THE RELATION BETWEEN ATOMIC AND MOLECULAR GAS: THE MAGELLANIC CLOUDS AND BEYOND

BY

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DISSERTATION

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Abstract

In this thesis, I employ two different observational techniques, ultraviolet spectroscopy and radio interferometry imaging, to study the atomic and molecular gas relation in the Large/Small Magellanic Clouds and 43 nearby galaxies. These galaxies demonstrate various galactic environments compared with the Milky Way and provide an ideal sample for testing the cloud-scale and galactic-scale models of the atomic-to-molecular transition and molecular cloud formation. From the absorption line analysis on archival data provided by the Far Ultraviolet Spectroscopic Explorer, I found the molecular hydrogen absorbers trace the diffuse and translucent cloud components in the Magellanic Clouds. Although the absorbers’ velocities generally agree with the large-scale kinematic structure revealed in HI 21cm emission, their physical properties are distinct from the gas revealed by the molecular gas emission in CO. The observed atomic-to-molecular gas relation derived from the absorbers, together with existing gas cloud models, suggest the possible existence of significant diffuse warm atomic gas along the ultraviolet absorption sight lines. In the second part of the thesis, I use high-resolution CO and HI 21cm observations of 45 nearby galaxies, including the Magellanic clouds, to analyze the spatial correlation of the interstellar gas in molecular and atomic phases and old stellar populations. The results suggest strong independent roles for galaxy metallicity and stellar-to-gas ratios in the atomic-to-molecular gas transition and are consistent with a self-regulation galaxy model of star formation and interstellar medium evolution. The model and observations highlight the importance of the diffuse atomic gas component in understanding the observed atomic and molecular gas relation at sub-kiloparsec and kiloparsec scales. I conclude that it is essential to incorporate diffuse cloud components into
theoretical models of galaxy ISM evolution and molecular cloud formation because of their important role in the galactic ecosystem.
# Table of Contents

List of Figures .......................................................... vi

Chapter 1  Introduction ................................................. 1

Chapter 2  Diffuse H$_2$ in the Magellanic Clouds ...................... 3
  2.1  Introduction ................................................................ 3
  2.2  Sample and Data ....................................................... 5
    2.2.1  UV Archival Data ................................................. 5
    2.2.2  Ancillary Radio Data ............................................. 6
  2.3  Analysis ............................................................... 9
    2.3.1  Physical and Instrumental Model for H$_2$/HI Absorptions .... 13
    2.3.2  Evaluating the Model Quality .................................. 15
    2.3.3  Iterative Fitting .................................................. 18
  2.4  Results ............................................................... 22
    2.4.1  H$_2$ Rotational/Excitation Temperature ......................... 25
    2.4.2  Large-Scale Velocity Field ..................................... 29
    2.4.3  ISM Structure .................................................... 34
  2.5  Interpretation of H$_2$ Abundances and Populations ................. 35
    2.5.1  An Analytical Cloud Model for H$_2$ Formation and Dissociation 39
    2.5.2  Comparisons with Previous Cloud Models ....................... 43
    2.5.3  Caveats ............................................................ 48
  2.6  Physical Properties of Absorbers Inferred from Cloud Models ....... 51
    2.6.1  Comparisons with the Two-phase Equilibrium model ............. 51
    2.6.2  Gas Volume Density .............................................. 54
    2.6.3  Radiation Field Near Absorbers ................................ 55
  2.7  Discussion ................................................................ 58
    2.7.1  WNM Contribution to Absorption ................................ 58
    2.7.2  Diffuse H$_2$ ....................................................... 60
  2.8  Summary and Conclusions ........................................... 64

Chapter 3  Spatially Resolved Atomic and Molecular Gas Distributions in
  Nearby Galaxies ......................................................... 66
  3.1  Introduction .......................................................... 66
  3.2  Sample and Data ....................................................... 69
    3.2.1  CARMA Survey Toward IR-Bright Nearby Galaxies (STING) .... 73
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.2.2 CO and HI Integrated Intensity Maps</td>
<td>85</td>
</tr>
<tr>
<td>3.2.3 Metallicity and Infrared Images</td>
<td>87</td>
</tr>
<tr>
<td>3.3 Analysis and Results</td>
<td>89</td>
</tr>
<tr>
<td>3.3.1 Gas and Stellar Surface Density Maps</td>
<td>90</td>
</tr>
<tr>
<td>3.3.2 Spatially Resolved Relation of Gas and Stellar Distributions: NGC4254</td>
<td>93</td>
</tr>
<tr>
<td>3.3.3 Atomic Gas Surface Density in Molecular-Rich Regions</td>
<td>99</td>
</tr>
<tr>
<td>3.3.4 Surface Density Correlations in Individual Galaxies</td>
<td>103</td>
</tr>
<tr>
<td>3.4 Discussion</td>
<td>105</td>
</tr>
<tr>
<td>3.5 Summary and Conclusions</td>
<td>109</td>
</tr>
<tr>
<td>Chapter 4 Summary and Future Work</td>
<td>112</td>
</tr>
<tr>
<td>Appendix A Empirical/Theoretical Models for the Atomic-to-Molecular Gas Transition</td>
<td>114</td>
</tr>
<tr>
<td>A.1 Empirical Relation Between $R_{\text{H}_2}$ and the Hydrostatic Pressure</td>
<td>114</td>
</tr>
<tr>
<td>A.2 Cloud-scale H$_2$ Formation/Dissociation and Pressure Equilibrium Models</td>
<td>115</td>
</tr>
<tr>
<td>A.3 Galactic-scale Thermal and Dynamical Equilibrium Model</td>
<td>122</td>
</tr>
<tr>
<td>Appendix B Weight Adjustment for Calibrated HI Data in CASA</td>
<td>125</td>
</tr>
<tr>
<td>Appendix C 21 cm Line Brightness with a Continuum Background</td>
<td>127</td>
</tr>
<tr>
<td>References</td>
<td>130</td>
</tr>
</tbody>
</table>
# List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>FUSE UV spectra from the FUSE Magellanic Clouds Legacy Project</td>
<td>7</td>
</tr>
<tr>
<td>2.2</td>
<td>Sky distribution of UV absorption sight lines</td>
<td>10</td>
</tr>
<tr>
<td>2.3</td>
<td>H$_2$ rotational diagram at the ground electronic-vibrational state (AzV 6)</td>
<td>11</td>
</tr>
<tr>
<td>2.4</td>
<td>Rotational temperature $T_{01}$ versus H$<em>2$ column density $N</em>{H_2}$</td>
<td>27</td>
</tr>
<tr>
<td>2.5</td>
<td>LMC velocity structure traced by gas emission and absorption</td>
<td>32</td>
</tr>
<tr>
<td>2.6</td>
<td>SMC velocity structure traced by gas emission and absorption</td>
<td>33</td>
</tr>
<tr>
<td>2.7</td>
<td>Emission and absorption comparison of atomic gas</td>
<td>36</td>
</tr>
<tr>
<td>2.8</td>
<td>Emission and absorption comparison of molecular gas</td>
<td>37</td>
</tr>
<tr>
<td>2.9</td>
<td>Structure function revealed by H$_2$ and HI absorbers</td>
<td>38</td>
</tr>
<tr>
<td>2.10</td>
<td>Predictions of the HI and H$_2$ column density relation</td>
<td>47</td>
</tr>
<tr>
<td>2.11</td>
<td>Observed HI and H$_2$ column density relation</td>
<td>52</td>
</tr>
<tr>
<td>2.12</td>
<td>Gas volume density derived from UV absorption observations</td>
<td>56</td>
</tr>
<tr>
<td>2.13</td>
<td>UV radiation field derived from absorption observations</td>
<td>57</td>
</tr>
<tr>
<td>3.1</td>
<td>CO $J = 1 - 0$ total flux comparisons of different CLEAN algorithms</td>
<td>79</td>
</tr>
<tr>
<td>3.2</td>
<td>HI 21cm global line profile</td>
<td>80</td>
</tr>
<tr>
<td>3.3</td>
<td>Luminosity-metallicity relation</td>
<td>88</td>
</tr>
<tr>
<td>3.4</td>
<td>Adopted $X_{CO}$ factors</td>
<td>91</td>
</tr>
<tr>
<td>3.5</td>
<td>Deprojected atomic, molecular, and stellar surface density maps of NGC 4254</td>
<td>94</td>
</tr>
<tr>
<td>3.6</td>
<td>HI surface density ($\Sigma_{HI}$) versus total gas surface density ($\Sigma_H=\Sigma_{HI}+\Sigma_{H_2}$) in NGC 4254.</td>
<td>96</td>
</tr>
<tr>
<td>3.7</td>
<td>Old stellar surface density ($\Sigma_*$) versus total gas surface density ($\Sigma_{HI}+\Sigma_{H_2}$) in NGC 4254.</td>
<td>98</td>
</tr>
<tr>
<td>3.8</td>
<td>$\Sigma_{HI}^M$ as a function of the galaxy characteristic metallicity.</td>
<td>101</td>
</tr>
<tr>
<td>3.9</td>
<td>$\Sigma_{HI}^M$ as a function of the galaxy stellar-to-gas ratio averaged over the molecular-rich regions</td>
<td>102</td>
</tr>
<tr>
<td>3.10</td>
<td>Stellar-to-gas mass ratio as a function of the galaxy characteristic metallicity.</td>
<td>105</td>
</tr>
<tr>
<td>3.11</td>
<td>Ratio of the predicted and observed atomic gas surface density versus the galaxy metallicity</td>
<td>110</td>
</tr>
<tr>
<td>3.12</td>
<td>Ratio of the predicted and observed atomic gas surface density versus the galaxy stellar-to-gas ratio in the regions with CO observations.</td>
<td>111</td>
</tr>
<tr>
<td>A.1</td>
<td>Predictions from the atomic-to-molecular transition model of MK10</td>
<td>121</td>
</tr>
<tr>
<td>C.1</td>
<td>HI absorption in NGC 4536</td>
<td>129</td>
</tr>
</tbody>
</table>
Chapter 1
Introduction

Molecular clouds are the building blocks for star formation in galactic environments because they provide the high-density cold gas necessary for the star-forming process (McKee & Ostriker 2007). Yet the majority of the gas in many galaxies is in the atomic phase, which also occupies a much larger volume in the interstellar medium (ISM). Because star formation has been a central question in extragalactic astronomy and galaxy evolution, understanding the relation between molecular and atomic gas, namely, how the atomic-to-molecular gas conversion plays a role in molecular cloud formation and consequent star formation, becomes an essential step to build a more comprehensive theoretical framework for galaxy evolution.

Although many observational facts have been discovered in the past regarding the physical and chemical properties of the atomic and molecular gas phases and theoretical models have been proposed to explain the atomic-to-molecular gas transition in individual clouds, we do not yet understand the net effects of those “microphysical” processes: how is the star-formation-related molecular gas mass determined in a galaxy? Answering this question will help us understand how the universe evolves across the cosmic time.

Observationally, answering this simple question could be challenging from several perspectives. Although the observational results at cloud scales (e.g., interactions between photoionization/dissociation radiation field and ISM near local H II regions and photo-dominated regions, or PDRs) were well-documented due to the presence of their bright emission features, the interface between atomic and molecular gas at the stage of the molecular cloud formation is poorly understood due to the difficulty of obtaining both HI and H$_2$ measurements in those relatively quiescent regions without prominent star formation.
activity. Many observations rely on indirect tracers, which could be difficult to interpret. Therefore, the existing evidence on the atomic-to-molecular transitions is almost built on information collected from local environments, which may not be representative of conditions in low-metallicity environments, e.g. those in the high-redshift galaxy.

In this dissertation, we carried out two separate studies to investigate the spatially resolved atomic and molecular gas relation and to understood their connection to the galactic environments on both large and small scales. Our approach is to collect and analyze data tracing the relation between atomic and molecular gas over a wide range of galactic environments from both microscopic and macroscopic points of view. In Chapter 2, we present the first study: a survey of H$_2$ ultraviolet (UV) absorption lines in the nearest two sub-solar metallicity galaxies, the Large and Small Magellanic Clouds (LMC/SMC). This project is an expansion of the study by Welty et al. (2012) and makes use of absorption lines to directly trace the column density of atomic and molecular gas (using Lyman-Werner band H$_2$ absorption and Lyman lines from HI) to probe the small-scale HI-H$_2$ relation, H$_2$ properties, and the interstellar radiation field (ISRF). The ancillary HI 21cm and CO $J = 1 - 0$ data allowed us to compare the results from absorption with those from emission-line tracers. In Chapter 3, we describe the second study: a high resolution nearby galaxy study in the CO and HI 21cm lines based on the galaxy sample of the CARMA$^1$ Survey Toward Infrared-Bright Nearby Galaxies (STING) and the publicly available HERA CO Line Extragalactic Survey (HERACLES) (Leroy et al. 2009), as well as high-resolution atomic and molecular gas data on the LMC and SMC. The metallicities of the entire sample span more than one order of magnitude, therefore providing an excellent sample to test different model predictions on the galactic-scale atomic-to-molecular gas transition. The summary of the entire thesis and future perspectives on the follow-up work are presented in Chapter 4.

$^1$Combined Array for Research in Millimeter-wave Astronomy (CARMA) is operated by the Universities of California (Berkeley), Chicago, Illinois, and Maryland, and the California Institute of Technology, under a cooperative agreement with the University Radio Observatory program of the National Science Foundation.
Chapter 2

Diffuse $\text{H}_2$ in the Magellanic Clouds

2.1 Introduction

The Large and Small Magellanic Clouds (LMC/SMC) are the two nearest gas-rich galaxies and serve as unique astrophysical laboratories for studies of the interstellar medium (ISM). Their proximity (50 and 62 kpc respectively, Monson et al. 2012; Scowcroft et al. 2015) allows us to resolve giant molecular clouds (GMCs) and their envelopes with the moderate spatial resolution typically available for common gas tracers such as the 21-cm line of HI and rotational lines of CO. The large-scale galactic dynamics and the cloud population characteristics can be also assessed without the distance ambiguities suffered in the Galactic plane. Their lower metallicities (especially SMC) are ideal to investigate physical/chemical processes in low metallicity environments, which are similar to those in the early universe.

Extensive survey studies have been carried out to image the Magellanic Clouds (MCs) at nearly all accessible wavelengths, mapping the stellar distribution (e.g., Zaritsky et al. 1997; Harris & Zaritsky 2009), the ionized/neutral/molecular gas (e.g., Smith & MCELS Team 1999; Kim et al. 2003; Stanimirovic et al. 2004; Mizuno et al. 2001a; Fukui et al. 2008; Wong et al. 2011; Muller et al. 2013), and the interstellar dust (e.g., Meixner et al. 2006, 2013) across each galaxy. These surveys reveal the interplay between stars and the ISM at different spatial scales in low metallicity and high radiation environments, and already improve our understanding on several key questions in galactic evolution: the effects of low metallicity environments on the atomic-to-molecular gas relation (e.g. Bolatto et al. 2011), the empirical conversion factor from CO luminosity to molecular gas mass (e.g. Leroy
et al. 2011), and the dust properties in low-metallicity systems (e.g. Galliano et al. 2011; Gordon et al. 2014). Supplementing the imaging surveys, spectroscopic measurements in the MCs (e.g., Tumlinson et al. 2002; Gordon et al. 2003; Maíz Apellániz & Rubio 2012) have also greatly improved our knowledge of the ISM physical and chemical properties. For example, Tumlinson et al. (2002) analyzed H$_2$ absorption against Magellanic Cloud hot stars using early FUSE observations and found high rotational excitation of H$_2$, which can be explained by high radiation fields and a low H$_2$ formation rate in the Magellanic system. More recently, Welty et al. (2012, hereafter W12) performed a comprehensive survey of HI and H$_2$ absorption features using archival Hubble Space Telescope (HST) and Far-Ultraviolet Spectroscopic Explorer (FUSE) spectra. That work systematically addressed the question of how gas-to-dust ratios and atomic and molecular gas abundances in the MCs compare with the Galaxy, using direct measurements of HI (Ly$_\alpha$), H$_2$ (Lyman-Werner, or LW bands), and dust extinction toward optical/UV background sources. Although these measurements sampled only limited regions that are necessarily biased against high extinction and lack the information on ISM structure provided by emission-based surveys (e.g. Roman-Duval et al. 2014), the directness and high sensitivity with which absorption-line analyses can probe the ISM allow unique insights into the physical and chemical properties of the gas and dust components of low-metallicity extragalactic environments.

Although W12 measured and compiled the column densities of HI and H$_2$ (hereafter $N_{\text{HI}}$ and $N_{\text{H}_2}$), as well as the rotational temperatures from the lowest two levels $T_{01}$ for the majority of sight lines with FUSE and/or HST observations, H$_2$ column densities were only measured for sight lines in which the damped profile fitting method was suitable ($N_{\text{H}_2} \gtrsim 10^{18}$ cm$^{-2}$). In addition, the rotationally excited H$_2$ lines from the LW bands were not systematically studied for deriving H$_2$ column densities at different rotational $J$-levels of the ground electronic-vibrational state, or $N_J$. In this subsequent study, we expand the work of W12 to a spectroscopic analysis of both ground and excited-state H$_2$ (up to $J = 5$) and Lyman HI lines, using the entire archival data set from the FUSE Magellanic Clouds Legacy
H$_2$ populations are directly related to UV pumping and H$_2$ formation, and can reveal the physical conditions and radiation environment of the absorbing gas, beyond its H$_2$ and HI column densities. Un-damped H$_2$ lines from excited $J$-levels also provide constraints on the absorber velocity structure at a moderate resolution ($\sim 20 – 30$ km s$^{-1}$) and clues how the absorbing gas is related to the gas seen in emission. In addition, Ly$\beta$ measurements available from some sight lines can augment the number of sight lines with both HI and H$_2$ absorption measurements.

We organized this chapter as follows. In Section 2.2, we describe the characteristics of the UV sight line sample in B09 and the UV and radio archival data used in this study. Sections 2.3 and 2.4 describe the UV spectroscopic analysis implemented in this study and direct observational results. In Sections 2.5 and 2.6, we present an analytical model to derive the gas and radiation field properties near absorbers using observables under several idealized assumptions, followed by the model-dependent results. We discuss the interpretation of the observational and model-dependent results in Section 2.7. Finally, Section 2.8 summarizes the conclusions of the work.

2.2 Sample and Data

2.2.1 UV Archival Data

The UV spectroscopic analysis presented in this study is entirely based on archival spectra compiled in the FUSE Magellanic Clouds Legacy Project. The data reduction and calibration were described in B09. The project includes 287 MC sight lines (187 for LMC and 100 for SMC), and the spectral coverage extends from $\sim 900$ to $1200$ Å at a resolution of $\sim 0.05$ Å (or FWHM $\sim 20$ km s$^{-1}$). All calibrated archival spectra were retrieved from the Multimission Archive at Space Telescope (MAST)$^1$, with separate FITS files covering three wavelength

$^1$http://archive.stsci.edu/prepds/fuse_mc
segments (910–1000, 990–1080, and 1090–1180 Å, respectively).

We summarized individual sight lines in Table 2.2, including star names, coordinates, and archive identifier\textsuperscript{2}. In this study, we excluded archival sight lines with complicated stellar continua or poor signal-to-noise from analysis due to difficulties in continuum estimation and line identifications, but still kept them in Tables 2.2 with corresponding data quality notes. We note the sample does include sight lines presented in Tumlinson et al. (2002, hereafter T02) and Cartledge et al. (2005), which constituted the majority of MC sight lines with previously published H$_2$ population measurements. We reanalyzed those sight lines for both MC and Galactic H$_2$/HI absorption. Because the archival spectra from B09 have been co-added from all usable FUSE data for each object, and processed with the final calibration pipeline with extensive updates (CalFUSE 3.2, Dixon et al. 2007), they include additional data taken subsequent to the earlier studies with possibly improved calibrations.

We present a complete overview of 1048–1056 Å absorption spectra from the MC FUSE archives in Figure 2.1. The 1D spectra are ordered by increasing declination of sight lines, with the color scale indicating the UV intensity. Argon and hydrogen lines from the MC (red tick marks) and the Milky Way (gray tick marks) can be clearly identified on this image, tracing the neutral gas components. The velocity difference between the LMC and SMC, as well as the velocity gradient within each galaxy, are easily apparent in this image. The velocities of the Galactic components do not change significantly across the spatial scale of each galaxy.

### 2.2.2 Ancillary Radio Data

To estimate the foreground Galactic contribution in the HI Lyman absorption lines and to calibrate the wavelength zero-point of the FUSE spectra (see more details in Section 2.3),

\textsuperscript{2}All stars names are known to SIMBAD, and their positions are from Skiff (2014) and verified to be within the FUSE apertures (either LWRS 30′′ × 30′′ or MDRS 4′′ × 20′′) based on the observation information provided in FITS headers. A number of FUSE observations apparently missed the designated UV sources, and their spectra were excluded in our analysis due to poor signal-to-noise.
Figure 2.1 Overview of the archival FUSE spectra from the FUSE Magellanic Clouds Legacy Project (Blair et al. 2009), covering the wavelength range from 1048 to 1056 Å. The spectra were presented in color scale, arranged with increasing declinations of sight lines from bottom to top. H$_2$ lines from the Lyman band 4 − 0 and or metal lines from Ar I and Fe II are identified at the top of the plot, near the Galactic (gray ticks) and LMC (red ticks) velocity. H$_2$ and metal lines from the Magellanic component clearly show a velocity gradient as the declination increases.
we retrieved the HI 21cm data from the Galactic All-Sky Survey\(^3\) (GASS, Kalberla et al. 2010). The data were provided in one spectral cube covering both the LMC, SMC, and the Magellanic Bridge, with a spatial resolution of 14.4′ and a velocity coverage of \(|v_{\text{LSR}}| < 468\, \text{km}\, \text{s}^{-1}\). The upper two panels of Figure 2.2 present the FUSE absorption line locations overlaid on the distributions of Galactic and Magellanic atomic gas (integrated over \(v_{\text{LSR}} = −70 \sim 70\) and \(70 \sim 350\, \text{km}\, \text{s}^{-1}\), respectively), showing the UV sight lines sample large parts of each galaxy. The foreground Galactic gas distribution is relatively smooth. A close examination of the 21cm spectra near UV sightline locations suggests a single velocity component near the Galactic absorption.

Absorption-based data from Lyα, LW bands of H\(_2\), and dust extinction measurements, provide a direct constraint on the ISM properties at small spatial scales. However, the environment of the HI and H\(_2\) gas measured in absorption can be better understood through ancillary emission-based multi-wavelength data covering adjacent regions, bearing in mind complications from line of sight confusion as demonstrated in W12. To assess the relation between the absorbers and their larger-scale ISM environments, we obtained the high-resolution \((\sim 60 − 100″)\) HI 21 cm data of the LMC and SMC from the ATCA+Parkes surveys\(^4\) (Kim et al. 2003; Stanimirovic et al. 1999) and 45″-resolution CO \(J = 1 − 0\) maps from the Magellanic Mopra Assessment (MAGMA) surveys\(^5\) (Wong et al. 2011; Muller et al. 2013). These data are able to reveal the atomic and molecular gas distributions near each sight line. Although the MAGMA surveys only cover CO-bright clouds and their nearby regions, their relatively high resolution compared with previous CO surveys is valuable for comparisons with absorption-based gas properties revealed at very small scales. Despite their limited spatial coverage, they already cover a significant fraction of the entire sample \((\sim 1/3\) of the sight lines with \(N_{\text{H}_2}\) measurements or upper limit).

In order to compare gas properties between Galactic and Magellanic absorbers, we com-

\(^3\)http://www.astro.uni-bonn.de/hisurvey/gass
\(^4\)http://www.atnf.csiro.au/research/HI/mc/queryForm.html
\(^5\)http://mmwave.astro.illinois.edu/magma/DR3
piled previously published Galactic HI and H$_2$ absorption measurements, some with H$_2$ population distributions$^6$. These Galactic measurements are taken toward either Galactic or extragalactic background sources (including the MC sample in this work). Most of $N_{\text{HI}}$ and $N_{\text{H}_2}$ measurements are from early Copernicus observations (e.g. Savage et al. 1977; Bohlin et al. 1978) and more recent FUSE observations (e.g. Rachford et al. 2002, 2009; Jensen et al. 2010) toward nearby stars (within $\sim 1 \text{kpc}$), supplemented with results from the FUSE high Galactic latitude ($|b| > 20^\circ$) sight lines toward AGNs (Gillmon et al. 2006; Wakker 2006). In the bottom panel of Figure 2.2, we shown the locations of compiled UV sight lines with both Galactic HI and H$_2$ measurements, overlaid on the all-sky HI 21cm map from the Leiden/Argentine/Bonn (LAB) survey (Kalberla et al. 2005). We only use the absorbers with $|v_{\text{LSR}}| < 70 \text{ km s}^{-1}$ as the comparison sample. They generally probe the diffuse or translucent clouds in the Galactic disk.

2.3 Analysis

The primary goal of our UV spectroscopic analysis is to measure H$_2$ populations at individual $J$-levels in the FUSE sample with a uniform procedure. Traditionally, the curve-of-growth (COG) technique is preferred for analyzing H$_2$ lines from $J \geq 2$ states. While the COG method is still adequate for lower-$J$ H$_2$ lines from absorbers with $N_{\text{H}_2} < 10^{18} \text{ cm}^{-2}$, a line profile fitting method is commonly adopted to derive $N(0)$ and $N(1)$ for higher column density absorbers, when their damping wings are distinct and insensitive to the line Doppler broadening parameter ($b$-value). The instrumental line spread function (LSF) of the FUSE spectra is $\text{FWHM}_{\text{LSF}} = 20 \text{ km s}^{-1}$. Because high-$J$ H$_2$ transitions are not resolved, the apparent optical depth technique (Savage & Sembach 1991) is not applicable, despite its advantage of requiring no prior assumptions for the absorber velocity distribution.

$^6$The compilation is based on the online Galactic sight lines catalog from D. Welty at http://astro.uchicago.edu/~dwelty/coldens.html and several recent published works. The complete reference for the compilation is available at http://los.magclouds.org
Figure 2.2 Upper/middle panels: MC absorption line locations, overlaid on the distributions of the atomic gas from the Magellanic Clouds (integrated over $v_{\text{LSR}} = 70 - 350\ \text{km s}^{-1}$) and foreground Galactic ISM (integrated over $|v_{\text{LSR}}| < 70\ \text{km s}^{-1}$). The HI column densities (color-scale) were derived from the Galactic All-Sky Survey (GASS, Kalberla et al. 2010), presented in a Cartesian projection. The foreground Galactic HI distribution is relatively smooth and weak towards both galaxies ($\sim 3 \times 10^{20}$ and $\sim 5 \times 10^{20}\ \text{cm}^{-2}$ for the SMC and LMC foregrounds, respectively). Bottom panel: UV sightline locations of the comparison sample in Galactic coordinates, overlaid on the all-sky 21cm map from the Leiden/Argentine/Bonn (LAB) survey (Kalberla et al. 2005) in an Aitoff projection.
Figure 2.3 H$_2$ rotational diagram for the absorber along the SMC sight line AzV 6. The statistically weighted column densities at different $J$-levels in the ground electronic-vibration stated are plotted against their corresponding energy levels. The H$_2$ population distribution can be roughly represented by two temperatures, one for $J \leq 2$ at $\sim 80$ K, and another higher temperature of $\sim 500$ K for $J \geq 3$. 

$T_{01}$=88K  
$T_{12}$=77K  
$T_{36}$=543K
The COG method requires measuring the equivalent widths of multiple H$_2$ lines from the same energy state, and it does not depend on the spectral resolution. The profile fitting method demands a reliable continuum fit and exclusion of unrelated spectral features in the broad damping wings. In practice, these two methods are complementary and commonly used together for H$_2$ absorption line surveys (e.g. Tumlinson et al. 2002; Jensen et al. 2010). However, compared with high-latitude or Galactic FUSE sight lines, analyzing UV spectra from MC sight lines becomes more difficult for two main reasons. First of all, the sight lines are typically toward MC stars which lack the simplicity of AGN continua frequently available for high-latitude samples, making continuum estimation difficult. Second, the MC sight lines show numerous absorption features contributed by the neutral and ionized ISM from MCs and Milky Way, as well as the UV background sources themselves (e.g., stellar winds and photospheres). Although the FUSE spectral resolution is sufficient to resolve velocity differences between the MC and Galactic lines, many MC lines suffer from blending with Galactic lines at a slightly longer rest wavelength. Without a precise velocity structure as prior, it would be extremely difficult to unambiguously decompose individual line components and evaluate their equivalent widths or line profiles.

To overcome the above difficulties, we developed an IDL-based package, which we have named htau. The package measures H$_2$ and HI absorber properties by directly fitting an absorber physical model and an instrument model to the observed UV spectra. Because the physical model incorporates multiple velocity components of H$_2$ and HI, all “hydrogen-related” spectral features can be fitted simultaneously, provided that a reliable continuum is obtained and spectral features from other species are excluded from the fitting.

In this section, we describe in detail the analysis strategies implemented in htau, with some specific procedures designed for analyzing the MC sight lines. We first introduce the physical and instrumental model implemented in htau, which is used to simulate normalized H$_2$ and HI line profiles. Then we explain how we evaluate the quality of the fits based on an approach similar to the continuum reconstruction method (e.g. Howk et al. 1999).
This is followed with additional details on the iteration model fitting. Finally, we compare our method with other techniques and discuss the uncertainties in the derived H$_2$ and HI properties.

### 2.3.1 Physical and Instrumental Model for H$_2$/HI Absorptions

We assume a simple physical model in htau, with H$_2$ and HI contributed by several diffuse clouds along the line of sight. The molecular and atomic hydrogen gas in each cloud is assumed to have a Gaussian turbulence field. Therefore, hydrogen-related lines can be modeled with a limited number of physical parameters, namely, the population distribution of absorbing H$_2$ at different energy states $N_J$, the HI column density $N_{\text{HI}}$, and their velocity structure (e.g. gas systemic velocity and turbulent dispersions). The physical parameters of the cloud model are summarized in Table 2.1. We adopted a single $b$-value and systemic velocity $v$ for H$_2$ at different $J$-levels as well as HI. Although this assumption is not relevant for HI (all Lyman lines are broad with damped wings), $b$–values can in principle vary among different $J$-levels (e.g. Lacour et al. 2005; Noterdaeme et al. 2007). For simplicity, we prefer to assume a single $b$-value as a prior assumption for modeling MC sight lines, because $J$-dependent $b$–values or velocity structures barely improve model fitting considering the moderate data quality in the FUSE MC sample (see related discussions on a Galactic sample in Jensen et al. 2010).

For a direct comparison between the physical model and observed FUSE spectra, we include an instrument model in which the absorption predicted by the physical model is convolved with a Gaussian instrumental LSF. We also shift the convolved model spectra by a small fitted offset (typically < 0.2Å) to compensate for the absolute wavelength calibration error commonly seen in FUSE archival spectra. Finally, the shifted model is resampled to the wavelength grid of the FUSE data in a flux conservative approach. Because the wavelength zero-point error is generally detector-dependent, a wavelength correction for each spectrum is necessary.
Table 2.1. Parameterized Model for Predicting Observed H$_2$/HI Absorption Profile

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical Model</td>
<td>Each velocity component</td>
<td></td>
</tr>
<tr>
<td>$N_J$</td>
<td>cm$^{-2}$</td>
<td>$N_{H_2}$ at the rotational level $J$ in the ground electronic-vibration state</td>
</tr>
<tr>
<td>$N_{HI}$</td>
<td>cm$^{-2}$</td>
<td>HI column density</td>
</tr>
<tr>
<td>$b$</td>
<td>km s$^{-1}$</td>
<td>Doppler broadening parameter</td>
</tr>
<tr>
<td>$v$</td>
<td>km s$^{-1}$</td>
<td>Component systemic velocity in the heliocentric frame</td>
</tr>
<tr>
<td>Instrumental Model</td>
<td>Each spectrum</td>
<td></td>
</tr>
<tr>
<td>$\Delta \lambda$</td>
<td>Å</td>
<td>Wavelength shift for a spectral segment</td>
</tr>
<tr>
<td>FWHM[$\phi$]</td>
<td>Å</td>
<td>FWHM of the instrumental line spread function</td>
</tr>
</tbody>
</table>

Although simulating absorptions from H$_2$ and HI is straightforward, the practical procedure could be time-consuming for iterative fitting. The major obstacle is that the total hydrogen-contributed optical depth should be derived by summing optical depth Voigt profiles of all H$_2$ and HI lines at a sufficient resolution for preserving numerical precision. To improve the efficiency, we followed McCandliss (2003) and developed a new H$_2$/HI optical depth template library in htau. For generating the optical depth templates, we used the up-to-date atomic and molecular data implemented in the meudon PDR code (Le Petit et al. 2006). The templates cover all H$_2$ and HI features from 900–1350 Å, with a fine logarithmic wavelength grid spacing\(^7\) to preserve adequate numerical precision in cases of small $b$-values. The $b$-value is sampled from 0.8 to 25 km s$^{-1}$ with $\Delta b = 0.1$ km s$^{-1}$ to cover common cold ISM conditions. With the set of parameters in Table 2.1, a simulated normalized hydrogen absorption spectrum can be generated from the pre-calculated optical depth templates as,

$$I_n = G \left\{ P \ast \exp \left[ - \sum \frac{N_i}{N_f} \tau_i \right] \right\}, \quad (2.1)$$

where $N_i$ is the column density of a species (either HI or the H$_2$ at a specific $J$-level) from one velocity component. $N_f$ is the fiducial value at which the optical depth templates were calculated, and $\tau_i$ represents the corresponding optical depth template of the species.

\(^7\)The grid spacing is $\log(\lambda_{i+1}/\lambda_i) = 1.0 \times 10^{-6}$ and $3.0 \times 10^{-6}$, for $b < 2.0$ km s$^{-1}$ and $b > 2.0$ km s$^{-1}$, respectively.
under the assumed $b$-values (after Doppler shifting to the systemic velocity). The sum was performed over all species at different velocities. The result was convolved with the assumed LSF function of $P^8$. $G$ is the operation required for the wavelength calibration offset adjustment and spectral regridding to match the wavelength grid of the observations. Although htau does not allow for non-Gaussian velocity profiles, any absorber which can be decomposed into several Gaussian turbulent clouds can still be modeled. The above operation can be performed very efficiently with the pre-calculated templates because it only involves template scaling and resampling.

### 2.3.2 Evaluating the Model Quality

A simulated $\mathrm{H_2}/\mathrm{HI}$ absorption model describing the observed spectra will correspond to the physical properties of $\mathrm{H_2}$ and HI along the line of sight. However, a quantitative measure for the model quality requires continuum evaluation because the physical model only provides the flux transmission $I_n = \exp(-\tau)$. Because the absorption model in htau only incorporates $\mathrm{H_2}$ and HI absorption, we also have to exclude the spectral features contributed by other species when comparing models and observations.

Continuum fitting is usually done in a piecewise fashion by interpolating the assumed local continuum, identified as line-free regions near transmission maxima with sufficient signal-to-noise. Therefore, its reliability becomes degraded for low S/N or low-resolution data, with the fractional continuum error propagated into the uncertainty of measured line properties. The process, together with line exclusion, usually requires human intervention and is time-consuming, especially for targets with complicated continuum structure and many absorption features. To reduce subjectivity in the model fitting procedure, we adopted a semi-automated method to perform both line exclusion and continuum fitting in each fitting iteration.

For each simulated normalized hydrogen absorption profile, we define a wavelength ex-

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8FWHM$_{\text{LSF}}$ is assumed to be 20 km s$^{-1}$ or 25 km s$^{-1}$, for LiF and SiC channels, respectively.
clusion mask based on a list of non-hydrogen features, using on their rest wavelength and expected systemic velocity. Each component of the mask has a typical width of $\sim 1\Delta\lambda^9$, which accommodates the uncertainty in the actual line velocity difference from H$_2$. The mask is used to identify all wavelength intervals containing only hydrogen features and stellar continua. In Table 2.4, we summarize the excluded features, including prominent stellar features, non-hydrogen interstellar absorption, and terrestrial atmospheric lines (airglow). These features are compiled by comparing the archival spectra with various UV spectral atlases (e.g., Feldman et al. 2001; Danforth et al. 2002; Pellerin et al. 2002; Walborn et al. 2002; Willis et al. 2004; Smith 2010, 2012) and examining their general physical properties (e.g. species abundance and oscillator strength). The rest wavelengths and atomic data are from Morton (2003).

For continuum fitting, we first divide the observed spectrum by the line model $I_n$ to create a pseudo reconstructed continuum. We define “effective” continuum regions by excluding the regions identified by the exclusion mask and regions with SNR $< 4$. Then we applied an automated B-spline fitting algorithm from idlutils to fit a global continuum in each spectrum. The typical adopted B-spline order is 4. Besides the standard procedure offered idlutils (e.g. outlier rejections), we implement an adaptive method to determine the locations of B-spline knots in htau. The typical knot spacing is set to be $\sim 4\Delta\lambda$, but the spacing is automatically increased near broad hydrogen features (e.g. Ly$\beta$ or Ly$\gamma$) or decreased if the stellar continua show complicated structures. The knot spacing should be wider than any hydrogen feature, otherwise, an absorption feature will be fitted with both a highly variable continuum model and hydrogen line model.

In our sample, the background continua of some later-type stars are too complex to model using a B-spline. For a limited number of such cases, we approximate the continuum

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$^9$We assumed any ISM metal lines have similar velocity from H$_2$ and stellar lines are located near the velocity of the MC absorber. Some spectral features could be broader and originate at a different velocity from the H$_2$ gas or stellar velocity (e.g. ionized species like O VI). The corresponding mask components are expanded to accommodate these uncertainties.
based on a synthetic UV stellar model spectrum from the TLUSTY\textsuperscript{10} or CMFGEN\textsuperscript{11} O/B star model grid (Lanz & Hubeny 2003, 2007; Hillier & Miller 1998; Palacios et al. 2010). The model grid provides high-resolution UV model spectra at the LMC and SMC metallicity. A model stellar spectrum is chosen with a similar stellar/luminosity type to the background star (specified as the effective temperature, $T_{\text{eff}}$, and the surface gravity, log $g$ in the grid), and convolved with a projected rotational broadening of $v \sin i = 150$ km s$^{-1}$ or previously published values (e.g. Massey et al. 2004, 2005, 2009, 2013). Then we divide the pseudo continuum model by the stellar model (without UV extinction correction) before proceeding with B-spline fitting. The final stellar continuum fit will be a “hybrid” of the adopted stellar model and the B-spline.

The final model fitting quality is evaluated using the Poisson likelihood ratio (PLR, e.g. Dolphin 2002; Humphrey et al. 2009; Erwin 2015),

$$C = 2 \sum_i (M_i - D_i + D_i \ln D_i - D_i \ln M_i),$$

where $D_i$ is the number of detected counts in the $i$-th spectrum sampling point and $M_i$ is the model prediction. The “$C$-statistic” is preferred over the standard $\chi^2$ minimization because it better describes the statistics in the low signal-to-noise regions, which is common near H$_2$ and HI absorptions in the FUSE archival spectra. The sum was done over all wavelength intervals after excluding non-hydrogen features. Therefore, the relative value of the $C$-statistic reflects the modeling quality of both hydrogen absorption and continuum, a quantitative alternative to the relatively subjective evaluation of fit quality in the continuum reconstruction method.

\textsuperscript{10}http://nova.astro.umd.edu/index.html
\textsuperscript{11}http://pollux.graal.univ-montp2.fr
2.3.3 Iterative Fitting

We adopted a Levenberg-Marquardt algorithm implemented in IDL (MPFIT, Markwardt 2009) to minimize $C$ defined in Equation 2.2. In each fitting iteration, we use $N_J$, $b$, and $v$ from the last step (or first-order model) to simulate the observed spectra along the line of sight. The value of $C$ and its derivatives are numerically evaluated to find a model better describing the observed spectra, until no significant $C$ improvement can be achieved.

In rare occasions, the default mask generated by the program might not capture all non-hydrogen spectral features, which will lead to a continuum model bias. Some complicated continuum features might also be difficult to fit in both normal B-spline or “hybrid” fitting. For such cases, we add extra mask components to remove spectral or continuum features which cannot be reasonably fit by $htau$, and also divide the spectrum into smaller chunks for a piecewise continuum fitting during each iteration. Because the fitting process can be reproduced given the same input and the results can be visualized directly, the spectral fitting can be improved incrementally and efficiently during a model re-fitting.

In practice, any iterative fitting algorithm requires a proper prior model, because a global minimum of $C$ in a nonlinear, multi-dimension parameter space is not guaranteed. Additionally, not all modeling parameters can be constrained by the FUSE spectra alone. To assist the iterative fitting, we introduce prior assumptions and constraints for the modeling of each sight line, which come from previous work and non-FUSE data. In addition, we also adopt a reasonable first-order model from the initial spectra examination. All of these constraints can be flexibly incorporated into the spectral fitting of $htau$.

Velocity Structure and Wavelength offsets

Despite good relative wavelength calibration, the error in the absolute wavelength calibration of FUSE archival data can be as large as 0.2Å. In B09, the co-adding of multiple observations was done for each individual channel with a cross-correlation-based alignment shift to avoid any wavelength misalignment from multiple observations. However, the absolute wave-
length calibration is uncertain due to technical reasons (e.g. thermally-induced distortions or mispointing toward target stars).

In our instrument model, we add a wavelength shift \( \Delta \lambda = \lambda_{\text{obs}} - \lambda_{\text{hel}} \) to the model, before resampling the wavelength grid to that of in the archival spectra. Considering the requirement of wavelength correction, the line centroid in the archival spectra \( \lambda_{\text{obs}} \) will be related with the line rest wavelength \( \lambda_0 \) as,

\[
\lambda_{\text{obs}} - \Delta \lambda = \lambda_{\text{hel}} = \left( \frac{v_{\text{hel}}}{c} + 1 \right) \lambda_0,
\]

(2.3)

Here \( \Delta \lambda \) is the wavelength correction for an individual spectrum and \( v_{\text{hel}} \) is the absorber heliocentric velocity. Technically, if we can measure the line centroids of multiple different lines believed to be at the same velocity (e.g., \( \text{H}_2 \) lines from the same \( J \)-level), both \( v_{\text{hel}} \) and \( \Delta \lambda \) can be derived by fitting the \( \lambda_{\text{obs}}-\lambda_0 \) correlation. Although this approach has been demonstrated in \textit{Wakker} (2006), it would be difficult for \( \text{H}_2 \) absorption in MC sight lines because uncontaminated \( \text{H}_2 \) lines usually only span a limited wavelength range in a spectrum from a single detector. To simplify the procedure, we make the prior assumption that the Galactic HI and \( \text{H}_2 \) absorption components have the same velocity\(^\text{12} \) as the HI gas seen in the GASS 21cm survey. Then the wavelength correction in the instrumental model and absorber velocity in the physical model will be tied to this velocity as an absolute reference, and solved simultaneously during the model fitting.

For most sight lines, our model consisted of two velocity components from the Magellanic Cloud and Milky Way, respectively. However, we added additional absorber components for sight lines showing multiple distinct components near the Magellanic Cloud velocity, leading to a maximum number of 3 components in modeling. The LMC and SMC \( \text{H}_2 \) absorptions are located near \( v_{\text{LSR}} \sim 260 \pm 40 \text{ km s}^{-1} \) and \( \sim 160 \pm 40 \text{ km s}^{-1} \), respectively, with the Galactic components within \(|v_{\text{LSR}}| < 30 \text{ km s}^{-1} \). The wavelength centroid of narrow unblended \( \text{H}_2 \)

\(^{12}\text{We performed a double Gaussian decomposition for the 21cm emission and define the velocity of the component with narrower FWHM and higher brightness temperature peak as the } \text{H}_2 \text{ absorber velocity.} \)
lines and atomic ISM lines (e.g. Fe II λ1096.88) provide the first-order systemic velocity of each absorption component. But their final value, together with the wavelength correction, were derived from the iterative fitting.

**HI and H₂ Column Density**

The MC and Galactic HI absorption lines are broad and blended, and their corresponding column densities cannot be constrained simultaneously. Following W12, we adopt the Galactic HI gas column density from the GASS survey (assuming optically thin) in the absorption model fit. Therefore, the Galactic contribution to the Lyman lines are accounted for in our data analysis. In the *FUSE* wavelength coverage, Lyβ is the most prominent feature from HI. However, Lyβ is usually contaminated by H₂ lines and metal lines (e.g. O VI), yielding less reliable measurements of $N_{\text{HI}}$ compared with Lyα. We generally adopted the Lyα-based $N_{\text{HI}}$ value from W12, and attempted to fit $N_{\text{HI}}$ contributed by the MC gas only when it is not measured in W12. However, the Lyβ fitting procedure was only performed when a reasonable continuum reconstruction was obtained around the line. A comparison between Lyα and Lyβ fitting results for a sub-sample of W12 suggests a reasonable agreement within 0.2 dex.

Welty et al. (2012) have measured $N_{\text{H₂}}$ and $T_{01}$ for a majority of the high column density sample using the line profile fitting method. For those sight lines, we build an initial-guess H₂ population model by assuming: $N_{\text{H₂}} = \sum_j N_j$, $T_{12} = T_{01}$, and $T_{23} = T_{34} = T_{45} = 300$ K, with the $b$-value assumed to be 5 km s$^{-1}$. When previous measurements are not available, the initial model will still be based on the above assumption, with $N_{\text{H₂}} = 10^{19}$ cm$^{-2}$ and $T_{01} = 100$ K.

**Uncertainty**

Although the iterative fitting in *htau* is adequate to provide the best-fit absorber model, the parameter uncertainties directly provided by the *mpfit* algorithm are generally not realistic.
They are based on numerically evaluated derivatives or the covariance matrix, which can vary significantly between the best-fit model and the corresponding value at an offset of 1σ. The correlations between fitting parameters are also ignored. In the iterative fitting, \( b \)-value is constrained mainly by the relative line strengths among multiple lines from the same energy state, while the column density \( N_J \) is constrained by the absolute line strengths or line profiles under the same \( b \)-value. The uncertainties in \( N_J \) and \( b \) could be strongly correlated if most of measured lines are located on the flat part of COG. Therefore, the output from MPFIT is generally a lower limit to the true uncertainty.

To give a realistic estimation of the confidence level in each fitted parameter, we adopted a \( \Delta C \) criterion in HTAU, which is similar with the method used in T02. Specifically, we generate a set of simulated models covering the adjacent parameter space around the best-fit model by randomly varying all free parameters included in the fitting. We assume that \( C - C_{\text{best}} \) is approximated as a \( \chi^2 \) distribution with \( N \) degrees of freedom. Then we define a threshold value of \( \Delta \chi^2_c \) corresponding to 1σ confidence in the \( \chi^2 \) distribution. The maximum parameter variation from the simulated models having \( \Delta C < \Delta \chi^2_c \) is used to define the uncertainties of individual fitting parameters. This approach not only yields conservative uncertainty estimations, but also helps to confirm the best-fit from iterative fitting as a global \( C \) minimum by exploring a larger parameter space.

Most sight lines presented in this work have been analyzed in W12 using the line profile fitting method to derive the \( \text{H}_2 \) column densities for the lowest two rotational levels \( N(0) \) and \( N(1) \). A significant fraction of them was measured with corresponding atomic gas column density (see W12 and references therein). A smaller number of sight lines were also studied in Tumlinson et al. (2002) and Cartledge et al. (2005), with higher-\( J \) column densities. We compared the new results with previous COG-based results and found a general agreement of \( N_J \) and \( b \)-values within the measurement uncertainties, without systematic bias. The consistency degrades for sight lines with poor SNR and complicated stellar continua.
2.4 Results

We summarize measured H$_2$ and HI properties of the Magellanic and Galactic absorbers along $FUSE$ sight lines in Table 2.2. The table content includes: H$_2$ column density at each $J$–level (up to 6) in the ground electronic-vibrational state, $b$–value, and absorber component velocity. We note that some results are directly compiled from W12 (e.g. $N_{\text{HI}}$ from Ly$\alpha$), depending on the data availability and quality. In this section, we present major new results from these measurements.
Table 2.2. H$_2$ and HI Properties: SMC Sight Lines

<table>
<thead>
<tr>
<th>Star</th>
<th>Data ID</th>
<th>RA (J2000)</th>
<th>DEC</th>
<th>$N_{HI}$ cm$^{-2}$</th>
<th>$v_{HEL}$</th>
<th>$N_{HI}$ cm$^{-2}$</th>
<th>$N(0)$ cm$^{-2}$</th>
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<td>00 43 36.9</td>
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<tr>
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<td>11</td>
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<td>16.87+0.44</td>
<td>16.39+0.90</td>
<td>15.01+0.90</td>
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<tr>
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<td>10</td>
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<td>10</td>
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<td>&lt;13.87</td>
<td>K10/X15</td>
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</table>

Note. — Only a portion of the table (first 10 sight lines) is shown here for guidance regarding its form because of the large size of the content. An up-to-date complete version of this table is available at http://lincs.mpia.de, complemented with additional metadata (e.g. $E(B-V)$, stellar type, etc.) for individual sight lines. A comparison sample of Galactic sight lines is also available, compiled from previous studies. Some contents of the online table are based on the UV sight line database maintained by D. Welty (http://astro.wi.edu/~dwelty/coldens.html). References: X15, this work; W12, Welty et al. (2012); K10, Kalberla et al. (2010).
### Table 2.3. H$_2$ and HI Properties: LMC Sight Lines

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<tr>
<th>Star</th>
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<th>$v_{HEL}$ km s$^{-1}$</th>
<th>$b_{DPH}$ km s$^{-1}$</th>
<th>$N(H_2)$ cm$^{-2}$</th>
<th>$N(0)$ cm$^{-2}$</th>
<th>$N(1)$ cm$^{-2}$</th>
<th>$N(2)$ cm$^{-2}$</th>
<th>$N(3)$ cm$^{-2}$</th>
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<td>14.6±0.35</td>
<td>14.5±0.48</td>
<td>K10/X15</td>
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Note. — Only a portion of the table (first 10 sight lines) is shown here for guidance regarding its form because of the large size of the content. An up-to-date complete version of this table is available at [http://ioa.igloo.org](http://ioa.igloo.org), complemented with additional metadata (e.g., $E(B-V)$, stellar type, etc.) for individual sight lines. A comparison sample of Galactic sight lines is also available, compiled from previous studies. Some contents of the online table are based on the UV sight line database maintained by D. Welty ([http://astro-uchicago.edu/~welty/voldena.html](http://astro-uchicago.edu/~welty/voldena.html)). References: F86, Fitzpatrick (1986); X15, this work; W12, Welty et al. (2012); K10, Kalberla et al. (2010).
2.4.1 \( \text{H}_2 \) Rotational/Excitation Temperature

\( \text{H}_2 \) rotational temperatures in the ground electronic-vibrational state, defined by the population distribution as,

\[
\frac{N_u}{N_l} = \frac{g_u}{g_l} \exp \left( -\frac{\Delta E_{lu}}{kT_{lu}} \right),
\]

are determined by several different physical mechanisms. The higher-\( J \) levels are mainly populated by radiative excitation or \( \text{H}_2 \) formation. The lowest two \( J \)–levels, with the statistical weights ratio \( g_1/g_0 = 9 \) and \( \Delta E_{01}/k = 171 \text{ K} \), are mainly determined by collision excitation. If the density is higher than the critical density, \( T_{01} \) could reveal the kinetic temperature of the \( \text{H}_2 \) gas. Figure 2.3 presents a typical \( \text{H}_2 \) rotational diagram in the \( v = 0 \) vibrational level of the \( \text{H}_2 \) ground electronic state, with two distinct temperatures fitted among the lower and higher \( J \)-levels. This is common behavior toward many Galactic and Magellanic sight lines, which agrees with the fact that high-\( J \) states are populated by UV pumping and \( \text{H}_2 \) formation processes.

In Figure 2.4, we present the relation between \( T_{01} \) and \( N_{\text{H}_2} \) for different sight line groups. The top panel shows the correlation for the MC absorbers measured in this work and W12. The bottom panel shows the same correlation for the Galactic absorbers, compiled from previous studies (see the online version of Table 2.2 for the references). Although the correlations show significant scatter and measurement uncertainties, the result indicates an overall similar relation between \( T_{01} \) and \( N_{\text{H}_2} \) for both samples: \( T_{01} \) is distributed between 40 ~ 200 K for sight lines with \( N_{\text{H}_2} \gtrsim 10^{18.5} \text{ cm}^{-2} \), with higher \( T_{01} \) at lower \( N_{\text{H}_2} \). For sight lines with \( N_{\text{H}_2} \gtrsim 10^{18.5} \text{ cm}^{-2} \) and \( T_{01} \) uncertainty less than 50 K, we found \( < T_{01} > = 68 \pm 16 \text{ K} \) and \( 73 \pm 20 \text{ K} \) for the MC and Galactic sample (excluding Galactic sight lines with \( |b| > 20^\circ \)), respectively. This result is consistent with the measurements from T02 and their comparison with the Galactic values \( < T_{01} > = 77 \pm 17 \text{ K} \) from the \textit{Copernicus} \( \text{H}_2 \) survey (Savage et al. 1977) and 67 \pm 14 K from the \textit{FUSE} Galactic survey (Rachford et al. 2009). Shull & Woods (1985) suggested that the equilibrium gas temperature should be nearly independent
Table 2.4. Excluded Lines in Spectral Fitting

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Note. — Only a portion of the table (from 1010 to 1075Å) is shown here for guidance regarding its content. An online version of this table is available http://uvline.magclouds.org
Figure 2.4 Rotational temperature $T_{01}$ plotted against $N_{\text{H}_2}$ for the Magellanic Clouds (Top) and Galactic (Bottom) absorbers. The Magellanic Clouds absorber results are from UV absorption observations targeting LMC or SMC hot stars. The Galactic results are from measurements toward Galactic stars (MW) and high-latitude extragalactic objects (ExG), compiled from previous studies. We find large scatters in $T_{01}$ for sight lines with $N_{\text{H}_2} < 10^{18}$ cm$^{-2}$ in all samples. At higher H$_2$ column densities, $T_{01}$ is distributed between 50–140 K for both the MC and Galactic absorbers, with similar median values.
of metallicity as both heating (UV photoelectric heating by dust grains) and cooling (primarily by the [C II] 158 µm line) depend on metallicity, provided that the ratio of UV field and gas density does not change and the cloud is diffuse. This may indicate this ratio does not change significantly in regions where H$_2$ resides across the Magellanic clouds and the Milky Way, despite the atomic-to-molecular gas ratio being generally higher in the MCs.

To quantitatively evaluate the relation between $T_{01}$ and $N_{H_2}$ for the sight lines with $N_{H_2} \gtrsim 10^{18.5}$ cm$^{-2}$, we calculated the rank correlation coefficient, which is a nonparametric measure of statistical dependence between two variables. The result indicates an anti-correlation between $T_{01}$ and $N_{H_2}$ for the MC and Galactic absorbers, with a correlation coefficient of $-0.45$ and $-0.32$, respectively, and significant departure (above 3σ) from the null hypothesis. This anti-correlation is expected, considering higher gas column density may provide greater UV shielding from dust and H$_2$, leading to cooler gas on average along the line of sight. A similar trend between $T_{01}$ and reddening is also found in Rachford et al. (2009).

Gillmon et al. (2006) found a systemically higher $T_{01}$ in their high latitude sample, with

Table 2.5. References for Previous HI and H$_2$ Measurements

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<th>Code</th>
<th>Reference</th>
<th>Code</th>
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a mean value of 124 ± 8 K. We also find that high latitude H$_2$ sight lines have slightly higher $T_{01}$ when compared with Galactic disk sight lines with similar $N_{\text{H}_2}$, presumably due to a lower volume density and less efficient cooling. But the systemically higher $T_{01}$ in Gillmon et al. (2006) also appears to be caused by a sample bias toward lower H$_2$ column density.

2.4.2 Large-Scale Velocity Field

We present the large-scale velocity field traced by absorbing H$_2$ gas and 21cm/CO emissions in Figures 2.5 and 2.6. In each row, the first gray-scale image shows the distribution of HI emission (Stanimirovic et al. 1999; Kim et al. 2003) or CO emission (Wong et al. 2011; Muller et al. 2013) in position-position space, after integrating along the velocity axis. The image is in the sinusoidal projection of an Equatorial J2000 coordinate system, with the projection center, reference pixel position, and image dimensions summarized in Table 2.6. Six images at the right show the distribution of HI emission in the velocity-$y$ ($v-y$) space (integrated along the projected $x-$axis) in individual regions divided by the dotted lines. Red circles present the velocities of individual absorbers.

Both LMC and SMC are known to show disrupted HI kinematic structure at large-scale. Although the LMC is dynamically close to being a rotating disk galaxy with a velocity gradient from south to north, a high-velocity component exists in the southeast part of the galaxy, near the molecular ridge. This is evident in the 1st and 2nd $v-y$ plot, with two kinematic components converging near the 30 Doradus region at the north end of the molecular ridge. Several bubbles are also evident (in 3rd/5th/6th panels), with both higher and lower velocity gas away from the main kinematic component. The SMC exhibits even more complicated kinematic structure (e.g. Stanimirovic et al. 1999). Scowcroft et al. (2015) also report that the SMC is tilted with its eastern side up to 20 kpc closer than its western side. Two kinematic components are distinct in nearly every $v-y$ plot, with a velocity convergence in the 4th and 5th p-v plots (tracing the region near the SMC “bar”).

The velocity comparison between HI 21cm and absorbers suggests that the detected
absorbers generally trace the overall velocity gradient in the LMC. This agrees with the result from Danforth et al. (2002), which found a velocity similarity between the LMC P II absorption and HI 21cm. However, a significant number of sight lines also show slightly lower velocity (e.g. 3rd v-y plot) that is not associated with prominent HI emission. This indicates that H₂ gas revealed by the absorption lines does not necessarily trace the gas in the LMC disk. The velocity comparison between CO and H₂ absorption shows similar results as indicated by the 21cm-absorber comparison. Since the CO clouds are generally associated with stronger 21cm emission, a significant number of sight lines show up in regions of position-velocity space where no CO is detected at all.

In the SMC, our comparison reveals that most absorbers are generally associated with the lower velocity component except in the northern regions where only higher velocity structure exists. This general result has been reported in Welty et al. (2012), suggesting the lower velocity component is at the near side, although the exact depth of individual background stars can vary. The MAGMA CO survey of the SMC is largely incomplete because the CO emission is intrinsically weak and the survey was limited to the region where strong CO has been detected at lower resolution (Mizuno et al. 2001b). The detected CO resides in both kinematic components in the SMC. Although the majority of sight lines reside in the region not covered by the MAGMA survey, we found several absorbers showing velocity roughly consistent with CO clouds, although they are generally not centered on the sky positions of CO clouds.

The velocity comparison highlights the difficulty in comparing the gas absorption and emission in a general sense, as the absorbing gas may just trace a cloudlet at the near side even when a molecular cloud is along the line of sight. Overall, the absorbers are not guaranteed to trace the main gas component in each galaxy and could instead trace lower-latitude halo gas. On the other hand, we indeed found more than half of sight lines showing coherence in both angular and velocity space with the emission at or near the sightline location, suggesting that they may trace the edges of the molecular clouds or nearby diffuse
<table>
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<th>SMC</th>
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</table>

clouds in the same large-scale kinematic structure. A similar conclusion is also revealed by the column density comparison between emission and absorption tracers, illustrated in the following section.
Figure 2.5 LMC velocity field traced by absorbers and 21cm/CO emission. In each row, the first image shows the sky distribution of HI 21 cm emission (Kim et al. 2003) or CO $J = 1 - 0$ emission (Wong et al. 2011), after integrating along the velocity axis. Both the HI and CO images are in the sinusoidal projection of an Equatorial J2000 coordinate system, with the projection center, reference pixel position, and image dimensions summarized in Table 2.6. The images to their right show the gas emission distribution in the velocity-position space (integrated along the image x-axis) within individual regions divided by the dotted lines. Cyan circles present the H$_2$ absorber velocity of individual UV sight lines.
Figure 2.6 SMC velocity field traced by absorbers and 21cm/CO emission.
2.4.3 ISM Structure

W12 presents a comparison of emission and absorption based $N_{\text{HI}}$, showing a reasonably good agreement between those two values if the comparison is limited to the velocity interval showing absorption. The remaining difference is presumably due to the spatial variation of $N_{\text{HI}}$, because absorption lines trace much smaller spatial scales than 21 cm observations do ($60 - 90''$). We present here an updated comparison between the emission and absorption column density, with additional measurements of velocity and gas column density.

Figure 2.7 shows the 21cm integrated intensity at the resolution of 90'' versus the HI column density of UV absorbers at small scales. The 21cm line brightness is derived by integrating radio spectra over the expected velocity range of each galaxy (top panel) or over the velocity range within $\pm 15 \text{ km s}^{-1}$ of the detected H$_2$ absorber. This velocity integration restriction improves the correlation between $N_{\text{HI,21cm}}$ and $N_{\text{HI,UV}}$ (especially for SMC), although the scatter remains significant and significantly larger than the observational uncertainties.

Figure 2.8 presents the CO $J = 1 - 0$ integrated intensity at a resolution of 45'' versus the absorber H$_2$ column density at small scales. To reduce the influence of noise, the CO $J = 1 - 0$ intensity is derived by integrating the CO $J = 1 - 0$ spectrum from the MAGMA surveys over the velocity range $\pm 15 \text{ km s}^{-1}$ of the absorber velocity rather than integrating over the entire velocity interval with 21cm emission. In contrast to the comparison between HI absorbers and 21cm emission, we do not find a correlation between these two, and their ratio is significantly lower than the expectation from $X_{\text{CO}}$ factors usually defined at larger scales. We note that UV absorption becomes difficult to observe in high extinction (molecular rich) regions and limited sensitivity makes it difficult to detect low column densities in CO. Therefore, the H$_2$ absorber is likely tracing edges of molecular clouds or diffuse clouds, with the CO-based column density representing an average over the small-scale, clumpy structure.
In Figure 2.9, we present the structure function of \( N_{\text{H}_2} \) and \( N_{\text{HI}} \) at different spatial scales. This represents the column density difference of two sight lines as a function of their separation in projected distance. Red and gray circles represent the sight line pairs for which the velocity separation is larger or smaller than 20 km s\(^{-1}\), a conservative estimation of the \( \text{H}_2 \) absorber velocity uncertainties. Open circles show the sight line pairs for which the velocity difference is not available (usually for sight lines without \( \text{H}_2 \) velocity measurements). A large velocity separation at a short length scale is usually an indication the pair does not trace the same continuous structure. For the sight line pairs with consistent velocity, the variation of \( N_{\text{HI}} \) is very small at all scales below 50 pc except for a few red points in the LMC. This suggests HI structure is rather smooth at scales as small as 50 pc. We note that the region probed by absorbers is rather limited and biased toward regions where the gas column is not high enough to create opaque 21cm emission. However, \( N_{\text{H}_2} \) shows larger column density variations than \( N_{\text{HI}} \). At smaller angular separations, the variations become smaller while these spatial scales are poorly sampled by the absorption lines. In the LMC, somewhat larger variations on small scales are contributed by several adjacent sight lines near the N11 H II region. The enhanced small-scale structure may be due to feedback effects from young stars and varying line-of-sight placements of clouds and background stars. After a close examination, we found that most \( N_{\text{H}_2} \) variations below 100 pc come from sight lines near molecular clouds. The sight lines in diffuse regions do not show much variation at these scales, presumably because of smooth radiation field and density structure.

## 2.5 Interpretation of \( \text{H}_2 \) Abundances and Populations

The abundance of \( \text{H}_2 \) and its population at individual ground-state \( J \)-levels are known to be highly influenced by local ISM environments. However, physically interpreting observational results is not straightforward, because the procedure involves calculations of both radiative transfer of UV photons and \( \text{H}_2 \) formation/dissociation in a poorly constrained cloud struc-
Figure 2.7 *Upper panel:* 21cm integrated intensity at 90" resolution versus the absorber HI column density at small scales. The 21cm line brightness is derived by integrating 21cm spectra over the full velocity range with signal detections. *Lower panel:* the same as the top panel except the integration is restricted to the velocity range within ±20 km s⁻¹ of absorber velocity.
Figure 2.8 CO $J = 1 - 0$ integrated intensity at 45″ resolution versus the absorber H$_2$ column density at small scales. The CO $J = 1 - 0$ intensity is derived by integrating CO $J = 1 - 0$ spectra from the MAGMA surveys over a velocity range ±15 km s$^{-1}$ of the absorber velocity.

In this section, we review basics of the HI-to-H$_2$ transition in a diffuse ISM cloud and detail a simple analytical 1D cloud model for interpreting our data. This 1D homogenous model is mainly based on recent theoretical work from Sternberg et al. (2014), but includes a H$_2$ self-shielding prescription from Draine & Bertoldi (1996, hereafter, DR96). The model is able to help constrain the physical conditions in individual sight lines without the complexity of numerical modeling. We compare this approach with previous models and prescriptions, and stress that it provides a more general solution for interpreting H$_2$ abundances in diffuse clouds, without requiring the optically thin or thick assumption. We also demonstrate that the proposed method agrees with numerical modeling results and offers comparable constraints on UV field and gas density using the same observable inputs. Finally, we note the caveats of using this method (or any similar approach) to derive ISM physical properties based on H$_2$ formation and dissociation equilibrium.
Figure 2.9 Structure function of $N_{\text{H}_2}$ and $N_{\text{HI}}$ revealed by absorbers at different spatial scales. The column density difference of two sight lines is plotted against their separation in projected distance. Red and Gray circles present the sightline pairs of which the velocity separation is larger or small than 20 km s$^{-1}$. Open circles show the sight lines pairs of which the velocity differences are not available.
2.5.1 An Analytical Cloud Model for H\textsubscript{2} Formation and Dissociation

The balance between H\textsubscript{2} formation and destruction at any location within a cloud in chemical equilibrium can be described as,

\[ n_{\text{HI}}n_{\text{H}}R = n_{\text{H}_2}D. \] (2.5)

\( D \) is the free-space H\textsubscript{2} photo-dissociation rate from ultraviolet radiation in s\textsuperscript{-1} \((D \simeq 0.11\beta, \) where \( \beta \) is the photo-absorption rate). \( n_{\text{H}} \) and \( n_{\text{HI}} \) are the number densities of hydrogen nucleons and atoms, respectively. The H\textsubscript{2} formation rate \( R \) is predominantly determined by grain surface reactions (Hollenbach & Salpeter 1971), with a value of \( \sim 3 \times 10^{-17} \) cm\textsuperscript{3}s\textsuperscript{-1} observed in typical Galactic diffuse interstellar cloud conditions (Jura 1975b). Following Sternberg et al. (2014), the equilibrium dissociation rate can be rewritten as,

\[ D = \frac{n_{\text{HI}}n_{\text{H}}R}{n_{\text{H}_2}} = n_{\text{H}}R \frac{dN_{\text{HI}}}{dN_{\text{H}_2}}. \] (2.6)

If the cloud is 1D and subjected to a beamed incident field from one side, the local dissociation rate can also be described as,

\[ D = D_0f_{\text{shield}}(N_{\text{H}_2})e^{-\sigma_d(2N_{\text{H}_2}+N_{\text{HI}})} s^{-1}. \] (2.7)

Here \( D_0 \) is the dissociation rate at the cloud edge where the UV incident radiation comes from. \( f_{\text{shield}}(N_{\text{H}_2}) \) is the H\textsubscript{2} shielding function, and \( \sigma_d \) is the dust cross-section in units of cm\textsuperscript{2} in FUV. Substituting \( D \) from Equation 2.7 into Equation 2.6 and integrating over \( N_{\text{HI}} \) and \( N_{\text{H}_2} \) respectively, Sternberg et al. (2014) established the following relation between \( N_{\text{H}_2} \)
and \( N_{\text{HI}} \):

\[
D_0 \int_0^{N_2} f_{\text{shield}}(N'_2) \, e^{-2\sigma_d N'_2} \, dN'_2 = R n_H \int_0^{N_1} e^{\sigma_d N'_1} \, dN'_1 = \frac{R n_H}{\sigma_d} (e^{\sigma_d N_1} - 1).
\]

(2.8)

The above equation indicates that the predicted \( \text{H}_2 \) abundance in diffuse and translucent clouds might vary significantly depending on the functional form of \( f_{\text{shield}} \). Although \( f_{\text{shield}} \) requires a self-consistent numerical calculation of UV attenuation and \( \text{H}_2 \) formation/destruction at each depth of the cloud, we can adopt an analytical prescription for \( f_{\text{shield}} \) from Draine & Bertoldi (1996, their Eq. 37),

\[
f_{\text{shield}}(N_{\text{H}_2}) = 0.965 \left(1 + \frac{x}{b_5}\right)^2 + \frac{0.035}{\sqrt{1 + x}} \exp \left(-8.5 \times 10^{-4} \sqrt{1 + x}\right),
\]

(2.9)

where \( x = N_2/5 \times 10^{14} \, \text{cm}^{-2} \) and \( b_5 = b/10^5 \, \text{cm} \, \text{s}^{-1} \) (\( b \) is the Doppler parameter describing the cloud turbulence in \( \text{km} \, \text{s}^{-1} \), as previously defined). This analytical form of \( f_{\text{shield}} \) was derived from numerical modeling in Draine & Bertoldi (1996), and realistically represents line-overlapping effects of \( \text{H}_2 \) self-shielding. It was also verified by Sternberg et al. (2014) using the meudon PDR code (Le Petit et al. 2006). A more recent study from Liszt (2015) also adopted the same prescription to model the \( \text{H}_2 \) abundance in the Milky Way and damped/sub-damped Ly\( \alpha \) systems (DLAs). A variant form was used in Gnedin & Draine (2014) for application to supersonic turbulence on larger scales.

Using Equations 2.8 and 2.9, the relation between \( N_{\text{HI}} \) and \( N_{\text{H}_2} \) can be determined in terms of several ISM properties, including \( \sigma_d \), \( b \), and a dimensionless parameter \( \alpha^{13} \), defined in Sternberg et al. (2014) as,

\[
\alpha \equiv \frac{D_0}{R n_H}.
\]

(2.10)

In other words, this method also provides a constraint on \( \alpha \) from observed \( N_{\text{H}_2} \) and \( N_{\text{HI}} \),

\[13\text{The value of } \alpha \text{ is essentially the atomic-to-molecular density ratio at the cloud edge (see Equation 2.5).} \]
given assumed $\sigma_d$ and $b$ values. Although $\sigma_d$ depends on the dust properties and abundance, Sternberg et al. (2014) presented an effective value over the LW band based on the Galactic value and the metallicity-dust scaling relation,

$$\sigma_g = 1.9 \times 10^{-21} \phi_g Z' \text{ cm}^2,$$

(2.11)

in which $Z'$ is the metallicity normalized by the solar value. $\phi_g$ is of order unity depending on the grain composition and size distribution, with $\phi_g$ smaller ($\sim 0.5$) for an extinction curve less steep toward the UV. $b$ describes the cloud turbulence and influences the self-shielding by affecting the H$_2$ line optical depth. However, our numerical testing found $b$ values ranging from 2 to 10 km s$^{-1}$ only affect the molecular abundance within a factor of 2. Therefore, we adopted a value of 5 km s$^{-1}$ for the following analysis. Based on the above assumptions, we can derive $\alpha$ from the observed $N_{\text{HI}}$ and $N_{\text{H}_2}$ using Equations 2.8 and 2.9.

We note that an estimated value of $\alpha$ defined in Equation 2.10 does not directly provide constraints on either the local UV radiation field strength or gas density. However, the analytical approach presented in Jura (1975a) can provide an independent evaluation of the product of density and H$_2$ formation rate $n_H R$. This approach relies on the fact that the LW photons that dissociate H$_2$ are also responsible for exciting the high-$J$ levels. Based on the steady-state equation for $J = 4$ (Jura 1975a, their equations 2a) and the H$_2$ formation and dissociation equilibrium (Equation 2.5 here), the H$_2$ population distribution should satisfy,

$$2.75 \times 10^{-9} n(4) = R n_H n_{\text{HI}} \left[ 2.36 \frac{n(0)}{n_{\text{H}_2}} + 0.19 \right]$$

(2.12)

Assuming that the cloud has a constant hydrogen nucleon density and $n(0)/n_{\text{H}_2}$ does not vary significantly across the cloud, namely $n(0)/n_{\text{H}_2} \approx N(0)/N_{\text{H}_2}$, the volume density-based
relation can be represented as a column density relation,

\[ R_{nH} = 2.75 \times 10^{-9} \frac{N(4)}{N_{HI}} \left[ 2.36 \frac{N(0)}{N_{H_2}} + 0.19 \right]^{-1}. \] (2.13)

We note that this is essentially the same equation used in Lee et al. (2002) (see also Welty et al. 2006), except there \( N_{H_2} \) and \( N_{HI} \) were replaced with \( N(0) + N(1) \) and \( N_H \), respectively, which are valid in optically thick clouds with low molecular fraction. This relation provides a constraint on the gas density \( n_H R \) and is independent of Equation 2.8.

Using Equations 2.8 and 2.13, we are able to derive both \( D_0 \) and \( R_{nH} \) from observables measured from UV absorptions of HI and \( H_2 \). They are directly related to two important ISM properties: the interstellar UV field strength and gas number density. The interstellar radiation field (ISRF) is commonly presented as \( I_{UV} \), in units of the local “standard” ISRF described in Draine (1978). From the analytical description of \( I_{UV} \) presented in Draine (1978), Sternberg et al. (2014) estimated the relation between \( D_0 \) and \( I_{UV} \) to be

\[ D_0 = 5.8 \times 10^{-11} I_{UV} \text{s}^{-1}. \] (2.14)

On the other hand, deriving gas volume density requires an assumption for the \( H_2 \) formation rate \( R \), because only the product \( R_{nH} \) appears in Equations 2.8 and 2.13. \( R \) is believed to be closely related to the dust abundance because \( H_2 \) formation proceeds by grain surface reactions and the grain surface area per H is proportional to the dust abundance. Browning et al. (2003) suggested a lower \( R \)-value in the low metallicity environments of the LMC and SMC by comparing their \( H_2 \) population models with the observed abundance patterns from Tumlinson et al. (2002), which is consistent with the expected metallicity dependence of \( R \).

The \( H_2 \) formation rate also depends on the dust properties and gas/dust temperature (see Hollenbach & McKee 1979), because these affect the collision rate and sticking coefficient.

\[^{14}\text{We note that the UV radiation field is also often presented in units of the integrated field described in Habing (1968), denoted as } G_0. G_0 = 1.7 \text{ is comparable to the local field strength described in Draine (1978).}\]
of the atomic gas with grains (e.g. Hollenbach & Salpeter 1971; Cazaux & Tielens 2004). For a first-order approximation, we derived the gas density in this work by assuming a value of $R$ based on the canonical Galactic H$_2$ formation rate from Jura (1975b) and a metallicity/temperature-based scaling relation:

$$R = 3 \times 10^{-17} Z' \text{ cm}^3 \text{s}^{-1}. \quad (2.15)$$

We note that the ratio of the incident UV field strength and diffuse cloud density $\zeta$ is related to $\alpha$ and $R$ as,

$$\zeta = \frac{I_{\text{UV}}}{n_H} = \frac{\alpha R}{5.8 \times 10^{-11} \text{s}^{-1}}, \quad (2.16)$$

which is a similar definition adopted in the models of Wolfire et al. (2003) and Krumholz et al. (2009).

### 2.5.2 Comparisons with Previous Cloud Models

In Section 2.5.1, we outlined an analytical approach to establish a relation between the dimensionless parameter $\alpha$ and the atomic and molecular gas column density, based on Sternberg et al. (2014). We note that similar procedures and formulae were developed and used by previous studies (Jura 1974; Lee et al. 2002; Krumholz et al. 2009; Jorgenson et al. 2010). In this section, we demonstrate that our adopted method based on Sternberg et al. (2014) and Draine & Bertoldi (1996) is fundamentally a more general solution for modeling the HI and H$_2$ transition, suitable for diffuse/translucent clouds.

As Sternberg et al. (2014) points out, the H$_2$ self-shielding function is defined as,

$$f_{\text{shield}} = \sigma_g \frac{dW_d}{dN_2}, \quad (2.17)$$

in which $\sigma_g$ is the total effective dissociation cross section in units of cm$^2$ Hz, and $W_d$ is the "equivalent band-width" of radiation absorbed in H$_2$ dissociation. Because $W_d$ is contributed
by individual absorption lines, the value will also loosely go through a “linear/flat/square-root” relation with \( N_2 \) similar to the curve-of-growth for a single absorption line. However, a significant difference in a multi-line system across the LW band is that the line-overlapping effect will suppress the growing of \( W_d \) compared with the square-root law of a single absorption line when \( N_{\text{H}_2} \) reaches \( \sim 10^{20} \text{ cm}^{-2} \) (as illustrated in Figure 6 of Draine & Bertoldi 1996).

In Jura (1974, 1975a) (also Lee et al. 2002), an optically thick cloud model was assumed with no dust extinction. Under similar assumptions, we can neglect the dust extinction (\( \sigma_d \rightarrow 0 \)) and assume \( W \propto N_2^{0.5} \) or \( f_{\text{shield}} \propto N_2^{-0.5} \) (Equation A3 of Jura 1974) in Equation 2.8. This approximation is equivalent to the square-root part of the single-line COG. If the molecular fraction is small (\( f_{\text{H}_2} \ll 1 \)), the \( N_{\text{H}_2} \)-\( N_{\text{HI}} \) relation from Equation 2.8 will be,

\[
\frac{N_2}{N_1} \propto \frac{R^2 N_1^2 n_{\text{H}_2}^2}{D_0^2} \tag{2.18}
\]

This is essentially the same as Equation A8 of Jura (1974) or Equation 20 from Lee et al. (2002). More recent work from KMT09 presented a spherical cloud-scale atomic-to-molecular transition model by incorporating UV shielding from both dust and \( \text{H}_2 \). Beyond the different cloud geometry, they adopted a simplification that is equivalent as simplifying the \( \text{H}_2 \)-shielding treatment as (see Equations 1–8 in Krumholz et al. 2008),

\[
f_{\text{shield}} = e^{-<f_{\text{diss}} \sigma_{\text{H}_2}>} N_{\text{H}_2}, \tag{2.19}
\]

in which \( \sigma_{\text{H}_2} \) is the effective cross section for UV absorption from a hydrogen molecule and \( f_{\text{diss}} \) is the fraction of absorbed UV photons that lead to dissociation of \( \text{H}_2 \). However, because \( f_{\text{diss}} \) and \( \sigma_{\text{H}_2} \) vary within the PDR (Draine & Bertoldi 1996), an effective value of \( f_{\text{diss}} \sigma_{\text{H}_2} \) value is not accurate enough to describe the UV dissociation flux at a specific location. Although this model successfully explains the metallicity dependence of the column density...
of the atomic layer around molecular clouds from large-scale surveys (Wong et al. 2013), this simplification may lead to a large deviation in the diffuse cloud regime (e.g. Welty et al. 2012), where the H$_2$ abundance in the HI-dominated cloud is very sensitive to the H$_2$ self-shielding effect.

For optically thin clouds, previous studies adopted different sets of assumptions for modeling the H$_2$ abundance. Jorgenson et al. (2010) used the H$_2$ abundance to derive the ISM physical properties of high-redshift DLAs. As DLAs are usually optically thin in UV with low molecular fraction, they assumed a H$_2$ self-shielding function following Hirashita & Ferrara (2005) of the form:

$$f_{\text{shield}} = \left( \frac{N_{\text{H}_2}}{10^{14}\text{cm}^{-2}} \right)^{-0.75}.$$  

(2.20)

An even more simple optically thin approximation, in which $f_{\text{shield}} \approx 1$, was presented in Jura (1974) and adopted in Gillmon et al. (2006). Equation 2.8 will be simplified and lead to a molecular fraction of,

$$f_{\text{H}_2} = \frac{2nR}{D}.$$  

(2.21)

To compare the atomic-to-molecular transitions predicted by different methods, we used them to calculate the H$_2$ column density as a function of the total gas column density $N_H$ under the same “typical” Galactic cloud conditions. Following KMT09, we adopted the radiation-to-density ratio from the Galactic two-phase pressure equilibrium ISM model of Wolfire et al. (2003)$^{15}$. The results are presented in Figure 2.10. Our comparison shows that the optically thick dust-free approximation from Jura (1974, their Equation A8) only loosely agrees with our analytical approach in molecular fraction within a factor of $\sim 4$ for $N_H > 10^{20.5}$ cm$^{-2}$ clouds, and overestimates the UV shielding at lower densities. On the other hand, the optically thin approximation in Jura (1974) is consistent with the solution when $N_{\text{H}_2} < 10^{19.5}$ cm$^{-2}$. We note that most UV sight lines presented in this work are located in the regime where $N_H$ is between $10^{20}$ and $10^{22}$ cm$^{-2}$. The model of KMT09 (dashed line) suggests

$^{15}\zeta = 0.044$ or $\alpha = 7.6 \times 10^4$, see Section 6.1 for more details
a rather steep HI-to-H$_2$ transition after the total gas column density exceeds $\sim 2 \times 10^{21}$ cm$^{-2}$. However, this model is designed to predict the cloud-averaged H$_2$ abundance, and adopts a different geometry compared with other analytical models.

Besides analytical models, detailed numerical models have been developed to estimate the FUV radiation field and gas density from the observed H$_2$ abundance or other ISM species (e.g., C I or C II). For example, Browning et al. (2003) studied a large sample of FUSE Galactic and MC sight lines by numerically modeling H$_2$ populations. Previous studies (e.g. Gry et al. 2002; Boissé et al. 2005; Nehmé et al. 2008b; Jensen et al. 2010) have also used the MEUDON PDR model to model several well-studied Galactic sight lines. To examine the consistency between these numerical models and our analytical method, we use the H$_2$ abundance/populations predicted by MEUDON to derive the gas density and radiation field for those sight lines, by applying our analytical model. Then we compare the values with the MEUDON model inputs.

For three Galactic sight lines presented in Gry et al. (2002), we found that the estimated $n_{H}R$ value from Equation 2.13 is within the model input by a factor of 3, comparable to the observational uncertainties. The derived UV field from Equation 2.8 is about the solar neighborhood value, roughly consistent with the model input of $I_{UV} = 1$ in Gry et al. (2002). For two sight lines modeled in Jensen et al. (2010), we also derived UV field and $n_{H}R$ using the predicted $N_{J}$ and $N_{HI}$ of the best fit MEUDON PDR models. The results were found to be in excellent agreement (a factor 2) with the PDR model inputs.

These comparisons suggest a consistency between the numerical and analytical approach in the prediction of physical properties from observable results. Considering the complexity of the PDR model inputs (often requiring additional constraints and dust properties not available for MC sight lines) and the consistency between the numerical and analytical prediction of $\alpha$ and $nR$ under similar assumptions, we suggest the analytical model described in Section 5.1 provides a simple alternative for interpreting observed $N_{HI}$ and $N_{H2}$ compared to detailed numerical modeling.
Figure 2.10 Predicted $N_{\text{H}_2}$-$N_{\text{H}}$ relations from different gas cloud models for the HI-H$_2$ transition. The predictions are derived under the typical Galactic condition described in Section 2.5.2, with the same UV field strength and gas density. The solid black line represents the results from the improved model presented in Section 5.1. The dotted lines present the results of optically thin and thick approximations. The prediction from the model of MK10 is shown as a dashed line, which is averaged over a spherical cloud geometry. The molecular fraction of 100% is presented as the gray diagonal line. The comparison suggests that the improved model provides a general description to relate the H$_2$ and HI gas components in diffuse/translucent clouds without optically thin or thick assumptions.
Table 2.7. Analytical and Numerical Modeling Comparisons

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<th>Stars</th>
<th>$N_{\text{HI}}$ cm$^{-2}$</th>
<th>$N_{\text{H}_2}$ cm$^{-2}$</th>
<th>$N(0)$ cm$^{-2}$</th>
<th>$N(4)$ cm$^{-2}$</th>
<th>$I_{\text{UV}}$ ISRF</th>
<th>$n_{\text{H}}$ cm$^{-3}$</th>
<th>$I_{\text{UV}}/n_{\text{H}}$</th>
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<td>700</td>
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<td>20.40</td>
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<td>10</td>
<td>500</td>
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<td>Jensen et al. (2010)</td>
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<td>7</td>
<td>2000</td>
<td>$3.5 \times 10^{-3}$</td>
<td>Jensen et al. (2010)</td>
</tr>
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</table>

Note. — The ISRF strength is presented in units of the local “standard” field described in Draine (1978).

2.5.3 Caveats

We note that any similar method using H$_2$ formation/dissociation equilibrium models to estimate radiation field and gas density will be only valid if all assumptions about the cloud geometry (1D) and structure (homogenous) are satisfied. Although the analytical method provides a general solution to interpret the observed results (e.g. H$_2$ population and abundance), it is important to understand the uncertainties in the derived $n_{\text{H}}$ and $I_{\text{UV}}$ before any further interpretation. We explore the uncertainties contributed from the observations and modeling below.

First the observational column density uncertainties will directly lead to a large error budget in the estimation of $Rn_{\text{H}}$ and $I_{\text{UV}}$. A conservative estimate of observational uncertainties would be $\sigma(\log N_{\text{H}_2, \text{HI}}) = 0.2$, roughly the maximum error in observational measurements. Then the statistical uncertainties of $Rn_{\text{H}}$, $\alpha$, and $I_{\text{UV}}$, are expected to be at least 0.2–0.3 dex. Because $n_{\text{H}}$ and $R$ are degenerate in the modeling, the adopted value of $R$ will directly affect the derived $n_{\text{H}}$. Although the canonical Galactic value of $R \sim 3 \times 10^{-17}$ from early Copernicus UV observation was confirmed later by FUSE observations within an uncertainty of less than a factor of 2 (Gry et al. 2002), Wolfire et al. (2008) find the H$_2$ formation rate could be lower by a factor of $\sim$3 in the Galactic sight lines with low column density ($A_V \lesssim 0.25$, but the author noted that this rate could be underestimated due to different cloud geometry as-
sumptions). On the other hand, Habart et al. (2004) found $R$ could be higher in dense PDR regions exposed to high UV radiation. More recent theoretical investigation from Le Bourlot et al. (2012) also suggested a higher $R$ than the adopted astronomical “standard” value. Because the H$_2$ formation process depends on the dust properties and gas/dust temperature (e.g. Cazaux & Spaans 2004), which are poorly understood for individual UV sight lines, $R$ could vary by a factor of 5 in individual sight lines from our adopted value. Conservatively, any description of $n_{H}$ derived in this approach will bear a similar uncertainty level to $R$ in this work.

On the other hand, the uncertainties contributed by the idealized models might be a dominant factor when we interpret the derived ISM physical properties because they may cause systematical bias in large samples. Previous detailed modeling has suggested that a single component cloud model might not be able to produce both low-$J$ and high-$J$ H$_2$ abundances for some sight lines. For example, the H$_2$ models from Browning et al. (2003) have difficulty fitting H$_2$ abundances at lower and high J using a single isothermal slab model. They concluded that gas layers with different temperatures might help explain the observed results. Boissé et al. (2005) and Nehmé et al. (2008b) modeled two sight lines. Their results suggested the presence of warm H$_2$ associated with the diffuse clouds or matter in the vicinity of stars as a possible explanation for the high-$J$ excitation, with the low-$J$ H$_2$ abundance contributed by cold translucent clouds. Jensen et al. (2010) also found a single-cloud model was not able to explain the observed H$_2$ abundance and populations for two translucent Galactic sight lines. They also suggested that a “concatenated model” consisting of multiple clouds might be an alternative solution for the discrepancy between cloud models and observational results. Although a quantitative evaluation in our entire sample is impossible because of the limited information available for individual sight lines, the question of how the derived $n_{H}$ and $I_{UV}$ would be biased can still be addressed qualitatively.

Following the “concatenated” model suggested in Browning et al. (2003) and Jensen et al. (2010), we present two idealized models to explore the physical meaning of the derived $Rn_{H}$
and $D$ following the scheme described Section 2.5.1, in more complicated conditions rather than a single cloud component along the line of sight.

In the first scenario, we consider the observed absorber consists of two components: a cold diffuse cloud in the CNM contributing most $\text{H}_2$ along the line of sight, and a WNM-type atomic gas component with much lower volume density. With both components illuminated by a typical Galactic UV field, the prediction from Equation 2.8 will provide an upper limit to $\alpha$ for the cold cloud component because the WNM component does not contribute $\text{H}_2$ gas. At the same time, Equation 2.13 will lead to a lower limit of $Rn_\text{H}$ for the cold cloud component. The estimation of $I_{\text{UV}}$ is generally not affected because it is not sensitive to the observed $N_{\text{HI}}$ if the gas cloud is optically thin in the UV. If the cloud is optically thick, the derived value of $I_{\text{UV}}$ will over-predict the ISRF to the cold cloud when the $\text{H}_2$-free warm component blends in.

In the second situation, we consider the absorbing materials consist of two components with similar column and volume density ($N_\text{H}$ and $n_\text{H}$). However, one component is exposed to much higher $I_{\text{UV}}$ than the other and does not contribute significant $\text{H}_2$ along the line of sight. In this case, the prediction of $\alpha$ from Equation 2.8 will overestimate the actual value in the cloud exposed to lower $I_{\text{UV}}$. Because of dramatically different UV excitation, the $\text{H}_2$ population distribution can be very different in the two components along the line of sight. This scenario is similar to the modeling study results from Boissé et al. (2005) and Nehmé et al. (2008a) for two Galactic sight lines. We note that although these two Galactic sight lines apparently invalidated the single cloud assumption, it is not known whether they represent the majority of UV sight lines.

Although the real situation could be a mixture of those two cases, the above two simple scenarios outline the possible complications in the interpreting the observed $N_{\text{H}_2}$ abundance and population, which will be discussed later.
2.6 Physical Properties of Absorbers Inferred from Cloud Models

2.6.1 Comparisons with the Two-phase Equilibrium model

The atomic and molecular gas relation presented in W12 (see their Figure 17) show a different H$_2$ abundance pattern between the Galactic and Magellanic clouds sample. Specifically, the HI-to-H$_2$ transition happens at a higher gas column density. Recent theoretical work of Krumholz et al. (2009, hereafter KMT09) suggested the difference could be mainly caused by metallicity, or specifically, different UV shielding from interstellar dust and H$_2$ for the same amount of gas. However, its quantitative comparison with UV absorption data is difficult.

The model from KMT09 was optimized to predict the cloud-averaged molecular gas fraction, corresponding to a spherical dense cloud model immersed in an ISM environment governed by CNM/WNM pressure equilibrium (Wolfire et al. 2003). Meanwhile, UV absorption usually traces the physical properties of small-scale diffuse ISM structure due to the bias of the observation technique: most UV absorption sight lines are located in HI-dominated regions.

The introduction of a gas cloud model in Section 2.5.1 provides a new opportunity to compare the observed H$_2$ abundance with the prediction from the two-phase equilibrium model of Wolfire et al. (2003). Because this cloud model emphasizes accurate modeling of H$_2$ self-shielding effects in atomic-dominated clouds, it provides a better prescription for the H$_2$ abundance in diffuse clouds. We describe the comparison in detail below.

One important implication of the CNM/WNM equilibrium model introduced in KMT09 is that the ratio between the ISRF and the gas density in the CNM, $\zeta_{\text{CNM}}$, is restricted to a narrow range and depends weakly on the metallicity. For the coexistence of CNM and WNM, this ratio should satisfy,

$$\zeta_{\text{CNM}} = \frac{1 + 3.1Z^{0.365}}{31\phi_{\text{CNM}}}.$$ (2.22)
Figure 2.11  Top panel: $N_{\text{H}_2}$ versus $N_{\text{HI}}$ of the MC absorbers towards the LMC (red) and SMC (blue) stars. Bottom panel: $N_{\text{H}_2}$ versus $N_{\text{HI}}$ of the Galactic absorber measured towards the Galactic stars (gray) and extragalactic objects (cyan). The dotted hyperbolic curves present total gas column densities of $10^{20}$, $10^{21}$, and $10^{22}$ cm$^{-2}$, and the diagonal dashed lines show the molecular-to-atomic gas ratio $R_{\text{H}_2} = 1$, 0.1, and 0.01. The hatched regions present the predicted $N_{\text{H}_2}$/$N_{\text{HI}}$ relation from the cloud model presented in Section 2.5.1 under the two-phase pressure equilibrium described in Wolfire et al. (2003).
Here $\phi_{\text{CNM}}$ is a dimensionless parameter confined between 1 and 10. From Equation 2.22, the equivalent value of $\alpha$ in the CNM could be written as

$$\alpha_{\text{CNM}} = 5.6 \times 10^4 \frac{1 + 3.1Z^{0.365}}{\phi_{\text{CNM}}Z'}.$$  \hspace{1cm} (2.23)

Therefore, we can use Equation 2.8 and 2.23 to predict the $N_{\text{H}_2}$ vs. $N_{\text{HI}}$ relation for the CNM, provided that the WNM is negligible and does not contribute a significant amount of HI.

Figure 2.11 presents the predictions and observations of the $N_{\text{H}_2}$ vs. $N_{\text{HI}}$ relation in the SMC, LMC, and Milky Way as hatched areas (blue, red, and gray, respectively). We choose to plot $N_{\text{H}_2}$ versus $N_{\text{HI}}$ to present the atomic-molecular gas relation rather than the commonly used molecular-to-atomic gas ratio $R_{\text{H}_2}$ or molecular fraction $f_{\text{H}_2}$, to ensure that each axis is from independent measurements. For the model prediction, we assumed three different metallicities for the individual galaxies ($0.2 Z_\odot$, $0.5 Z_\odot$, and $1.0 Z_\odot$ for the SMC, LMC, and Galactic samples, respectively) with the dust opacity relation from Equation 2.11. The KMT09 model predictions for the $N_{\text{H}_2}$ vs. $N_{\text{HI}}$ relation are shown as thick dashed lines. As pointed out in W12, the KMT09 model appears to underpredict the molecular fraction at the low column density range, with a sharp atomic-molecular transition at a particular HI saturation column evident as a vertical prediction. The explanation for the different predictions has been discussed in Section 2.5.1.

The observed $N_{\text{H}_2}$ vs. $N_{\text{HI}}$ relation presented in Figure 2.11 is based on this work or W12 (for MC absorbers) and on previous studies toward Galactic stars and high-latitude extragalactic objects (see Section 2.2.2). We note that all points are based on direct absorption columns measured for both species. The observational results show that most of the MC and Galactic UV sight lines have $R_{\text{H}_2} < 1$. A steep increase of $\text{H}_2$ abundance is also evident from $\text{H}_2$ self-shielding: $N_{\text{H}_2}$ increases by a factor of 8 when $N_{\text{HI}}$ increases from $10^{20}$ to $10^{22}$ cm$^{-2}$. As previously shown in Figure 17 of W12, the atomic gas column density appears to be
significantly higher in the MCs when we compare MC and Galactic sight lines with a similar amount of H\textsubscript{2}. This might be an indication that H\textsubscript{2} self-shielding happens at a higher gas column density in the MCs, as expected based on the model for a lower metallicity and/or higher radiation field environment. We also note that MC absorbers show large scatter, presumably because the sample sight lines are located in a wide range of environments in each galaxy, unlike the Galactic sample, which probes the gas in the Galactic disk or lower halo. We note that UV absorption lines do not probe regions where H\textsubscript{2} is dominant due to the inability to observe UV background sources given limited sensitivity. These molecular rich regions are better studied in emission lines (e.g. HI 21cm or CO rotation lines in millimeter). On the other hand, emission tracers are subjected to various observational effects (e.g., optical depth or brightness-to-mass conversions) and could thus be unreliable to study the HI and H\textsubscript{2} content at small scales.

From the comparison presented in Figure 2.11, we find the prediction from the new cloud model shows a similar abundance pattern to the observed results. The majority of Galactic absorbers fall into the predicted hatched parameter space, demonstrating an improvement compared with the prescription provided by KMT09. However, a significant number of MC absorbers are located to the right of their predicted regime, indicating that the model overpredicts the H\textsubscript{2} abundance in those cases.

### 2.6.2 Gas Volume Density

Using the single cloud model presented in Section 2.5.1, we are able to derive gas density from Equation 2.13 for individual absorbers. Figure 2.12 presents the derived gas volume density as functions of the atomic and molecular gas column density. We have not found strong correlations between \( n_{\text{H}} \) and \( N_{\text{H}} \) in both samples. However, a trend of increasing \( n_{\text{H}} \) exists when \( N_{\text{H}_2} \) reaches above \( 10^{20} \text{cm}^{-2} \), consistent with the Galactic result based on CO absorption analysis (Goldsmith 2013).

Most MC absorbers appear to have gas volume densities similar with or smaller than
the values of the Galactic diffuse and translucent clouds. However, we note that the values can be underestimated and only represent the average density of the gas along the line-of-sight that can contributed by both the CNM and WNM. Based on a more direct density tracer [C I], the Galactic study by Jenkins & Tripp (2011) suggests a pressure value of \( \log(P/k) = 3.58 \pm 0.18 \text{ cm}^{-3} \text{ K} \) in the diffuse CNM of the Milky Way. For the galactic sightline sample we compiled, we find a gas density of \( n_{\text{H}} \sim 10^2 \text{ cm}^{-2} \) and \( T_{\text{rot}} \sim 90 \text{ K} \), indicating a slightly higher pressure, but still within the measurement uncertainties. Recent CO or [C II] study also shows similar values in the Galactic plane (Goldsmith 2013; Gerin et al. 2015). We note that the density value presented here is based on the H\(_2\) formation rate assumed in Equation 2.15, while the methods using weaker atomic fine structure lines is more direct. Rather than depending on the less certain H\(_2\) formation and dissociation process, they relay on the collisional excitations (e.g. Jenkins & Tripp 2001; Wolfire et al. 2008; Jorgenson et al. 2010; Jenkins & Tripp 2011). We note that H\(_2\) and C I shares the similar photo-dissociation/ionization energy. Therefore, the H\(_2\)-based method should provide similar results as the C I method in diffuse clouds, provided the assumptions of gas clouds can be applied.

### 2.6.3 Radiation Field Near Absorbers

We present the radiation field as a function of column density in Figure 2.13. In both samples, the derived \( I_{\text{UV}} \) is between 1 and 10 for all sight lines below \( 10^{20} \text{ cm}^{-2} \). For MCs, this estimation is lower than the suggestion from T02 based on limited number of sight lines, in which a radiation field of \( I_{\text{UV}} \sim 10 - 100 \) was expected to produce the abundance pattern. We recalculated the sight lines included in T02 and found \( I_{\text{UV}} = 50 \pm 30 \). Therefore, the different statistics may come from the fact that high-UV sight lines were included in their subsample.

The Galactic sight lines against disk stars show a wild range of the \( I_{\text{UV}} \) distribution from 1 to 100, similar to the results from the LMC. The UV field strength from the high-latitude Galactic sight lines spans from \( \sim 1 \) to 10. We found a weak correlation between \( I_{\text{UV}} \) and
Figure 2.12  Gas volume density $n_H$ derived from constant-density cloud models versus absorber H$_2$ (top panels) and total (H$_2$ and HI, bottom panels) column density. *Left panels:* the Magellanic Clouds absorbers; *Right panel:* Galactic absorbers. We found $n_H$ increases when $N_{H_2}$ reaches above $10^{20}$ cm$^{-2}$ in the Galactic absorbers, although this trend is less clear in the Magellanic sample. We have not found correlations between $n_H$ and $N_H$ in both samples. Most MC absorbers appear to have gas volume densities similar with the Galactic diffuse and translucent clouds, although the values could be underestimated and only represents the average density of the line-of-sight of gas contributed by both the CNM and WNM.
Figure 2.13 UV field derived from the HI-H$\textsubscript{2}$ transition models versus the absorber H$\textsubscript{2}$ (top panels) and total (H$\textsubscript{2}$ and HI, bottom panels) column density. **Left panels:** the Magellanic Clouds absorbers; **Right panel:** Galactic absorbers.
but a strong correlation between $I_{UV}$ and $N_{HI}$. Considering the massive young stars providing the UV dissociation are usually located near dense cloud, the later correlation is not surprising. As we discussed before, our radiation field estimation is not sensitive to the single-cloud assumption in the optically thin regime. The relative moderate $I_{UV}$ values indicate that majority sight lines are not in the vicinity of massive OB stars, even some of them are near the star-formation activities in the sky projections.

2.7 Discussion

2.7.1 WNM Contribution to Absorption

In Figure 2.11, we show a comparison between the observed $H_2$ abundance pattern (data points) and the prediction from the analytical cloud model (hatch regions). We note that the model predictions were derived using the radiation-to-density ratios expected from the CNM/WNM equilibrium model of Wolfire et al. (2003). Although the majority of Galactic sight lines agrees well with the predictions, a significant number of MC sight lines are located to the right of the predicted hatch area in the $N_{H_2}$-$N_{HI}$ relation.

One possible simple explanation for the discrepancy is that those sight lines have radiation-density ratios higher than the expectations from the CNM/WNM equilibrium model. In other words, the value of $\phi_{CNM}$ in Equation 2.22 will be below unity, contradicting the model. Because the majority of MC sight lines show $I_{UV} < 10$ which is comparable with the Galactic sight lines, a higher radiation-density ratio can be only interpreted as lower gas densities in this scenario. However, as shown in Figure 2.12, this explanation will lead to a unrealistic length scale ($> 100$ pc) based on the ratios of observed column densities and the volume densities derived from HI-$H_2$ transition models. In the LMC and SMC, the projected gas distribution does not support the existence of such cloud structure. The structure function analysis for UV absorbers also shows growing HI column density variation above 50 pc.

To explain the discrepancy, we propose an alternative to the constant-density cloud
model: a significant fraction of atomic gas traced by UV absorption is contributed by WNM rather than CNM in the Magellanic clouds. The low-density WNM is inefficient for forming H$_2$ and a sight line showing H$_2$ absorptions can pass through irrelevant HI gas in the WNM, which contributes a H$_2$ free gas component. If the LMC and SMC stellar distribution could be considered as a thin structure along the line of sight, then our observation towards MC hot stars will create a viewing point more similar to the Galactic high-latitude sight lines, tracing WNM absorbers from lower galactic halo. Cormier et al. (2015) presented a recent FIR fine-structure cooling lines study in a large sample of low-metallicity line dwarf galaxies. The diagnostic line ratios and line-to-FIR ratios also suggest a more porous structure in dwarf galaxies with diffuse gas filling a large volume, which could also represent the ISM structure in MCs.

Although this WNM scenario can easily explain the discrepancy between the model and observations, distinguishing the WNM and CNM is difficult in observations. The classifications of WNM and CNM are also a simplified representation of the continuous density ISM structure. Most of our knowledge on low-density WNM ($<0.1$ cm$^{-3}$) were from observations using HI 21cm absorption and emission pairs. A limited examples have suggested a significant WNM fraction in the Galactic and extragalactic environments (e.g. Heiles & Troland 2003; Dickey et al. 1994; Borthakur et al. 2014; Stanimirović et al. 2014). Assume that $N_{H_2}$ observed in absorptions are contributed from the CNM component in which the radiation-density ratio is predicted from the CNM/WMN models, the column density of the WNM component is expected to be $N_{HI,WMN}=N_{HI}-N_{HI,CNM}$. If the CNM component can still be represented by a constant-density cloud model described before, we will be able to estimate the value of $N_{HI,CNM}$ from the observed $N_{H_2}$. By adopting a fiducial condition in the cloud model described before ($\phi_{CNM} \sim 1-10$), our analysis following the above scheme found a 20%-80% WNM gas fraction is required to describe the H$_2$ abundance pattern which we see in Figure 2.11.
Table 2.8. Atomic/Molecular Mass and CO brightness

<table>
<thead>
<tr>
<th></th>
<th>LMC</th>
<th></th>
<th>SMC</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>full</td>
<td>MAGMA</td>
<td>CO-bright</td>
<td>full</td>
</tr>
<tr>
<td>$M_{\text{HI,21 cm}}$</td>
<td>$3.6 \times 10^6$</td>
<td>$6.8 \times 10^7$</td>
<td>$2.1 \times 10^7$</td>
<td>$3.0 \times 10^8$</td>
</tr>
<tr>
<td>$M_{\text{H}_2,\text{diffuse}}$</td>
<td>$1.7 \times 10^2$</td>
<td>$2.3 \times 10^6$</td>
<td>$6.4 \times 10^5$</td>
<td>$9.3 \times 10^6$</td>
</tr>
<tr>
<td>$M_{\text{H}_2,\text{CO}}$</td>
<td>$2.6 \times 10^7$</td>
<td>$2.0 \times 10^7$</td>
<td>$1.8 \times 10^7$</td>
<td>$5.1 \times 10^7$</td>
</tr>
<tr>
<td>$L_{\text{CO}}$</td>
<td>$7.2 \times 10^5$</td>
<td>$5.4 \times 10^7$</td>
<td>$4.7 \times 10^7$</td>
<td>$9.3 \times 10^5$</td>
</tr>
<tr>
<td>$M_{\text{dust}}$</td>
<td>$4.1 \times 10^5$</td>
<td>$1.8 \times 10^5$</td>
<td>$7.0 \times 10^4$</td>
<td>$4.2 \times 10^4$</td>
</tr>
</tbody>
</table>

Note. — All masses are the estimated hydrogen mass in units of $\odot$ (excluding Helium) and the CO $J = 1 - 0$ brightness is in units of K km s$^{-1}$ arcsec$^2$. For each galaxy, we derived the HI and H$_2$ masses different by their integration regions: entire HI coverage (full), the regions observed in the MAGMA surveys (MAGMA), or the pixels with high-confident CO detections above 4σ (CO-bright). The HI mass is based on the integrated 21cm line brightness restricted to regions selected from a “smooth-mask” signal detection algorithm, but without opacity corrections. The quoted total integrated CO brightness for each galaxy is from the NANTEN surveys (Mizuno et al. 2001b; Fukui et al. 2008), as they provide a comprehensive coverage of each galaxy. The quoted ‘MAGMA’ mass is derived from the spectral cube data products of the MAGMA surveys (Wong et al. 2011; Muller et al. 2013) after applying the same noise masking algorithm as the 21cm data, as well as the CO-bright regions. The CO-based H$_2$ mass $M_{\text{H}_2,\text{CO}}$ are derived based on the assumed Canonical $X_{\text{CO}}$ values of $4 \times 10^{20}$ for the LMC and SMC.

### 2.7.2 Diffuse H$_2$

The molecular content in the Magellanic Clouds has been extensively studied in millimeter CO rotational lines and mid-/far-infrared dust emissions. However, both methods are based on indirect H$_2$ tracers. The CO brightness to molecular mass conversion factor $X_{\text{CO}}$ is known to be dependent on the ISM metallicity and referred spatial scales (Bolatto et al. 2013). Determining H$_2$ mass from dust emissions relies on spatially-resolved dust emission modeling, estimating local dust-to-gas ratios (DGRs), and removing HI contributions to the total gas mass. The first two steps could be challenging in a HI-dominated environment as the Magellanic systems (Gordon et al. 2014; Roman-Duval et al. 2014), and the accuracy of derived H$_2$ values could be compromised. Nevertheless, previous observational efforts have established two qualitative conclusions. First, the MC molecular clouds are associated with weaker CO emissions when compared with their counterparts in higher metallicity systems, therefore corresponding with larger $X_{\text{CO}}$ factors (Mizuno et al. 2001b; Fukui et al. 2008; Leroy et al. 2011; Hughes et al. 2013, etc.). We note that these results are based on CO
observations in which the clouds are unresolved or partly resolved and the derived $X_{\text{CO}}$ values depend on the observation resolutions and the estimation techniques. Second, DGRs in both LMC and SMC are lower compared with the Galactic values, roughly linearly scaled with the metallicity. This result is based on comparing the dust and gas emissions in the atomic-dominated phase ISM (Roman-Duval et al. 2014) and direct absorption-based gas and dust tracers along UV sight lines (Welty et al. 2012). Our H$_2$ absorption analysis suggests most H$_2$ absorbers in the MCs show similar gas temperature and UV fields compared with those of the Galactic diffuse or translucent clouds. However, they are associated with higher HI gas column densities at a specific $N_{\text{H}_2}$. The H$_2$ gas component revealed in absorptions likely resides in HI clouds as defined in the CNM or atomic envelope near the molecular cloud edge. They are too diffuse to produce detectable CO emissions in the MCs.

The exact role of the detected diffuse H$_2$ gas is not clear at galactic scales: the diffuse H$_2$ component could be accounted for the CO-dark H$_2$ mass in the LMC and SMC; the atomic-dominated environment where it resides might provide raw material and initial conditions for molecular cloud formation as a gas reservoir; it is also possible that the diffuse H$_2$ arises from transient gas structures in the turbulent ISM, which is not related to star formation at all. An estimate of the diffuse H$_2$ mass budget in each galaxy may help answer these questions.

To estimate the expected diffuse H$_2$ mass in the MCs, we adopted a similar method presented in T02 to derive synthetic diffuse H$_2$ maps. Specifically, each pixel in the HI 21cm maps was assigned with a H$_2$ column density from one UV sight line. This UV sight line is randomly chosen from a subsample of UV sight lines within a ±0.1 dex $N_{\text{HI}}$ bin centered around the 21cm-based $N_{\text{HI}}$ value of that pixel$^{16}$. The rationale behind this approach is that the $N_{\text{H}_2}$-$N_{\text{HI}}$ relation derived from absorbers (seen in Figure 2.11) could represent a general relation between the atomic gas and diffuse H$_2$ gas in the entire galaxy. Then, we can use

$^{16}$For SMC, as the 21cm data show two major dynamics components over a large fraction of the regions. We divided the 21cm $N_{\text{H}_2}$ by a factor of 2 to derive the $N_{\text{H}_2}$ map and then multiple 2 to get the final synthetic map.
the HI 21cm maps and this relation to extrapolate diffuse \(N_{\text{H}_2}\) down to a sensitivity level which is not reachable from observations of CO or dust emissions. The extrapolated \(N_{\text{H}_2}\) provide a lower limit of the total \(\text{H}_2\) mass undetected in CO, because \(\text{H}_2\) absorbers do not trace the same materials revealed by CO emissions. Although the derived diffuse \(N_{\text{H}_2}\) maps contain “noise” because of discrete sampling from randomly selected UV sight lines, the integrate \(\text{H}_2\) mass over a large region should give a rough estimation of diffuse \(\text{H}_2\) budget. This result should be independent from other emission-based gas mass tracer (e.g. CO or dust emissions).

We used the synthetic diffuse \(\text{H}_2\) maps to derive total \(\text{H}_2\) and HI masses from three types of integration regions: the entire HI map of each galaxy; the limited region observed in the MAGMA surveys; and the MAGMA regions restricted to the pixels where CO is detected above 4\(\sigma\). For each type of integration, we derived three hydrogen masses: the atomic hydrogen mass from 21cm data; the diffuse \(\text{H}_2\) mass from synthetic \(\text{H}_2\) maps; and the CO-based \(\text{H}_2\) virial mass based on the CO brightness, assuming canonical \(X_{\text{CO}}\) values of \(4 \times 10^{20} \text{ cm}^{-2} (\text{K km s}^{-1})^{-1}\) for both the LMC and SMC. Table 2.8 summarizes different estimations of \(\text{H}_2\) or HI masses, labeled as Full, MAGMA, and CO-Bright, respectively.

For the atomic gas mass, we used the 21cm maps from Stanimirovic et al. (1999); Kim et al. (2003) after applying a noise-masking algorithm, with the optically thin approximations (no optical depth correction). Therefore, the values quoted here is slightly different from previous works. The adopted \(X_{\text{CO}}\) value is about twice the canonical Galactic value and consistent with previous results of high-resolution resolved studies of the virial mass and CO brightness in each galaxy (Israel et al. 2003; Bolatto et al. 2003; Pineda et al. 2009; Wong et al. 2011). Therefore, the CO-based mass here only accounts for the \(\text{H}_2\) mass coexisting with CO emissions. It is important to note that previous studies based on virial mass of unresolved CO maps or dust emission techniques usually led to higher \(X_{\text{CO}}\) values, as the referred \(\text{H}_2\) mass is a dynamic or total (diffuse+bright) mass estimation at larger spatial scales beyond the CO-bright clumps (e.g. Mizuno et al. 2001b; Fukui et al. 2008; Bolatto
et al. 2011; Bot et al. 2010; Leroy et al. 2011). The CO integrated brightness of the entire galaxies are directly quoted from the result of the NANTEN surveys (Mizuno et al. 2001b; Fukui et al. 2008), with the MAGMA and CO-brightness results derived from the MAGMA CO maps (Wong et al. 2011; Muller et al. 2013), after applying the same noise masking algorithm as the HI maps. We note that all mass listed here exclude the contribution from Helium.

Integrated over the entire galaxy, the mass estimates in Table 2.8 suggest that only a small fraction of the total hydrogen mass lies in the diffuse H$_2$ phase, with molecular-to-atomic gas ratios less than 2% and 10% for the SMC and LMC, respectively. Although this result is consistent with the finding from T02, we found higher integrated diffuse H$_2$ mass compared with those from T02, by a factor of $\sim 2$ and $\sim 5$ for LMC and SMC, respectively. We note that this result is based on the entire FUSE MC H$_2$ absorption line sample, including more highly reddened sight lines with $(E(B-V) \gtrsim 0.2)$ compared with T02 and sampling the entire $N_{\text{HI}}$ dynamical range offered by the 21 cm data. Therefore, the higher diffuse H$_2$ mass we found can be caused by the fact that we included the top end of the $N_{\text{HI}}$-$N_{\text{H}_2}$ relation for the extrapolation.

Notably, the diffuse H$_2$ mass $M_{\text{H}_2,\text{diffuse}}$ is surprisingly comparable with the CO-based H$_2$ mass $M_{\text{H}_2,\text{CO}}$ over entire galaxy, and even exceeds the CO-based mass by a factor of $\sim 3$ in the SMC. Although the CO-based H$_2$ estimation depends on $X_{\text{CO}}$ and the referred spatial scales, the comparison illustrates the importance of diffuse H$_2$ mass in the molecular budget in each galaxy at large scales. When we compare molecular mass restricted to the MAGMA or CO-bright regions, the diffuse H$_2$ mass become much less significant in the H$_2$ mass enclosed in these regions. The atomic and CO-based molecular mass becomes comparable in the LMC although HI mass is still dominant in SMC. It is worth to note that the CO brightness from the entire galaxy is only slightly smaller than the values recovered from the MAGMA surveys, even though neither survey spatially covered the entire galaxy and only 10-20% atomic mass of entire galaxy lies in those regions. In a contrast, the HI mass is
decreasing as we restrict the integration to the MAGMA or CO-bright regions due to the more extended HI emission morphology.

This trend found in three types of integration regions is somewhat expected as our diffuse H$_2$ mass is extrapolated from HI 21cm emission and the atomic-to-molecular gas relation in diffuse clouds. So the diffuse H$_2$ follows the more extended distribution of HI. However, the physical picture is consistent with the finding of larger $X_{\text{CO}}$ factor in unresolved CO map. If we define $X_{\text{CO}}$ to take account of all H$_2$ mass, the value of $X_{\text{CO}}$ will be a strong function of the spatial scale because the diffuse H$_2$ mass make a significant contribution at larger spatial scales. For example, we found a factor of $\sim$20 difference in the diffuse and CO-based molecular gas estimates in the entire SMC. We note that we used a $X_{\text{CO}}$ value of $4 \times 10^{20}$ cm$^{-2}$ (K km s$^{-1}$)$^{-1}$ in deriving CO-based molecular gas. Therefore, we need to increase $X_{\text{CO}}$ by a factor of $\sim$ 20 to match the diffuse H$_2$ estimation. Such increasing of $X_{\text{CO}}$ will lead to a value more likely consistent with the finding in dust techniques (Bolatto et al. 2011; Roman-Duval et al. 2014), which does not distinguish diffuse and CO-bright molecular gas.

As indicated from their high temperature and low volume density, the diffuse H$_2$ gas does not constitute the immediate gas supply for star formation. However, if the galaxy SFR depends on the fraction of dense ISM gas or the probability distribution function of the gas volume/column density (Lee et al. 2015), modeling the SFR in the galaxy ecosystem will require a better understanding of the diffuse gas components in galactic environment because their significant roles in the mass budgets.

2.8 Summary and Conclusions

In this study, we have estimated the physical properties of H$_2$ and HI gas in the Magellanic clouds by measuring their UV absorption lines from the FUSE archival data offered by the FUSE Magellanic Clouds Legacy Project (Blair et al. 2009). We also compiled similar
measurements from previous studies.

We found the absorber velocity roughly traces the large-scale kinematic structure of each galaxy revealed in HI and CO emissions. However, the velocity discrepancy remains at small-scale in a significant number of UV sight lines.

The absorption-based $N_{\text{H}_2}$ is not correlated with the CO emission reveal in the MAGMA surveys at 45' resolutions. The CO brightness is lower than the expected CO brightness based on $N_{\text{H}_2}$ and Galactic $X_{\text{CO}}$ value with a few exceptions. A similar comparison between absorption-based $N_{\text{HI}}$ and 21cm emission show a distinct correlation with significant scatters. The difference suggested a clumpy structure of the molecular gas and also demonstrated the difficulty of observing molecular emission in the extragalactic diffuse or translucent clouds.

We found the constant-density diffuse cloud model with a two-phase pressure equilibrium assumption is not able to fully explain the observed the $\text{H}_2$-HI relation from absorbers in the LMC and SMC. It also does not provide a realistic gas density constraint. The decreased metallicity alone cannot explain the high amount of HI associated with diffuse $\text{H}_2$ gas in both galaxies, compared with their counterparts in the Galactic environment. The discrepancy suggests the existence of WNM components in a significant fraction of UV sight lines.

The radiation field estimated from $\text{H}_2$ population distribution suggest a comparable UV field in MC sight lines with the Galactic diffuse cloud at similar $\text{H}_2$ column densities in the statistical sense. However, we also find the UV field increases for a small number of sight lines near the star-forming regions.

The absorber measurements indicate the existence of an extended diffuse $\text{H}_2$ gas component in the Magellanic clouds, which is largely not detectable in the emission-based surveys due to low column density. This diffuse $\text{H}_2$ component, not confused from denser CO-bright $\text{H}_2$ molecular clouds, is expected to include a significant of $\text{H}_2$ in overall mass budgets. A galaxy modeling taking account of diffuse gas mass (both molecular and atomic) is necessary to better predict star formation.
Chapter 3

Spatially Resolved Atomic and Molecular Gas Distributions in Nearby Galaxies

3.1 Introduction

Cold gas in galaxies provides the fuel for star formation (McKee & Ostriker 2007). Understanding its physical and chemical properties is necessary to improve our knowledge of galaxy formation and evolution across cosmic time. Among the interstellar medium (ISM) phases, molecular gas has the highest volume density and lowest temperature, and is observationally found to be closely correlated with tracers of recent star formation (e.g. Hα, UV, or mid-infrared emission) both locally and at high redshift (e.g. Wong & Blitz 2002; Kennicutt et al. 2007; Bigiel et al. 2008; Leroy et al. 2008; Genzel et al. 2010; Tacconi et al. 2013). On the other hand, the correlation between star formation and the spatially more extended diffuse atomic gas (HI) was found to be poor, even in HI-dominated galaxies or the outskirts of H2-rich galaxies (e.g. Bolatto et al. 2011; Schruba et al. 2011). Therefore, it is important to understand the differences in physical properties and spatial distribution of the atomic and molecular gas across a variety of galactic environments. This will help reveal the mechanisms that determine how molecular clouds are formed from atomic gas, and help us understand what determines the fraction of dense and cold gas mass in a galaxy, which is the gas most relevant to star formation. It will also provide a more realistic prescription for modeling star formation and stellar feedback in a cosmological context. Until recently, most cosmological and galaxy evolution models did not model different gas phases separately and assumed a star formation rate dependent on the total gas content.

The microphysics of H2 dissociation and formation has been studied extensively in the
past (e.g. van Dishoeck & Black 1986; Draine & Bertoldi 1996; Browning et al. 2003). However, modeling of the large-scale (∼0.1–1 kpc) atomic and molecular gas relation was only carried out in recent years, by incorporating both microphysics and new knowledge of ISM properties at galactic scales. Although implementing a detailed time-dependent model of the atomic-to-molecular transition remains challenging in galaxy-sized simulations (e.g. Pelupessy & Papadopoulos 2009; Glover et al. 2010), the emergence of physically-motivated H$_2$ formation/dissociation equilibrium models at cloud scales have identified several potential links relating the molecular gas fraction to global galaxy properties.

For example, Krumholz et al. (2008) (see also Sternberg et al. 2014) emphasized that the atomic-to-molecular transition happens in cold atomic-molecular complexes when the total gas column density reaches a characteristic value (∼ 10$ M_\odot$ pc$^{-2}$ in a typical Galactic environment). This transition threshold is roughly determined by two factors: (1) ISM metallicity, which is related to the extent of UV shielding from dust and H$_2$ formation, and (2) the ratio between radiation field and gas volume density in the atomic shielding layers of cloud complex. The model of Krumholz et al. (2008) also implied that the column density of HI appears to saturate as the total gas column density increases and H$_2$ becomes dominant in the complex. These H$_2$ dissociation/formation equilibrium models were later expanded by incorporating the Cold-Neutral-Medium (CNM) and Warm-Neutral-Medium (WNM) pressure equilibrium model developed in Wolfire et al. (2003). Krumholz et al. (2009, hereafter KMT09), as well as McKee & Krumholz (2010, hereafter MK10), suggested that the atomic-to-molecular transition threshold is mainly determined by ISM metallicity, because the ratio between radiation field and volume density is restricted to a predictable narrow range by the CNM/WNM pressure equilibrium. The simple physically motivated solution from KMT09/MK10 provided a shortcut for implementing the HI-H$_2$ transition in galaxy simulations, producing results which can be compared with observational results on H$_2$ fractions or star formation rate (e.g. Kuhlen et al. 2012).

Additional evidence for HI column density saturation and its metallicity dependence has
been provided by several recent observational studies of both the Galactic and nearby galaxy environments (e.g. Wong et al. 2013; Lee et al. 2012). However, because the cloud complex model in KMT09 did not predict the amount of atomic gas residing in the surrounding medium (presumably in the CNM/WNM), whether the observed HI column density at a coarser resolution (typically > 200 kpc for extragalactic studies) reflects the predicted HI layer saturation near the molecular cloud scale (≲ 100 pc) is still questionable. As the validity of both the CNM/WNM pressure and H$_2$ chemistry equilibrium in a general galaxy environment is still a subject of debate (e.g. Motte et al. 2014), Ostriker et al. (2010, hereafter OML10) proposed a different model in which all neutral gas is partitioned into a diffuse component (atomic) and a dense gravitationally bound component (atomic and molecular), with the properties of diffuse component (e.g. density and mass) constrained by thermal (e.g. UV heating from star formation and line cooling) and dynamic (e.g. gravitational potential provided by stars, gas, and dark matter) equilibrium. The model accounts for the empirical correlation between molecular-to-atomic gas ratio $R_{H_2}$ and the hydrostatic mid-plane pressure in spiral galaxies, which was found in Blitz & Rosolowsky (2006, hereafter BR06) at kpc scales. The models emphasized a different and maybe more realistic large-scale ISM structure, rather than presuming that most ISM mass is contained in atomic-molecular cloud complexes and ignoring the WNM mass contribution. The predicted diffuse component surface density also has a metallicity-dependence at fixed total gas and stellar surface densities, which could potentially also explain the metallicity-dependent atomic gas saturation seen in Wong et al. (2013).

Nevertheless, what is required are more robust comparisons between model predictions and observations in a variety of galactic contexts and at physical scales close to atomic/molecular cloud structures. This will be challenging for extragalactic observations in terms of both spatial resolution and sensitivity.

The present study expands upon Wong et al. (2013) by carrying out a spatially resolved study of the atomic and molecular gas distributions for a wide range of galaxies with high-
resolution CO and HI images. The sample includes 45 galaxies from the CARMA Survey Toward IR-bright Nearby Galaxies (STING) (Rahman et al. 2011, 2012; Wong et al. 2013) and the HERA CO-Line Extragalactic Survey (HERACLES) (Leroy et al. 2009, 2012), as well as the Large and Small Magellanic Clouds (LMC/SMC). We used the CO/HI lines and ancillary mid-infrared (MIR) images to examine the dependence of atomic and molecular surface density on different galactic properties (i.e., metallicity, stellar mass surface density), and to compare observational results from this diverse sample with predictions of several theoretical and empirical models for both local and global $H_2$ fractions.

In Section 3.2, we describe the observations and data used in this study. Observational results are presented in Section 3.3, followed by the discussion of the results in Section 3.4. In Section 3.5, we summarize this work and present our conclusions.

### 3.2 Sample and Data

We selected a sample of 45 galaxies from the STING and HERACLES CO surveys for this work based on the availability of high-resolution HI maps. In addition, we included the LMC and SMC, whose proximity and low metallicity environments offer us the only opportunity to study both atomic and molecular gas at a physical resolution that could resolve individual giant molecular clouds (GMC). Overall, the entire sample in this work includes a diverse collection of galaxies from large spirals to dwarf galaxies, with significant spatial coverage in CO lines at angular resolutions better or comparable with HI maps. We summarize the sample galaxies in Table 3.1.

For the galaxies from the STING survey, the CO $J = 1 - 0$ data were obtained as part of the project using the Combined Array for Research in Millimeter-wave Astronomy (CARMA)\(^1\), with spatial coverage extending to $0.25 \sim 0.5R_{25}$ at a resolution of $\sim 3'' - 4''$.

\(^1\)Combined Array for Research in Millimeter-wave Astronomy (CARMA) is operated by the Universities of California (Berkeley), Chicago, Illinois, and Maryland, and the California Institute of Technology, under a cooperative agreement with the University Radio Observatory program of the National Science Foundation.
For the corresponding HI data, we assembled and reduced all usable archival HI 21cm data available from the Karl G. Jansky Very Large Array (VLA). In addition, we carried out new observations using the upgraded VLA at B and CnB configurations in December 2013 to supplement the existing archival data in both resolution and sensitivity for 6 galaxies. The STING CO $J = 1 - 0$ images have been presented in previous studies, mainly focusing on the Kennicutt-Schmidt star formation law on (sub-)kpc scales (Rahman et al. 2011, 2012; Fisher et al. 2013), in addition to the preliminary study related to the topic here by Wong et al. (2013). We note that providing both HI and CO $J = 1 - 0$ data products is also a major effort in this work. The observations and reduction of both CO and HI data have not been systematically presented in Wong et al. (2013) and preceding work. Therefore, we describe the details in Sections 3.2.1 and 3.2.1.

For galaxies selected from the HERACLES survey, we generally used the existing CO and HI data products provided by the HERACLES project and the HI Nearby Galaxy Survey (THINGS, Walter et al. 2008) for data analysis, and refer the reader to the corresponding references for full details of the observations and data products. The HERACLES CO $J = 2 - 1$ nearby galaxy survey (Leroy et al. 2009) was carried out using the IRAM 30-m telescope. Most galaxies have multi-wavelength data from far/mid-infrared, optical, and UV imaging, and have been presented in a number of studies mainly focusing on the star formation law, star formation efficiency, and the CO-to-H$_2$ conversion factor (Bigiel et al. 2008, 2010, 2011; Schruba et al. 2011, 2012; Leroy et al. 2013b; Sandstrom et al. 2013).

We note that five galaxies are included in both the STING CO $J = 1 - 0$ and HERACLES CO $J = 2 - 1$ surveys (NGC 0337, NGC 2976, NGC 3198, NGC 4254, and NGC 5713). The inner part of NGC 5194 (or M51a, selected from the HERACLES survey) has also been recently observed by the Plateau de Bure Interferometer Arcsecond Whirlpool Survey (PAWS) in CO $J = 1 - 0$ at a high physical resolution (Schinnerer et al. 2013). All six galaxies were included in the THINGS survey. However, we adopted the HI data from our independent reduction (including new observations) for those galaxies, instead of using the...
data products from THINGS. Although the availability of multiple CO maps for a single galaxy offers opportunities for comparisons between different line transitions (CO $J = 1 - 0$ vs. CO $J = 2 - 1$), we did not attempt them in this work due to systematic uncertainties and different spatial coverages for those galaxies. Instead, we adopted a preferred line ratio (see Section 2) to convert CO $J = 2 - 1$ line brightness to that of CO $J = 1 - 0$, and treated the two data sets for a single galaxy separately in our analysis.

NGC 4254 and NGC 4536 (selected from the STING survey) have been mapped by the Nobeyama 45-m telescope in CO $J = 1 - 0$ (Kuno et al. 2007), as well as the Five College Radio Astronomy Observatory (FCRAO) 14-m (Chung et al. 2009b). For these two galaxies, we compared the total fluxes of our data with the public maps from the Nobeyama survey\(^2\), which show remarkably good consistency within 10% (see Table 3.2). However, the single-dish map from the Nobeyama survey shows less dynamic range after we smoothed the CARMA map to the same angular resolution (either in integrated intensity images or spectral cubes). We note that a similar brightness temperature difference was also implied in Table 5 of Leroy et al. (2009), when their HERACLES CO $J = 2 - 1$ maps were compared with the CO $J = 1 - 0$ maps from the Nobeyama survey and the BIMA Survey of Nearby Galaxies (SONG, Helfer et al. 2003), separately. A similar case was also found by Wilson et al. (2009) when they compared the BIMA SONG images of NGC 4321 and NGC 4569 with the images from Kuno et al. (2007). One possible explanation is that the gridding function used to generate the single-dish maps resulted in the loss of some higher spatial frequency information compared with smoothed high-resolution interferometer maps.

We used the data products from the Magellanic Mopra Assessment (MAGMA) surveys of the LMC and SMC (Wong et al. 2011; Muller et al. 2013) and the high-resolution HI maps from Kim et al. (2003) and Stanimirovic et al. (1999) for studying the atomic and molecular gas relation. Before this work, a CO and HI comparison was carried out in the LMC by Wong et al. (2009) using the low-resolution CO $J = 1 - 0$ map from Fukui et al.

\(^2\)http://www.nro.nao.ac.jp/~nro45mrt/html/COatlas
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(2008). The availability of the MAGMA data gives us an unprecedented opportunity to test atomic-to-molecular transition models in sub-solar metallicity environments with resolution better than 10 pc.
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3.2.1 CARMA Survey Toward IR-Bright Nearby Galaxies (STING)

Over the past few decades, the HI 21 cm line and CO rotational lines have been the primary methods to study the atomic and molecular gas components in the ISM of nearby galaxies. The inference of atomic gas mass from HI 21 cm brightness is straightforward, except in some cases where the optical depth is significant or radio continuum background sources exist. The primary challenge is systematically mapping the line in nearby galaxies with the necessary angular resolution and sensitivity. Recent such efforts include the Westerbork HI Survey of Irregular and Irregular and Spiral Galaxies (WHISP) (van der Hulst et al. 2001), the Westerbork SINGS survey (Braun et al. 2007), the THINGS survey of star-forming galaxies (Walter et al. 2008), and the VIVA survey of the Virgo Cluster (Chung et al. 2009a). All of them are made with radio interferometers using the aperture synthesis...
Table 3.2. Flux Density Comparison in CO $J = 1 - 0$

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Note. — All values are in units of Jy km s$^{-1}$.
* Chung et al. (2009b) noted a limited coverage and baseline issue for NGC 4536.

Technique. Studying molecular gas in CO lines rather than H$_2$ lines is necessary due to the lack of emission features from cold H$_2$. Although H$_2$ can be directly studied in infrared (IR) quadrupole emissions or Lyman-Werner absorption (see Section 3), the requirement of special excitation conditions (Dalgarno 1995) or strong UV background sources, respectively, make both methods unsuitable for mapping molecular gas in nearby galaxies. Because a single dish observation in CO $J = 1 - 0$ does not offer sufficient resolution to reveal clumpy structures of molecular gas at a couple of Mpc distance, recent studies have exploited aperture synthesis using millimeter arrays (e.g., Helfer et al. 2003; Koda et al. 2009), or scan mapping using single-dish telescopes in higher-$J$ CO transitions (e.g., Leroy et al. 2009; Wilson et al. 2009). Another work-around is using a total gas tracer (e.g. dust emission) and an atomic gas tracer (HI 21 cm) to calculate the mass contribution of molecular gas. This approach has been demonstrated in some recent works (e.g. Leroy et al. 2007; Lee et al. 2012), despite the loss of kinematical information.

The CARMA Survey Toward Infrared-Bright Nearby Galaxies (STING) is a recent effort to study the molecular gas properties in a sample of 23 nearby star-forming galaxies. The sample is specifically chosen to cover a wide range of associated galaxy properties (star formation rate, color, luminosity, metallicity, etc.), with a distance from $\sim 4 - 40$ Mpc. Supplementing the STING CO data with ancillary multi-wavelength data from the UV to IR, the spatially resolved star formation law for nearly the entire STING sample has been
studied by Rahman et al. (2012). With ancillary high-quality HI 21cm images, the molecular gas data from the STING survey can also be used to study the spatially resolved atomic and molecular gas relation at larger than typical GMC scales. The range of galaxy properties in the sample makes it valuable for testing the HI-to-H$_2$ transition model from KMT09.

**HI Observations and Data Reduction**

We searched the NRAO Science Data Archive$^3$ for VLA HI data for each galaxy in the STING survey and found 21 of 23 have usable and calibratable visibility data. Table 3.3 summarizes the observing setup of those archival programs, as well as observation details (e.g. observation date, project ID, integration time on source and velocity coverage), illustrating the diversity of the archival HI data. We also list the publication reference when available. In addition, Table 3.3 also includes 27 hrs of new VLA observations carried out specifically for this work under VLA program 13B-363. To synthesize the data obtained from both archival programs and new observations and facilitate the reduction of such a heterogeneous dataset, we built a data reduction pipeline implemented in the CASA$^4$ software package (McMullin et al. 2007), for reprocessing the entire dataset in a uniform and repeatable procedure. We briefly describe the implemented calibration and imaging procedures below.

For each VLA observation, the uncalibrated visibility data were retrieved from the data archive in either the VLA archive format or as a CASA Measurement Set (MS). We first inspected the data and identified the target, flux calibrator (also used as bandpass calibrator) and phase calibrator, and imported visibilities into an MS after excluding auto-correlation data. Bad data from interference or instrument glitches were located and examined using the CASA tasks `plotms` and `viewer`, and later flagged with the shadowed data. In addition, the edge channels of each spectral window were also flagged if the bandpass response is below 0.5. All flagging information is saved in the pipeline to facilitate reprocessing. After

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$^3$http://archive.nrao.edu

$^4$http://casa.nrao.edu
flagging, the flux calibrator visibility model was set using \texttt{setjy}, and we computed the bandpass and gain tables with flux scaling bootstrapped from the flux and gain calibrator data, using tasks \texttt{BANDPASS}, \texttt{GAINCAL}, and \texttt{FLUXSCALE}. All calibration tables were later applied to the data to create the calibrated visibility dataset, with the task \texttt{APPLYCAL}. For each galaxy, the calibrated visibility data from different observations can be combined and imaged to create the final imaging products. However, because of different observing setups and changes in instrumentation spanning the archival and new observations, the calibrated visibilities from individual observations usually have different velocity coverage and resolution (e.g., NGC 3147 in Table 3.3). The visibility weighting implemented in CASA can also result in different weight scalings between datasets due to a lack of full information to derive an estimate of the theoretical visibility noise. To solve this problem, we performed several procedures to adjust the weight scaling and channelization before concatenating each observation into a joint visibility set for imaging (see more details in Appendix B).

We performed continuum subtraction in the visibility domain using the task \texttt{UVCONTSUB}\(^5\) on calibrated visibilities from individual observations. A linear fit was used to estimate the continuum emission from line-free channels, although a zero-order fitting was used in some rare cases where line-free channels were only available at one end of the spectral window. The visibility data containing line emission from each track were combined using the task \texttt{CONCAT} with scaled weights. The CASA task \texttt{CLEAN} was used to image and \texttt{CLEAN} the combined visibility data using the ROBUST weighting algorithm (Briggs 1995, ROBUST parameter \(R = 0.5\)). We set the \texttt{CLEAN} depth to a flux level of 2.5 times the noise r.m.s derived from the line free regions of the dirty cube. A \texttt{CLEAN} mask was also defined bounding regions with primary beam response above 0.2. This approach avoids picking up model components

\(^5\) For some cases, the spectral line cube was created using task \texttt{IMCONTSUB} in the image domain. This is preferred if line emission exists in all channels in the UV domain, but line-free channels are still available towards the target direction in the image domain. It is also preferred if there are strong continuum sources away from the phase center. In addition, \texttt{IMCONTSUB} could also help to eliminate the problem of unstable continuum subtraction (e.g., line-free channels are only available at one edge), because bad subtraction in visibilities could have more severe impacts on overall image quality, causing channel-dependent strips rather than bad pixels in specific regions
in regions where a signal is unlikely to be detected and eliminates a slow convergence of the 
clean process when the clean flux threshold is not specified in advance. We note that 
most STING galaxies have HI disks much smaller than the VLA primary beam of $\sim 32'$ at the 
$L$-band. Continuum emission was also imaged using line-free channels from the calibrated 
visibleibilities, using the same pipeline. However, continuum images constructed from the full 
1 GHz bandwidth of the new VLA system are not included in this work for the 6 galaxies 
with new observations.

We utilized the multi-scale clean (msclean) (Cornwell 2008) option implemented in 
CASA to better recover extended structure in both spectral line and continuum imaging. 
Tests on our data indicate that this option is able to recover low-level extended emission 
around emission peaks without increasing the clean depth. This is particularly important 
given our strategy of smoothing the data for improving signal detections in spectral cubes 
as described in Section 3.2.2. For all clean products, we generate corresponding error 
cubes/images based on the noise characteristics derived from emission-free regions and the 
systematic noise pattern in both spectral and spatial domain caused by the effective primary 
beam and channel response.

We summarize the STING HI data products in Table 3.4, including the sensitivity, syn-
thesizerd beam size, velocity coverage/resolution, and cube dimensions. Because our focus is 
deriving the atomic gas surface density at high resolution, we include all archival data with 
spectral resolution better than 25 km s$^{-1}$ to enhance the sensitivity at the possible expense 
of velocity resolution. This strategy differs from the approach of other systematic HI surveys 
(e.g. Walter et al. 2008; Haan et al. 2008; Chung et al. 2009a; Hunter et al. 2012), for which 
archival data were also compiled for some of the same galaxies included in the STING survey. 
To address the uncertainties in absolute flux calibration and the missing flux problem due 
to a lack of the total power constraints from the VLA, we examine the HI global line profile 
from the VLA maps and compare them with single-dish spectra from the Cornell Digital 
HI Archive (Springob et al. 2005), the HI Parkes All Sky Survey (HIPASS) (Barnes et al.
2001), or published results available at the NASA/IPAC Extragalactic Database (NED). To make the VLA-based global profile comparable with the single-dish spectra without pointing offset and extended source corrections, we simulated the single-dish beam response on the high-resolution VLA maps and extract the global profile from its pointing center.

The comparison is presented in Figure 3.2, showing a good agreement in the HI flux and line profiles except for NGC 3147 and NGC 5713. The discrepancy for NGC 5713 is attributed to an intergalactic gas flow between NGC 5713 and NGC 5719 (roughly 11′ to the east of NGC 5713). While the single-dish data cover their line emissions, the VLA image does not provide reliable continuum subtraction towards NGC 5719 due to the limited velocity coverage. For NGC 3147, the disagreement is likely related to the poor quality and large baseline uncertainty in the single-dish spectra.
Figure 3.1  CO $J = 1 - 0$ total flux comparisons between the data products generated by the multi-scale clean (Cornwell 2008) and Steer-Dewdney-Ito CLEAN (Steer et al. 1984) algorithms implemented in CASA and MIRAID, respectively.
Figure 3.2 HI 21cm global line profile comparisons between the single-dish (blue line) and VLA data (shadow).
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Notes. — Comments on columns: We only included data with resolution better than 20 km s\(^{-1}\). Column 1: galaxy name; Column 2: VLA configuration; Column 3: program code (13B-363: new observations from this work; AW0605: THINGs; AH927: Little THINGs; others: archival data); Column 4: observing date; Column 5: time on source (min, before flagging); Column 6: channel width in km s\(^{-1}\); Column 7: velocity coverage in barycentric (heliocentric, before flagging); Column 8: reference: (1) Little THINGs (Hunter et al. 2012) (2) THINGs (Walter et al. 2008) (3) VIVA (Chung et al. 2009a) (4) This work (5) Adam’s project (6) Mundell et al. (1999) (7) Emily Richards, private communication (8) KING-FISH Walter (9) Johnson et al. (2012) (10) Haan et al. (2008) (15) del Rio et al. (2003)

Notes on individual galaxies: NGC 337: we performed the continuum subtraction in the image domain because of the existence of non-related HI emission beyond the velocity coverage. NGC 772: the data taken in the D configuration suffered minor solar interference in the visibilities; NGC 1156: the archival data don’t contain any no line-free channels, and the HI detection could be underestimated; NGC 1569: foreground Galactic emission exists and absorptions were seen in some channels; NGC 2782: absorption seen in the galaxy center; NGC 2976: foreground Galactic emission exists; NGC 4151: absorption seen in the galaxy center; NGC 4536: absorption seen in the galaxy center; NGC 4554: imcontsub() used because another galaxy is in the primary beam but with line emissions beyond the correlator setup. NGC 5713: imcontsub() used because another galaxy is in the primary beam but with line emissions beyond the correlator setup. It is connected with NGC 5719 via an atomic gas bridge.

### CO \(J = 1 - 0\) Observations and Data Reduction

Most CO \(J = 1 - 0\) data presented in this work are obtained as part of the STING survey with CARMA, supplemented by a small amount of data obtained with the Berkeley-Illinois-Maryland Array (BIMA), which is now part of CARMA. The entire survey includes CO \(J = 1 - 0\) observations toward 23 galaxies. The CARMA observations were performed using a 19 pointing hexagonal mosaicing pattern with \(~26''\) separation, and the data were taken between 2005 and 2010.

The visibilities from individual observations were calibrated in MIRIAD (Sault et al. 1995), and later imported into CASA for imaging. We used the same pipeline mentioned in Section 3.2.1 for imaging the calibrated visibilities, without continuum subtraction required. The same mscl ean algorithm is adopted, with a CLEAN mask used to exclude regions where the sensitivity falls below 0.25 times that in the mosaicing center. The final products have synthesized beams ranging from \(~2'' - 5''\), and generally better resolution than VLA HI maps. However, the spatial coverage of CO \(J = 1 - 0\) observations is limited to 0.25–0.5

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\(^6\) The calibrated MIRIAD data preserve full information required for theoretical visibility noise estimations and it is not required for the weights scaling described in Appendix B.
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<td>10.2 x 9.64</td>
<td>83</td>
<td>20.8</td>
<td>726.4–2940.4</td>
<td>2</td>
<td>640</td>
<td>0.3</td>
</tr>
<tr>
<td>NGC 4254</td>
<td>9.7 x 8.6</td>
<td>73</td>
<td>10.4</td>
<td>2214.8–2578.8</td>
<td>2</td>
<td>320</td>
<td>0.3</td>
</tr>
<tr>
<td>NGC 4273</td>
<td>15.4 x 14.3</td>
<td>-2</td>
<td>20.8</td>
<td>1855–2957.4</td>
<td>2</td>
<td>320</td>
<td>0.8</td>
</tr>
<tr>
<td>NGC 4536</td>
<td>9.3 x 8.6</td>
<td>46</td>
<td>20.8</td>
<td>1581.2–2059.6</td>
<td>2</td>
<td>640</td>
<td>0.2</td>
</tr>
<tr>
<td>NGC 4605</td>
<td>5.8 x 5.2</td>
<td>72</td>
<td>20.8</td>
<td>1.6–313.6</td>
<td>2</td>
<td>320</td>
<td>0.2</td>
</tr>
<tr>
<td>NGC 4654</td>
<td>16.8 x 16.2</td>
<td>49</td>
<td>10.4</td>
<td>810.6–1372.2</td>
<td>4</td>
<td>320</td>
<td>0.4</td>
</tr>
<tr>
<td>NGC 5371</td>
<td>85.3 x 42.7</td>
<td>82</td>
<td>20.8</td>
<td>2310–2850.8</td>
<td>12</td>
<td>160</td>
<td>0.3</td>
</tr>
<tr>
<td>NGC 5713</td>
<td>16.8 x 15.6</td>
<td>2</td>
<td>20.8</td>
<td>1653.2–2048.4</td>
<td>4</td>
<td>320</td>
<td>0.2</td>
</tr>
<tr>
<td>NGC 6951</td>
<td>9.5 x 9.0</td>
<td>-62</td>
<td>20.8</td>
<td>1172–1650.4</td>
<td>4</td>
<td>320</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Note. — (1) galaxy name; (2) the beam sizes from the data products generated with a briggs weighting of robust=0.5; (3) the beam position angle; (4) channel width in $\text{km s}^{-1}$; (5) velocity coverage in $\text{km s}^{-1}$; (6) imaging pixel size in $''$; (7) Image size; (8) noise levels. Note: Several galaxies are covered by the existing or on-going H I nearby galaxy survey: THINGs (Walter et al. 2008): NGC 1569 and NGC 3198; VIVA (Chung et al. 2009a): NGC 4254, NGC 4536, NGC 4654; Little THINGs (Hunter et al. 2012): NGC 1156, NGC 1569.
times of the galaxy optical radius \( R_{25} \), defined as the 25 mag arcsec\(^{-2}\) \( B \)-band isophote).

### 3.2.2 CO and HI Integrated Intensity Maps

To construct atomic and molecular gas surface density maps, we derived CO and HI integrated-intensity maps from the available spectral cubes assembled from individual surveys using a uniform procedure.

Since it is common to apply a signal mask to exclude noise before deriving integrated intensity maps (Rupen 1999), several different algorithms have been used for identifying signals in spectral cubes. For example, previous CO and HI extragalactic surveys (e.g. Helfer et al. 2003; Walter et al. 2008) have adopted signal masks derived from a spatially smoothed spectral cube. The CPROPS package developed by Rosolowsky & Leroy (2006) expands the signal mask from regions above a specified intensity threshold and allows some extra spillover (also known as the dilated mask method) in channel integration for robust signal identifications. Several previous studies (e.g. Schruba et al. 2011; Pety et al. 2013) have also used HI and its velocity field information as a prior to define the region for integrating CO spectra, which is based on the observational evidence that CO emissions are mostly associated with detectable HI emissions. In this work, we adopt an approach of creating a signal mask by combining the strengths from the first and second methods mentioned above: we smooth a spectral cube in both spatial and spectral dimensions, then identify continuous 3D regions above a flux threshold (usually \( 4\sigma_{\text{rms}} \)), and extend each region to adjacent pixels above \( 2\sigma_{\text{rms}} \) in the smooth data to create a signal mask.

The rationale behind the smoothing procedure is that signal identification of extended sources could be improved in the smoothed data, provided that the original image is oversampled. Assuming that a source with a Gaussian spatial distribution is embedded in a noise background and the pixel noise is correlated at the spatial scale of the synthesis beam, the signal and noise levels near the source center will roughly obey the relation below: the
local signal-to-noise ratio (SNR) near the source center will roughly obey the relation below:

\[
\text{Signal} \propto \frac{1}{s^2 + r^2 + g^2} \\
\text{Noise} \propto \frac{1}{\sqrt{r^2 + g^2}}
\]  

(3.1) \hspace{2cm} (3.2)

Here, \( r, s, \) and \( g \) are the angular sizes of the synthesis beam, the source, and the adopted smoothing kernel, respectively.

Therefore, smoothing an image to a resolution similar to the characteristic scale of expected emissions will enhance the local SNR for source identifications if the pixel size is not changed. This approach can be applied to both spatial and spectral dimensions, to better recover extended low-intensity emission (e.g. near inter-arm regions) and broad low brightness line features (e.g. near the galaxy center, where the rapidly-changing velocity field and beam smearing effect may cause a broad low-intensity line profile). On the other hand, expanding from \( 4\sigma_{\text{rms}} \) regions in all dimensions is based on the reasoning that one could reduce the potential flux bias from a brightness-based cutoff by padding around the pixels with robust signal detections. We chose slightly different smoothing scales for CO and HI data, depending on the expected typical angular scale of emission features in individual velocity frames.

We implemented our adopted procedures along with other commonly used algorithms mentioned above into a publicly available IDL package\(^7\), and experimented with different methods on the STING CO maps. We performed cross-correlation comparisons between the results and Spitzer/IRAC 8\( \mu \)m images, which is a high-resolution tracer of Polycyclic Aromatic Hydrocarbons (PAHs) and known to be associated with molecular gas (Regan et al. 2006). The results indicated that the adopted technique indeed shows advantages of picking up genuine weak emission without HI prior information. One drawback of all masking approaches is that it does not give an upper limit on the integrated intensity for

\(^7\)https://www.github.com/r-xue/moments
spatial pixels without signal identification. To calculate a conservative error map for image analysis, we used the quadratic sum of the errors from individual integrated channels but adopted a minimal pixel error equivalent with the value expected from integrating over 15 km s$^{-1}$ (CO) or 30 km s$^{-1}$ (HI).

We used the procedure mentioned above to derive integrated intensity maps and associated error images for both CO and HI spectral cubes assembled from different surveys. Although most public data releases from these surveys do provide integrated intensity maps, they usually do not provide error images (except for HERACLES).

### 3.2.3 Metallicity and Infrared Images

We collected the metallicity measurements of each galaxy from previous studies, as the equilibrium models from KMT09 and Sternberg et al. (2014) pointed out the strong influence of metallicity on H$_2$ formation / UV shielding and atomic-to-molecular transition. The majority of the galaxies are included in Moustakas et al. (2010), with direct nebular strong-line based metallicity measurements at different galactocentric radii. The characteristic metallicity (defined as the value at 0.4$R_{25}$ or an overall averaged value in Moustakas et al. 2010) is summarized in Table 3.1. As discussed in Moustakas et al. (2010), different emission line calibration methods (empirical or theoretical) could create an uncertainty as large as 0.6 dex. We adopted the average value from two methods in this work and expect this systematic difference will not play a role when we compare the relative metallicities among individual galaxies. For the rest of the galaxies, we collected the measurements from various published individual studies and converted the observed line ratio to metallicity using the calibration presented in Moustakas et al. (2010), or used their $B$-band luminosities and the luminosity-metallicity relation from Moustakas et al. (2010) for estimating the characteristic metallicity, which has greater uncertainty. We plot the characteristic metallicity as a function of $B$–band luminosity in Figure 3.3. The metallicity for the entire sample spans from 12+log(O/H)=7.4 to 9.0.
Figure 3.3 The metallicity and absolute $B$–band magnitude for 45 galaxies selected from the STING and HERACLES surveys. The dotted lines present the luminosity-metallicity ($L-Z$) relation derived by Moustakas et al. (2010), using two different strong-line metallicity calibration methods from Kobulnicky & Kewley (2004) (KK04) and Pilyugin & Thuan (2005) (PT05). The solid line present the average of two. The symbol colors denote difference references from which the metallicity measurements are collected, although most values are from Moustakas et al. (2010). We note that the filled blue diamonds indicate the metallicity values based on the averaged $L-Z$ relation from Moustakas et al. (2010) for the galaxies without direct emission line measurements. Their error bars show the value differences from the theoretical (KK04) and empirical calibration (PT05) approaches. The sample metallicities span from $\sim 7.5$ to $\sim 9.0$, with the value increasing as the $B$–band magnitudes. However, the metallicity for individual galaxies could vary as large as $\sim 0.3$ dex depending on resolved regions referred in the galaxy or the calibration methods. The solar, LMC, and SMC characteristic metallicity were marked as the horizontal dashed lines, respectively.
Although recent theoretical development has focused on the metallicity effects on atomic-to-molecular transition, the hydrostatic pressure models in disk galaxies (e.g. Elmegreen 1993, BR06) suggested that both stellar and gas mass play an important role in the overall status of the ISM. Therefore, we obtained ancillary Spitzer/IRAC 3.6 and 4.5 µm images for our galaxy sample, which provides a tracer of the stellar content. Most of our target galaxies are included in the Spitzer Survey of Stellar Structure in Galaxies (S^4G) (Sheth et al. 2010), which offers both calibrated images and foreground star masks. For galaxies not included in the S^4G survey, we obtained the images provided by the Spitzer Heritage Archive\(^8\), from contributed enhanced products of the Spitzer Infrared Nearby Galaxies Survey (SINGS) (Kennicutt et al. 2003), the Spitzer Local Volume Legacy Survey (LVL) (Dale et al. 2009), or post-BCD data. In addition, we used the data products from the Surveying the Agents of a Galaxy’s Evolution (SAGE) survey (Meixner et al. 2006; Gordon et al. 2011) for estimating the stellar surface density of LMC/SMC.

### 3.3 Analysis and Results

In this section, we compare the spatially resolved atomic/molecular gas surface density \((\Sigma_{\text{HI}}/\Sigma_{\text{H}_2})\) and stellar mass surface density in individual galaxies and across the entire sample. The relation between the ISM and stellar distribution will help uncover the physical mechanisms determining the molecular or dense gas fraction, which links to star formation. We first present the method of estimating the surface density maps. Then we will illustrate the spatially resolved relation between gas and stellar surface density using the example of NGC 4254, and reveal their dependence on galaxy global properties. Finally, we present the correlations among different surface density within individual galaxies.

\(^8\)http://irsa.ipac.caltech.edu/applications/Spitzer/SHA/
3.3.1 Gas and Stellar Surface Density Maps

The gas density maps were derived from the CO and HI integrated intensity maps presented in Section 3.2.2. The column density of HI was estimated from the integrated intensity of HI using the optically thin approximation:

\[
\frac{N_{\text{HI}}}{I_{21\text{cm}}} = 1.82 \times 10^{18} \text{ cm}^{-2} \frac{\text{K km s}^{-1}}{\text{T}}. \tag{3.3}
\]

For CO images, we adopted the following CO intensity to H\textsubscript{2} column density conversion, or X\textsubscript{CO} factor:

\[
\frac{N_{\text{H}_2}}{I_{\text{CO} J=1-0}} = 1.34 \times 10^{20} \exp\left(\frac{0.4}{Z'}\right) \text{ cm}^{-2} \frac{\text{K km s}^{-1}}{\text{T}}. \tag{3.4}
\]

Those relations are based on the canonical CO \( J = 1 - 0 \) conversion factor of the Milky Way (\( X_{\text{CO}}=2 \times 10^{20} \text{ cm}^{-2} \text{ K}^{-1} \text{ km}^{-1} \text{ s} \)) and the estimated unresolved \( X_{\text{CO}} \) scaling relation with metallicity (see Equation 31 of Bolatto et al. 2013, assuming a typical GMC surface density of \( \sim 100 M_\odot \text{ pc}^{-2} \)).

In Figure 3.4, we show the adopted \( X_{\text{CO}} \) values of individual galaxies with CO detections. We note that the values were directly derived from their metallicity. For some galaxies with metallicity gradient measurements, the adopted \( X_{\text{CO}} \) values vary significantly from galaxy centers to outskirts, which correspond to the vertical lines on the mean values. For most galaxies, the pixel-averaged \( X_{\text{CO}} \) values are below \( 5 \times 10^{20} \text{ cm}^{-2} \text{ K}^{-1} \text{ km}^{-1} \text{ s} \). Only the SMC and NGC 1569 have higher mean values because they are the only two galaxies with significantly lower metallicity but still detected in CO.

We note that the adopted CO-to-H\textsubscript{2} conversion is empirical and only valid after averaging over typical GMC scales. Although we attempted to correct for the metallicity-dependence of \( X_{\text{CO}} \) in Equation 3.4, it may still be subject to systematic uncertainties. To estimate the CO \( J = 1 - 0 \) line brightness in the HERACLES maps, we assume a typical line ratio

---

\(^9\)We note that the HI brightness-to-mass conversion could be compromised by opacity effects at small scales (e.g. Braun 2012).
Figure 3.4  Adopted $X_{\text{CO}}$ values for individual galaxies. For some galaxies with metallicity gradient measurements, the adopted $X_{\text{CO}}$ values vary from galaxy centers to outskirts, which correspond to the vertical lines on the mean values.

of $R_{21} = I(\text{CO } J = 2 - 1)/I(\text{CO } J = 1 - 0) \approx 0.7$ (Leroy et al. 2012). The line ratio of $I(\text{CO } J = 2 - 1)/I(\text{CO } J = 1 - 0)$ generally decreases away from the center in large spirals (e.g. Sawada et al. 2001). We note that any atomic and molecular gas surface density reported later is based on the HI and H$_2$ column densities derived from Equations 3.3 and 3.4, excluding the helium contribution in the gas mass.

The stellar density maps were estimated based on the Spitzer infrared images. For those Spitzer images without foreground star masks, we generated masks for point sources from flux calibrated images and exposure time / weight images using SExtractor (Bertin & Arnouts 1996), following the same procedure described in Sheth et al. (2010). We performed flat background subtraction using the median pixel value derived from emission-free regions surrounding our targets for all Spitzer images, and further used the statistical noise from emission-free regions and weight images to derive conservative error maps after tak-
ing account of an estimated systematic flux uncertainty of 10%. We adopted the empirical relation\(^{10}\) between stellar mass and 3.6/4.5\(\mu\)m flux derived by Eskew et al. (2012):

\[
\frac{\Sigma_*}{M_\odot \text{ pc}^{-2}} = 179 \times \left( \frac{I_{3.6}}{\text{MJy sr}^{-1}} \right)^{2.85} \left( \frac{I_{4.5}}{\text{MJy sr}^{-1}} \right)^{-1.85}.
\]

(3.5)

Although the recent study from S\(^4\)G also provided the stellar-only 3.6\(\mu\)m images based on Independent Component Analysis (ICA, Querejeta et al. 2014), we did not use them here because not all galaxies here were included in S\(^4\)G. For six spiral galaxies, Meidt et al. (2012) concluded that the PAHs and hot dust could contribute 5% – 15% of the 3.6\(\mu\)m integrated light. However, Querejeta et al. (2014) found the empirical relation from Eskew et al. (2012) based on both 3.6 and 4.5\(\mu\)m flux to be comparable with the results from the ICA approach.

To study the spatially resolved relation of the observed gas and stellar surface density, we first deprojected different surface density maps of each galaxy, as well as point spread functions (PSFs) and error maps, using the galaxy inclination and position angle listed in Table 3.1. The brightness and error maps were properly scaled by \(\cos(i)\) to create “face-on” images. Then we matched the resolution of all images to a minimum circular beam, oversampled and regridded them to the same astronomical frame. In image processing, pixel values of error maps were scaled by considering the quadratic sum error propagation and noise covariance of adjacent pixels. For the masked regions of stellar maps, we replaced the missing data using the median value of adjacent pixels. For the molecular gas surface density maps derived from the STING survey, we padded regions out of the observation coverage with zero value during image convolution. Following a similar procedure adopted in Leroy et al. (2011), we used a hexagonal grid spaced by half of the common resolution to select noise-independent pixels from the deprojected images. We measured atomic, molecular, and stellar surface densities and their other traits (e.g. surface density uncertainties, metallicity, galactocentric distance, etc.), and collected them across the entire galaxy sample for the

\(^{10}\)A simplified approach is adopted in Muñoz-Mateos et al. (2013) using only 3.6\(\mu\)m images, see also Wong et al. (2013).
3.3.2 Spatially Resolved Relation of Gas and Stellar Distributions: NGC 4254

We use NGC 4254 as an example to demonstrate general observational results with regard to the atomic/molecular/stellar mass distributions in spiral galaxies, which consist of a large fraction of the sample.

NGC 4254 is an unbarred spiral galaxy located in the Virgo cluster at a distance of \( \sim 16 \) Mpc, with a less tightly wound outer arm extended to a stream linking to the massive HI region VIRGO HI 21\(^{11}\). Despite the peculiar morphology in the outskirt region, Nakanishi et al. (2006) found the overall molecular gas fraction is similar with field galaxies and did not show H\(_2\) fraction enhancement exhibited by other galaxy members in the cluster center. This suggested that NGC 4254 might be a new cluster member, and external mechanisms (such as ram pressure) had not stripped its gas yet. Rahman et al. (2011) also used NGC 4254 for the STING pilot study to understand the systematic effects (e.g. choices of star formation tracers, fitting methods with a range constrained from signal-to-noise cuts, etc.) on the spatially-resolved Kennicutt-Schmidt law.

Figure 3.5 shows the deprojected atomic/molecular/stellar surface density \( (\Sigma_{\text{HI}}/\Sigma_{\text{H}_2}/\Sigma^*) \) map set of NGC 4254 at a resolution of \( \sim 800 \) pc, presented in physical coordinates. In this example, the lower contrast of \( \Sigma_{\text{HI}} \) is clearly visible compared with the molecular or stellar surface density maps. \( \Sigma_{\text{HI}} \) is also much more extended. The bulge structure in the galaxy center is noticeable from the stellar map. In some regions, the gas component is slightly offset from the stellar mass component. However, all surface density maps still trace a similar spiral structure at kpc scales.

\(^{11}\)We detected some high-velocity HI gas in the expected extension region, but the stream is not detected due to the limited sensitivity and velocity coverage. VIRGOHI 21 itself might be a tidal tail of NGC 4254 (Haynes et al. 2007) or a so-called dark galaxy (Minchin et al. 2005).
Figure 3.5 Deprojected atomic (21cm-based), molecular (CO-based), and stellar surface (Spitzer/IRAC-based) density maps of NGC 4254 in a linear color scale, at a same resolution of \( \sim 800\) pc. All images are shown in the same physical scale, which were based on the galaxy distance and angular size. In each panel, the cyan solid contours present the molecular gas surface density, and the dashed contour outlines the observation coverage of the STING CO \( J = 1 - 0 \) map (distorted due to the deprojection), from which \( \Sigma_{H_2} \) is derived. The filled circle denotes the density map resolution. In the middle panels, we show individual sampling locations at which the physical properties are measured and analyzed.

We present the atomic gas surface density \( \Sigma_{HI} \) as a function of the total gas surface density \( \Sigma_H = \Sigma_{HI} + \Sigma_{H_2} \) in Figure 3.6. Individual sampling points are color-coded based on their galactocentric distance in units of \( R_{25} \), with the model predictions from KMT09 shown as a solid curve and gray shadow\(^\text{12}\). The points are from two groups of data: one is from a map set which consists of our VLA HI map and the CARMA STING CO \( J = 1 - 0 \) maps (filled circles); the other is based on a map set including the HI map and the HERACLES CO \( J = 2 - 1 \) image with a larger spatial coverage (up to \( R_{25} \)) at a slightly worse resolution (open circles). As shown in Figure 3.6, the relation between \( \Sigma_{HI} \) and \( \Sigma_H \) from both data are almost identical, except that \( \Sigma_{H_2} \) at the galaxy center are slightly smaller from the VLA/HERACLES map set (measured at a worse resolution, \( \sim 1.4 \) pc versus \( \sim 0.8 \) pc).

It is clear from the trend that \( \Sigma_{HI} \) shows the “saturation” behavior predicted by the KMT09 model: \( \Sigma_{HI} \) stays near \( \sim 12M_\odot\) pc\(^{-2}\) even \( \Sigma_H \) reaches \( \sim 100 - 200M_\odot\) pc\(^{-2}\).\(^{12}\)

\(^{12}\)We assumed the mean metallicity value measured in the CO observation field of view and the model parameter \( \phi_{CNM} = 1 \sim 10 \) (see the discussion of \( \phi_{CNM} \) in KMT09).
though this finding is not surprising given the lower dynamical range of the $\Sigma_{\text{HI}}$ map in Figure 3.5, it is remarkable that most data points fell into the gray shadowed region predicted from the model, and were generally scattered near the preferred fiducial model condition (gray curve) discussed in KMT09. However, the y-axis scatter around the model curve is much larger than the observational error in $\Sigma_{\text{HI}}$. For high gas column density regions (higher $\Sigma_{\text{H}}$ values), the observed $\Sigma_{\text{HI}}$ are systematically below the fiducial model. These pixels are mostly contributed by sampling pixels located in the center of the galaxy, where the stellar surface density and the metallicity are higher.

In Figure 3.6, we also present the expected $\Sigma_{\text{HI}}$-$\Sigma_{\text{H}_2}$ relation from BR06. Following the procedure details in the Appendix, we adopted a typical gas velocity dispersion $\sigma_{\text{gas}} = 8\text{ km s}^{-1}$ and a stellar scale height $h_*$ of 700 pc (roughly the median value found in three nearby galaxies in Yim et al. 2014), and additionally assumed that stellar surface density was linearly scaled with the total gas surface density by a factor of $\sim 5.5$ (see the justification in Figure 3.7). Caldú-Primo et al. (2013) found a slightly higher mean value of $\sigma_{\text{gas}} \sim 11 - 12\text{ km s}^{-1}$ in 12 nearby spiral galaxies using stacking techniques to trace low intensity gas emissions. They also found there was no significant correlation between $\sigma_{\text{gas}}$ and $\Sigma_{\text{HI}}$ or $\Sigma_{\text{H}_2}$ (or galactocentric radius) within the optical radius of each galaxy. The BR06 model also roughly predicts the saturation of $\Sigma_{\text{HI}}$ at higher gas column densities as KMT09. In addition, it creates a $\Sigma_{\text{HI}}$ turnover feature after $\Sigma_{\text{H}}$ reaches over $\sim 80M_\odot \text{ pc}^{-2}$. We note that the relation from BR06 is empirical and requires several input parameters (e.g. $\sigma_{\text{gas}}$ and $h_*$ mentioned above), which are not directly observed in most cases.

The pressure-dependent HI-H$_2$ transition model (e.g. BR06) argued the importance of vertical gravitational potential (from gas/stars/dark matter) in disk galaxies. Understanding how the observable stellar and gas masses are spatially coupled in the disk would be important, considering their ratio will tell you the hydrostatic pressure in a unit gas mass following Equation A.2. In Figure 3.7, we show the old stellar surface density $\Sigma_*$ derived from Spitzer/IRAC images as a function of the gas surface density $\Sigma_{\text{H}}$. This turns out to
Figure 3.6 Atomic gas surface density ($\Sigma_{\text{HI}}$) as a function of the total gas surface density ($\Sigma_{\text{HI}}=\Sigma_{\text{HI}}+\Sigma_{\text{H}_2}$) in NGC 4254. Filled circles represent the sampling points measured from a map set consists of the CARMA STING CO $J=1-0$ map and the VLA HI map reduced from archival data and our new observations. Open circles show the sampling measurements from a map set including the HI map and the HERACLES CO $J=2-1$ image, with a larger spatial coverage (up to $2R_{25}$) and at a slightly worse resolution. Each data point is color-coded with the galactocentric distance of its contributing sampling point in the images. The diagonal black (dashed) line presents the gas purely atomic (half molecular). The dotted line shows the typical $3\sigma$ sensitivity level contributed by $\Sigma_{\text{H}_2}$ measurements, so any data points falling into the region between the solid diagonal and dotted lines are from sampling pixels without significant CO detections. The gray shadow (as well as the gray curve) and dashed gray curve are the model predictions from MK10 and BR09, with details and assumptions explained in are compared and discussed in Section 3.
be a nearly linear strong correlation in NGC4254 at the high resolution provided by the CARMA CO $J = 1 - 0$ map and the new VLA 21cm map (filled circles). However, the data from the HERACLES map (open circles) show a steeper slope. We did a test by reprocessing original images of the STING-based dataset to the HERACLES map resolution and further comparing the result with the HERACLES-based data points. After removing data points out of the STING coverage, we found a better agreement. This suggested that the different slopes are partly due to differences in resolution and also gas clumpiness.

We note that a vertical color gradient is evident in Figure 3.7, suggesting a lower stellar-to-gas ratio (SGR) from sampling pixels at larger radii when compared with regions with similar gas column densities but near the galaxy center. Because we use spatially resolved (or pixel-by-pixel) analysis, a lower SGR at larger radii truly reflects a change in the gas-stellar relation as a function of galactocentric distance down to the $\sim 800$ kpc resolution. Previous azimuthally-averaged analysis on spiral galaxies also showed a similar trend. However, the integrated SGR at each radius bin actually represents a gas-mass weighted average value of local SGRs in resolved regions and is likely affected by different filling factors of stellar and gas components in the galactic structure. We adopted a metallicity independent $X_{\text{CO}}$ value and re-analyzed the data. The result still suggested a systematically lower SGR at large galactocentric radii. The CO $J = 2 - 1$ to CO $J = 1 - 0$ ratio of $R_{21}$ is usually expected to be higher at small radii (Sawada et al. 2001; Druard et al. 2014). Therefore, we can rule out the possibility that the apparent lower SGR in galaxy outskirts was an artifact of the assumed constant $R_{21} = 0.7$.

In Figure 3.6, we presented the expected $\Sigma_{\text{HI}}$-$\Sigma_{\text{H}_2}$ relation from BR06 based on a constant SGR of 5.5. However, the assumption breaks down in the outskirts of NGC 4254 as seen in Figure 3.7. A lower SGR will lead to a lower molecular fraction prediction in the BR06 model.
Figure 3.7  Old stellar surface density ($\Sigma_*$) as a function of the total gas surface density ($\Sigma_{\text{HI}}+\Sigma_{\text{H}_2}$) in NGC 4254. Filled circles represent the sampling points measured from a map set consists of the CARMA CO $J = 1 - 0$ map and VLA HI 21cm map. Open circles show the sampling measurements from a map set including the VLA map and the HERACLES CO $J = 2 - 1$ map, with a larger spatial coverage (up to $R_{25}$) but at a worse resolution. Each data point is color-coded with its galactocentric distance. The old stellar surface density measurements are based on the Spitzer/IRAC 3.6/4.5$\mu$m images. For the HERACLES and STING-based data sets, we derived the median value of $\Sigma_*$ in each $\Sigma_{\text{H}}$ bin separately, shown as black filled or circles, respectively, with the error bars indicate the lower and upper quartiles. Two diagonal black lines present a linear $\Sigma_*$-$\Sigma_{\text{H}}$ relation with a stellar/gas ratio of 1 and 5.5, respectively. A ratio of 5.5 roughly passes near most binned data points from the high-resolution data set, which covers the galaxy inner $\sim 0.5R_{25}$ region. The dotted line shows the typical $3\sigma$ sensitivity level of $\Sigma_{\text{H}}$. 

98
3.3.3 Atomic Gas Surface Density in Molecular-Rich Regions

The behavior of HI saturation illustrated in Figure 3.6 is common for most spiral galaxies with CO detections. This behavior becomes less clear in irregular galaxies (including the LMC and SMC), where CO is intrinsically weak and H$_2$ mass is not dominant. Nevertheless, there is no clear evidence that $\Sigma_{\text{HI}}$ is correlated with $\Sigma_{\text{H}}$ or $\Sigma_{\text{H}_2}$ where CO is detected.

Considering the typical sensitivity of $\Sigma_{\text{HI}}$ is better than $\Sigma_{\text{H}_2}$ (except for the LMC and SMC), we can define a characteristic atomic gas surface density $\bar{\Sigma}_{\text{HI}}^M$ in molecular rich regions for each galaxy, by adopting the median of observed HI in CO-detected regions. This definition is biased because of the CO-based selection criteria. However, it is a good estimator on how much atomic gas is associated with molecular clouds in each sampling pixel. Because $\Sigma_{\text{HI}}$ shows only small variations in CO-detected regions, choosing this definition or a spatial-/mass-weighted mean of $\Sigma_{\text{HI}}$ (Leroy et al. 2013a) in the same regions does not significantly influence the resulting characteristic $\Sigma_{\text{HI}}$ values.

Because $\bar{\Sigma}_{\text{HI}}^M$ is related to the typical gas column density where the atomic-to-molecular transition happens, we examined its correlation with two galaxy global properties: metallicity and SGR. Those two quantities are important determining factors in the metallicity and pressure dependent transition models, respectively.

In Figure 3.8, we present $\bar{\Sigma}_{\text{HI}}^M$ as a function of the characteristic galaxy metallicity\footnote{For the galaxies with measurements of the galactocentric metallicity gradient, we derived a local metallicity estimation in each pixel and chose the mean value in the CO observation coverage as the characteristic value.} summarized in Table 3.1. The red points present the galaxies with CO detections. The error bars of $\bar{\Sigma}_{\text{HI}}^M$ show the 10% and 90% percentiles of the $\Sigma_{\text{HI}}$ distribution in CO-detected regions. For the galaxies without CO detections, we also derived the characteristic value of $\Sigma_{\text{HI}}$ (blue triangles) following a similar definition of $\bar{\Sigma}_{\text{HI}}^M$ but based on the $\Sigma_{\text{HI}}$ detections in the entire HI observation field (we denoted it as $\bar{\Sigma}_{\text{HI}}^A$ for clarity). Figure 3.8 suggests that many galaxies showed significant discrepancy from the preferred fiducial model from MK10 ($\phi_{\text{CNM}}=3$, see the discussion in KMT09), despite that NGC 4254 (see Figure 3.6)
showed good agreement with the model prediction without introducing a clumping factor larger than 1. However, the values of $\Sigma_{\text{HI}}^{M}$ are indeed negatively correlated with galaxy characteristic metallicity, roughly consistent with the predicted metallicity dependence of the “saturation” $\Sigma_{\text{HI}}$ values from KMT09. Also, most galaxies are still within the shadowed region constrained by the model. The galaxies without CO detections are all below the model prediction range, which agree with the model because the prediction suggested that their typical HI surface density is not high enough for UV shielding on molecule formation. This is consistent with the conclusion from Wong et al. (2013) from a smaller sample based on the STING survey, showing that the typical $\Sigma_{\text{HI}}$ in the CO detected regions are correlated with the local metallicity. As a matter of prudence, we marked the galaxies with inclination larger than $65^\circ$ or those observed compared at a physical resolution $> 1.5$ kpc using open symbols.

We note that high inclination will make the surface density inclination correction and 21cm-to-$\Sigma_{\text{HI}}$ conversion unreliable due to opacity effects and error propagations. Meanwhile, observations done at physical resolutions $> 1$ kpc are less likely to trace the real density fluctuation in atomic gas structure (e.g. Leroy et al. 2013a). Therefore, these data points are potentially biased rather than presenting the typical HI column density in molecular rich regions. We note that the observed correlation between $\Sigma_{\text{HI}}^{M}$ and the metallicity is not affected by the adopted $X_{\text{CO}}$ because it is defined based on HI 21cm measurements.

In Figure 3.9, we present the $\Sigma_{\text{HI}}^{M}$ of each galaxy as a function of SGR. The gray region in Figure 3.9 shows the prediction of $\Sigma_{\text{HI}}$ from the empirical $R_{\text{H}_2}$ pressure relation of BR06. To estimated the range of $\Sigma_{\text{HI}}$ at a fixed SGR, we varied several model input parameters to derive all possible values: $\sigma_g = 8 - 15$ km s$^{-1}$, $h_*= 300 - 100$ pc, and $\Sigma_{\text{H}_2} = 3 - 200 M_\odot$ pc$^{-2}$. The parameter coverages are based on empirical observational results for $\sigma_g$ and $h_*$, and our $\text{H}_2$ detection sensitivity for $\Sigma_{\text{H}_2}$. From this figure, we saw a clear trend with lower $\Sigma_{\text{HI}}^{M}$ for galaxies at higher SGR. For the region with CO gas detection, HI appears to be saturated at lower column density. However, the trend is evidently scattered from the empirical prediction shown as gray shadow regions.
Figure 3.8 $\Sigma_{\text{HI}}$ (see the definition in the main text) as a function of the galaxy characteristic metallicity. The gray region presents the predicted HI saturation limit from the preferred fiducial model prediction of MK10 ($\phi_{\text{CNM}}=3$). The range indicated different clumping factor of the model atomic-molecular complex at the observation resolution, and the upper and lower boundaries correspond $c=1$ and 10, respectively. Red and blue data points present the galaxies with and without CO detections, respectively. Open symbols indicate the galaxies with an observational physical resolution $> 0.75$ kpc or inclination above 65°. The y-axis error bars present the 10 and 90 percentiles of $\Sigma_{\text{HI}}$ in molecular-detected regions of individual galaxies.
Figure 3.9 $\Sigma_{\text{HI}}^M$ as a function of the galaxy stellar-to-gas ratio averaged over the molecular-detected regions. The symbols have the same definition as Figure 3.8. The gray region presents the prediction of $\Sigma_{\text{HI}}$ from the empirical $R_{\text{H}_2}$pressure relation from BR06. We vary several input parameters of the model to derive all possible $\Sigma_{\text{HI}}$ values at a specific SGR: $\sigma_g = 8 - 15 \text{km s}^{-1}$, $h_* = 300 - 700 \text{pc}$, and $\Sigma_{\text{H}_2} = 3 \sim 200 \text{M}_\odot \text{pc}^{-2}$. The parameters coverages are based on empirical observational results (for $\sigma_g$ and $h_*$), and our H$_2$ detection sensitivity (for $\Sigma_{\text{H}_2}$).
The association of \( \Sigma_{\text{HI}}^{M} \) with both metallicity and SGR raises the question of whether one of these two properties is just a mediator. To explore this possibility, we plotted SGR as a function of the metallicity in Figure 3.10. The results show barely any trend for the galaxy from 12+log(O/H)=8.4 to 9.3. To test the significance of the above associations, we calculated the Spearman rank correlation coefficient among three quantities: 12+log(O/H), SGR, and \( \Sigma_{\text{HI}}^{M} \). This approach does not depend on any prior assumptions about the nature of variable relations. As we expected, both 12+log(O/H) and SGR show a strong negative correlation with \( \Sigma_{\text{HI}} \) with a Spearman coefficient \( r_s = -0.60 \) and -0.52, respectively. The null hypothesis is rejected at \( \sim 99.7\% \) confidence level. On the other hand, the correlation between 12+log(O/H) and SGR is very weak (\( r_s = 0.16 \)). This suggested that both metallicity and the stellar-to-gas ratio is anti-correlated with \( \Sigma_{\text{HI}}^{M} \). Therefore, they require separate physical explanations and it is unlikely that one acts as the mediator for another in their correlation with \( \Sigma_{\text{HI}}^{M} \) (at least for the sample with 12+log(O/H)>8.4). We further used the partial rank correlation coefficient to quantify the significance of the relation between the metallicity and \( \Sigma_{\text{HI}}^{M} \), with the effects of SGR removed (Akritas & Siebert 1996). This partial coefficient \( r_{Z-\text{HI}, \text{SGR}} \) is defined as,

\[
r_{Z-\text{HI}, \text{SGR}} = \frac{r_{Z-\text{HI}} - r_{Z-\text{HI}}r_{\text{HI}, \text{SGR}}}{\sqrt{(1 - r_{Z-\text{HI}}^2)(1 - r_{\text{HI}, \text{SGR}}^2)}},
\]

(3.6)

where \( r_{Z-\text{HI}}, r_{Z-\text{SGR}}, \) and \( r_{\text{HI}, \text{SGR}} \) are the individual Spearman rank correlation coefficient from different variable pairs. The results showed the \( Z - \Sigma_{\text{HI}} \) correlation becomes slightly stronger while holding SGR constant, with \( r_{Z-\text{HI}, \text{SGR}} = -0.62 \).

### 3.3.4 Surface Density Correlations in Individual Galaxies

As shown in Figure 3.6 and previous observational evidence, the gas surface density is the most important factor in determining the atomic-to-molecular transition. The analysis presented in the last section also suggested that both the galaxy metallicity and SGR are
related to the gas surface density above which the ISM becomes quickly molecular dominated. However, those second order effects were presented by comparing the integrated properties among individual galaxies.

To examine the potential second-order effects mentioned above within individual galaxies, we performed a serial of statistical tests among the three surface density properties ($\Sigma_{\text{HI}}$, $\Sigma_{\text{H}_2}$, and SS), local metallicity (when the metallicity gradient is available), and galactocentric radii. We summarized the results in Table 3.5, including two rank order correlation coefficients and three partial correlation coefficients to describe the gas/density/metallicity relations in each galaxy. A few conclusions are evident from Table 3.5. First of all, the correlation between $\Sigma_{\text{H}_2}$ and $\Sigma_{\text{H}}$ is strong across all galaxies with CO detections, which is consistent with the fact that $\Sigma_{\text{H}}$ is the first-order factor determining $\Sigma_{\text{H}_2}$. Second, although we see a strong correlation between $\Sigma_*$ and $\Sigma_{\text{H}}$ in the example case of NGC 4254, this is not always the case. For example, NGC 628 and NGC 2403 indicate no correlation. We note that the local SGR variation was averaged (weighted by gas mass) when we derived the characteristic SGR for individual galaxies in the last section. However, the variation is indicated in the error bars shown in Figure 3.9 and 3.10, respectively. We listed two partial rank coefficients $r_{Z-\text{HI}}$ and $r_{\text{SGR}-\text{HI}}$, describing the correlation of $Z$ or SGR with $\Sigma_{\text{HI}}$ after the first order effects from $\Sigma_{\text{H}}$ are removed. The result indicates a strong anti-correlation between $\Sigma_{\text{HI}}$ and $Z$ or SGR, provided the same gas column density. This is consistent with the results we found among the galaxy sample, shown in Figures 3.8 and 3.9. In the last column of Table 3.5, we present the partial rank correlation $r_{\text{HI}-R,H_2}$, which describe the correlation between $\Sigma_{\text{HI}}$ and galactocentric radii $R$ when $\Sigma_{\text{H}_2}$ is restricted to similar values. Most of the galaxies show positive values of $r_{\text{HI}-R,H_2}$, indicating $\Sigma_{\text{HI}}$ in molecular rich regions is higher at larger radius when compared to regions with a similar amount of molecular gas at small radii. This result may not be easily illustrated from an azimuthally averaged $\Sigma_{\text{HI}}$ (e.g. Figure 1 of Bigiel & Blitz 2012). Because the azimuthally-averaging is area-weighted and strongly affected by the gas filling factor in each annulus, it suppress local variation.
and largely present the filling factor of galactic structures rather than local cloud properties (Rahman et al. 2011).

### 3.4 Discussion

All observational evidence points out anti-correlations of both ISM metallicity and SGR with the characteristic $\Sigma_{\text{HI}}$ saturation limits in the molecular rich regions across different galaxies and within individual galaxies.

The metallicity-$\Sigma_{\text{HI}}^M$ dependence are successfully predicted by the equilibrium models from KMT09, but it can not explain 1) the offset between the data point with the preferred fiducial models; 2) the scatter between the model and data (see Figure 3.8). If the overall offset of the observed and predicted $\Sigma_{\text{HI}}$ was interpreted as a change of clumping factor in the context of KMT09, we would expect galaxies observed at lower physical resolutions would be systematically below the model, which is not seen in Figure 3.8. This scenario also
Table 3.5. Rank Correlations of $\Sigma_{\text{HI}}$, $\Sigma_{\text{H}_2}$, $Z$, and $\Sigma_*$

<table>
<thead>
<tr>
<th>Galaxy</th>
<th>$r_{\text{H}_2-\text{H}}$</th>
<th>$r_{\text{Stellar}-\text{H}}$</th>
<th>$r_{Z-\text{HI},\text{H}}$</th>
<th>$r_{\text{SGR}-\text{HI},\text{H}}$</th>
<th>$r_{\text{HI}-r,\text{H}_2}$</th>
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<td>...</td>
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<td>...</td>
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</tr>
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</tr>
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</tr>
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</tr>
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</tr>
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<td>−0.55</td>
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</tr>
<tr>
<td>NGC4736</td>
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<td>−0.09</td>
<td>−0.18</td>
<td>−0.17</td>
</tr>
<tr>
<td>NGC5055</td>
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<td>0.74</td>
<td>−0.71</td>
<td>−0.70</td>
<td>0.61</td>
</tr>
<tr>
<td>NGC5194</td>
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<td>−0.84</td>
<td>−0.59</td>
<td>0.79</td>
</tr>
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<td>−0.84</td>
<td>−0.77</td>
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<td>...</td>
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<tr>
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<td>−0.79</td>
<td>−0.40</td>
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<tr>
<td>NGC6951</td>
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<td>0.69</td>
<td>...</td>
<td>...</td>
<td>0.52</td>
</tr>
</tbody>
</table>
contradicts the result of Leroy et al. (2013a), which suggested a very smooth HI structure below 1 kpc scale. We note that the KMT09 model does not provide any constrain on the mass fraction of the WNM, which should also be included in the observed $\Sigma_{\text{HI}}$. However, adding the WNM mass component in the model context will still lead to an offset between predictions and observations, considering we found the model is over-predicting in most cases.

The importance of stellar mass content on the atomic-to-molecular gas transition is empirically evident in BR06, from which we expected an anti-correlation between $\Sigma^M_{\text{HI}}$ and SGR. The stellar-to-gas ratios are also correlated with $\Sigma^M_{\text{HI}}$. We note that SGR is essentially a strong pressure estimator at a specific gas surface density (see Equation A.2, assuming a fixed $\sigma_g$ and $h_\star$, this correlation is intrinsically linked to the relation found between the hydrostatic pressure estimator and $R_{\text{H}_2}$ in BR06. For a specific total gas column density which $\text{H}_2$ is already become significant component, a higher SGR will lead to a higher value of the pressure estimator in Equation A.2, therefore BR06 will predict a higher $R_{\text{H}_2}$ or lower HI. This is exactly what we found in Figure 3.9 from the CO detected regions. In addition, we found this argument will hold in individual galaxies through a pixel-by-pixel analysis, indicated by a significant negative $r_{\text{SGR-HI}}$. SGR is essentially a quality describing in mid-plane hydrostatic pressure at a fixed gas surface density. Because both metallicity and SGR dependence requires independent physical explanations, a model describing galactic-scale atomic-to-molecular gas relation should synergistically include both effects, and are compatible with other existing observational results (e.g. different clumping structures for molecular and atomic gas).

However, there is no clear indication that SGR and metallicity are dependent for the sample above $12+\log(O/H)> 8.5$, illustrating their separate physical influences on determining the $\Sigma_{\text{HI}}$ threshold for atomic-to-molecular transition. In other words, both of them should be both implemented in the atomic-to-molecular transition recipes. We discuss a comparison with one such model below, which were originally presented in Bolatto et al.
(2011), based on the theoretical work of Ostriker et al. (2010).

Ostriker et al. (2010) proposed a model partitioning the ISM gas into the diffuse and dense gravitationally bound components. In this model, the predicted diffuse component surface density (presumably atomic) $\Sigma_{\text{diff}}$ also has a metallicity-dependence at a fixed total gas and stellar surface densities. The relative fraction of diffuse and dense components are self-regulated by star formation under thermal and dynamic equilibrium requirements. This could potentially also explain the dependence of $\Sigma_{\text{HI}}^M$ on the SGR and metallicity. However, OML10 did not provide the prediction of the atomic gas surface density, as both diffuse and dense components include atomic gas.

Bolatto et al. (2011) described a hybrid model for the molecular-to-atomic gas ratio prediction in the SMC. They referred the model as OML10ph, therefore we follow the notation. Based on several observables as the OML10 model inputs, they first predicted the diffuse/dense gas mass ratio $\Sigma_{\text{diff}}/\Sigma_{\text{gbc}}$ and then adopted the KMT09 model to estimate the atomic and molecular gas ratio in gravitational-bound clouds (GBC). The final predicted observed atomic and molecular gas surface density will be:

$$\Sigma_{\text{HI}} = \Sigma_{\text{diff}} + (1 - f_{\text{H}_2})\Sigma_{\text{gbc}} \quad (3.7)$$

$$\Sigma_{\text{H}_2} = f_{\text{H}_2}\Sigma_{\text{gbc}} \quad (3.8)$$

This model is physically motivated and appears to be a more realistic representation of very different different distributions of atomic and molecular clouds at various physical scales. It successfully explained the observed molecular-to-atomic gas ratio in the SMC, as well as the star formation rate. Similar predictions can be also verified using our observational results.

We summarized the implementation of the OML10 model in the Appendix A.3. In short, the model parameters from observations includes the gas and stellar surface density, as well as several empirical-based fiducial parameters. For deriving the mid-plane stellar mass volume density, we assumed a stellar scale height of $\sim 700 \, \text{pc}$ for all galaxies, despite that the
scale heights of the stellar disk could vary (e.g. Yim et al. 2014). Although some galaxies from the THINGS survey do have observational constrains on the dark matter profile, For an first-order approximation, we included the dark matter contribution in the mid-plane total pressure by adopting a spherical pseudo-ISO halo using the scaling relation from Kormendy & Freeman (2004). We assumed the dense component consists of individual atomic-to-molecular gas complex (as defined in KMT09) with a characteristic surface density of \( \sim 100 \, M_\odot \, pc^{-2} \), the typical values in the Milky Way and local group, so the observed \( \Sigma_{H_2} \) defines the cloud projected area in individual sampling points.

Using the observational input (\( \Sigma_* \) and \( \Sigma_{H=\Sigma_{HI}+\Sigma_{H_2}} \)) and the above assumption, we numerically solved the \( \Sigma_{diff} \) and \( \Sigma_{gbc} \) using the OML10 models for each pixel in our dataset, and then derive \( \Sigma_{H_2} \) and \( \Sigma_{HI} \) using Equations 3.7 and 3.8. We compared the model and observations by evaluate the predicted and integrated HI mass and observed \( \Sigma_{HI} \) in individual galaxies. The ratio of individual galaxies as a function of the metallicity is presented in Figure 3.11. We also present this ratio as a function of SGR in Figure 3.12. The result suggests that the model reasonably predict the HI mass (or HI mass fractions) in all galaxies, and the ratio is close to 1 by 0.3 dex for most galaxies. In addition, the model normalization removed all metallicity or SGR dependence.

### 3.5 Summary and Conclusions

The availability of both HI 21cm and CO maps at high angular resolutions from the STING and HERACLES surveys allowed us to perform a systematical study of the molecular gas and atomic gas transition in a large sample of galaxy with wide variety.

1. We presented the new HI 21cm observation and ancillary data for the CARMA STING survey.

2. Following the pilot study from Wong et al. (2013), we found most galaxies in our samples exhibited the appeared HI saturation as the prediction from KMT09. However,
Figure 3.11 Ratio of the predicted and observed atomic gas surface density versus the galaxy metallicity. The prediction is based on the OML10ph model presented in Bolatto et al. (2011).

the preferred fiducial model from KMT09 apparently over-predicts the gas column density threshold for the atomic-to-molecular transition threshold in a significant number of galaxies.

3. We measured an estimator of the HI saturation threshold $\bar{\Sigma}_{\text{HI}}$ for each galaxy. This value is defined as the statistical median value of $\Sigma_{\text{HI}}$ in the regions detected with CO emission. We found this value is strongly correlated with both the galaxy characteristic metallicity and stellar-to-gas ratio derived in the same region.

4. The partial correlation analysis indicates that both the metallicity and stellar-to-gas ratio are also important second-order factors affecting the gas phase transition within each galaxy. Because the metallicity and stellar-to-gas ratio are two quantities not intrinsically related in the galaxy sample with $12+\log(O/H) > 8.4$, their separate correlation requires different physical explanations.
Figure 3.12  Ratio of the predicted and observed atomic gas surface density versus the galaxy stellar-to-gas ratio in the regions with CO observations. The prediction is based on the OML10ph model presented in Bolatto et al. (2011).

5. We examine the model from Ostriker et al. (2010) and Bolatto et al. (2011), which is physically-motivated and incorporated both metallicity and stellar mass as environment factors determine the atomic-to-molecular gas transition. The model successfully predict the observed dependence of the ISM metallicity and stellar mass.
Chapter 4

Summary and Future Work

Recent theoretical investigations suggested the formation of molecular hydrogen (H$_2$) might not be vital to star formation, rather, it is a consequence of increasing density, UV shielding, and cooling, which also happen to be the same prerequisites of star formation (see a review discussion in Mac Low 2013). One implication of this argument is that molecular gas and star formation could become decoupled at some extreme conditions (e.g. high-redshift and low-metallicity environments) because the H$_2$ formation time scale could be longer than the star formation time scale (Krumholz 2012). However, despite the limited direct physical connect between H$_2$ and star formation, it is still critical to understand how the conversion from atomic to molecular gas is related to ISM physical/chemical properties and global galactic properties, e.g., metallicity.

Using correction interpretations, observing atomic and molecular gas actually provides a powerful tool to study gas density structures and UV radiation field, both of which can help us identify how dense structures and stars formed in turbulent galactic ISM environments. This is demonstrated in this dissertation. Our UV H$_2$ and HI absorption line analysis suggests a significant amount of diffuse H$_2$ exists in the Magellanic Clouds and a large fraction of HI gas might reside in the gas phase similar as the Warm Neutral Medium. The radio data from nearby galaxies CO and HI surveys indicate that the HI surface density in molecular-rich regions is correlated with both ISM metallicity and stellar-to-gas ratio. The results are consistent with the model presented in Ostriker et al. (2010) and Bolatto et al. (2011), in which the relative fraction of diffuse and dense ISM components are self-regulated by star formation under thermal and dynamic equilibrium requirements.
For the UV absorption line study, we plan to release a comprehensive multi-wavelength database and atlas, not only for HI and H$_2$ absorbers but also on their large-scale environments. Many non-hydrogen spectral features have not been fully explored in the FUSE UV data of the Magellanic Clouds sample. It becomes easy to expand the current work to study those features now because H$_2$ and HI absorptions can be modeled using the existing results. In the STING survey, we will generate a public dataset for HI maps of 21 nearby galaxies. The ancillary high-resolution radio continuum images of 5 galaxies from recent VLA HI observation could be used to study star formation activity.

With the advice and help from my supervisor and colleagues, I have developed new techniques of UV spectroscopic analysis and radio interferometer imaging for large-volume data in the dissertation work. The experience and codebase will definitely benefit future research projects using similar methods.
Appendix A

Empirical/Theoretical Models for the Atomic-to-Molecular Gas Transition

A.1 Empirical Relation Between $R_{H_2}$ and the Hydrostatic Pressure

Observational results on the spatially resolved CO and HI relation across significant samples (e.g. Wong & Blitz 2002; Blitz & Rosolowsky 2004, 2006) indicated that the atomic-to-molecular ratio, defined as

$$R_{H_2} \equiv \frac{\Sigma_{H_2}}{\Sigma_{HI}},$$

in spiral galaxies could be attributed by the hydrostatic pressure variation in the disks, which is largely due to the stellar surface density and gas surface density changes (although the stellar surface density is usually dominated). The is based on the theoretical argument from Elmegreen (1993), which considering $R_{H_2}$ is not sensitive to the radiation field and metallicity at a given pressure level. Blitz & Rosolowsky (2006) derived an empirical relation of $R_{H_2}$ as a function of $P_{\text{ext}}$:

$$R_{H_2} = \left[ \frac{P_{\text{ext}}/k}{4.3 \times 10^4} \right]^{0.92},$$

(A.1)

based on those observational evidence that those two values are strongly correlated in various galactic environments. Here $P_{\text{ext}}$ is the interstellar gas pressure and expressed as,

$$\frac{P_{\text{ext}}}{k} = 272 \text{ cm}^{-3} \text{ K} \left( \frac{\Sigma_g}{M_\odot \text{ pc}^{-2}} \right) \left( \frac{\Sigma_*}{M_\odot \text{ pc}^{-2}} \right)^{0.5}$$

(A.2)

$$\times \left( \frac{v_g}{\text{ km s}^{-1}} \right) \left( \frac{h_*}{\text{ pc}} \right)^{-0.5}. \quad \text{(A.3)}$$
$v_g$ is the gas dispersion in km s$^{-1}$ (assumed to be 8 km s$^{-1}$ in Blitz & Rosolowsky 2006), $\Sigma_*$ is the stellar surface density in $M_\odot$ pc$^{-2}$, and $h_*$ is the stellar disk scale height. One observational-based argument from this empirical relation is that because $P_{\text{ext}}$ is determined by the gas velocity dispersion and stellar scale height and is not strongly varied across different galaxies, the stellar surface density where $R_{\text{HI}}$ should be a constant for different galaxies and not be a strong function of galactocentric radius (as shown in Figure 1 of Blitz & Rosolowsky 2004).

This prediction was based on several observational empirical relations which require explanation by themselves. Also, the approximation in this expression requires that the stellar surface density is dominant compared with the neutral gas surface density. The hydrostatic pressure and $R_{\text{H}_2}$ relation supported an earlier model by Elmegreen (1993) in which the atomic-to-molecular transition is mainly governed by the interstellar pressure determines and secondarily affected by the radiation field. To ensure that both axes are from independent observational measurements, we choose to present the atomic and molecular gas relation in the $\Sigma_{\text{H}_2}$ vs. $\Sigma_{\text{HI}}$ domain, rather than the commonly adopted molecular fractions or molecular-to-atomic gas ratio, defined as:

$$R_{\text{H}_2} = \frac{2N_{\text{H}_2}}{N_{\text{HI}}} \quad \text{(A.4)}$$

and

$$f_{\text{H}_2} = \frac{2N_{\text{H}_2}}{2N_{\text{H}_2} + N_{\text{HI}}} \quad \text{(A.5)}$$

### A.2 Cloud-scale H$_2$ Formation/Dissociation and Pressure Equilibrium Models

The galactic scale HI-H$_2$ transition model proposed by Krumholz et al. (2008, 2009, hereafter KMT08/09) (KMT09) and McKee & Krumholz (2010, hereafter MK10), is based on the
chemical equilibrium of $H_2$ formation and dissociation, including radiative transfer of Lyman-Werner (LW) photons in a pressure-equilibrium mute-phase ISM complex structure. Their models were essentially based on semi-analytic chemical equilibrium models including the radiative transfer of UV photons, and predict: 1) the galaxy metallicity is the dominating factor on the atomic and molecular gas relation; 2) that there is an upper limit of HI surface density that can be reached for a cloud complex. We review some basic concepts and solutions from the model, and refer readers to original works for more details.

- **Radiative Transfer and $H_2$ Formation/Dissociation**

  The radiative transfer in a HI/$H_2$ cloud complex can be written as,

  \[
  \frac{dI^*_\nu}{ds} = -n_H \left( \sigma_{d,\nu} + \frac{1}{2} f_{H_2} \sigma_{H_2,\nu} \right) I^*_\nu, \tag{A.6}
  \]

  in which $\sigma_{d,\nu}$ and $\sigma_{H_2,\nu}$ are the dust and $H_2$ cross sections per H nucleus respectively, at the frequency $\nu$. $n_H$ is the hydrogen nuclei number density of the HI/$H_2$ mixture, with a molecular fraction of $f_{H_2}$. $I^*_\nu = I_\nu / (h\nu)$ is the photon number intensity. On the other hand, if we assume the $H_2$ formation and dissociation are in equilibrium, the total molecular fraction of the gas will be determined by the balance,

  \[
  f_{HI} n_H^2 R = \frac{1}{2} n_H f_{H_2} \int d\Omega \int_{\nu_1}^{\nu_2} d\nu I^*_\nu \sigma_{H_2,\nu} f_{\text{diss},\nu}, \tag{A.7}
  \]

  where $R$ is the $H_2$ formation rate coefficient on dust grain surfaces, and $f_{\text{diss},\nu}$ is the fraction of absorbed UV photons that yield dissociation of $H_2$ rather than decay back to a bound state ($\sim 0.11$)\(^1\). The integration covers the wavelength of the LW photons related to photodissociation, from 912 Å to 1108 Å.

\(^1\) $f_{\text{diss},\nu}$ and $\sigma_{H_2,\nu}$ actually varied when integrated over frequency and over positions in a PDR (Draine & Bertoldi 1996). The $H_2$ self-shielding simplification here is less realistic from the numerical results of (Draine & Bertoldi 1996) and its analytical approximation Sternberg et al. (2014, see also). This is one reason for the sharp atomic-to-molecular transition seen in their prediction. And
1D and Spherical Cloud Complex Solution

After substituting Equation (A.7) into (A.6) and eliminating the frequency dependence, KMT09 demonstrated that there will be a characteristic HI column density required to shield the H$_2$ gas in a 1D plane-parallel condition. Assuming the atomic and molecular gas transition zone is infinitely sharp, the cloud dust optical depth in the UV at that characteristic column density of HI will be approximately given by,

$$\tau_{ch} = \ln (1 + \chi),$$  \hspace{1cm} (A.8)

in which $\chi$ is a dimensionless parameter defined as,

$$\chi \equiv \frac{f_{diss} \sigma_d c E_0^*}{n_H R}.$$  \hspace{1cm} (A.9)

Here $E_0^*$ is the photon number density outside of the cloud complex. Physically, $\chi/f_{HI}$ is approximately the ratio of the number of Lyman-Werner photons absorbed by dust to the number absorbed by H$_2$. Therefore, there will be an upper limit to the HI surface gas density for a cloud complex that can be reached,

$$\Sigma_{HI, ch} = \frac{\mu_H}{\sigma_d} \ln (1 + \chi),$$  \hspace{1cm} (A.10)

in which $\mu_H$ is the mass of H nucleus. The major work of KMT09 and MK10 is actually giving a more general analytical solution of the atomic fraction $f_{HI}$ for a spherical atomic/molecular cloud complex placed in an isotropic radiation field. They suggested that the value of $f_{HI}$ in a spherical cloud complex was a function of the cloud averaged dust optical depth $\tau_c$ (or cloud averaged gas surface density $\Sigma_H$), which can be presented as,

$$f_{HI} \simeq \left(\frac{3}{4}\right) \frac{s}{1 + 0.25s}.$$  \hspace{1cm} (A.11)
\[ s = \frac{\ln(1 + 0.6\chi + 0.01\chi^2)}{0.6\tau_c}, \quad (A.12) \]

\[ \tau_c \equiv \frac{3}{4} \left( \frac{\Sigma_H\sigma_d}{\mu_H} \right), \quad (A.13) \]

In the Galaxy, \( \sigma_d \) is \( \sim 10^{-21} \text{ cm}^2 \) and the \( \text{H}_2 \) formation rate coefficient is \( \mathcal{R} \simeq 10^{-16.5} \text{ cm}^3 \text{ s}^{-1} \) (Draine & Bertoldi 1996).

- **Approximation based on the Muti-phase Pressure-Equilibrium ISM Arguments**

The solution for the above cloud complex model requires the values of \( \chi \) and the dust properties. To constrain the value of \( \chi \), which is difficult to evaluate from observations, KMT09 introduced a first-order approximation of \( \chi \) from the cold neutral medium and warm neutral medium (CNM/WNM) pressure equilibrium model of Wolfire et al. (2003),

\[ \chi = 3.1 \left[ \frac{\sigma_{d,-21}}{\mathcal{R}^{-16.5}(\phi_{\text{CNM}}/3)} \right] \left( 1 + 3.1Z'^{0.365}/4.1 \right), \quad (A.14) \]

in which \( \phi_{\text{CNM}} \) is the density ratio between the CNM volume density \( n_H \) in the complex and the minimal possible volume density determined by the two-phase equilibrium \( (\phi_{\text{CNM}} = n_{\text{CNM}}/n_{\text{min}}) \). The metallicity relative to solar is proportional to the O/H ratio in KMT09:

\[ \log Z' = [\log(O/H) + 12] - 8.76 \quad (A.15) \]

Plugging Equation A.14 into either 1D or spherical cloud solution, one finds that the atomic gas fraction is a simple function of the gas surface density \( \Sigma_H \), the metallicity related to the solar value \( Z' \), and \( \phi_{\text{CNM}} \) for an additional adjustment of \( \chi \) beyond the effects contributed from the metallicity. They adopted a fiducial value of \( \phi_{\text{CNM}} = 3 \) (1 \( \sim \) 10).

Krumholz (2013) further expand the framework of KMT09/MK10 to HI-dominated
regions to have a "floor" value of $f_{\text{H}_2}$. Basically, $\chi$ will not follow the prescription of Wolfire et al. 2003 and is determined by the hydrostatic balance of CNM (giving $n_{\text{cmn}}$) and a SFR-dependent radiation field strength. The full numerical solutions can be derived from Eq.8-15 of Krumholz (2013), but an approximated analytical solution at the $\text{H}_2$-poor limit can be described below.

In a $\text{H}_2$-poor condition, the gas deletion time will be,

$$t_{\text{dep,hd}} \equiv \frac{\Sigma}{\Sigma_s} \approx \frac{3.1 \text{ Gyr}}{\Sigma_0^{1/4}} + \frac{100 \text{ Gyr}}{(f_c/5) Z' \rho_{\text{sd},-2} \Sigma_0}$$

(A.16)

for the case in which the stellar and dark matter gravity is dominated, where $\rho_{\text{sd},-2} = \rho_{\text{sd}}/0.01\odot \text{ pc}^{-3}$ and $\Sigma_0 = \Sigma_{\text{comp,obs}}/1\odot \text{ pc}^{-2}$. If the pressure contribution from gas is dominant, then we will have

$$t_{\text{dep,hd,\text{gas}}} \equiv \frac{\Sigma}{\Sigma_s} \approx \frac{3.1 \text{ Gyr}}{\Sigma_0^{1/4}} + \frac{360 \text{ Gyr}}{(f_c/5) Z' \Sigma_0^{1/2}}.$$ 

(A.17)

However, the star formation law will give,

$$\dot{\Sigma}_s = f_{\text{H}_2} \epsilon_{\text{ff}} \frac{\Sigma}{t_{\text{ff}}},$$

(A.18)

where $\epsilon_{\text{ff}} \approx 0.01$ and $t_{\text{ff}}$ is the free-fall time of the molecular gas with a prescription of,

$$t_{\text{ff}} \approx \frac{\pi^{1/4}}{\sqrt{8}} \frac{\sigma_g}{G(\Sigma_{\text{GMC}}^3/\Sigma)^{1/4}} \approx 31 (f_c \Sigma_0)^{-1/4} \text{ Myr.}$$

(A.19)

So we will have,

$$f_{\text{H}_2} = \frac{t_{\text{ff}} \dot{\Sigma}_s}{\epsilon_{\text{ff}} \Sigma} = \frac{t_{\text{ff}}}{\epsilon_{\text{ff}} t_{\text{dep}}}$$

(A.20)

Note: it looks like some assumptions will still not work for diffuse medium (see Appendix B of Krumholz 2013). In diffuse medium, $G_0$ might be not nicely correlated
with local star formation rate because photons could come from somewhere far away due to low optical depths. This will create a larger $G_0$, or a value of $\chi$ compared that of Krumholz (2013), and leads to a smaller $f_{H_2}$ compared with the prediction (which I already see from UV data).

- **Predicted $\Sigma_{HI}$ and $\Sigma_{H_2}$ Relations**

  Fiducial values: $a = 0.2$, $\phi_{mol} = 10$, $\phi_{CNM} = 3$ or $(1 \sim 10)$

Both 1D plane-parallel and spherical clouds give predictions of the relation between $\Sigma_{HI}$ and $\Sigma_{H_2}$ as a function of the solar-normalized metallicity $Z'$ and $\phi_{CNM}$. The behavior of different models at three $Z'$ values (color coded) are tested and shown in Figure A.1.

The solid lines and dotted lines are from the 1D solutions with $\phi_{CNM} = 3$ and 8, respectively. The spherical cloud solutions with $\phi_{CNM} = 3$ are displayed as dashed lines. A typical value of $\phi_{CNM} = 6 \sim 10$ was found in the recent work of Lee et al. (2012), which treat $\phi_{CNM}$ as a free parameter that they constrain with sub-pc resolution observations in the Perseus cloud. The left and right panels show the same predicted relation but plotted in different ways: Left:, $\Sigma_{HI}$ vs. $\Sigma_{H_2} + \Sigma_{HI}$; right, $\Sigma_{H_2}$ vs. $\Sigma_{HI}$.

From the comparison of KMT09 predictions under different conditions, we obtain the following general conclusions:

- In the spherical solutions, after most of the UV photons have been absorbed by dust or $H_2$, $\Sigma_{HI}$ becomes a weak function of $\Sigma_H$ on a log-log scale and molecular gas becomes dominant.

- $\Sigma_{HI}$-$\Sigma_H$ or $\Sigma_{H_2}$-$\Sigma_{HI}$ relations predicted from spherical cloud solutions are not clearly distinguishable from the 1D solution with the same $\phi_{CNM}$ and $Z'$ values. The difference
Figure A.1 KMT09/MK10 predictions of the atomic and molecular gas relation at metallicities of $0.2 \times$ (red), $1.0 \times$ (green), and $5.0 \times$ (blue) solar value (generally representing the SMC, typical Galactic conditions, and metal-rich ISM environment, respectively). **Left Panel:** $\Sigma_{\text{HI}}$ vs. $\Sigma_{\text{H}_2} + \Sigma_{\text{HI}}$; **right:** $\Sigma_{\text{H}_2}$ vs. $\Sigma_{\text{HI}}$. The solid and dotted lines are from the spherical cloud complex models with $\phi_{\text{CNM}}=3$ and $\phi_{\text{CNM}}=8$, respectively. The dashed line is from the 1D model with $\phi_{\text{CNM}}=3$, showing a clear $\Sigma_{\text{HI}}$ saturation limit. The gray shadow highlights the region below the assumed $\Sigma_{\text{HI}}$ and $\Sigma_{\text{H}_2}$ detection limits of $1\sigma = 1M_\odot\text{ pc}^{-2}$, which are typical from high resolution extragalactic CO $J = 1 - 0$ (using a typical galactic $X_{\text{CO}}$ factor) and HI observations. The diagonal line in the right panel shows a molecular or atomic fraction of 50%.
is small compared with the sensitivity level of most high-resolution extragalactic HI 21cm surveys (Walter et al. 2008).

- A higher $\phi_{\text{CNM}}$ or higher $Z'$ have similar effects on the $\Sigma_{\text{HI}}-\Sigma_{\text{H}}$ or $\Sigma_{\text{H}_2}-\Sigma_{\text{HI}}$ relation. In other words, a higher $\phi_{\text{CNM}}$ or $Z'$ is not distinguishable from the model predictions. Although the metallicity is observable, the variation of $\phi_{\text{CNM}}$ is poorly understood. The results from Bolatto et al. (2011) suggest a value of $\phi_{\text{CNM}}=3$ generally agrees with the SMC observations. However, Lee et al. (2012) found $\phi_{\text{CNM}} \sim 6 - 10$ in the Perseus Molecular Clouds at sub-pc scales. So it is still unclear whether $\phi_{\text{CNM}}$ can be assumed universal, varies significantly at different metallicity systems or changes based on spatial scales.

### A.3 Galactic-scale Thermal and Dynamical Equilibrium Model

Ostriker et al. (2010) proposed a galactic-scale thermal and dynamical equilibrium model for determining star formation rate in disk galaxies. In this model, all neutral gas is partitioned into a diffuse component and a dense gravitationally bound component. The properties of diffuse component (e.g. density, mass fraction in total gas) is constrained by thermal (e.g. UV heating from star formation and line cooling) and dynamic (e.g. gravitational potential provided by stars, gas, and dark matter) equilibrium. It explains the empirical near linear relation between molecular-to-atomic gas ratio $R_{\text{H}_2}$ and the hydrostatic mid-plane pressure in disk galaxies from Blitz & Rosolowsky (2006).

In the model of Ostriker et al. (2010) (see also Bolatto et al. 2011), the surface density of the diffuse and gravitational components can be determined by solved their Equations 10
Here $x$ is the fraction of gas in the diffuse phase. $\Sigma_{\text{gas}}$, $\Sigma_{\text{diff}}$, and $\Sigma_{\text{gbc}}$ are the large-scale averaged surface densities of total, diffuse, and gravitationally-bound gas, respectively (in units of $M_\odot \text{pc}^{-2}$). $\rho_{sd}$ is the midplane volume density of stars and dark matter (in units of $M_\odot \text{pc}^{-3}$). The equations include several normalization parameters and fiducial values: $\Sigma_0 \approx 10 M_\odot \text{pc}^{-2}$, $\Sigma_{\text{SFR},0} \approx 2.5 \times 10^{-9} M_\odot \text{pc}^{-2}\text{yr}^{-1}$, $\alpha \approx 5$, $f_w \approx 0.5$, and $\tau_{\text{dep}} \approx 2 \times 10^9 \text{yr}$. They are respectively: the gas surface density and the star formation rate near the solar neighborhood, the ratio of total to thermal pressure, the diffuse gas mass fraction in the warm phase, and the gas depletion time in the gravitationally-bound component (empirically from spiral galaxies). The physical meaning of $y$ is the normalized thermal $P_{\text{th}}$ pressure, $y \equiv (P_{\text{th}}/k)/3000 \text{K cm}^{-3}$ where $k$ is Boltzmann’s constant. $Z_d$ and $Z_g$ are the dust-to-gas ratio and the gas phase metallicity normalized to the solar neighborhood values, respectively. We expect $Z_d \approx Z_g$. We note that Equation A.24 is from the modification of Bolatto et al. (2011), which is to take account of different dust attenuation per gas column at different metallicity.

We listed their main formal The models emphasized a different and maybe more realistic large-scale ISM structure, rather than presuming that most ISM mass is constrained in the atomic-molecular cloud complexes like KMT09 and ignoring the WNM mass contribution. The predicted diffuse component surface density also has a metallicity-dependence at a fixed
total gas and stellar surface densities, which could potentially also explain the metallicity-dependent atomic gas saturation seen in Wong et al. (2013).
Appendix B

Weight Adjustment for Calibrated HI Data in CASA

The theoretical visibility noise for each visibility record can be estimated as,

$$\sigma_{i,j}^2 = \frac{(Jy/K)^2 \left[T_{sys,i}T_{sys,j}\right]}{2\Delta t \Delta \nu}$$ \hspace{1cm} (B.1)

where Jy/K is the antenna efficiency, $T_{sys}$ is the system temperature, $\Delta t$ is the integration time, $\Delta \nu$ is the bandwidth or channel width, and $(i,j)$ denote two different antennas. A natural weighting during imaging will assign the data weights as,

$$w_{i,j} = \frac{1}{\sigma_{i,j}^2}$$ \hspace{1cm} (B.2)

In practical, the noise or weight estimation can be off by a scaling factor in the calibrated visibilities due to the lack of full information required for the calculation in Equation B.1 from raw visibilities data. Although imaging individual observations is not affected by the absolute scaling of $\sigma_{i,j}^2$, additional scaling of the weights may be required to image data from multiple observations or different instruments. In our case, this problem appears to be most severe when imaging a galaxy having data obtained during the VLA-EVLA transition phase, or observed with both the old and new VLA backends.

To solve this problem, we performed several procedures to adjust the weight scaling before concatenating visibilities from different observations: First we regrid the calibrated visibilities to the desired velocity frame (barycentric for HI observations) for imaging, with the channelization set by the largest channel width present in the observations for that
galaxy, and a velocity range spanning all observations. This step also reduces the computing resource required for imaging considering the clean task works interactively in both the image and visibility domain for model component searching and subtraction, respectively. Then we derive a weight scaling factor by comparing the existing noise estimate in the CASA MS with the statistical visibility noise derived by the CASA task statwt using the line-free channels. Although the noise estimation from statwt is not robust for individual visibility records\(^1\), the ratio between the statistical median value of \(\sigma_{i,j,\text{stat}}\) and the present noise estimate \(\sigma_{i,j,\text{cal}}\) in the calibrated visibility data will still be a robust estimator of the scaling factor required for combining multiple observations. We note that this calculation must be done before continuum subtraction.

For the CO \(J = 1 - 0\) data from CARMA, we verified that the visibility weights were properly calculated and preserved when MIRIAD exported calibrated visibility into the UVFITS format which we later imported into CASA for imaging. Although during pre-imaging spectral regridding, the channel-wise weights were still not properly rescaled in the statistically correct sense in current CASA tasks, it doesn’t affect the CO \(J = 1 - 0\) imaging because all data were observed in the same original spectral resolution.

\(^{1}\)Ideally, the noise for individual records can be estimated over a subset data nearby in the time frame of which the systematic time-dependent noise variation can be ignored. Such feature is not implemented in statwt as for CASA v4.2.
Appendix C

21 cm Line Brightness with a Continuum Background

Two basic assumptions for using Equation 3.3 to derive HI column density $N_{\text{HI}}$ are that the optical depth is small and the HI spin temperature $T_s$ is constant along the line of sight. $N_{\text{HI}}$ will be underestimated if either assumption breaks down. The issue is more likely to occur for high inclination galaxies, where the sight line may pass through several atomic clouds with different temperatures. On the other hand, the presence of strong continuum background source will also significantly decrease the brightness of HI line emission. A simple linear conversion using Equation 3.3 will underestimate $N_{\text{HI}}$ or totally fail in the case of the line being seen in absorption. The problem is simply demonstrated below:

For an isothermal HI cloud with a 21 cm line optical depth $\tau \ll 1$, the line brightness temperature will be

$$T_b = T_s \tau \propto N_{\text{HI}}, \quad (C.1)$$

in which $T_s$ is the spin temperature. The existence of an extended continuum background source will change the line brightness temperature to,

$$T_b^* = (T_s - T_c) \tau, \quad (C.2)$$

where $T_c$ is the continuum source brightness temperature. So the presence of the continuum source will lead to an underestimate of $N_{\text{HI}}$ by a factor of $F = 1 - T_c/T_s$ using Equation 3.3. A much higher $T_c$ will create absorption features. Several STING galaxies indeed showed such features. One example (NGC 4536) is shown in Figure C.1. An HI absorption feature is evident at the galaxy center against a strong continuum source. A large telescope beam...
size can depress the absorption features because of beam smoothing or even make it undetectable. However, using Equation 3.3 will still lead to underestimation. Considering the typical dynamic range of our HI maps is $\sim 30$, we would like to have a value of $F \gtrsim 0.9$ to avoid any significant ($>3\sigma$) underestimation, which requires $T_c/T_s \lesssim 0.1$. Assuming a typical spin temperature of 40$\sim$400 K (Dickey et al. 2009), a continuum brightness temperature $T_c > 40$ K may create large relative uncertainties in deriving $N_{\text{HI}}$. 
Figure C.1 *Top panel*: Integrated HI intensity map of NGC 4536 (color scale and red contours). The red contour levels are 8, 14 and 20σ. The blue solid contours show the 1.5 GHz radio continuum map at levels of 100, 200, 250, and 300 K in brightness temperature. The dashed blue contour presents the effective field of view of CARMA CO $J = 1 − 0$ observations. *Bottom panel*: Position-velocity diagram along the major axis of NGC 4536 (the southeast to northwest direction). The velocity is in the barycentric velocity frame. The blue contours show the absorption, at levels of -3 and -8σ. The red contours are the emission, at levels of 4, 16, and 32σ.
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133


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