spectroscopic information.

GT has been widely tested in numerical simulation and observation, spanning from diffuse transparent atomic gas (González-Casanova & Lazarian 2019; Hu et al. 2020c) to molecular self-absorbing dense gas (Hsieh et al. 2019; Hu et al. 2019a, 2019c; Alina et al. 2020). Several studies also extend the GT to estimate the magnetization level (Lazarian et al. 2018a) and the sonic Mach number (Yuen & Lazarian 2020), distinguishing shocks (Hu et al. 2019b), and identifying the self-gravitating regions in molecular clouds (Hu et al. 2020b). GT can employ either the density gradient or the velocity gradient. However, the statistics of density in supersonic turbulence can significantly differ from velocities (Beresnyak et al. 2005; Kowal et al. 2007). Nevertheless, the study in Beresnyak et al. (2005) revealed that for most of the supersonic turbulent volume, the density passively follows the velocity fluctuations, the notable exceptions being shocks. Thus, we expect that for subsonic and a significant portion of the supersonic turbulent volume, the density gradients will behave similarly to the gradients of velocity. This constitutes the theoretical justification of intensity gradients (IGs; Hu et al. 2019b) that we also employ in this paper.

The challenge that we address here is related to the application of the GT to PDRs. For instance, for the PDRs at the cloud boundaries, the anisotropic properties of turbulence might be distorted by the transition from atomic gas to molecular gas. Therefore, it is essential to study the effect of turbulence on the chemical structure of interstellar clouds and the performance of the GT in PDRs. In this work, we focus on the turbulence’s properties of H1-to-H2 transition produced by photodissociation at the cloud boundaries (Bialy et al. 2017b, 2019). We generate synthetic H1 and H2 cubes in chemical balance by post-processing numerical MHD simulations.

For extracting the density information, we employ the intensity map (i.e., moment-0 map, Yuen & Lazarian 2017b; Hu et al. 2019b), the velocity centroid map (i.e., moment-1 map; González-Casanova & Lazarian 2017; Yuen & Lazarian 2017a), and the velocity channel map (Lazarian & Yuen 2018a) to obtain the velocity information in spectroscopic data. In this work, we explore the ability of gradients of higher-order centroids to trace the magnetic field. In particular, we use the gradients of second-order velocity centroids, which we term VC2Gs, to distinguish from the traditional velocity centroid gradients (VCGs). We use this modification to trace the magnetic field and make a comparison with the one obtained from moment-0 and moment-1 maps.

In what follows, we illustrate the theoretical foundation of the GT in terms of MHD turbulence in Section 2. We give details about the analytical model of the H1-to-H2 transition and the numerical simulations used in this work in Section 3. In Section 4, we describe the full algorithm in probing the magnetic fields through GT. In Section 5, we analyze the properties of turbulence in PDRs through the energy spectrum and structure function. We compare the ability of the GT to trace the magnetic field using different moment maps. In Sections 6 and 7, we give our discussion and conclusions.

2. Theoretical Consideration

2.1. MHD Turbulence Theory

MHD turbulence theory is at the GT’s foundations, and it capitalizes on the advancements of this theory. The understanding that MHD turbulence is anisotropic came through theoretical and numerical work several decades ago (Montgomery & Turner 1981; Matthaeus et al. 1983; Shebalin et al. 1983; Higdon 1984). In this section, we briefly explain the basic elements of the theory that are essential for understanding the GT. An in-depth discussion of the properties of MHD turbulence can be found in the monograph by Beresnyak & Lazarian (2019).

A crucial boost to the theory of MHD turbulence was given by Goldreich & Sridhar (1995, hereafter GS95). GS95 explicitly derived that the turbulence eddies are elongating along the magnetic field, showing the scaling relation

\[ k_\perp \propto (k_\parallel)^{2/3}, \]

where \( k_\perp \) and \( k_\parallel \) are wavenumbers perpendicular and parallel to the magnetic field, respectively. The cornerstone of the GS95 theory is the concept of a “critical balance” between parallel and perpendicular timescales \( k_\parallel v_\perp \sim k_\perp v_\parallel \), where \( v_\parallel \) is the rms speed of turbulence at the scale \( l \) and \( V_A \) is the Alfvénic speed. However, the GS95 anisotropy scaling is derived in the global, i.e., mean magnetic field, reference frame, in which the predicted scaling is not valid. To understand the actual dynamics, it is useful to consider the eddy-based picture of strong MHD turbulence that is based on the concept of turbulent reconnection. Lazarian & Vishniac (1999, hereafter LV99) demonstrated that the turbulent reconnection process is fast and the timescale for the reconnection of the corresponding eddies equal to the eddy turnover time. This result meant that turbulent motions were not constrained by fluid motion perpendicular to the local magnetic field. Therefore, one can conclude that hydrodynamic-type eddy motions are not affected by magnetic field back-reaction if the eddy rotations are aligned with the direction of the magnetic field surrounding the eddy.

For our present, the latter is the fundamental property at the foundation of the GT. In other words, the alignment of eddies with the local magnetic field means that if we detect the eddy’s preferential rotation direction, we can determine the magnetic field direction at the eddy location. Therefore, using velocity gradients, one can map the magnetic field direction in turbulent media.

Continuing with our picture of MHD turbulence as a collection of eddies aligned with the magnetic field, we can

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5 The symmetry of Alfvénic perturbations in terms of velocity and magnetic field entails that the magnetic fluctuations also share the same property. This gave rise to the development of the magnetic field tracing based on synchrotron intensity gradients (SGGs; Lazarian et al. 2018b) and synchrotron polarization gradients (SPGs; Lazarian & Yuen 2018b). We do not discuss these promising techniques in this paper.

6 The IGs should not be confused by the histogram of relative orientations (HRO) proposed by Soler et al. (2013). While both techniques employ IGs, the IGs use the set of procedures from the velocity gradient technique (VGT) to obtain the magnetic field direction. On the contrary, the HRO gets the magnetic field via polarization measurements and compares those with the magnetic field in order to determine a critical density at which the change of the gradients and polarization occurs in molecular clouds. A detailed comparison of IGs and HRO is presented in Hu et al. (2019b).
state that turbulent cascade, which gets minimal resistance for the mixing perpendicular to the magnetic field, directs most of the cascading energy. In this case, the critical balance is the natural consequence of equality of the time of eddy turnover: $l_\perp/v_L$ and the period of the Alfvén wave $l_\parallel/V_A$. Note that we use notations $l_\parallel$ and $l_\perp$ and not wavenumber notation. This is to stress that the measurements are done in the local reference system and not the reference system related to the mean field.

Incidentally, for the calculations in LV99 provided for Alfvén Mach number $M_A < 1$, where $M_A$ is the ratio of the injection velocity $V_{inj}$ to the Alfvén speed $V_A$, the relation between the parallel and perpendicular scales of the eddies is as follows:

$$ l_\parallel \simeq L_{inj} \left( \frac{l_\perp}{L_{inj}} \right)^{2/3} M_A^{1/3}. $$

where $L_{inj}$ is the injection scale of turbulence and $l_\perp$ denotes the eddies’ scale perpendicular to the magnetic field. Note that this scaling relation is measured in the eddies’ local reference frame, rather than the mean magnetic field used in GS95. This universal scale-dependent anisotropy of Alfvénic turbulence in the local magnetic field reference frame has been demonstrated in Cho & Vishniac (2000), Cho et al. (2002), and Maron & Goldreich (2001). Indeed, the local system of reference is critical for understanding the GT. For tracing the magnetic field using either density or velocity field, it is essential that the density fluctuation or velocity fluctuation is oriented with respect to the local magnetic field’s direction, instead of the global mean magnetic field; see Figure 1.

Combining Equation (2) and the “critical balance” expressed in the local reference frame, i.e., $l_\parallel V_A \sim l_\perp v_L$, one can get the scaling relation for velocity fluctuations (see LV99):

$$ v_L \simeq v_L \left( \frac{l_\perp}{L_{inj}} \right)^{1/3} M_A^{1/3}. $$

where $v_L$ is the injection velocity of turbulence. By taking the square on both sides, Kolmogorov’s scaling relation $v_L^2 \propto (l_\perp)^{2/3}$ is recovered.

The fluctuation induced by turbulence is more complicated in terms of the stochastic density field. Cho & Lazarian (2003) derived that the density $\rho_k$ of the eddy at scale $k$ in Fourier space can be expressed as

$$ |\rho_k| = \frac{\rho_0 v_L}{c} |\hat{k} \cdot \hat{\zeta}|, $$

where $\rho_0$ is the mean density; $\hat{\zeta}$ is the unit vector for the Alfvénic mode, fast mode, or slow mode; $c$ is the propagation speed of the corresponding mode; and $v_L$ is the turbulence’s velocity at scale $k$ in Fourier space. The density fluctuation $\rho_k$ in real space is therefore obtained from the inverse Fourier transform:

$$ \rho_l = \mathcal{F}^{-1}(\rho_k) = \frac{\rho_0 v_L}{c} \mathcal{F}^{-1}(|\hat{k} \cdot \hat{\zeta}|). $$

Explicitly, since the anisotropic relation indicates $l_\parallel \ll l_\perp$, the velocity gradient and density gradient scale as (Yuen & Lazarian 2020; Hu et al. 2020a).
\[ \nabla \rho_l \propto \frac{\rho_l}{l_z} \propto \frac{\rho_l}{c} \mathcal{F}^{-1}(\mathbf{k} \cdot \mathbf{\xi}) \nabla v_l \]
\[ \nabla v_l \propto \frac{v_l}{l_{\text{inj}}} \left( \frac{l_z}{l_{\text{inj}}} \right)^{-\frac{3}{2}} M_t \]
\[ \nabla v_l^2 \propto \frac{v_l^2}{l_{\text{inj}}} \left( \frac{l_z}{l_{\text{inj}}} \right)^{-\frac{3}{2}} M_t^2. \]

The gradients induced by both velocity and density fluctuations increase, respectively, as \( v_l/l_z \sim t^{-2/3} \) and \( \rho_l/l_z \sim t^{-2/3} \). The direction of gradients is perpendicular to the local directions of the magnetic field (Maron & Goldreich 2001; Cho & Vishniac 2000). Also, this means that the smallest eddies resolved in observations provide important contributions for the gradients. This consideration is at the core of the GT.

2.2. Gradient of Moment Maps

In observation, the gas distribution in a given spectral line is defined in position–position–velocity (PPV) cubes toward some direction on the sky and at a given LOS velocity \( v \), rather than in the real space \( \vec{r} = (x, y, z) \). The LOS component of velocity \( v \) at the position \( (x, y) \) is a sum of the turbulent velocity \( \mu(\vec{r}) \) and the residual component due to thermal motions. This residual thermal velocity \( v - \mu(\vec{r}) \) has a Maxwellian distribution:

\[ \Phi(v - \mu(\vec{r})) = \frac{1}{\sqrt{2\pi \beta(\vec{r})}} \exp \left[ -\frac{(v - \mu(\vec{r}))^2}{2\beta(\vec{r})} \right], \]  

where \( \beta(\vec{r}) = k_B T(\vec{r})/m \), with \( m \) being the mass of atoms. The temperature \( T(\vec{r}) \) depends on point to point if the emitter is not isothermal.

The relation between the gas distribution \( \rho(x, y, v) \) in PPV cubes and \( \rho(\vec{r}) \) in real space is given by Lazarian & Pogosyan (2004):

\[ \rho(x, y, v) = \int \rho(\vec{r}) \Phi(v - \mu(\vec{r})) d\vec{r}, \]  

where \( \Phi(v - \mu(\vec{r})) \) is the Maxwell distribution of the thermal component of LOS velocity and \( \mu(\vec{r}) \) is the LOS turbulent velocity.

For the gas distribution \( \rho(x, y, v) \), we can define the moment-0 map \( f_0(x, y) \) (i.e., the intensity or the average intensity) and the moment-\( n \) map \( f_n(x, y) \) as

\[ f_0(x, y) = \int \rho(x, y, v) dv = \int \rho(\vec{r}) d\vec{r} \int \Phi(v - \mu(\vec{r})) dv \]  
\[ = \int \rho(\vec{r}) d\vec{r}, \quad f_n(x, y) = \int v^n \rho(x, y, v) dv \int \rho(x, y, v) dv, \quad n \geq 1. \]

The moment corresponding to \( n = 1 \) is called the “velocity centroid,” representing the averaged LOS velocity when density is constant. The constructions with \( n > 1 \) will call “higher-moment centroids.”

Applying the gradient operator \( \nabla_{2D} = \left( \frac{\partial}{\partial y}, \frac{\partial}{\partial x}, 0 \right)^T \) to \( f_0(x, y) \), the gradient amplitude can be expressed as (Yuen & Lazarian 2020)

\[ |\nabla_{2D} f_0(x, y)| \propto \int |\nabla_{2D} \rho(\vec{r})| d\vec{r} \]
\[ = \langle |\nabla_{2D} \rho(\vec{r})| \cos \gamma \rangle \sqrt{N l_{\text{inj}}^2}, \]

in which we assume that there are \( N = L/l_{\text{inj}} \) eddies along the LOS with distance \( L \) and the density gradient follows a random walk summation. \( \langle \cdots \rangle \) denotes the average value, the 3D gradient operator is \( \nabla_{3D} = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)^T \), and \( \gamma \) is the relative angle between the gradient and the plane-of-the-sky (POS) with \( \cos \gamma = |\nabla_{2D} \rho(\vec{r})|/|\nabla_{3D} \rho(\vec{r})| \). Note that this summation of gradient amplitude as random walk is only valid when \( \tan(\gamma/4) > M_t/\sqrt{3} \) (Lazarian et al. 2020). The direction of the gradient is then

\[ \nabla_{2D} f_0(x, y) = U \cdot \sum_{i=1}^N \nabla_{3D} \rho_i(\vec{r}), \]  

where \( U \) is the projection operator:

\[ U = \begin{pmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \]

The direction of \( \nabla_{2D} f_0(x, y) \) is therefore the vector summary of the density gradient along the LOS. As for the moment-\( n \) map \( f_n(x, y) \), in the limit of constant density distribution, \( f_n(x, y) \) provides the value of \( \mu(\vec{r})^n \) averaged along the LOS. In particular, for moment-1 and moment-2 maps, we have

\[ f_1(x, y) = \int \rho(\vec{r}) d\vec{r} \int v \Phi(v - \mu(\vec{r})) dv \int \rho(z) d\vec{r} \propto \int \rho(\vec{r}) \mu(\vec{r}) d\vec{r} \int \rho(\vec{r}) d\vec{r} \]
\[ f_2(x, y) = \int \rho(\vec{r}) d\vec{r} \int v^2 \Phi(v - \mu(\vec{r})) dv \int \rho(\vec{r}) d\vec{r} \propto \int \rho(\vec{r}) \mu^2(\vec{r}) d\vec{r} \int \rho(\vec{r}) d\vec{r}. \]

Note that if we consider also the regular gas flow due to Galactic rotation \( v_{\text{gal}}(\vec{r}) \), the residual thermal velocity becomes \( v - v_{\text{gal}}(\vec{r}) - \mu(\vec{r}) \), which has a Maxwellian distribution. This introduces one more velocity term \( \int \frac{\rho(\vec{r}) v_{\text{gal}}(\vec{r}) d\vec{r}}{\rho(\vec{r}) d\vec{r}} \) to \( f_1(x, y) \) and \( \frac{\int \rho(\vec{r}) v_{\text{gal}}^2(\vec{r}) d\vec{r}}{\rho(\vec{r}) d\vec{r}} \) to \( f_2(x, y) \), which can be considered as constant for an individual cloud owing to the little variation in \( v_{\text{gal}}(\vec{r}) \).

As shown in Figure 2, we produce a synthetic PPV cube from the MHD simulation A3 (see Section 3 for details), using a unity density field while keeping the original velocity field \( M_{\text{S}} = 10.54 \) unchanged. We calculate three moment maps from the PPV cube and project the density field \( \rho(\vec{r}) \) and velocity field \( \mu(\vec{r}) \) along the z-axis. We find that moment maps...
exhibit very similar structures to the projected density and velocity maps. In particular, these structures are elongating along the magnetic field. This agrees with our theoretical consideration. In the rest of the paper, when we study the various moment projections in H I-to-H2 gas, we take into account fluctuations in both the density and the velocity.

The gradients of corresponding $f_1(x, y)$ and $f_2(x, y)$ can be written as

$$
\nabla_{2D} f_1(x, y) \propto \frac{\int \nabla_{2D}[\rho(\vec{r})\mu(\vec{r})]d\vec{r} - f_1(x, y) \int \nabla_{2D}\rho(\vec{r})d\vec{r}}{f_0} = \frac{U}{f_0} \sum_{i=1}^{N} \left[ (\mu_i - f_1)\nabla_{3D}\rho_i + \rho_i\nabla_{3D}\mu_i \right],
$$

$$
\nabla_{2D} f_2(x, y) \propto \frac{\int \nabla_{2D}[\rho(\vec{r})\mu^2(\vec{r})]d\vec{r} - f_2(x, y) \int \nabla_{2D}\rho(\vec{r})d\vec{r}}{f_0} = \frac{U}{f_0} \sum_{i=1}^{N} \left[ (\mu_i^2 - f_2)\nabla_{3D}\rho_i + \rho_i\nabla_{3D}\mu_i^2 \right].
$$

The subscript $i$ indicates the variable of the $i$th eddy. The directions of $\nabla_{2D} f_1(x, y)$ and $\nabla_{2D} f_2(x, y)$ consist of the contribution from both density and velocity field. In the limit of constant density distribution, the density gradient can be erased, but only the velocity gradient gives a contribution. Note that in the case of a large-scale study in which $v_{\text{gal}}(\vec{r})$ cannot be assumed as constant, one has to consider the gradients of the $v_{\text{gal}}(\vec{r})$ term. Nevertheless, considering the flux freezing condition, the magnetic field is expected to follow the radial direction of regular gas flow caused by Galactic rotation. Coincidentally, the gradients, in this case, are still perpendicular to the magnetic field, showing a different scaling relation from Equation (6). Similarly, the gradient amplitude is summed in a random walk manner:

$$
|\nabla_{2D} f_1(x, y)| \propto \frac{\sqrt{NL_{i_{\text{ij}}}}}{f_0} \left[ ((\mu - f_1)\nabla_{3D}\rho + \rho \nabla_{3D}\mu)\cos \gamma \right],
$$

$$
|\nabla_{2D} f_2(x, y)| \propto \frac{\sqrt{NL_{i_{\text{ij}}}}}{f_0} \left[ ((\mu^2 - f_2)\nabla_{3D}\rho + \rho \nabla_{3D}\mu^2)\cos \gamma \right].
$$

Note that here we assume that the density gradient and velocity gradient exhibit the same relative angle $\gamma$ with respect to the POS, as both gradients are perpendicular to the magnetic field. Following similar steps, we can extend the calculation to the unnormalized moment maps $F_n(x, y)$:

$$
F_1(x, y) = \int v\rho(x, y, v)dv \propto \int \rho(\vec{r})\mu(\vec{r})d\vec{r},
$$

$$
F_2(x, y) = \int v^2\rho(x, y, v)dv \propto \int \rho(\vec{r})\mu^2(\vec{r})d\vec{r}.
$$

$$
\nabla_{2D} F_1(x, y) \propto U \cdot \sum_{i=1}^{N} \left[ (\mu_i\nabla_{3D}\rho_i + \rho_i\nabla_{3D}\mu_i) \right],
$$

$$
\nabla_{2D} F_2(x, y) \propto U \cdot \sum_{i=1}^{N} \left[ (\mu_i^2\nabla_{3D}\rho_i + \rho_i\nabla_{3D}\mu_i^2) \right],
$$

$$
|\nabla_{2D} F_1(x, y)| \propto \sqrt{NL_{i_{\text{ij}}}} \left[ ((\mu\nabla_{3D}\rho + \rho \nabla_{3D}\mu)\cos \gamma \right],
$$

$$
|\nabla_{2D} F_2(x, y)| \propto \sqrt{NL_{i_{\text{ij}}}} \left[ ((\mu^2\nabla_{3D}\rho + \rho \nabla_{3D}\mu^2)\cos \gamma \right].
$$
Comparing with Equation (13), we can see that the magnitude of the density gradient is suppressed in the normalized moment maps. Nevertheless, as we discussed in Section 2.1, for incompressible turbulence, the scaling of the density gradient is similar to that of the velocity gradient (see Equation (6)). Therefore, we can expect that the gradient of moment maps exhibits exactly the velocity gradient properties in the incompressible limit, i.e., the direction of moment maps’ gradients is expected to be perpendicular to the projected magnetic field.

A particular case for GT is the presence of strong shocks. The density gradient is preferentially perpendicular to the shock front owing to the rapid jump of density and velocity. Coincidentally, the magnetic field tends to be perpendicular to the shock front as well in the ISM (Xu et al. 2019). It results from the shock waves propagating along the magnetic field. The magnetic field suppresses the compression in the perpendicular direction so that the fluid presidency follows the magnetic field line. Therefore, the shock compression in supersonic turbulence produces the perpendicular structures. Consequently, the density gradient becomes parallel to the magnetic field, instead of being perpendicular (Yuen & Lazarian 2017b; Hu et al. 2019b). As for the velocity gradient, the situation changes. As shown in Figure 2, the projected supersonic velocity field is still parallel to the magnetic field, rather than being perpendicular. The corresponding velocity gradient is always perpendicular to the magnetic field in both the subsonic and supersonic environments.

We know that $\nabla_2D_f(x, y)$ consists of only density gradient; see Equation (11). The gradient of moment 0 is, therefore, sensitive to shocks. However, from Equation (13), we know that $\nabla_2D_f(x, y)$ and $\nabla_2D_f(x, y)$ are projected from the summation of 3D velocity and density gradients along the LOS. To see this change of the gradient’s direction requires the shock to be strong enough so that the density’s contribution gets dominated.

### 3. Numerical Data

#### 3.1. MHD Simulations

We perform 3D MHD simulations through the ZEUS-MP/3D code (Hayes et al. 2006), which solves the ideal MHD equations in a periodic box. We use single-fluid, operator-split, solenoidal turbulence injections and a staggered grid MHD Eulerian assumption. To emulate a part of an interstellar cloud, we use the barotropic equation of state, i.e., these clouds are isothermal with temperature $T = 50.0$ K, sound speed $c_s = 0.42$ km s$^{-1}$, and cloud size $L = 10$ pc. The sound-crossing time $t_s = L/c_s$ is $\sim 23.2$ Myr, which is fixed owing to the isothermal equation of state. This allows a natural extension of the isothermal H-I to H$_2$ transition model proposed in Sternberg et al. (2014) and Bialy & Sternberg (2016) into the turbulent regime, similarly to the Bialy et al. (2017b, 2019) turbulent-chemical model.

MHD turbulence is characterized by sonic Mach number $M_s = \nu_l/c_s$ and Alfvénic Mach numbers $M_A = \nu_l/v_A$, where $\nu_l$ is the injection velocity and $v_A$ is the Alfvénic velocity. The turbulence is highly magnetized when the plasma’s magnetic pressure is larger than the thermal pressure, i.e., $M_A < 1$. The compressibility of turbulence is characterized by $\beta = 2\left(\frac{M_A}{M_s}\right)^2$.

We refer to the simulations in Table 1 by their model name. For instance, our figures or captions will have the model name indicating which data cube is used to plot the figure. As indicated in Table 1, all the simulations are highly compressible, so that the supersonic simulations ($M_s > 1$) develop strong density fluctuations. As we discuss below, these density fluctuations result in fluctuations in the abundances of H$_1$ and H$_2$ in the turbulent boxes.

#### 3.2. H$_1$ and H$_2$ Chemical Balance

At any cloud depth and for unidirectional radiation normal to the cloud surface, the H$_2$ formation—destruction steady-state balance is given by

$$R_{\text{HI}H_2} = \left(\frac{D_0}{2}\sigma_{\text{shield}}(N_{\text{HI}})e^{-\alpha N} + \zeta\right)x_{\text{HI}}.$$  \hspace{1cm} (16)

The left-hand side represents H$_2$ formation out of atomic H, where $R$ (cm$^3$ s$^{-1}$) is the H$_2$ formation rate coefficient, $n = n_{\text{H}} + 2n_{\text{H}_2}$ is the hydrogen nucleus volume density, and $x_{\text{HI}} \equiv n_{\text{HI}}/n$ and $x_{\text{H}_2} \equiv n_{\text{H}_2}/n$ are the H and H$_2$ relative abundances. The right-hand side represents H$_2$ destruction. The first term accounts for destruction by photodissociation, where $D_0$ (s$^{-1}$) is the free-space H$_2$ photodissociation rate, $\sigma_{\text{shield}}$ is the H$_2$ self-shielding function that depends on the accumulated H$_2$ column density $N_{\text{HI}}$ from the cloud edge to the point of interest, and $e^{-\alpha N}$ is the dust absorption attenuation term, where $\alpha$ (cm$^2$) is the dust absorption cross section per hydrogen nucleus integrated over the Lyman–Werner dissociation band (11.2–13.6 eV) and $N = N_{\text{HI}} + 2N_{\text{H}_2}$ is the total (atomic plus molecular) column density. The factor of 1/2 accounts for the absorption of half the radiation by the optically thick slab. The second term on the right-hand side of Equation (16) accounts for H$_2$ destruction by cosmic rays (through ionization that is followed up by a series of abstraction reactions and by recombination that leads to the formation of H; Bialy & Sternberg 2015), where $\zeta$ is the H$_2$ cosmic-ray ionization rate. Equation (16) is augmented by the mass conservation equation, $x_{\text{HI}} + 2x_{\text{H}_2} = 1$.

We calculate the H$_1$ and H$_2$ abundances in all the simulation boxes in the post-process, as follows. We use the density field from each simulation and calculate $x_{\text{HI}}$ and $x_{\text{H}_2}$ via Equation (16) assuming a unidirectional UV field and the standard parameter values: $D_0 = 5.8 \times 10^{-11}$ s$^{-1}$, $\zeta = 2 \times 10^{-16}$ s$^{-1}$, $R = 3 \times 10^{-17}$ cm$^3$ s$^{-1}$, and $\alpha = 1.9 \times 10^{-21}$ cm$^{-2}$. These values correspond to the local mean UV radiation field (Draine 1978), a standard dust-to-gas ratio, and H$_2$ formation rate in the cold neutral medium (CNM; Sternberg et al. 2014). For $f(N_{\text{HI}})$ we use Equation (37) from Draine & Bertoldi (1996). The H$_2$
abundances at different cloud depths are coupled through the H$_2$ self-shielding process.

To derive the H and H$_2$ abundances in each location, we follow a similar procedure to that in Bialy et al. (2017b, 2019). For each LOS (i.e., a pair of coordinates, $(x, y)$), we solve Equation (16) starting from cloud edge ($z = 0$) and progressively move inward. At the cloud edge, there is no attenuation, $f_{\text{shield}}(N_{\text{H}1})e^{-\sigma N} = 1$, and the H$1$ and H$_2$ abundances are readily given by Equation (16) (and the $x_{\text{H}1} + 2x_{\text{H}2} = 1$ constraint). We then make a (small logarithmic) step, $\Delta z$, into the cloud and calculate $x_{\text{H}1}$ and $x_{\text{H}2}$, where now the shielding is calculated with $N_z = n\Delta z X_{\text{H}1}$, $N = n\Delta z$. We continue this process until we reach the end of the simulation box, and we repeat it for all the LOSs. In each step, we interpolate the density as obtained from the MHD simulation onto the grid that is used for the calculation of the H$1$–H$_2$ balance (which is much finer and is logarithmic). Finally, we interpolate the resulting H$1$–H$_2$ abundances back onto the native simulation grid. In the conclusion of this process, we have $x_{\text{H}1}$ and $x_{\text{H}2}$ in each cell of each of the simulation boxes.

With increasing distance from cloud edge, the UV radiation is attenuated via dust absorption and absorption in the H$_2$ lines (i.e., H$_2$ self-shielding), and the gas undergoes a transition from atomic to molecular state. Following Bialy & Sternberg (2016), for a uniform-density gas, the H$1$-to-H$_2$ transition occurs at a column density

$$N_{\text{tran}} = 3.7 \times 10^{20} \ln \left[1 + \left(\frac{n}{59 \text{ cm}^{-3}}\right)^{-0.7}\right] \text{cm}^{-2}, \quad (17)$$

where we evaluated Equations (22) and (39) of Bialy & Sternberg (2016) assuming the standard parameter values. Because the H$1$–H$_2$ balance depends on the gas density, in a supersonic turbulent medium the transition point varies between sight lines, due to the strong density fluctuations (see, e.g., Figure 5 in Bialy et al. 2017b). Thus, Equation (17) does not hold for supersonic turbulence; however, it is still useful as an analytic estimate for the typical depth into the simulation where the H$1$-to-H$_2$ transition occurs (with $n$ replaced with the mean density in the simulation, $\langle n \rangle$).

In this work, we set $\langle n \rangle = 50 \text{ cm}^{-3}$ for all simulations. The mean column density $\langle N \rangle$ and $N_{\text{tran}}$ are therefore $\approx 1.40 \times 10^{21} \text{ cm}^{-2}$ and $\approx 2.80 \times 10^{20} \text{ cm}^{-2}$, respectively. Thus, on the one hand, the simulations have a sufficiently large column density to allow an H$1$-to-H$_2$ transition for most of the sight lines, thus allowing us to study the statistics of both phases. On the other hand, the typical width of the transition zone is sufficiently large (with the simulation resolution of 792$^3$, the transition zone is of order $\sim 100$ cells), allowing us to resolve substructure in the H$1$ layers.

4. Methodology

4.1. Implementation of the Gradient Technique

The theory of intensity fluctuations in PPV space was pioneered in Lazarian & Pogosyan (2000), and later Lazarian & Pogosyan (2008) explored the possibility of using the statistics of intensity fluctuations in PPV cubes to study velocity turbulence. To detect the anisotropy of intensity and velocity fluctuations that are induced by the magnetic field in PPV cubes, GT usually employs a statistical description of either a moment-0 map or moment-1 map (González-Casanova & Lazarian 2017; Yuen & Lazarian 2017a; Hu et al. 2019b).

The moment-0 map $I(x, y)$ presents intensity map $I(x, y)$, as it contains the information of intensity fluctuations. The normalized moment-1 map $f_1(x, y)$ reflects the velocity fluctuations and is, as we mentioned earlier, denoted as the velocity centroid map $C(x, y)$. The intensity map and normalized velocity centroid map are calculated as follows:

$$I(x, y) = f_0(x, y) = \int \rho(x, y, v)dv, \quad C(x, y) = f_1(x, y) = \frac{\int \rho(x, y, v)vdv}{\int \rho(x, y, v)dv}, \quad (18)$$

where $\rho$ is the gas density and $v$ is the radial velocity along the LOS. The applicability of $I(x, y)$ and $C(x, y)$ in tracing the magnetic field has been widely tested in both numerical simulation (González-Casanova & Lazarian 2017; Yuen & Lazarian 2017a; Hu et al. 2019b) and observation (Hu et al. 2019a, 2020a). In this work, we further explore how to trace the magnetic field using the normalized moment-2 map, or second-order centroids $S(x, y)$:

$$S(x, y) = f_2(x, y) = \frac{\int \rho(x, y, v)v^2dv}{\int \rho(x, y, v)dv}. \quad (19)$$

In Figure 3, we present the spectral line of each map along the LOS using simulation A3. For moment 0, the spectral line as a function of the LOS velocity is simply the mean intensity in each corresponding channel. The spectral lines of moment 1 and moment 2 are the mean intensity weighted by the corresponding LOS velocity and squared velocity, respectively. Given the spectral line, $I(x, y)$ is effectively the integration over the entire line width carried out to find intensity. $C(x, y)$ constructs the velocity-weighted moment of intensity over the entire line width. Part of the intensity information is removed, as the weighting can give the opposite sign. As for $S(x, y)$, the intensity of the central line becomes zero through the weighting of squared velocity. It emphasizes only the intensity in the surrounding of central lines.

The pixelized gradient map $\psi(x, y)$, which denotes the angle of the gradients on the POS, of each moment map is calculated from the convolution of individual 2D maps with $3 \times 3$ Sobel
kernels $G_x$ and $G_y$: \(^7\)
\[
\begin{align*}
\nabla_x f(x, y) &= G_x * f(x, y) \\
\nabla_y f(x, y) &= G_y * f(x, y) \\
\psi(g(x, y)) &= \tan^{-1}\left(\frac{\nabla_y f(x, y)}{\nabla_x f(x, y)}\right),
\end{align*}
\]
where $f(x, y)$ represents $I(x, y)$, $C(x, y)$, or $S(x, y)$. $\nabla_x f(x, y)$ and $\nabla_y f(x, y)$ are the $x$ and $y$ components of the gradient, respectively. An asterisk denotes the convolution.

Note that the perpendicular relative orientation of gradients and magnetic field only appears when the gradient sampling is enough, as the anisotropy of turbulent eddies concerning the local magnetic field is a statistical concept. Therefore, the raw gradient map $\psi(g(x, y))$ is not necessarily required to have any relation to the local magnetic field direction. The critical step after getting $\psi(g(x, y))$ is taking the average of the gradients' orientation within a sub-block of interest, i.e., the sub-block averaging method, which is proposed by Yuen & Lazarian (2017a). Because the gradients' orientation within a sub-block forms a Gaussian distribution, the expectation value of the Gaussian distribution reflects the statistical most probable anisotropic gradient. Therefore, to probe the local magnetic field, we first draw the histogram of the gradients’ orientation and take the expectation value of the Gaussian fitting. By rotating the resulting gradient $\psi(g(x, y))$ by $90^\circ$, we output the predicted local mean magnetic field. Without specification, we automatically rotate the gradient by $90^\circ$ to align with the magnetic field in the following.

4.2. Velocity Fluctuation in the Thin Velocity Channel

In Section 2, we derived that the moment-0 map consists of a pure density contribution, while moment-1 and moment-2 maps can be used to obtain both density and velocity information. Nevertheless, Lazarian & Pogosyan (2000) presented an alternative way to extract the velocity fluctuations in PPV cubes through the effect of velocity caustics. There it was shown that the velocity fluctuations are most prominent when the channel is sufficiently thin, i.e., the channel width $\Delta v$ satisfies
\[
\begin{align*}
\Delta v < \sqrt{2\delta v^2}, & \quad \text{thin channel} \\
\Delta v \geq \sqrt{2\delta v^2}, & \quad \text{thick channel},
\end{align*}
\]
where $\delta v$ is the velocity dispersion calculated from the velocity centroid (Lazarian & Pogosyan 2000). Based on this theory, the thin velocity channel map has been employed to obtain the velocity gradient for magnetic field tracing, which is named velocity channel gradients (VChGs; Lazarian & Yuen 2018a). For VChGs, only the thin central channel $Ch(x, y)$ is selected for calculation:
\[
Ch(x, y) = \int_{v_0 - \Delta v/2}^{v_0 + \Delta v/2} \rho(x, y, v)dv,
\]
where $v_0$ is the velocity of the averaged emission line maximum. The validity of VChGs has been widely tested in both numerical and observational studies (Lazarian & Yuen 2018a; Hu et al. 2019a, 2019c; Hu et al. 2019b) also give a detailed comparison of IGs and VChGs. Later, instead of using only the thin central channel, Hu et al. (2020c) extend the calculation of the velocity gradient to all thin channels in the PPV cube. This calculation introduces the pseudo-Stokes parameters and the principal component analysis (PCA). The detailed recipe is presented in Hu et al. (2018) and Hu et al. (2020c). Here we give only a brief review. The PCA uses an orthogonal linear transformation to convert a set of possibly correlated variables to a set of linearly independent variables called principal components. For the implementation of PCA, the PPV cube $\rho(x, y, v)$ is assumed as a probability density function (pdf) of three random variables $(x, y, v)$. We first calculate the covariance matrix and its corresponding eigenvalue equation (Brun & Heyer 2002a, 2002b; Hu et al. 2018):
\[
M(v_i, v_j) = \int dx dy \rho(x, y, v_i) \rho(x, y, v_j) - \int dx dy \rho(x, y, v_i) \int dx dy \rho(x, y, v_j)
\]
\[
M \cdot \mathbf{u} = \lambda \mathbf{u},
\]
where $M$ is the covariance matrix with matrix element $M(v_i, v_j)$, with $i, j = 1, 2, \ldots, n_v$, $n_v$ is the number of channels in PPV cubes, and $\lambda$ are the eigenvalues associated with the eigenvector $\mathbf{u}$. The eigenvalues correspond to the weight of each principal component. If the eigenvalue is small, then the contribution from its corresponding principal component is also small. We can therefore enhance the contribution from crucial components by projecting the original data set into the new orthogonal basis formed by the eigenvectors (Hu et al. 2018, 2020c). The projection of the PPV cube into the new orthogonal basis is operated by weighting channel $\rho(x, y, v_j)$ with the corresponding eigenvector element $u_{ij}$, in which the corresponding eigenchannel $I_i(x, y)$ is
\[
I_i(x, y) = \sum_j n_v u_{ij} \rho(x, y, v_j).
\]
Through this projection, we have a total of $n_v$ eigenchannels in the PCA space. The recipe of the gradient’s calculation and the sub-block averaging method (see Section 4) are applied to each eigenchannel, so that we have the eigengradient fields $\psi_{gi}(x, y)$ with $i = 1, 2, \ldots, n_v$. In analogy to the Stokes parameters of polarization, the pseudo-$Q_g$ and pseudo-$U_g$ of gradient-inferred magnetic fields are defined as
\[
Q_g(x, y) = \sum_{i=1}^{n_v} I_i(x, y) \cos(2\psi_{gi}(x, y))
\]
\[
U_g(x, y) = \sum_{i=1}^{n_v} I_i(x, y) \sin(2\psi_{gi}(x, y))
\]
\[
\psi_g = \frac{1}{2} \tan^{-1}\left(\frac{U_g}{Q_g}\right).
\]

The pseudo-polarization angle $\psi_g$ is then defined correspondingly, which gives a probe of the plane-of-sky magnetic field orientation after rotating $90^\circ$. Note that in constructing the $Q_g(x, y)$ and $U_g(x, y)$, the number of used eigenchannels $n_v$ can

\(^7\) The Sobel kernels are defined as:
\[
G_x = \begin{vmatrix}
-1 & 0 & +1 \\
-2 & 0 & +2 \\
-1 & 0 & +1
\end{vmatrix}, \quad G_y = \begin{vmatrix}
-1 & -2 & -1 \\
0 & 0 & 0 \\
+1 & +2 & +1
\end{vmatrix}
\]
be less than \( n_v \). In Hu et al. (2018), it was shown that only the first 20 eigenchannels are most important, and other eigenchannels are negligible and more sensitive to noise. Nevertheless, we still consider all eigenchannels when constructing the pseudo-Stokes parameter in this work. We use the abbreviation VGT+PCA to represent this method (see Hu et al. 2020c for the full recipe).

4.3. Alignment Measure

To quantify the relative alignment between the magnetic fields and rotated gradient angle, we utilize the alignment measure (AM):

\[
\text{AM} = 2 \left( \cos^2 \theta_r \right) - \frac{1}{2},
\]

where \( \theta_r \) is the angular difference of two vectors, while \( \langle \ldots \rangle \) denotes the average within a region of interest. In the case of a perfect alignment of the magnetic field and gradient, we get \( \text{AM} = 1 \), i.e., we have a perfect global alignment between gradients and the POS magnetic field. \( \text{AM} = -1 \) indicates that global gradients are perpendicular to the POS magnetic field, and \( \text{AM} = 0 \) indicates a globally random correlation. The standard error of the mean gives the uncertainty \( \sigma_{\text{AM}} \), that is, the standard deviation divided by the square root of the sample size \( N \):

\[
\sigma_{\text{AM}}^2 = \frac{\langle \cos^2 2\theta_r \rangle - \langle \cos 2\theta_r \rangle^2}{N}.
\]

The AM given by Equation (27) was introduced in González-Casanova & Lazarian (2017) and later was borrowed by other researchers doing their studies, e.g., the studies of the Rolling Hough Transform (Clark & Hensley 2019). Similarly, Jow et al. (2018) introduce the projected Rayleigh statistic (PRS) for characterizing relative orientations. For a set of \( N \) angles \( \theta_i \in [-\pi/2, \pi/2] \), the PRS \( Z_i \) and its uncertainty \( \sigma_{Z_i} \) are defined as

\[
Z_i = \frac{\sum^N \cos 2\theta_i}{\sqrt{N/2}} \quad \text{and} \quad \sigma_{Z_i}^2 = \frac{2\sum^N (\cos 2\theta_i)^2 - 2\left(\sum^N \cos 2\theta_i\right)^2}{N}.
\]

therefore, \( Z_i \gg 0 \) indicates strong parallel alignment, while \( Z_i \ll 0 \) indicates strong perpendicular alignment. When the sampling size \( N \) is large, compared with the PRS, the AM takes the average directly so that its value is bounded between \([-1, 1] \). In this work, we only use the AM to characterize the relative orientation.

5. Results

5.1. The Distributions of the HI and H2 Abundances

In this section, we discuss the distributions of the atomic and molecular fractions, \( x_{\text{HI}} \) and \( x_{\text{H2}} \), for nonhomogeneous turbulent gas. These distributions are shown in a set of three figures, Figures 4, 5, and 6. In these figures we show the 2D pdf’s of \( n \) versus \( x_{\text{HI}} \) and \( x_{\text{H2}} \), standard 1D pdf’s of \( x_{\text{HI}} \) and \( x_{\text{H2}} \), and a bar plot showing a statistical summary of the atomic and molecular fractions.

Examining the four panels in Figure 4, from left to right, we see that at small \( M_s \) the distribution is narrow in the \( y \)-direction, i.e., the dynamic range in the density is small, as expected for subsonic gas. With increasing \( M_s \), density fluctuations develop in the gas, and the density dispersion increases. At a given density, the dispersion of the HI and H2 pdf’s along the \( x \)-axis results from the transition from atomic (\( x_{\text{HI}} = 1 \)) to molecular state (\( 2x_{\text{H2}} = 1 \)). The dispersion increases with cloud depth. In
particular, the low values of $2\chi_{\text{H}_2}$ (and high values of $x_{\text{H}_2}$) correspond to regions near the cloud boundary where $\text{H}_2$ destruction is very efficient. With increasing column density (i.e., distance from cloud edge), the UV radiation is absorbed by dust, and in the $\text{H}_2$ lines ($\text{H}_2$ self-shielding), the $\text{H}_2$ photodissociation rate decreases and $x_{\text{H}_2}$ increases. Finally, at sufficient cloud depth, the gas becomes molecular. The $\text{H}_1$ fraction never falls to zero, as even in cloud interiors cosmic rays maintain a small $\text{H}$ population (Li & Goldsmith 2003).

The balance between $\text{H}_1$ formation via cosmic rays in cloud interiors and its destruction (to form $\text{H}_2$) gives rise to the diagonal shape seen at the lower end of the $\text{H}_1$ pdf’s in Figure 4. Following Equation (16), at large cloud depth the photodissociation term is negligible, $2\chi_{\text{H}_2} \approx 1$, and we get $x_{\text{H}_1} \propto 1/n$. Similarly, in all the panels, the diagonal shape of the $\text{H}_2$ pdf’s at their low end results from the balance of unshielded $\text{H}_2$ photodissociation and $\text{H}_2$ formation at the cloud edge. This results in $x_{\text{H}_2} \propto n$ (i.e., Equation (16) with $\zeta \ll D_0$ and with the shielding terms $\approx 1$). For a complementary discussion of 2D pdf’s of density and molecular abundances, see Bialy et al. (2019).

Throughout the box, the $\text{H}_2$ formation rate (= the $\text{H}_1$ destruction rates) increases with $n$. Thus, positive fluctuations in the density promote higher $\text{H}_2$ fractions and lower $\text{H}_1$, resulting in the observed correlation between $x_{\text{H}_1}$ and $n$. In cloud interiors, the dependence is not linear, as besides the $\text{H}_2$ formation rate (which is linear in $n$), the destruction of $\text{H}_2$ is strongly affected by $\text{H}_2$ self-shielding, which in turn depends on the accumulated $\text{H}_2$ column ($N_{\text{H}_2} = \int n_{\text{H}_2} d\zeta$), from the cloud edge to the point of interest (Bialy et al. 2017b). In addition, we observe that an artificial tail exists in the low values of $2\chi_{\text{H}_2}$ (or high values of $x_{\text{H}_2}$). This tail becomes more apparent in supersonic cases. This results from the finite resolution of the grid, and the tail corresponds to the $x_{\text{H}_2}$ at the cloud edge (see Figure 3 in Bialy et al. 2019 and discussion in Section 4.1). The transition occurs over very short length scales at high densities, which correspond to one unit grid or less. When examining the 2D plot from left to right at constant density, the $2\chi_{\text{H}_2}$ jumps from the value at the tail (cloud edge) to its maximum value $2\chi_{\text{H}_2} \approx 1$ in the cloud interior. At lower density, the transition is continuous, as many cells resolve the transition. That is also why there is a large volume fraction in the low values of $2\chi_{\text{H}_2}$.

Figure 5 shows 1D pdf’s of the $\text{H}$ and $\text{H}_2$ abundances. Here, again, we see how the $\text{H}_1$ and $\text{H}_2$ pdf’s broaden with increasing sonic Mach number. The two peaks correspond to the cloud-edge and inner-cloud regions. The region between the two peaks results mainly from intermediate cloud depth, where the transition from $\text{H}$ to $\text{H}_2$ takes place. At large sonic Mach numbers, the lower end of the $\text{H}_2$ pdf broadens owing to density fluctuations. Without them, the $\text{H}_2$ abundance at the cloud edge is single valued. With density fluctuations, $x_{\text{H}_2} \propto n$ at the cloud edge, and the low end of the pdf then reflects the density pdf, which is nearly lognormal. The effect of density fluctuations is also seen in the $\text{H}_1$ pdf, which broadens to smaller values with increasing $M_s$. This tail results from regions at deep cloud interiors where $\text{H}_1$ forms via the action of cosmic rays and is destroyed by the $\text{H}_2$ formation process. At large cloud interiors this results in $x_{\text{H}_1} \propto 1/n$, and thus high-density regions push the $\text{H}_1$ fraction to lower values.

In Figure 6, we show the interquartile range, mean value, and median value of the $x_{\text{H}_1}$ and $x_{\text{H}_2}$ distributions. As in the previous figures, again, we see the trend of an increasing dispersion with increasing $M_s$ as strong density fluctuations develop in the gas. In addition, we see that with increasing $M_s$, the median and mean values of $x_{\text{H}_2}$ decrease, while that of $\text{H}_1$ decreases.
increases. The medians’ trend may be understood in terms of the properties of the density \(n\) pdf in turbulent gas. Let \(x \equiv n/\langle n\rangle\). For non-self-gravitating, magnetized, and isothermal turbulence \(x\) follows a lognormal distribution (Vazquez-Semadeni et al. 1995; Robertson & Kravtsov 2008; Collins et al. 2012; Burkhart 2018), for which \(x_{\text{median}} < 1\) and \(x_{\text{median}}\) decreases with increasing \(M_s\). Physically, with increasing sonic Mach number, larger regions of the volume are filled with moderately low-density material, \(x < 1\), compensated by small volumes filled with very high \(x\), i.e., shocks. The abundant low-density regions result in lowered \(H_2\) abundances and increased \(H_1\), resulting in the trend seen in Figure 6. The means’ behavior is more involved, as the \(H_1\) and \(H_2\) abundances depend nonlinearly (and nonlocally) on the gas density.

### 5.2. Moment Maps of \(H_1\) and \(H_2\) Gas

The moment maps can carry the density information and velocity information of the turbulent medium. For example, the moment-0 map contains a pure density field, while moment-1 and moment-2 maps mix both density and velocity field (see Section 2). The moment maps shall exhibit similar anisotropic properties to the density and velocity field, i.e., elongating along with their local magnetic fields. In PDRs, however, the density field is likely changed owing to the formation of other molecules. This transition process also introduces velocity fluctuations. Nevertheless, the velocities induced by \(H_2\) formation are not turbulent, as they do not form any eddies. These velocities are differences of thermal velocities that disappear over just one mean free path length. Therefore, the velocity field is expected to be anisotropic in moment maps.

In Figure 7, we present the moment-0, moment-1, and moment-2 maps for each simulation. For subsonic moment-0 maps, we can see that the intensity structures are elongating along the vertical direction, i.e., the mean magnetic field’s direction. However, for the supersonic turbulence \(M_s > 1\), the anisotropic pattern becomes less significant owing to shocks. As explained in Xu et al. (2019), these dense shock structures are preferentially perpendicular to the magnetic field. Therefore, in supersonic turbulence, we can observe the dense structures being perpendicular to the magnetic field. However, in the process of \(H_1\)-to-\(H_2\) transition, the dense gas usually is sampled into \(H_2\) so that the \(H_2\) map contains more shocks than the \(H_1\) map. We therefore can expect the \(H_2\) map to be less anisotropic.

The anisotropic pattern that the structures elongate along the mean magnetic field’s direction can also be observed in moment-1 and moment-2 maps. The difference here is that moment-1 and moment-2 maps contain the velocity contribution, which is insensitive to shocks (see Section 2). The effect of shocks is hence diluted, and the moment-1/moment-2 maps can remain anisotropic even in supersonic cases.

#### 5.2.1. Characterize the Anisotropy by the Structure Function

The structure function is widely used to characterize the anisotropic properties of MHD turbulence. Here we apply the second-order structure function to the moment maps, which is defined as

\[
SF(R) = \langle (f(\vec{r}) - f(\vec{r} + \vec{R}))^2 \rangle,
\]

where \(\vec{r} = (x, y, z)\), \(\vec{R}\) is a lag vector, and \(f(\vec{r})\) can be replaced by \(I(\vec{r})\), \(C(\vec{r})\), or \(S(\vec{r})\). In terms of the structure function, the anisotropy appears on a small scale. We therefore typically constrain \(\vec{r}\) in the range of fewer than 60 pixels. Figure 8 shows how the structure function should behave in terms of the contour plot. We use \(r_\perp\) and \(r_\parallel\) to denote the real-space scales perpendicular and parallel to the mean magnetic field, respectively.

For the structure function of moment-0 maps, we can observe that in the case of subsonic turbulence the contours of both \(H_1\) and \(H_2\) are elongated along the \(r_\parallel\) direction, i.e., the mean magnetic field direction. The contours on a large scale are slightly misaligned from the \(r_\parallel\) direction because of the limited inertial range in numerical simulations (Yuen et al. 2018). For the trans-sonic turbulence \(M_s = 1.27\), as the turbulence’s compression starts its dominance, the large-scale contours start evolving to approximately isotropic, while the small-scale contours are still anisotropic. This phenomenon is more significant for the structure function of \(H_1\) supersonic moment-0 maps. For \(H_2\), we can still see the change of the structure functions. The contour is getting isotropic when \(M_s = 5.64\), while it elongates in the direction perpendicular to the magnetic field (vertical direction) at large scales when \(M_s = 10.54\). Beattie & Federrath (2020) also report a similar finding, which is in agreement with theoretical expectations in

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**Figure 6.** Statistical properties of \(x_{H_1}\) and \(2x_{H_2}\) distribution. The line along the y-axis give the range of \(x_{H_1}\) and \(2x_{H_2}\). The box indicates the interquartile range, and the red/blue segment represents the mean/median value. The entire vertical segment gives the range of \(x_{H_1}\) and \(2x_{H_2}\).
Figure 7. (a) Moment-0 maps, (b) moment-1 maps, and (c) moment-2 maps for each simulation listed in Table 1. For each panel, the H I maps are in the top row, while the H2 maps are in the bottom row.
Figure 8. Structure function of (a) moment-0 maps, (b) moment-1 maps, and (c) moment-2 maps for each simulation listed in Table 1. For each panel, the H I maps are in the top row, while the H$_2$ maps are in the bottom row. $r_\perp$ and $r_\parallel$ are the real-space scales perpendicular and parallel to the magnetic field, respectively. For all plots, $r_\perp$ and $r_\parallel$ are in scales less than 60 pixels.
Xu et al. (2019). The authors numerically demonstrated that for sub-Alfvén turbulence with $M_s < 4$, the anisotropy in the column density is dominated by striations aligned with the magnetic field. However, Bialy & Burkhart (2020) find 3D density structures to squeeze along the magnetic fields in moderately supersonic gas. The anisotropy is significantly changed by high-density structures that form perpendicular to the magnetic field for sub-Alfvén and highly supersonic turbulence. We observe that the moment-1 and moment-2 maps have different behavior. For moment-1 maps, the anisotropy is always parallel to the magnetic field. Different from the structure function of H I’s supersonic moment-0 maps, the structure functions of moment-1 and moment-2 maps are striated in the direction parallel to the magnetic field (vertical direction). In addition, the structure function of supersonic H I is more striated (i.e., a larger semimajor-axis-to-semiminor-axis ratio) than the one of H$_2$. The shock effect in H$_2$ is likely significant, although moment-1 and moment-2 maps partially dilute shock contribution. In any case, the anisotropic patterns of moment-1 and moment-2 maps are always aligned with the magnetic field. This supports one of the arguments at the core of the GT, namely, that the velocity fluctuations are more reliable tracers of the magnetic field than density fluctuations, i.e., compared to the studies of Soler et al. (2013), Clark et al. (2014), and Clark & Hensley (2019).

5.2.2. Energy Spectrum for Each Moment Map

Furthermore, we calculate the energy spectrum for each moment map. The results are presented in Figure 9. For moment-0 maps, dense H$_2$ contains more energy than H I. This difference is more significant in supersonic cases, as the majority of high-density contrasts induced by density fluctuation have been sampled into H$_2$. As for moment-1 and moment-2 maps, H I and H$_2$ occupy an

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Figure 9. Energy spectrum of the moment-0 maps (left column), moment-1 maps (middle column), and moment-2 maps (right column) for each simulation listed in Table 1. $\alpha$ is the fitted slope of the spectrum.
approximately equivalent fraction of energy in sub/trans-sonic turbulence. Also, similarly, H₂ gets more energy in supersonic moment-1 and moment-2 maps, which means that dense and small-scale structures are sampled into H₂.

We fit the slope $\alpha$ of the spectrum in the range of $8 \leq k \leq 60$. We find that the slope gets shallower with the increment of $M_s$. In subsonic cases, both HI and H₂ fit similar spectrum slopes for corresponding moment maps (moment-0 map: $\sim -2.9$; moment-1 map: $\sim -3.1$; moment-2 map: $\sim -2.9$). With the increment of $M_s$, the spectrum of H₂ moment-1 and moment-2 maps becomes shallower than the one of HI moment-1 and moment-2 maps. However, the spectra of HI and H₂ moment-0 maps always exhibit a similar slope value. The shallower spectrum can be caused by shocks, which was numerically demonstrated by Beresnyak et al. (2005). For instance, moment-0 maps are produced by integrating spectral lines in the full range (see Figure 3). The contribution from density and all shocks in supersonic turbulence is more significant in moment-0 maps. We therefore see a shallower slope in the energy spectrum. Also, the density fluctuation induced by supersonic turbulence produces a number of small-scale structures, as shown in Figure 2. These small-scale structures also make the spectrum shallower.

5.3. Tracing the Magnetic Field Using GT

In the above, we discussed the anisotropy of atomic HI and molecular H₂ species, which is the theoretical foundation of the GT. We can see that both HI and H₂ maintain the anisotropic property after the transition. In this section, we apply the GT to trace the magnetic field and compare its performance with the utilization of different moment maps. Note that we denote the gradients of the moment-0 map, or the intensity map, as IGs, those of the moment-1 map, or first-order centroid map, as VCGs, and those of the moment-2 map as VC₂Gs.

In Figure 10, we give a comparison of the magnetic field orientation probed by synthetic dust polarization and by the GT with a block size of 33 pixels. The plot is overlaid on the moment-0 maps (left), moment-1 maps (middle), and moment-2 maps (right). We use the HI (top) and H₂ (bottom) cubes produced by simulation A0 and denote the gradients of the moment-0 map as IGs, those of the moment-1 map as VCGs, and those of the moment-2 map as VC₂Gs.

We further study the alignment of gradients and the magnetic field in terms of tracing scale. In Figure 11, we vary the sub-block size from 11 to 66 pixels and calculate the AM correspondingly. In general, the AM is positively proportional to the sub-block size since a larger sub-block guarantees more sample vectors, so that the mean magnetic field inferred from the gradients is statistically better determined (Yuen & Lazarian 2017a; Lazarian & Yuen 2018a). Empirically, the minimum sub-block size for the analysis of synthetic simulations was found to be 20 pixels (Lazarian & Yuen 2018a), which provides a sufficient 400 samples for the Gaussian fit in the absence of noise. For the HI gradients, the subsonic and trans-sonic cubes give similar results, as the turbulence is dominating. As for supersonic cubes, theoretically, high-density shocks flip the density gradient by 90° being parallel to the magnetic field (Yuen & Lazarian 2017b; Hu et al. 2019b). Therefore, the alignment...
AMI is anticorrelated with $M_s$. The shocks’ effect is more apparent for H$_2$ gradients, particularly for VCGs and VCs. It is likely that H$_2$ samples more shocks than H I, so that velocity contribution in VCGs and VCs is diluted by the shock effect. Nevertheless, we find that the VC$_2$Gs of H I are the most stable tracers of the magnetic field in the presence of shocks.

Additionally, we examine our hypothesis about shocks. First, we calculate the AM in each sub-block instead of taking global averaging. We then sort out the AM values based on the ratio between their corresponding column density and global mean column density, i.e., $N_{H_2}/\langle N_{H_2} \rangle$ and $N_{H_2}/\langle N_{HI} \rangle$. The moment-0 map is segmented into seven groups based on the ratio. Note that as the range of $N_{H_2}/\langle N_{HI} \rangle$ and $N_{H_2}/\langle N_{HI} \rangle$ is not a fixed value but depends on the sonic Mach number, we do not keep a constant interval when doing segmentation for different maps. In each segmentation, we output the averaged AM value. In Figure 12, we plot the AM value versus $N_{H_2}/\langle N_{HI} \rangle$ and $N_{HI}/\langle N_{HI} \rangle$. The sub-block size is selected as 20 pixels, and the moment-0 map is also reduced to the same resolution before doing the segmentation.

For the subsonic H I case, we see that the AM is slightly increasing when the ratio of $N_{HI}/\langle N_{HI} \rangle$ is large. When $M_s$ is larger than 1, the AM starts decreasing but is still positively correlated with the $N_{HI}/\langle N_{HI} \rangle$ ratio. Similarly, for H$_2$ gradients, the AM is decreasing in supersonic cases but is negatively correlated with the $N_{HI}/\langle N_{HI} \rangle$ ratio. When $N_{HI}/\langle N_{HI} \rangle$ is close to its maximum value, the AM of IGs gets a minimum value around 0.6, 0, and $-0.2$ for $M_s = 1.27$, 5.64, and 10.54, respectively. The rapid decrease of AM in supersonic H$_2$ high-density regions confirms our theoretical consideration about shocks, i.e., shocks can flip the gradients’ direction. This agrees with the results in Hu et al. (2019b). Also, in Section 2, we derived that the IGs consist of the contribution from the density gradient, while VCGs and VC$_2$Gs employ both the density gradient and velocity gradient. We can see that VCGs, in general, get more resistance for shocks than IGs owing to the velocity contribution. As VC$_2$Gs contain one more velocity term than VCGs, VC$_2$Gs usually have better performance than VCGs in both subsonic and supersonic cases.

Furthermore, in Figure 12 we introduce the comparison of VChGs and VGT+PCA. We can see in the supersonic case that the AM of VChGs decreases with the increment of $N_{HI}/\langle N_{HI} \rangle$. This is expected, as the thin channel criterion given by Equation (21) only indicates that the velocity fluctuation is dominating over the density fluctuation, instead of pure velocity fluctuation. As we discussed above, IGs contain only the density contribution and are most sensitive to shocks. The additional velocity contribution in VCGs and VC$_2$Gs (see Section 2) guarantees them a better performance (higher AM). Most importantly, in any case, VChGs are superior to IGs, VCGs, and VC$_2$Gs. This means that VChGs definitely are dominated by the velocity contribution. The velocity contribution in the thin velocity channel is even more than that in the moment-2 map.

Nevertheless, we also see that the VGT+PCA gives the best performance in tracing the magnetic field. We expect three possible reasons. First of all, VChGs utilize only the central channel. It is likely that the central channel only contains part of the magnetic field’s information. Differently, the gradient from VGT+PCA is summed along the LOS for all velocity channels, so that all information in the PPV cube is taken into account. Also, the vector summation used in IGs, VCGs, VC$_2$Gs, and VChGs is different from the polarimetry, which employs the summation of Stokes parameters. However, the pseudo-Stokes parameters used in VGT+PCA are more similar to the polarimetry measurement. Additionally, the PCA technique enhances the most crucial components for constructing the gradient field. Noise is suppressed in this case (Hu et al. 2018).

Figure 11. Correlation between AM and the sub-block size, which is selected for the implementation of the sub-block averaging method. We denote the gradients of the moment-0 map as IGs, those of the moment-1 map as VCGs, and those of the moment-2 map as VC$_2$Gs.
6. Discussion

6.1. The Role of Density Fluctuation in the H I-to-H2 Transition

The conversion of atomic H I to molecular H2 is a basic process in the turbulent, magnetized ISM. This transition has been widely studied from various perspectives, including numerically and analytically absorbing the effects of turbulence (Xie et al. 1995; Willacy et al. 2002; Bialy et al. 2017b). In this paper, we generate synthetic H I and H2 cubes in chemical balance to study the turbulence’s properties of H I-to-H2 transition. We fix the mean volume density (n) ≈ 50 cm\(^{-3}\) and temperature T = 50 K, but varying the sonic Mach number \(M_s\) from 0.66 to 10.54. We find that in the case of supersonic turbulence, the distribution of H2 fraction \(x_{H2}\) and H I fraction \(x_{HI}\) is more dispersed than the one of subsonic turbulence. The increased dispersion reflects the growth of density fluctuation in supersonic turbulence (Bialy et al. 2017b, 2019). For supersonic turbulence, the density fluctuation produces significant high-density and low-density contrasts. The high-density contrasts are fully sampled into H2 so that the fraction of H I left is much lower, so that \(x_{HI}\) is more dispersed. Similarly, low-density contrasts are not sufficient for self-shielding, so that the fraction of H2 left is lower. This suggests that density fluctuations induced by turbulence can play a critical role in the formation of heavy molecular species.

6.2. Tracing Local Magnetic Fields Using Velocity Gradients

In addition to turbulence, the magnetic fields are also essential in regulating molecules’ formation. With the assistance of polarized dust emission, the projected magnetic field along the LOS can be accessed. However, it is still challenging to separate the foreground and probe the local magnetic fields in either the PDR or the molecular cloud.

A possible solution is provided by the GT, which has been developed as an advanced synergetic tool for studying the magnetic field (González-Casanova & Lazarian 2017; Yuen & Lazarian 2017a; Lazarian & Yuen 2018a; Hu et al. 2019b). This technique uses the fundamental properties of MHD turbulence, namely, it is a sum of anisotropic eddies aligned, revealing the direction of the magnetic field in their vicinity (Goldreich & Sridhar 1995; Lazarian & Vishniac 1999). Due to the turbulent eddies being elongated along with their local magnetic fields, the corresponding density and velocity gradients are perpendicular to the magnetic fields. One can therefore infer the magnetic field orientation by rotating the gradients by 90°.

One important advantage of the GT is that it can utilize multiple molecular emission lines to construct the local magnetic field model. For instance, by using \(^{12}\)CO, \(^{13}\)CO, and C\(^{18}\)O data, GT can probe the POS component of the magnetic field over three different volume density ranges, from 10\(^2\) to 10\(^4\) cm\(^{-3}\) (Hu et al. 2019a; Hsieh et al. 2019). A similar idea can be migrated to the PRD regions. Since the H2 usually samples denser gas than H I, GT can also be used to trace the magnetic field in either the H2 or H I region.

The performance of the GT has been tested in either pure atomic H I gas (Yuen & Lazarian 2017a; González-Casanova & Lazarian 2019; Hu et al. 2020c; Hu & Lazarian 2020a, 2020b) or pure molecular species (Hu et al. 2019a, 2019c; Hsieh et al. 2019). However, for the PDRs at the cloud boundaries, the transition from atomic gas to molecular gas could distort the turbulence’s anisotropic properties crucial for GT. Therefore, in this work we examine the effect of turbulence on interstellar clouds’ chemical structure and the GT’s performance in PDRs. We find that the anisotropy of pure density structures may be distorted in the transition process. The distortion depends on the spatial distribution of the gas and may affect the performance of the GT. However, the H2 formation that takes place in a turbulent flow induces the change of the mass of the particles in the flow but does not change the momentum and energy of the turbulent motions. The velocities induced by H2 formation are differences of thermal velocities that disappear over just one mean free path length. These velocities are not turbulent in this case, and they do not form any eddies. Also, Bialy et al. (2017b) showed that the H I-to-H2 transition occurs as UV Lyman–Werner photons are absorbed in the H2 line wings, which are far (in wavelength) from spectral line centers. The gas velocity shifts the line centers by a small amount.
compared to the spacing between the lines, thus barely affecting the \( \text{H}1 \)-to-\( \text{H}_2 \) transition. It is important only for small columns where the gas is predominantly atomic, i.e., the column density \( N \approx 10^{15}–10^{20} \text{cm}^{-2} \). Therefore, the turbulent velocity field is expected to be anisotropic, and the velocity gradient is still a reliable tracer.

6.3. Gradients of Moment Maps

To calculate the density or velocity gradients, GT usually employs the gradients of the intensity map (i.e., moment-0 map; Yuen & Lazarian 2017, b; Hu et al. 2019b), velocity centroid map (i.e., moment-1 map; González-Casanova & Lazarian 2017; Yuen & Lazarian 2017a), and thin velocity channel map (Lazarian & Yuen 2018a). In this work, we introduce the second-order centroid map calculated from the PPV cube. We derive and confirm that the 2D gradient field of the intensity map carries only the information of turbulent density, while the 2D gradients of the velocity centroids contain the contribution from both the density and velocity fields. We find that the velocity contribution improves the performance of the GT in tracing the magnetic field. This corresponds to theoretical expectations. If the density fluctuations are associated with the entropy variations, they can be passively transformed by the anisotropic velocity cascade and therefore reflect the velocity scaling properties. This can happen in subsonic turbulence, while in supersonic MHD turbulence the properties of density and velocity can be very different (Beresnyak et al. 2005; Kowal et al. 2007). In this situation, the magnetic field tracing with IGs is not reliable because of the presence of shocks.

According to the theory in Lazarian & Pogosyan (2000), velocity fluctuation can also be obtained from a thin velocity channel map. This has been developed as a branch of the GT for studying the magnetic field (Lazarian & Yuen 2018a). However, the issue of what is measured in \( \text{H}1 \) channel maps has been debated recently. Some researchers believe that the striations observed in such maps are actual density filaments (Clark et al. 2014). The density, as we discussed earlier, for the velocity field can passively carry subsonic MHD turbulence. Therefore, the density filaments can be aligned parallel to the magnetic field (Xu et al. 2019). However, it is also well known from the theory (Lazarian & Pogosyan 2000) and numerically demonstrated by different groups (see, Clarke et al. 2018; Yuen & Lazarian 2020) that turbulent velocities produce the filaments in channel maps. Therefore, the pure density filament model is not tenable, and the actual question is the relative importance of turbulent densities and velocities for the observed striation. We note that by challenging the turbulent velocity origin of filaments, Clark et al. (2019) provided a series of arguments, the validity of which was seriously questioned in Yuen et al. (2019). Although several authors also argue that thin velocity channel maps observed in \( \text{H}1 \) emission are dominated by the CNM (Murray et al. 2020; Kalberla & Haud 2020), this issue will be discussed in detail elsewhere.

6.4. Thermal Phases of the ISM

In this work, we use isothermal MHD simulations to study the chemical balance of the \( \text{H}_1 \)-to-\( \text{H}_2 \) transition. The isothermal \( \text{H}_1 \)-to-\( \text{H}_2 \) transition model was proposed by Sternberg et al. (2014) and Bialy & Sternberg (2016) in the absence of turbulence. Analytically and numerically, Bialy et al. (2017b, 2019), as well this work, extend the transition into an isothermal turbulent-chemical model. The isothermal assumption \( (T = 50 \text{ K}) \) mimics a single-phase CNM. The cooling/heating processes in a real scenario, however, introduce a thermal instability resulting in a multiphase medium, including both the CNM and the warm neutral medium (WNM; Field et al. 1969; Wolfe et al. 1995, 2003; Bialy et al. 2019; Bellomi et al. 2020). In addition to the isothermal model, several authors also numerically considered the heating–cooling processes and found bimodal pdf’s of volume density, with a nonnegligible mass within the region of intermediate temperatures (Piontek & Ostriker 2007; Walch et al. 2011; Saury et al. 2014). The significance of heating–cooling processes on the chemical balance depends on the mixing scale of CNM/WMN structures (Bialy et al. 2019). In the case that the characteristic CNM scale \( \lambda_c \) is much less than the scale of cloud \( L_c \), the CNM and WNM are well mixed on small scales so that each cloud contains both phases. As a consequence, there would be less \( \text{H}_2 \) gas compared to the pure CNM case. However, when \( \lambda_c \gg L_c \), the transition samples only the higher CNM densities, which is similar to our isothermal numerical setting (see Bialy et al. 2019 for a detailed discussion).

For the calculation of moment maps, the nonlinear spectroscopic mapping between PPP space and PPV space does not require an isothermal environment (see Equation (7)). The temperature can vary from point to point in a multiphase medium. The integration along the LOS for moment maps eliminates the effect of temperature, so that the gradients are only regulated by gas density and turbulent velocity. Therefore, the moment-1 map and moment-2 map are not contaminated by thermal broadening (see also Esquivel & Lazarian 2005; Kandel et al. 2017). In a multiphase scenario, the presence of gas temperature variations can complicate the velocity distributions. However, as the temperature is a passive scalar, in the sub-Alfvénic environment, we expect its pattern to be similar to that of velocity, i.e., elongating along with the magnetic fields. In particular, the temperature is usually negatively proportional to the gas density (Wolfe et al. 1995). The temperature distribution thus can reduce the shock effect in a supersonic environment. On the other hand, the transition from WNM to CNM may occur in velocity divergence regions, which triggers the thermal instability. Consequently, the temperature differences may have a negative effect since the MHD turbulence structure may get changed.

6.5. Distinguish Shocks and Identify Self-gravitating Regions

The existence of shocks or regions of gravitational collapse is a particular case for applying the GT. The GT is founded on the fact that the turbulent velocity and magnetic field eddies are elongating along the magnetic field. As we discussed earlier, in MHD turbulence, the density statistics are different from turbulent velocity. As a result, it is not surprising that several authors have reported that the anisotropy is significantly changed by high-density filaments that form perpendicular to the magnetic field for sub-Alfvén and highly supersonic turbulence (Xu et al. 2019; Hu et al. 2019b; Beattie & Federrath 2020; Bialy & Burkhardt 2020). In the density gradient’s picture, its direction in front of shocks flips by 90º, becoming parallel to the magnetic field instead of perpendicular. This change comes from the rapid jump condition of density, so that there is no particular universal
density at which the change happens (Hu et al. 2019b). At the same time, the anisotropy of the velocity field is not sensitive to shocks (see Section 2). Therefore, shocks do not degrade the corresponding velocity gradient’s performance in tracing the magnetic field, and combining velocity and density gradients, one can identify shocks.

The gravitational collapse may also change the turbulence’s picture. In the vicinity of gravitational collapse, the gravitational pull produces the most significant acceleration of the plasma in the direction parallel to the magnetic field, and the density and velocity gradients are parallel to the magnetic field (Hu et al. 2020b). Unlike shocks, the collapse is unbounded by the sonic Mach number $M_s$, and it induces a significantly high gradient amplitude. As a result, we get the condition to distinguish shocks and identify self-gravitating regions: (i) for shocks, we have the low-amplitude velocity gradient being perpendicular to the magnetic field and the low-amplitude density gradient being parallel to the magnetic field; (ii) for gravitational collapse, we have both high-amplitude density and velocity gradients being parallel to the magnetic field. The corresponding recipe for identifying the gravitational regions with the GT is presented in Hu et al. (2020b).

7. Conclusion

The PDRs have a vital role in the formation of molecular clouds. They process the chemical transition from atomic gas to most of the molecular gas. For example, through the essential H I-to-H$_2$ transition, the formation of other heavy molecules is achievable. The role of turbulence and magnetic field in PDRs is not well understood, and it requires further studies. We explore the possibility of studying magnetic fields of the PDRs by performing MHD simulation with numerical cubes in H I–H$_2$ chemical balance. We study the properties of turbulence by calculating the energy spectrum and structure function. This work also suggests the promise of using multiple moment maps to probe magnetic fields. We summarize our results as follows:

1. Using the synthetic H I and H$_2$ cubes in chemical balance, we confirm the following:
   (a) The density fluctuation induced by turbulence can disperse the distribution of H$_2$ and H I fraction.
2. Analogous with IGS and VCGs, we introduce the gradients of the moment-2 map, denoted as VCGs, to trace the magnetic fields. In particular, we show that in an isothermal environment the following applies:
   (a) VCGs are more accurate than VCGs and IGS in tracing the magnetic field orientation.
   (b) VCGs, VCGs, and IGS tend to be parallel to the local magnetic fields when getting close to the dense shock front in the absence of gravity.
   (c) VCGs are less sensitive to shocks than IGS. VCGs have the advantage of tracing the magnetic field in supersonic turbulence.

3. We show that the synergy of the VGT and PCA improves the accuracy of magnetic field tracing.

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Software: Julia (Bezanson et al. 2012), ZEUS-MP/3D (Hayes et al. 2006), Paraview (Ahrens et al. 2005).

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