Abstract

To build bottom-up models of galaxies and their evolution, it is necessary to understand the many processes that take place in the interstellar medium (ISM). This thesis addresses properties of two ISM processes: how dust chemistry changes with metal enrichment and how spiral structure affects ISM dynamics.

Observational studies of dust emission from galaxies with sub-solar metallicities have shown that below a critical metallicity, the abundance of dust decreases faster than the abundance of metals. This is interpreted as evidence of reduced dust formation rates at low metallicities. These observations depend on a scale factor that has been calibrated in the Milky Way and could plausibly depend on metallicity. To provide an independent test for these results, I use ultraviolet absorption spectroscopy to measure gas and dust abundances in the Large and Small Magellanic Clouds (LMC and SMC). The LMC and SMC are satellites of the Milky Way and have metallicities $\frac{1}{2}$ and $\frac{1}{5}$ of solar, respectively. The dust abundances I measure for the LMC and SMC using absorption spectroscopy are consistent with dust abundances measured using dust emission, validating the use of the Milky Way scale factor at lower metallicities.
There are two main theories of spiral structure: stationary density wave theory and transient spiral structure theory. These theories predict qualitatively different ISM dynamics and, through those dynamics, different effects on star formation. There is not yet a consensus on which kind of spiral structure is present in the Milky Way. A useful observable that has not been available in the Milky Way is the spatially resolved velocity field of its ISM. I have developed two techniques for deriving the line-of-sight velocity of interstellar matter as a function of distance. Using these techniques, I have produced the first spatially resolved maps of ISM motions in the Milky Way. By comparing these maps with simulations of galaxies with different kinds of spiral structure, I show that the Milky Way is more likely to have transient, rather than density wave, spiral structure.
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Chapter 1

Introduction

Galaxies build up their in situ stellar populations and metal contents through the cycle of star formation and destruction. The interstellar medium (ISM) is the location of key steps in this cycle. It is what the stellar populations form from and what dying stars enrich with dust and metals. This thesis focuses on understanding how ISM conditions influence different stages of this cycle and vice versa.

The first aspect of this cycle I have studied is the effect of metal enrichment on ISM chemistry. This work focuses on dust abundances and composition in galaxies with sub-solar metallicities. The second aspect I have studied is the initiation of star formation. This work focuses on the effect of galactic structure on gas dynamics. Structure-induced gas flows are a potential mechanism for the formation of the sites of star formation, dense molecular clouds. The rest of this chapter provides introductions to aspects of ISM chemistry at sub-solar metallicity (Section 1.1) and spiral structure and its possible effects on gas dynamics (Section 1.2).
1.1 ISM chemistry at sub-solar metallicity

1.1.1 Interstellar dust

Interstellar dust consists of small, sub-micron size solid particles. It has generally been hypothesized that interstellar dust grains can be split by composition into two categories: silicate and carbonaceous grains (e.g. Draine and Li 2007). Silicates consist mostly of oxygen, silicon, magnesium, and iron and can be informally described as fine sand. Carbonaceous grains consist mostly of carbon and can be informally described as fine soot. Other categories of dust grains have been proposed, such as a pure iron dust grain category (Zhukovska, Henning, and Dobbs, 2018) or a carbon-coated silicate dust grain category (e.g. Jones et al. 2013).

Dust is a small fraction of the interstellar medium by mass but is extremely important from both astrophysical and observational perspectives (Galliano, Galametz, and Jones, 2018). It scatters or absorbs and re-radiates much of the light emitted by stars and others sources. It is an important source of heating and cooling for interstellar gas. Its surfaces are the site of the most efficient formation pathways of many molecules, including H₂ (Hollenbach and Salpeter, 1971; van Dishoeck and Blake, 1998). The details of how these processes happen depend on the properties of dust: its abundance, size distribution, and composition distribution.

Our understanding of how dust forms, evolves, and is destroyed is only partially complete. The best-understood ways of forming dust require high temperatures and densities. These conditions can be found in the ejecta of
some types of supernovae (Dwek and Werner, 1981; Dwek and Arendt, 2015) and in the outer layers of evolved stars, particularly asymptotic giant branch (AGB) stars (Gehrz and Woolf, 1971). Dust grains in dense, cold environments become coated in ices and stick together (Dominik and Tielens, 1997; Gibb et al., 2004).

Dust can be destroyed or broken up by being shattered in collisions with other dust grains, sublimated through sputtering by gas particles and heating by photon absorption, and exploded by internal electrostatic forces as a result of charging by electrons and energetic photons (Tielens et al., 1994; Jones et al., 1994; Fruchter, Krolik, and Rhoads, 2001). Shocks driven by supernovae are thought, and tentatively observed, to be particularly efficient sources of gas particles capable of sublimating dust through sputtering (Barlow, 1978; Andersen et al., 2011; Lakićević et al., 2015). Explosive charging requires large concentrations of X-ray photons and hence is likely to be irrelevant except near highly energetic sources.

Attempts to calculate the amount of dust that should be present in a location using the dust formation and destruction mechanisms described above give predictions that are up to an order of magnitude lower than what is observed (Zhukovska, Henning, and Dobbs, 2018). The currently most popular proposed solution for this imbalance is that dust must also form or grow outside of hot, dense environments by accreting material from the gas phase. Calculations that incorporate this additional source of dust mass can produce the required extra dust (Asano et al., 2013; Zhukovska, Henning, and Dobbs, 2018). However, the parameters of the accretion model are not known.
a priori and have to be adjusted to produce the correct result.

The abundance and properties of dust depend on elemental abundances in its environment. The simplest possible dependence is one in which the amount of dust of a given type linearly scales with the abundance of that type’s elemental constituents. The fraction of available heavy elements that is in the form of dust is called the dust-to-metals ratio (DMR). A linear scaling of dust abundance with metallicity would mean that the DMR does not depend on metallicity.

Observational studies of the DMR in nearby galaxies have shown that it is approximately constant at metallicities greater than $\frac{1}{5}$ of the solar metallicity ($Z_\odot$). Below this threshold metallicity, the DMR declines as metallicity decreases (Rémy-Ruyer et al., 2014; De Vis et al., 2017). One proposed explanation for this scaling is that dust growth through accretion is less efficient at lower metallicity (Asano et al., 2013; Zhukovska, Henning, and Dobbs, 2018). An alternative explanation is that the dependence of the DMR on metallicity emerges from the dependence of both metallicity and DMR on the rate at which a galaxy expels its metal- and dust-rich ISM and accretes metal- and dust-poor gas from the cosmic web (Feldmann, 2015).

The observational studies discussed above use dust and gas emission to determine dust and gas masses. However, the conversion between an amount of dust emission and a dust mass includes a calibration factor that may itself depend on metallicity. This calibration factor is known as the dust’s wavelength-dependent absorption cross section. The cross section is an intrinsic property of dust that depends on its composition, size, and structure (e.g.
Jones et al. (2016). If the proposal that the change in DMR is due to a change in the predominant mode of dust mass growth is true, it is plausible that this differently-grown dust would have different properties and hence a different absorption cross section. Given that other characteristics of dust emission have been found to change with metallicity (Meixner et al., 2010; Gordon et al., 2014; Roman-Duval et al., 2017; Chastenet et al., 2017), measurements of dust abundances at sub-solar metallicities based on other observables are necessary to confirm the emission-based findings.

The absorption cross section of dust in the Milky Way is calibrated by measuring dust emission and abundances of elements in dust in the same location (e.g. Compiègne et al. 2011). The abundance of an element in dust is computed by comparing measurements of the element’s gas phase abundance with its independently measured intrinsic, total abundance. The difference between the two is the abundance of the element in dust. The solid phase abundances of the different constituents of dust can then be converted to masses using the elements’ precisely measured atomic weights.

The quotient of the gas phase abundance of an element by the total abundance is called the depletion. By convention, studies of dust composition based on gas phase abundances phrase results in terms of depletions rather than solid phase abundances. The gas phase column densities needed for computing depletions are measured using ultraviolet absorption spectroscopy. This is done because all of the major constituents of dust, many elements that are present in dust in trace amounts, and atomic and molecular hydrogen all have absorption features in the ultraviolet.
Before the work described in Chapter 2, most depletion measurements had been made in either the Milky Way or in damped Lyman-α absorbers (DLAs). Decades of observations in the Milky Way were summarized by Jenkins (2009), who found that the depletions of all observable elements are connected. This connection can be expressed as a set of linear relations, one for the depletion of each element, with a single abscissa, referred to by Jenkins (2009) as the depletion parameter. This depletion parameter is a unitless effective description rather than a physical quantity. It has, however, been shown to correlate with the volume density of gas along a sightline.

DLAs are extragalactic systems detected in absorption whose atomic hydrogen column densities are greater than $2 \times 10^{20}$ cm$^{-2}$. In almost every case, the only measurement available of a DLA are the column densities of different elements along a single sightline through the system. Estimating depletions in a DLA requires imputing intrinsic abundances from a single set of (depletion-affected) gas phase abundances. There are empirically informed relations, modeled after the Milky Way relation discussed above, that attempt to do this imputation (e.g. De Cia et al. 2016). However, detailed studies of elemental abundances in DLAs and their possible analogues have shown that there is significant variation in relative intrinsic elemental abundances from DLA to DLA (Berg et al., 2015; Skúladóttir et al., 2018). This variation is not captured by currently existing empirical relations.

A pair of low metallicity environments in which it is possible to independently measure intrinsic and gas phase abundances are the Large and Small Magellanic Clouds (LMC and SMC). The metallicities of the LMC and SMC
are approximately $\frac{1}{2}$ and $\frac{1}{5}$ of $Z_\odot$, putting the SMC at the transition metallicity found in emission-based studies. Before 2015, there had been eleven sightlines through the Magellanic Clouds along which the depletions of multiple elements had been measured and 40 sightlines along which the depletion of a single element, titanium, had been measured (Roth and Blades, 1997; Welty et al., 1997; Welty et al., 2001; Sofia et al., 2006; Welty and Crowther, 2010). These studies provided hints that some elements, in particular silicon and titanium, were less depleted in the Magellanic Clouds than in the Milky Way.

In Tchernyshyov et al. (2015), I measured depletions of phosphorus and iron along 84 sightlines and depletions of silicon, zinc, and chromium along 16 sightlines through the Magellanic Clouds. I showed that depletion relations analogous to those of Jenkins (2009) exist in the Magellanic Clouds, though the parameters describing these relations are not the same in the Magellanic Clouds and Milky Way. The differences are clearest in the SMC, where there is less iron and silicon depletion at a given zinc or phosphorus depletion. I produced the first emissivity-independent estimate of the GDRs and DMRs of the LMC and SMC. Except along the least depleted sightlines in the SMC, the DMRs of the Magellanic Clouds are consistent with that of the Milky Way. Along those least depleted sightlines, the DMR is approximately 70% of the DMR of the Milky Way. This work is reproduced in this thesis as Chapter 2.

1.1.2 Techniques for the analysis of absorption spectra

The depletion studies described above are based on column density measurements made using restframe UV and optical absorption spectroscopy.
Absorption spectroscopy is also widely used in other studies of the chemistry and physical conditions of interstellar (and beyond) gas. A variety of techniques have been developed for measuring column densities from absorption spectra.

As more computing power has become available and as Bayesian statistics has been accepted in astronomy, people have started adapting existing techniques to the Bayesian statistical framework and developing new ones entirely within it. For the depletion study introduced above and for subsequent work on the chemistry of the ISM, I have developed several techniques for Bayesian analysis of absorption spectra.

The purpose of developing these Bayesian techniques is that they can be more robust than the existing, loosely frequentist, techniques when confronted with low quality spectra. Even if point estimates are not more precise, it is more straightforward to accurately estimate uncertainties in the context of a specified model in the Bayesian formalism than in the frequentist formalism. Low quality spectra can have low signal-to-noise ratios or can be affected by systematics such as unresolved spectral lines, blending of absorption features from different species, or difficult to disentangle background source continua.

Most existing Bayesian absorption spectroscopy tools are implementations of profile fitting. The assumption behind profile fitting is that spectral lines can be broken up into contributions from some number of distinct components. These components have different velocities, widths, and total column densities. The standard approach is to decide on a number of components and find the set of parameters that minimizes the square discrepancy between the
observed spectrum and the model spectrum synthesized from the parameters. Bayesian profile fitting tools, such as BayesVP (Liang, Kravtsov, and Agertz, 2018), Starfish (Czekala et al., 2015), and sick (Casey, 2016) instead compute the posterior probability distribution function over the the parameters. Computing the posterior probability distribution makes it possible to marginalize over parameters that are uncertain but important. This way, uncertainty in the parameters of interest due to uncertainty in the marginalized parameters is straightforwardly and correctly accounted for.

The first of the tools I have developed is also a Bayesian implementation of profile fitting. What differentiates it from the ones described above is that it treats the number of absorption components as a parameter, rather than having this be a user-specified quantity. Correctly determining the number of components present in an absorption feature is important because a large number of unresolved high-column density components can appear similar to a small number of resolved low-column density components. Assuming as small a number of components as possible can therefore bias column density estimates to systematically lower values. When a high resolution spectrum that can be used as a guide to the component structure in a lower resolution spectrum is not available, marginalizing over all possible component structures can, with carefully chosen priors, account for this source of uncertainty.

The depletion study described in the previous section was done using spectra whose resolution is known to be too low to resolve absorption lines arising in neutral and molecular gas. I developed this technique to account for this potential systematic. When those measurements were later compared
with ones obtained using higher resolution spectra, they were found to be consistent within uncertainties (Jenkins and Wallerstein 2017, Roman-Duval private communication). This technique is described in detail in Section 2.7.1.

The second tool I have developed is a way of treating the continuum of the source towards which a spectrum is taken. In most Bayesian and classical absorption spectroscopy tools, the continuum is a linear combination of functions such as polynomials. The parameters describing the continuum are the coefficients of the linear combination. In existing Bayesian tools, these coefficients are marginalized over numerically. Because the model spectrum depends linearly on the coefficients, it is actually possible to marginalize over them analytically. Analytic marginalization can be more computationally efficient than numerical marginalization. It also makes it possible to straightforwardly marginalize over different possible continuum parametrizations. This technique is described in detail in Chapter 3.

1.2 Gas dynamics and spiral structure in the Milky Way

Most low redshift disk galaxies, including the Milky Way, have spiral structure. With contemporary instrumentation, it has been possible to map the disks of a large number of spiral galaxies at wavelengths ranging from the radio to the ultraviolet with sufficient resolution to separate individual molecular clouds. Despite this wealth of data, two foundational questions about spiral structure remain unsolved.

The first question is known as the winding problem. In most galaxies, the
rotation curve is flat outside of a small central region. This means that the angular rotation velocity decreases with increasing radius. Therefore, if spiral arms are material features, their pitch angle must decrease over time until the arms become indistinguishable. Why, then, is spiral structure so common?

The second question is on the effect of spiral structure on star formation. Spiral arms are often particularly clear in tracers of young stars and dense, molecular gas. Do spiral arms induce this star formation at a level beyond being overdensities of interstellar matter? Put another way, do spiral arms affect the mass of stars formed per unit gas mass, the star formation efficiency, or do they just redistribute star formation that would have happened elsewhere anyway?

There are two categories of solution to the winding problem. Either spiral arms are not material and hence not subject to winding or there is a mechanism that can quickly replace wound-up or otherwise disrupted spiral arms. The first solution is realized in stationary density wave theory, in which spiral arms are stable traveling waves (Lin and Shu, 1964; Lin and Shu, 1966). The second solution is realized in transient spiral structure theories, which invoke a variety of spiral arm replenishment mechanisms. These mechanisms include swing amplification, self-perpetuation of material spiral arms, and self-perpetuation of non-stationary density waves (Goldreich and Lynden-Bell, 1965; Sellwood and Carlberg, 1984; Baba, Saitoh, and Wada, 2013; D’Onghia, Vogelsberger, and Hernquist, 2013; Sellwood and Carlberg, 2014). Density wave theory and the transient spiral structure theories make different predictions for gas dynamics and the role of spiral structure in star formation.
In classical density wave theory, spiral arms induce a quasi-stationary spiral shock along most of the length of a spiral arm (Roberts, 1969). In simulations that include feedback and/or more sophisticated treatments of (magneto)hydrodynamics than the classical theory, the spiral shock is perturbed but still present along much of the arm (e.g. Dobbs, Bonnell, and Pringle 2006; Kim, Kim, and Ostriker 2010; Kim, Kim, and Elmegreen 2015). The shock compresses gas as it passes through, inducing molecular cloud formation or collapse and, downstream, to star formation (Roberts, 1969; Shu et al., 1972; Dobbs et al., 2008). The resulting sequence of offsets between spiral arms as seen in old stars, gas, and young stars is a key prediction of density wave theory.

In transient spiral structure theories, the velocity field of gas around a spiral arm is, inherently, time dependent. Unlike in density wave theory, there is not a single, clear velocity field signature. A general qualitative prediction is that gas converges on the stellar spiral arm during the arm formation phase and diverges from the stellar spiral arm during the arm destruction phase (Dobbs and Bonnell, 2008; Pettitt et al., 2014; Baba et al., 2016). The divergence can happen as part of a redistribution of interstellar matter from an old, disappearing set of spiral arms to the next generation of spiral arms. Because there is no strong, large scale shock, no significant enhancement in star formation efficiency is predicted (Baba, Morokuma-Matsui, and Saitoh, 2017). Because interstellar matter collects in the arm rather than flowing through it, there is no expectation of an offset between the old stellar, gaseous, and young stellar spiral arms.
While it is clear from measurements of the positions of young stars and star forming regions show that there are spiral arms in the Milky Way (Morgan, Sharpless, and Osterbrock, 1952), there is no consensus around its nature. Precise measurements by the \textit{Gaia} mission of the stellar velocity field have been used as evidence in favor of both density wave theory Michtchenko et al. 2018; Xu et al. 2018; Dias et al. 2019 and transient spiral structure theories (e.g. Quillen et al. 2018; Hunt et al. 2018; Baba et al. 2018). This is despite the fact that many of these studies focus on the same collection of well-known moving groups.

Measurements of spatially resolved gas dynamics in the Milky Way may help break this impasse. In addition to predicting different offsets between gas and stellar spiral arms, the two categories of spiral structure theory also predict different offsets in gas and stellar velocity fields. The gas velocity field is, in some ways, simpler to interpret than the stellar velocity field because gas is collisional. The presence or absence of one-sided large scale shocks—a collisional phenomenon—along spiral arms, for example, provides a clear distinction between theories of spiral structure.

To provide this constraint, I developed two ways of mapping the line-of-sight velocity of interstellar matter as a function of position throughout the Galaxy. The first method is based, conceptually, on matching features between three-dimensional dust maps and line emission maps. In Chapter 4, I describe how to implement this idea using regularized non-linear least-squares optimization and apply it to produce a velocity field map. To test this map, I compare it with the velocities of high mass star formation regions.
with parallax measurements. Outside of the inner several kiloparsecs of the Galaxy, the velocities of the map and star formation regions agree.

The second method is based on building a consistent description of line absorption towards stars throughout the Galactic disk. The spectra used for this work are taken from the SDSS APOGEE survey. These spectra contain absorption from a diffuse interstellar band at 1.527 μm that is known to be a linear tracer of total column outside of dense molecular clouds (Zasowski et al., 2015). After producing this second map and showing that it and the first map are mutually consistent, I compare the two maps with simulations of different kinds of spiral structure. I find that the maps are more consistent with simulations of transient spiral structure than with simulations of density wave spiral structure. This work is reproduced in this thesis as Chapter 5.
Chapter 2

Depletions in the Magellanic Clouds

1We present a study of the composition of gas and dust in the Large and Small Magellanic Clouds (LMC and SMC, together – the MCs) as measured by UV absorption spectroscopy. We have measured P II and Fe II along 85 sightlines toward the MCs using archival FUSE observations. For 16 of those sightlines, we have measured Si II, Cr II, and Zn II from new HST COS observations. We have combined these measurements with H I and H₂ column densities and reference stellar abundances from the literature to derive gas-phase abundances, depletions, and gas-to-dust ratios (GDRs). 80 of our 84 P measurements and 13 of our 16 Zn measurements are depleted by more than 0.1 decades, suggesting that P and Zn abundances are not accurate metallicity indicators at and above the metallicity of the SMC. The maximum

1Adapted from a paper that originally appeared in The Astrophysical Journal (Tchernyshyov et al., 2015). The chapter includes two corrections to the source material: I have corrected the assumed intrinsic phosphorus abundances of the Magellanic Clouds and I now no longer treat H I column density upper limits as detections. I have excluded sightlines with H I upper limits from the depletion analyses and have updated tables and figures to reflect this. The exclusion had a negligible effect on the results. I would like to thank Dan Welty for pointing out these errors.
P and Zn depletions are the same in the MW, LMC, and SMC. Si, Cr, and Fe are systematically less depleted in the SMC than in the MW or LMC. The minimum Si depletion in the SMC is consistent with zero. Our depletion-derived GDRs broadly agree with GDRs from the literature. The GDR varies from location to location within a galaxy by a factor of up to 2 in the LMC and up to 5 in the SMC. This variation is evidence of dust destruction and/or growth in the diffuse neutral phase of the interstellar medium.

2.1 Introduction

From different types of observations of dust in the Milky Way (MW) and other galaxies, we know that the gas-to-dust ratio (GDR) varies within and between galaxies. Dust evolution models seek to explain and quantitatively reproduce these variations. Most of these models treat the dust evolution problem averaged over a galaxy, and follow the basic template set by Audouze and Tinsley (1976) in which different species (e.g. hydrogen or a specific metal) travels between well-mixed states (e.g. gas-phase outside of a galaxy or solid-phase in the dense molecular medium in a galaxy) according to a set of differential equations. The current generation of dust evolution models (e.g., Dwek and Cherchneff, 2011; Zhukovska, 2014; Feldmann, 2015) include a more comprehensive and relatively well-constrained set of dust production and destruction mechanisms than the original, but are still focused on reproducing galaxy-averaged properties. As the number of destruction and production parameters that need tuning is quite large, there is more than one way to correctly reproduce a galaxy-averaged dust-to-gas ratio. The
current-generation models listed above can all reproduce trends that have been observed between the metallicity and GDR of a galaxy while disagreeing on what the most important mechanism for dust evolution is. One possible way to break this degeneracy is to increase the number of constraining observations by attempting to reproduce GDRs averaged over different phases of the interstellar medium (ISM) of each galaxy.

Computing an ISM-phase-averaged GDRs over a galaxy requires taking a comprehensive inventory of gas and dust over multiple phases, which requires observations of different gas mass tracers with sufficiently high spatial resolution to resolve the dense molecular phase. Some of the most complete necessary datasets are available for the Large and Small Magellanic Clouds (LMC and SMC, together – the MCs), which are two nearby, sub-solar metallicity (1/2 and 1/5 of the solar metallicity, respectively) dwarf galaxies. The dust content of the MCs has been extensively studied as part of the SAGE (Meixner et al., 2006; Gordon et al., 2011) and HERITAGE (Meixner et al., 2013) programs. As part of these programs, dust mass (Gordon et al., 2014) and GDR (Roman-Duval et al., 2014) maps of the LMC and SMC have been made.

When these GDR maps are binned by ISM phase, one finds different GDRs in diffuse neutral gas and dense molecular gas. However, the difference between these GDR values is not quantitatively accurate. Due to degeneracies that are explored in detail in Roman-Duval et al. (2014), it is not currently possible to accurately compute dust masses in dense molecular gas from dust emission. One way to resolve some of these degeneracies is to measure GDRs in various environments in the LMC and SMC using a method whose
systematic uncertainties are different from those of the dust emission method. One of the aims of this study is to measure GDRs in the LMC and SMC using elemental depletions derived from ultraviolet (UV) absorption spectroscopy. A depletion is the difference between an element’s gas-phase abundance and its intrinsic (i.e. combined gas-phase and solid-phase) abundance. If one makes the assumption that the missing amount is entirely in dust, which is a reasonable assumption in the molecule-poor diffuse neutral medium (DNM) through which UV spectroscopy is possible, depletions can be converted to solid-phase abundances. Combining the solid-phase abundances of the main constituents of dust yields a GDR.

Almost all depletion studies to date have focused on the DNM of the MW. The two main astrophysical results of the ensemble of MW depletion studies are that in a single location, elements with higher condensation temperatures tend to be more depleted (Field, 1974) and that the depletions of every element track each other and the volume density of the gas they are associated with in a consistent and continuous way (Jenkins, 2009). The latter result also implies that the gas volume density and GDR in a small amount of DNM are correlated. The SMC is the next-best studied galaxy after the MW, with four sightlines along which some or all of Mg, Si, and Fe have been measured (Welty et al., 1997; Welty et al., 2001; Sofia et al., 2006). These four measurements hint at possible differences between the composition of dust in the SMC and MW, but are inconclusive.

No other system has depletion measurements of multiple important dust
constituents along more than two sightlines. There have been several one-to-two sightline studies of local galaxies (James et al. 2014 and references therein) and many single sightline studies of damped Lyman-\(\alpha\) systems (DLAs) (Rafelski et al. 2012 and references therein). Because intrinsic elemental abundances in most local galaxies and all DLAs are not available, these studies have relied on MW depletion patterns to interpret their observed gas-phase abundances. The present study will provide depletion patterns for two more galaxies at sub-solar metallicities, which may be more appropriate contexts for the interpretation of gas-phase abundances in low-metallicity systems.

In this chapter, we present new measurements of silicon (Si II), phosphorus (P II), chromium (Cr II), iron (Fe II), and zinc (Zn II) column densities in the LMC and SMC. These measurements are made using 16 new and 84 archival spectra. Our sample, observations, and data reduction are described in Section 2.2. Our data analysis, which involves measuring column densities and computing gas-phase abundances, depletions, solid-phase abundances, and GDRs, is described in Sections 2.3 and 2.4. A discussion of our results and a comparison of gas-phase abundances in the MCs and DLAs is presented in Section 2.5. Our results are briefly summarized in Section 2.6.

### 2.2 Observations and archival data

The spectra presented in this study are a combination of new observations from the Cosmic Origins Spectrograph (COS; Green et al., 2012) on the *Hubble Space Telescope* (HST) along 16 sight lines and supplementary archival spectra for these 16 and 69 additional sight lines from the Far Ultraviolet Spectroscopic
<table>
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<tr>
<th>Target</th>
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<th>RA (J2000)</th>
<th>DEC (J2000)</th>
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<th>E(B-V)</th>
<th>log$_{10}$ NHI</th>
<th>log$_{10}$ NH$_2$</th>
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<td>0.13</td>
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<td>21.41</td>
<td>15.95</td>
</tr>
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<td>-72.0373</td>
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<td>0.13</td>
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<td>14.79</td>
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</tr>
<tr>
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<td>18.4269</td>
<td>-73.2915</td>
<td>O6.5 V</td>
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<td>0.23</td>
<td>21.85</td>
<td>20.95</td>
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<td>-65.8759</td>
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<td>-71.0695</td>
<td>O4-5 III(f)</td>
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<td>-66.3598</td>
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<td>-69.1324</td>
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<td>0.15</td>
<td>21.34</td>
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<td>18.69</td>
</tr>
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<td>-68.9171</td>
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<td>0.26</td>
<td>21.60</td>
<td>19.87</td>
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Table 2.1: Locations, stellar parameters, and ISM parameters of the COS sample. All values from Welty, Xue, and Wong (2012) and references therein.
Figure 2.1: H I column density maps of the LMC (left) and SMC (right). The positions of the 42 LMC and 46 SMC archival FUSE sightlines used in this study are marked with dots. The 8 LMC and 8 SMC sightlines that also have new COS observations are emphasized with large, open circles.

Explorer (FUSE Sahnow et al., 2000). Figure 2.1 shows the positions of these sight lines in the galaxies.

2.2.1 COS Observations

The COS spectra of the Magellanic Cloud sight lines presented here were obtained between the dates of 2012 October 12 and 2013 August 19 as part of HST program number 13004. All successfully acquired targets were faint enough to use the primary science aperture, and were dithered with all 4 FP-POS positions to improve the limiting signal-to-noise ratio (SNR). During the observation of target AzV 388, HST was unable to acquire the guide star, resulting in a mis-pointing and a failed observation. Observations were conducted with the near-UV (NUV) G185M grating at central wavelengths of 1921 and 1953 Å and a spectral resolution of 17 km sec$^{-1}$.
2.2.2 COS Targets

Table 2.1 lists the 8 SMC and 8 LMC stars along the lines of sight targeted in our new COS observations with their sky coordinates, spectral types, V, E(B-V), and HI and H$_2$ column densities as reported in Welty, Xue, and Wong (2012). These targets will be referred to as the COS sample.

The COS sight lines were chosen from a set of 285 Magellanic Cloud targets with HI and/or H$_2$ column densities measured from archival HST and FUSE spectra presented in Welty, Xue, and Wong (2012). In order to explore the dependence of depletion on the column density ($N$) and phase of gas, sight lines were chosen to most completely cover the $2N$(H$_2$)/($N$(HI)+2$N$(H$_2$)) vs. $N$(HI)+2$N$(H$_2$) parameter space. The targets sample a range of total neutral hydrogen column densities from $N$(HI) + 2$N$(H$_2$) of $\sim 10^{20.5}$ to $\sim 10^{22}$ cm$^{-2}$ and molecular hydrogen fraction, $2N$(H$_2$)/($N$(HI)+2$N$(H$_2$)), of $\sim 50\%$ to $\ll 1\%$. Few sight lines with high molecular fractions exist in the original sample of 285, so our COS sample is dominated (14/16) by those with molecular fractions of $< 10\%$.

2.2.3 FUSE Targets

Data for the 69 supplementary sightlines, of which 32 are towards the LMC and 37 are towards the SMC, were downloaded from the FUSE MC Legacy Project archive (Blair et al., 2009) and analyzed with no further processing. The FUSE MC Legacy Project archive contains spectra towards a total of 287 stars. From these, we selected stars whose continuum SNRs in the region from 1140 to 1155 Å were greater than 5 and towards which Welty, Xue, and
Wong (2012) had detected H I and H$_2$. These targets will be referred to as the FUSE-only sample.

2.2.3.1 Ancillary literature column densities

Two of the LMC and four of the SMC targets in the FUSE-only sample have been observed and analyzed before (Roth and Blades, 1997; Welty et al., 2001; Sofia et al., 2006). All of these targets have Zn and Cr measurements and three of the four SMC targets have Si measurements. Spectra towards Sk 155 and Sk 108 has been separately analyzed by both Welty et al. (2001) and Sofia et al. (2006). We adopt the values of the latter when they are given and the former otherwise. We note that this work is the first to use these measurements to compute depletions relative to hydrogen; the original authors did not have access to the hydrogen absorption measurements of Welty, Xue, and Wong (2012).

2.2.4 Data Reduction

Figures 2.2 and 2.3 show spectra towards SK $-65$ 22 in the LMC and SK 116 in the SMC. Labels and vertical lines indicate the typical wavelengths of absorption lines of interest; FUSE and COS line spread functions (LSFs) are shown at the bottom left of each panel (Kruk et al., 2002; Ghavamian et al., 2009). The relative velocities assumed for LMC and SMC absorption are based on the ranges given in Brüns et al., 2005. Most of the other spectra in this study resemble the ones described above.

The continua of SK $-68$ 135 and SK $-65$ 22 contain broad absorption and
Figure 2.2: FUSE (top two panels) and COS (bottom three panels) observations of the LMC O6 Iaf+ star Sk-65 22. Labels show the locations of ISM absorption features of interest. The instrumental LSF for each wavelength range is shown at the bottom left of each panel.
Figure 2.3: FUSE (top two panels) and COS (bottom three panels) observations of the SMC O9 Iabw star Sk 116. Labels show the locations of ISM absorption features of interest. The instrumental LSF for each wavelength range is shown at the bottom left of each panel.
emission lines, including some which overlap with absorption lines of interest. In some of the FUSE spectra, the absolute flux level between 1140 and 1150 Å is decreased relative to the flux level at nearby wavelengths due to a shadow from a repeller grid falling on part of the FUSE detector. All of our Fe II lines fall within this region; spectra where the shadow is especially strong are only marginally usable and have been excluded. There are absorption lines due to gas between the MW and LMC in half of the observations towards the LMC. This gas has relative velocities which range from 100 to 180 km sec$^{-1}$, has been observed before (Lehner, Staveley-Smith, and Howk, 2009), and can usually be distinguished from MW and LMC absorption.

The resolutions of FUSE and COS are $\sim$ 13 km sec$^{-1}$ (Kruk et al., 2002) and $\sim$ 15 km sec$^{-1}$ (Ghavamian et al., 2009), respectively. Isolated lines in higher resolution ($\sim$ 3 km sec$^{-1}$) spectra of the diffuse neutral medium in the MCs have widths of order a km sec$^{-1}$ (Roth and Blades, 1997; Welty et al., 1997), implying that all of the absorption we see is almost certainly unresolved.

### 2.3 Quantitative analysis: gas-phase

We compute four measurements of gas-phase metal content, which are listed below in order of increasing distance from the data. From the spectra, we measure column densities for P II, Zn II, Si II, Cr II and Fe II. Normalizing these column densities by the hydrogen column density gives us ion abundances. If we had measurements of a single element in more than one ionization state, we would compute an ionization correction for each sightline. Instead, we
check that the ionization corrections for most of our sightlines should be negligible and adopt the ion abundances and elemental abundances. Normalizing these elemental abundances by reference, or total gas- and solid-phase, abundances gives us elemental depletions. Finally, we analyze the distribution of depletions in each galaxy using the formalism from Jenkins (2009). This formalism gives us a concise summary of an element’s depletion trends each galaxy and allows us to impute partially missing data, such as Zn, Si, and Cr depletions for sightlines in the FUSE-only sample. Below, we describe each of these steps in moderate detail; the detailed mechanics of steps with relatively complex implementations are described in the appendices.

<table>
<thead>
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<th>Target</th>
<th>Galaxy</th>
<th>$\log_{10} N$ P II [cm$^{-2}$]</th>
<th>$\log_{10} N$ Fe II [cm$^{-2}$]</th>
<th>$\log_{10} N$ H [cm$^{-2}$]</th>
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</thead>
<tbody>
<tr>
<td>AzV 6</td>
<td>SMC</td>
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<tr>
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<td>&lt; 21.80</td>
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<td>(\log_{10} N_{\text{Fe II}}) [cm(^{-2})]</td>
<td>(\log_{10} N_{\text{H}}) [cm(^{-2})]</td>
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<td>13.73 ± 0.07</td>
<td>15.22 ± 0.06</td>
<td>21.42</td>
</tr>
<tr>
<td>SK 157</td>
<td>SMC</td>
<td>13.73 ± 0.11</td>
<td>15.16 ± 0.07</td>
<td>21.19</td>
</tr>
<tr>
<td>SK 159</td>
<td>SMC</td>
<td>13.71 ± 0.02</td>
<td>14.94 ± 0.01</td>
<td>21.16</td>
</tr>
<tr>
<td>SK 160</td>
<td>SMC</td>
<td>13.81 ± 0.05</td>
<td>14.95 ± 0.01</td>
<td>21.48</td>
</tr>
<tr>
<td>AzV 491</td>
<td>SMC</td>
<td>13.60 ± 0.09</td>
<td>14.56 ± 0.05</td>
<td>21.40</td>
</tr>
<tr>
<td>PGMW 3120</td>
<td>LMC</td>
<td>14.49 ± 0.32</td>
<td>15.27 ± 0.05</td>
<td>21.39</td>
</tr>
<tr>
<td>SK-66 35</td>
<td>LMC</td>
<td>13.84 ± 0.04</td>
<td>14.88 ± 0.04</td>
<td>20.64</td>
</tr>
<tr>
<td>SK-70 69</td>
<td>LMC</td>
<td>13.28 ± 0.10</td>
<td>14.61 ± 0.03</td>
<td>&lt; 20.50</td>
</tr>
<tr>
<td>SK-68 52</td>
<td>LMC</td>
<td>13.91 ± 0.04</td>
<td>15.17 ± 0.05</td>
<td>21.41</td>
</tr>
<tr>
<td>SK-69 104</td>
<td>LMC</td>
<td>12.66 ± 0.18</td>
<td>14.06 ± 0.03</td>
<td>&lt; 20.68</td>
</tr>
<tr>
<td>SK-68 73</td>
<td>LMC</td>
<td>14.40 ± 0.15</td>
<td>15.44 ± 0.05</td>
<td>21.63</td>
</tr>
<tr>
<td>SK-67 101</td>
<td>LMC</td>
<td>13.19 ± 0.05</td>
<td>14.82 ± 0.05</td>
<td>&lt; 20.61</td>
</tr>
<tr>
<td>SK-67 104</td>
<td>LMC</td>
<td>13.16 ± 0.06</td>
<td>14.72 ± 0.02</td>
<td>&lt; 20.48</td>
</tr>
<tr>
<td>SK-67 105</td>
<td>LMC</td>
<td>13.42 ± 0.05</td>
<td>14.85 ± 0.06</td>
<td>21.48</td>
</tr>
<tr>
<td>BI 170</td>
<td>LMC</td>
<td>13.27 ± 0.13</td>
<td>15.07 ± 0.06</td>
<td>&lt; 20.90</td>
</tr>
<tr>
<td>SK-66 100</td>
<td>LMC</td>
<td>13.28 ± 0.05</td>
<td>14.83 ± 0.02</td>
<td>&lt; 20.50</td>
</tr>
<tr>
<td>SK-69 142a</td>
<td>LMC</td>
<td>13.75 ± 0.05</td>
<td>14.94 ± 0.07</td>
<td>20.90</td>
</tr>
<tr>
<td>SK-67 144</td>
<td>LMC</td>
<td>13.59 ± 0.06</td>
<td>14.92 ± 0.03</td>
<td>20.80</td>
</tr>
<tr>
<td>BI 184</td>
<td>LMC</td>
<td>14.00 ± 0.15</td>
<td>15.34 ± 0.07</td>
<td>21.42</td>
</tr>
<tr>
<td>SK-69 175</td>
<td>LMC</td>
<td>13.69 ± 0.04</td>
<td>14.81 ± 0.03</td>
<td>&lt; 21.08</td>
</tr>
<tr>
<td>SK-67 166</td>
<td>LMC</td>
<td>13.39 ± 0.01</td>
<td>14.30 ± 0.00</td>
<td>&lt; 20.50</td>
</tr>
<tr>
<td>SK-67 167</td>
<td>LMC</td>
<td>13.46 ± 0.03</td>
<td>14.25 ± 0.01</td>
<td>&lt; 20.50</td>
</tr>
</tbody>
</table>
Table 2.2: Logarithmic ion column densities towards LMC and SMC targets in the FUSE sample. Hydrogen column densities are from Welty, Xue, and Wong (2012) and references therein. Sightlines for which hydrogen column densities are upper limits are not used in any of the analyses in this work.

<table>
<thead>
<tr>
<th>Target</th>
<th>Galaxy</th>
<th>log$_{10}$ N P II [cm$^{-2}$]</th>
<th>log$_{10}$ N Fe II [cm$^{-2}$]</th>
<th>log$_{10}$ N H [cm$^{-2}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>SK-67 191</td>
<td>LMC</td>
<td>13.76 ± 0.03</td>
<td>15.11 ± 0.09</td>
<td>20.76</td>
</tr>
<tr>
<td>SK-69 191</td>
<td>LMC</td>
<td>14.00 ± 0.05</td>
<td>15.49 ± 0.08</td>
<td>21.18</td>
</tr>
<tr>
<td>MACHO 81.8763.8</td>
<td>LMC</td>
<td>14.01 ± 0.04</td>
<td>15.49 ± 0.03</td>
<td>21.62</td>
</tr>
<tr>
<td>SK-67 211</td>
<td>LMC</td>
<td>13.99 ± 0.02</td>
<td>15.04 ± 0.01</td>
<td>20.76</td>
</tr>
<tr>
<td>Brey 64</td>
<td>LMC</td>
<td>14.22 ± 0.15</td>
<td>15.35 ± 0.10</td>
<td>21.78</td>
</tr>
<tr>
<td>BI 237</td>
<td>LMC</td>
<td>14.42 ± 0.14</td>
<td>15.25 ± 0.04</td>
<td>21.64</td>
</tr>
<tr>
<td>SK-68 129</td>
<td>LMC</td>
<td>14.78 ± 0.40</td>
<td>15.28 ± 0.10</td>
<td>21.75</td>
</tr>
<tr>
<td>SK-69 220</td>
<td>LMC</td>
<td>14.01 ± 0.06</td>
<td>15.15 ± 0.05</td>
<td>21.28</td>
</tr>
<tr>
<td>BI 253</td>
<td>LMC</td>
<td>14.36 ± 0.08</td>
<td>15.54 ± 0.04</td>
<td>21.61</td>
</tr>
<tr>
<td>SK-68 137</td>
<td>LMC</td>
<td>14.37 ± 0.06</td>
<td>15.63 ± 0.26</td>
<td>21.56</td>
</tr>
<tr>
<td>SK-69 246</td>
<td>LMC</td>
<td>14.06 ± 0.02</td>
<td>15.78 ± 0.01</td>
<td>21.43</td>
</tr>
<tr>
<td>SK-68 140</td>
<td>LMC</td>
<td>14.35 ± 0.22</td>
<td>15.32 ± 0.08</td>
<td>21.76</td>
</tr>
<tr>
<td>SK-71 50</td>
<td>LMC</td>
<td>14.03 ± 0.06</td>
<td>15.58 ± 0.05</td>
<td>21.25</td>
</tr>
<tr>
<td>SK-68 155</td>
<td>LMC</td>
<td>14.46 ± 0.21</td>
<td>15.47 ± 0.06</td>
<td>21.64</td>
</tr>
<tr>
<td>BI 272</td>
<td>LMC</td>
<td>13.55 ± 0.02</td>
<td>14.89 ± 0.02</td>
<td>&lt; 21.00</td>
</tr>
</tbody>
</table>

2.3.1 Ion column densities

The analysis of an absorption spectrum can generally be divided into two steps – continuum fitting and column density recovery. In a typical continuum fitting procedure, one interpolates over ISM absorption using neighboring parts of the spectrum as a guide. We do this interpolation using Gaussian process regression (Rasmussen and Williams, 2006). A Gaussian process is a probability distribution over functions. Regression is a procedure for choosing a function that has a high probability of having produced a set of observations.
Figure 2.4: Profile fit of the observation towards Sk 116 in the SMC for the different ions. Listed next to the ions is the rest frame ($v = 0$) wavelength of the absorption line. Circles represent the data; light and dark grey regions are the 68 and 95% credible regions about the median fit; the dashed line is the median continuum level.
Figure 2.5: Metal ion column density plotted against the total column density of atomic and molecular hydrogen. LMC sightlines are denoted in red, SMC sightlines are in blue. Sightlines without COS data are shown without errorbars.
<table>
<thead>
<tr>
<th>Target</th>
<th>Galaxy</th>
<th>log$_{10}$ N P II [cm$^{-2}$]</th>
<th>log$_{10}$ N Zn II [cm$^{-2}$]</th>
<th>log$_{10}$ N Si II [cm$^{-2}$]</th>
<th>log$_{10}$ N Cr II [cm$^{-2}$]</th>
<th>log$_{10}$ N Fe II [cm$^{-2}$]</th>
<th>log$_{10}$ N H [cm$^{-2}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>AzV 327</td>
<td>SMC</td>
<td>13.30 ± 0.13</td>
<td>12.75 ± 0.19</td>
<td>15.69 ± 0.04</td>
<td>11.74 ± 1.02</td>
<td>14.67 ± 0.02</td>
<td>20.93</td>
</tr>
<tr>
<td>SK 143</td>
<td>SMC</td>
<td>12.33 ± 0.99</td>
<td>12.57 ± 0.33</td>
<td>15.10 ± 0.11</td>
<td>11.49 ± 0.97</td>
<td>14.65 ± 0.03</td>
<td>21.43</td>
</tr>
<tr>
<td>AzV 47</td>
<td>SMC</td>
<td>13.77 ± 0.03</td>
<td>13.08 ± 0.03</td>
<td>15.74 ± 0.02</td>
<td>13.66 ± 0.03</td>
<td>15.43 ± 0.02</td>
<td>21.32</td>
</tr>
<tr>
<td>AzV 238</td>
<td>SMC</td>
<td>13.65 ± 0.04</td>
<td>13.05 ± 0.04</td>
<td>15.73 ± 0.02</td>
<td>13.31 ± 0.07</td>
<td>14.91 ± 0.02</td>
<td>21.41</td>
</tr>
<tr>
<td>AzV 95</td>
<td>SMC</td>
<td>13.77 ± 0.01</td>
<td>13.15 ± 0.03</td>
<td>15.86 ± 0.02</td>
<td>13.61 ± 0.04</td>
<td>15.30 ± 0.01</td>
<td>21.50</td>
</tr>
<tr>
<td>SK 116</td>
<td>SMC</td>
<td>13.83 ± 0.04</td>
<td>13.15 ± 0.02</td>
<td>15.95 ± 0.02</td>
<td>13.66 ± 0.02</td>
<td>15.36 ± 0.03</td>
<td>21.57</td>
</tr>
<tr>
<td>SK 9</td>
<td>SMC</td>
<td>13.09 ± 1.38</td>
<td>13.33 ± 0.02</td>
<td>16.04 ± 0.03</td>
<td>13.70 ± 0.04</td>
<td>13.91 ± 2.10</td>
<td>21.76</td>
</tr>
<tr>
<td>AzV 476</td>
<td>SMC</td>
<td>14.02 ± 0.04</td>
<td>13.38 ± 0.04</td>
<td>16.04 ± 0.04</td>
<td>13.75 ± 0.04</td>
<td>15.41 ± 0.04</td>
<td>21.95</td>
</tr>
<tr>
<td>SK-65 22</td>
<td>LMC</td>
<td>13.67 ± 0.01</td>
<td>12.69 ± 0.12</td>
<td>15.57 ± 0.02</td>
<td>13.10 ± 0.04</td>
<td>14.83 ± 0.01</td>
<td>20.58</td>
</tr>
<tr>
<td>SK-67 5</td>
<td>LMC</td>
<td>13.73 ± 0.02</td>
<td>13.03 ± 0.02</td>
<td>15.48 ± 0.02</td>
<td>13.22 ± 0.03</td>
<td>14.56 ± 0.02</td>
<td>21.02</td>
</tr>
<tr>
<td>SK-71 45</td>
<td>LMC</td>
<td>14.02 ± 0.01</td>
<td>13.17 ± 0.04</td>
<td>16.01 ± 0.01</td>
<td>13.61 ± 0.03</td>
<td>15.25 ± 0.01</td>
<td>21.09</td>
</tr>
<tr>
<td>SK-66 172</td>
<td>LMC</td>
<td>13.95 ± 0.03</td>
<td>13.07 ± 0.04</td>
<td>15.65 ± 0.02</td>
<td>13.10 ± 0.10</td>
<td>14.68 ± 0.04</td>
<td>21.25</td>
</tr>
<tr>
<td>SK-70 115</td>
<td>LMC</td>
<td>13.97 ± 0.02</td>
<td>13.16 ± 0.03</td>
<td>15.90 ± 0.01</td>
<td>13.67 ± 0.02</td>
<td>15.39 ± 0.02</td>
<td>21.34</td>
</tr>
<tr>
<td>BI 173</td>
<td>LMC</td>
<td>13.70 ± 0.02</td>
<td>13.13 ± 0.02</td>
<td>15.73 ± 0.02</td>
<td>13.54 ± 0.03</td>
<td>15.04 ± 0.02</td>
<td>21.34</td>
</tr>
<tr>
<td>BI 42</td>
<td>LMC</td>
<td>13.90 ± 0.11</td>
<td>13.24 ± 0.02</td>
<td>15.91 ± 0.09</td>
<td>13.52 ± 0.04</td>
<td>15.35 ± 0.08</td>
<td>21.51</td>
</tr>
<tr>
<td>SK-68 135</td>
<td>LMC</td>
<td>14.06 ± 0.05</td>
<td>13.36 ± 0.06</td>
<td>15.90 ± 0.06</td>
<td>13.76 ± 0.02</td>
<td>15.45 ± 0.03</td>
<td>21.62</td>
</tr>
</tbody>
</table>

*Table 2.3: Logarithmic ion column densities towards LMC and SMC targets in the COS sample*
Gaussian process regression, then, is a procedure for choosing a function that, on the one hand, has a high probability of having produced the observed points and, on the other, has a high probability according to the specified Gaussian process. The procedure also produces an estimate of the function’s pointwise uncertainty. This estimate includes correlations between neighboring values. Our chosen Gaussian process favors functions that resemble the sum of a second-order polynomial and a smooth (i.e. infinitely differentiable), zero-mean perturbation. For an example of what these continua look like over short wavelength ranges, see the dashed black line in Figure 2.4. For more details on this procedure, see Appendix 2.7.1.

The next step, column density recovery, requires a procedure for converting the observed amount of absorption into a column density or, if different parts of the absorption are caused by different absorbers, column densities. In our spectra, the absorption line corresponding to each transition appears at several Doppler velocities, each corresponding to a different line-of-sight object. In Figure 2.4, each absorption line appears near 0 km sec\(^{-1}\), which corresponds to gas in the MW, and 130 km sec\(^{-1}\), which corresponds to gas in the SMC (Brüns et al., 2005). Towards stars in the LMC, we see absorption at 0, 150, and 250 km sec\(^{-1}\) due to gas in the MW, intervening high velocity clouds (Lehner, Staveley-Smith, and Howk, 2009), and and the LMC. These shifts cause velocity components of some absorption lines, in particular the Cr II and Zn II lines near 2062 Å and the three Fe II lines near 1143 Å, to overlap. This can be seen in the second and third panels from the bottom of the right column of Figure 2.4 in which each absorption line has two broad velocity
components, but appears to have four.

To resolve the resulting confusion, we turn to a variation on Voigt profile fitting. In standard Voigt profile fitting, one models the observed absorption as coming from a series of coherent clouds. Each cloud has a central velocity and (Gaussian) velocity width and contains some amount of each species under investigation. One optimizes the central velocity, width, and amount of each species in each cloud by generating absorption spectra, comparing them to the observations, and minimizing the difference. The number of clouds is chosen in order to get an acceptable fit according to some criterion. We avoid choosing a set number of clouds and instead numerically integrate out the dependence on the number of coherent clouds using a transdimensional (i.e. operating over a parameter space of varying size) Markov Chain Monte Carlo (MCMC) procedure (Green, 1995). This procedure allows us to include the effects of different possible cloud decompositions in our quoted uncertainties. Additional information about our Voigt profile fitting implementation can be found in Appendix 2.7.1.

We have used these two procedures to measure ion column densities. These are plotted in Figure 2.5 and listed in Table 2.3 (COS sample) and Table 2.2 (FUSE-only sample).

2.3.2 Elemental abundances and ionization corrections

Next, we use the measured ion column densities to compute gas-phase elemental abundances. From our ion measurements and literature atomic and molecular hydrogen column densities (Welty, Xue, and Wong, 2012), we
\[ \log_{10}(N_{\text{H}}) - 12 - 10 - 8 - 6 - 4 - 2 + \log_{10}(f_{\text{H}_2}) - 0.5 - 0.4 - 0.3 - 0.2 - 0.1 + 0.0 \]

\[ \text{IC}(\text{Zn II}) = \varepsilon_{\text{gas}}(\text{Zn}) - \varepsilon_{\text{gas}}(\text{Zn II}). \]
The magnitude of the ionization correction depends on the element’s ionization potentials and the ISM phases present along the line of sight (Sembach et al., 2000). Based on models of the ionization structure of clouds with H I and H$_2$ column densities similar to those measured along our sightlines, we expect the ionization corrections to be negligible.

The ionization correction for the Zn II abundance is small when, on the one hand, most of the Zn that is spatially coincident with H I and H$_2$ is Zn II and, on the other hand, most of the Zn that is not spatially coincident with H I and H$_2$ is not Zn II. If the main ionizing source is the background star towards which we are observing and its neighbors, then both conditions for a small ionization correction will apply. Both conditions require radiation fields that should affect a qualitatively small fraction of the total gas. Because the ionization potential from H I to H II is lower than the ionization potential from Zn II to Zn III, the only way to miss some of the spatially coincident Zn is to attenuate the radiation field above the ionization potential from Zn I to Zn II. Since we can see non-negligible fluxes at and below the wavelength corresponding to this ionization potential, 1320 Å, the gas along the line of sight cannot contain significant amounts of Zn I. To violate the second condition, that Zn II be present without H I or H$_2$, we need a radiation field that is capable of ionizing H I but not Zn II. This requires photons with wavelengths between 690 Å and 912 Å, which corresponds to a fairly narrow shell within an H II region. The ionization potentials to and from the other ions in this study imply similar qualitative limits on the corresponding ionization corrections.
We can make these qualitative limits quantitative using models of clouds illuminated by UV-bright stars. We do not know the volume density of the gas along each sightline, so we have cloud models with constant volume densities of 0.1, 1, 10, and 100 particles per cm$^3$. The spectral types of our background stars range from B0 to O2, so we run each cloud model with a B0 star and with an O2 star in order to bracket the range of possible ionization corrections; the stellar spectra come from Lanz and Hubeny (2003). Stellar spectra, gas cooling, and gas shielding all depend on the metallicity, so we run each star-cloud pair at the LMC and SMC metallicities. These and other model parameters are listed and explained in Appendix 2.7.2. For each combination of spectral type, volume density, and metallicity, we use Cloudy (version 13.02, Ferland et al., 2013) to calculate the cloud ionization structure.

From the output of these calculations, we derive ionization corrections and molecular hydrogen fractions as a function of HI and H$_2$ column density, where the molecular hydrogen fraction $f_{H_2}$ is

$$f_{H_2} = \frac{2N(H_2)}{2N(H_2) + N(\text{HI})}. \quad (2.3)$$

Ionization corrections for P II and Zn II are shown in Figure 2.6, along with the positions of our observations in the hydrogen column-molecular fraction plane. These corrections are for an O2 star in the LMC. Almost all of the stars towards which we observe have later spectral types and, correspondingly, lower-magnitude P II corrections. The P II ionization corrections for this specific combination of metallicity and illuminating star have larger absolute values than the ionization corrections for any other ion in any other model. In
Table 2.4: Photospheric abundances in the LMC and SMC. Abundances are given in the form \( \log_{10}(X/H) + 12 \). The first uncertainty is the standard deviation of the abundance value; the second is the standard deviation of the star-to-star dispersion.

<table>
<thead>
<tr>
<th>Element</th>
<th>LMC abundance [cm(^{-2})]</th>
<th>SMC abundance [cm(^{-2})]</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>7.94 ± 0.10 ± 0.05</td>
<td>7.52 ± 0.10 ± 0.04</td>
<td>1, 2, 3, 5, 6, 7, 8, 10, 11</td>
</tr>
<tr>
<td>O</td>
<td>8.50 ± 0.11 ± 0.03</td>
<td>8.14 ± 0.08 ± 0.04</td>
<td>1, 2, 3, 5, 6, 9, 10, 12</td>
</tr>
<tr>
<td>Mg</td>
<td>7.26 ± 0.08 ± 0.04</td>
<td>6.88 ± 0.06 ± 0.03</td>
<td>1, 2, 4, 5, 6, 9, 10, 11, 12</td>
</tr>
<tr>
<td>Si</td>
<td>7.35 ± 0.10 ± 0.02</td>
<td>6.96 ± 0.07 ± 0.09</td>
<td>1, 2, 4, 5, 6, 9, 10, 12</td>
</tr>
<tr>
<td>P</td>
<td>5.1</td>
<td>4.7</td>
<td>0</td>
</tr>
<tr>
<td>Cr</td>
<td>5.37 ± 0.07 ± 0.03</td>
<td>4.92 ± 0.10 ± 0.05</td>
<td>1, 2, 4, 9, 11, 12</td>
</tr>
<tr>
<td>Fe</td>
<td>7.32 ± 0.08 ± 0.03</td>
<td>6.89 ± 0.08 ± 0.03</td>
<td>1, 2, 4, 6, 9, 11, 12</td>
</tr>
<tr>
<td>Ni</td>
<td>5.92 ± 0.07 ± 0.03</td>
<td>5.52 ± 0.18 ± 0.07</td>
<td>1, 2, 4, 9, 11</td>
</tr>
<tr>
<td>Zn</td>
<td>4.31 ± 0.15 ± 0.15</td>
<td>4.02 ± 0.20 ± 0.14</td>
<td>8, 9, 11</td>
</tr>
</tbody>
</table>

all cases other than P II at the LMC metallicity illuminated by an O2 star, the ionization corrections are similar in sign and magnitude to those of Zn II in Figure 2.6, whose largest magnitude in the part of the diagram occupied by our observations is less than 0.1 decades. To within our typical uncertainties, which are about 0.1 decades, our ion abundances should be equal to the gas-phase elemental abundances.
Figure 2.7: Elemental depletions relative to the ISM abundances of the LMC and SMC plotted against the total column density of atomic and molecular hydrogen. Depletions towards the LMC and SMC are shown in red and blue.
2.3.3 Depletions

The depletion $\delta(X)$ of an element $X$ is the fraction of the element’s assumed reference, or gas- and solid-phase total, abundance $\epsilon_{\text{ref}}$ that we observe in the gas phase:

$$\delta(X) = \log_{10} \left( \frac{\frac{N(X)}{N_H}}{\frac{N(X)}{N_H}^{\text{ref}}} \right)$$

$$= \epsilon(X)_{\text{gas}} - \epsilon(X)_{\text{ref}},$$  \hspace{1cm} (2.4)

where $\epsilon_{\text{gas}}$ is the observed gas-phase abundance. The more negative $\delta$ is, the more of the element is missing, presumably in the solid phase. This makes $\delta$ a proxy for the gas-to-dust ratio.

In order to compute depletions, we need reference abundances. The composition of a star’s photosphere is a superposition of the ISM composition at the star’s formation time with the effects of various enrichment processes. This makes recently-formed stars that have not yet undergone self-enrichment good proxies for the present-day ISM composition.

There have been a number of spectroscopic measurements of the composition of luminous stars in both MCs. Because no individual study includes all of the elements we are interested in, we have to combine their measurements. We believe that we cannot simply average measurements across the studies because of significant between-study differences, repeat observations and analyses of the same stars by multiple studies, and missing uncertainty information. Instead, we partially pool measurements across studies using a
Table 2.5: Abundance uncertainties and depletion parameters. We describe the abundance uncertainties $\sigma\epsilon$ in Section 2.3.3 and the depletion parameters $\delta(X)_{0}$ and $A_X$ in Section 2.3.4.

<table>
<thead>
<tr>
<th></th>
<th>LMC</th>
<th>SMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>P:</td>
<td>$\sigma\epsilon$</td>
<td>...</td>
</tr>
<tr>
<td>$\delta(P)_{0}$</td>
<td>$-0.01 \pm 0.06$</td>
<td>$0.12 \pm 0.05$</td>
</tr>
<tr>
<td>$A_P$</td>
<td>$-0.97 \pm 0.11$</td>
<td>$-0.86 \pm 0.09$</td>
</tr>
<tr>
<td>Zn:</td>
<td>$\sigma\epsilon$</td>
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</tr>
<tr>
<td>$\delta(Zn)_{0}$</td>
<td>$-0.09 \pm 0.06$</td>
<td>$-0.03 \pm 0.06$</td>
</tr>
<tr>
<td>$A_{Zn}$</td>
<td>$-0.61 \pm 0.06$</td>
<td>$-0.61 \pm 0.06$</td>
</tr>
<tr>
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</tr>
<tr>
<td>$\delta(Si)_{0}$</td>
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<td>$0.03 \pm 0.09$</td>
</tr>
<tr>
<td>$A_{Si}$</td>
<td>$-1.10 \pm 0.13$</td>
<td>$-1.07 \pm 0.16$</td>
</tr>
<tr>
<td>Cr:</td>
<td>$\sigma\epsilon$</td>
<td>0.07</td>
</tr>
<tr>
<td>$\delta(Cr)_{0}$</td>
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<td>$-0.34 \pm 0.06$</td>
</tr>
<tr>
<td>$A_{Cr}$</td>
<td>$-0.85 \pm 0.12$</td>
<td>$-0.99 \pm 0.12$</td>
</tr>
<tr>
<td>Fe:</td>
<td>$\sigma\epsilon$</td>
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</tr>
<tr>
<td>$\delta(Fe)_{0}$</td>
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<tr>
<td>$A_{Fe}$</td>
<td>$-1.14 \pm 0.11$</td>
<td>$-1.17 \pm 0.09$</td>
</tr>
</tbody>
</table>

multilevel linear model (Browne and Draper, 2006). The model is described in detail in Appendix 2.7.3. Our adopted reference abundances, abundance uncertainties, and estimated intrinsic (i.e. location-to-location) abundance variances are listed in Table 2.4. Figure 2.7 shows the depletions we obtain by assuming these reference abundances.

In the next section, we analyze how depletions vary from sightline to sightline.

### 2.3.4 Linear depletion relations

We would like to use the depletions derived in the previous section to estimate ranges of solid-phase elemental abundances in the MCs and compare them
Figure 2.8: Fits of the Jenkins parametrization to elemental depletions in the LMC ISM. Data points include our observations, our analysis of archival FUSE data, and measurements from Roth and Blades (1997). Shaded regions show 68% credible intervals about the median fit. The black line is the MW best fit from Jenkins (2009).
Figure 2.9: Fits of the Jenkins parametrization to elemental depletions in the SMC ISM. Data points include our observations, our analysis of archival FUSE data, and measurements from Roth and Blades (1997), Welty et al. (2001), and Sofia et al. (2006). Shaded regions show 68% credible intervals about the median fit. The black line is the MW best fit from Jenkins (2009).
with abundances in the MW. For these estimates to be robust, we need a representative sample of each MC’s diffuse neutral medium. The difference between the lowest and highest depletions of Fe and P, which we measure using FUSE spectra, is approximately equal to the same difference in the MW, suggesting that the FUSE sample is representative of the same range of diffuse neutral medium conditions as is covered by MW datasets.

In order to make the same depletion range estimates for the elements that are only available in the (unrepresentative) COS sample, we need a way of combining its elemental information with the FUSE sample’s population information. For this purpose, we use the Jenkins depletion parametrization (Jenkins, 2009). In this parametrization, the observed depletion \( \delta(X)_i \) of element X along a sightline i is given by

\[
\delta(X)_i = \delta(X)_0 + A_X F^*_i, \tag{2.6}
\]

where \( \delta(X)_0 \) and \( A_X \) are the minimum and range of depletions of element X in the diffuse neutral medium, and \( F^*_i \) is a parameter representing the overall depletion level of sightline i. \( F^*_i \) is kept fixed for all elements along sightline i and \( \delta(X)_0 \) and \( A_X \) are kept fixed for an element X across all sightlines.

This model is underdetermined; we can rescale or shift combinations of parameters without changing the observers \( \delta(X)_i \). We can scale a set of slope parameters \( A_X \) by a constant \( C \) and scale the \( F^*_i \) values by \( 1/C \). At fixed \( A_X \), we can add a constant \( C \) to \( \delta(X)_0 \) and subtract a factor of \( C/A_X \) from the \( F^*_i \). We fix these two degeneracies and connect our \( F^*_i \) values with those of Jenkins (2009) by imposing the MW values as priors on \( \delta(Zn) \) and \( A_{Zn} \). We chose this
prior because its implied $F^*$ zero point location has a clear interpretation – $F^*$ is zero when the depletion of Zn is (up to uncertainty) zero. Since Zn is a volatile element in the MW, meaning that its minimum depletion in the DNM is zero, we expect it to continue to be volatile in more dust- and metal-poor galaxies such as the MCs.

Our priors on the remaining parameters are uninformative. We impose broad uniform priors on the other depletion zero points and slopes, a uniform prior with bounds $F^*_\min$ and $F^*_\max$ on the $F^*_i$, and uniform priors with bounds $(-3, 0.5)$ and $(0.5, 3)$ on, respectively, $F^*_\min$ and $F^*_\max$. The $F^*$ bounds are included as parameters because we do not a priori know how much of the possible $F^*$ range our observations will fill. For both MCs, the $F^*$ ranges ended up being approximately $(0, 1)$.

We implemented and generated samples from this model using the Bayesian statistical analysis module PyMC (Patil, Huard, and Fonnesbeck, 2010). Our fits to the LMC and SMC depletions are shown in Figures 2.8 and 2.9. For each element, the reference abundance uncertainties, depletion zero points $\delta(X)_{0}$, and depletion slopes $A_X$ are listed in Table 2.5. The depletion zero points of the refractory elements Si, Cr, and Fe are significantly less negative in the SMC than they are in MW or LMC. The minimum Si depletion is particularly notable, since it is consistent with 0. However, if we include the uncertainty of the reference Si abundance, the minimum Si depletion is also within 1σ of 0.13 in logarithmic units, which corresponds to 1/4 of the Si being out of the gas phase. The depletion slope of Cr in the LMC and SMC is similar and significantly smaller than in the MW. The other depletion slopes do not
change significantly between the three galaxies. In the common interpretation of depletion variations within a galaxy, depletion zero points are associated with the composition of the refractory dust cores while depletion slopes are associated with the rate at which dust mantles either grow or are destroyed. By this interpretation, the fractional gas-to-solid transfer rate is roughly constant between galaxies while the refractory core composition changes. We will discuss the implications of these zero point and slope changes further in Sections 2.5.3 and 2.5.4.

2.4 Quantitative analysis: solid-phase

In this section, we describe our derivation of solid-phase abundances and GDRs from measured gas-phase and assumed total ISM abundances.

2.4.1 Solid-phase abundances

We can reasonably assume that all of the metals that are missing from the gas-phase are in dust and can use this assumption to derive a solid-phase abundance $\varepsilon(X)_{\text{dust}}$:

$$\varepsilon(X)_{\text{dust}} = \log_{10} \left(10^{\varepsilon(X)_{\text{ref}}} - 10^{\varepsilon(X)_{\text{gas}}} \right) \quad (2.7)$$

$$= \log_{10} \left(10^{\varepsilon(X)_{\text{ref}}} \left(1 - 10^{\delta(X)} \right) \right), \quad (2.8)$$

where $\varepsilon(X)_{\text{ref}}$ is the reference (i.e. theoretical gas- and solid-phase total) abundance, $\varepsilon(X)_{\text{gas}}$ is the gas-phase abundance, and $\delta(X)$ is the depletion of the gas-phase abundance relative to the reference abundance. By combining the
depletion-based formulation of Equation 2.8 with the depletion parametrization described in Section 2.3.4, we can get a continuous empirical relation between \( F^* \) and the solid-phase abundance of an element. We explore solid-phase abundances and related quantities further in Sections 2.4.2 and 2.4.3.

### 2.4.2 GDRs

We can combine all of the elements’ solid-phase abundances to compute a gas-to-dust mass ratio:

\[
\frac{1}{GDR} = \frac{\Sigma_{\text{dust}}}{\Sigma_{\text{gas}}} \approx \frac{1}{m_H} \sum_X m_X 10^{\epsilon(X)}_{\text{dust}},
\]

where \( X \) ranges over all elements and \( m_X \) is the atomic mass of element \( X \). This expression can be rewritten in terms of depletions \( \delta(X) \):

\[
\frac{\Sigma_{\text{dust}}}{\Sigma_{\text{gas}}} \approx \frac{1}{m_H} \sum_X m_X 10^{\epsilon(X)}_{\text{ref}} \left( 1 - 10^{\delta(X)} \right).
\]

In the MW, the only elements that contribute significantly to this sum are C, O, Mg, Si, Fe, and Ni. All other elements have low reference abundances and/or negligible depletions. If we assume that the composition of dust in the MCs is even remotely like that of dust in the MW, we can restrict the sum in Equation 2.9 to those elements without missing much of the total dust mass.

Since most of our sightlines do not have Si measurements and all of our sightlines do not have C, O, Mg, or Ni measurements, we compute GDRs using the linear depletion relations from Section 2.3.4. We use our LMC and SMC relations for Si and Fe and the MW relations from Jenkins (2009) for C, O, Mg and Ni. GDRs derived from these combination of depletion
Figure 2.10: We show the surface mass GDR as a function of the over-all depletion level $F^*$, which increases from low depletion in all elements ($F^* = 0$) to high depletion in all elements ($F^* = 1$). The MW, LMC, and SMC are denoted by black, red, and blue. The solid lines are derived by applying Equation 2.10 to each galaxy’s best-fit reference abundances and the MW’s best-fit depletion relations (Jenkins, 2009). The shaded regions are derived by applying Equation 2.10 to each galaxy’s reference abundances and depletion relations, both with uncertainties. The vertical extent of the shaded regions represent the 84% posterior credible interval of the GDR at each value of $F^*$. 
relations are shown as red (LMC) and blue (SMC) shaded regions in Figure 2.10. For comparison, we show the MW’s GDR in black and GDRs derived by assuming MW depletions at LMC and SMC reference abundances as solid red and blue lines. We will refer to these GDRs as abundance-scaled MW GDRs to differentiate them from the first set, which we will refer to as the LMC and SMC GDRs.

We can make three main observations about this figure. First, regardless of which set of depletions we adopt, the GDR of all three galaxies changes by a factor of 2 from $F^* = 0$ to $F^* = 1$. This suggests that there is a significant amount of dust destruction and/or growth in the DNM of the LMC, SMC, and MW. Second, the GDRs of the LMC and the high-depletion part of the SMC are approximately the same as the corresponding abundance-scaled MW GDRs. Third, the GDR of the low-depletion part of the SMC is higher than the SMC-abundance-scaled MW GDR. The second observation may be an artifact of our assumptions, as the MC depletion relations that we do observe are always either as depleted or less depleted than the corresponding MW relations. This suggests that the depletions we are assuming for some or all of C, O, Mg, and Ni are too high and implies that even the GDRs which assume MC depletions for Si and Fe are most likely underestimates. The third observation suggests that the dust-to-metals ratio (DMR) decreases with decreasing metallicity.

At and above the metallicity of the SMC, the (galaxy-averaged) DMR is constant while below the SMC metallicity, the DMR ratio decreases with decreasing metallicity (Rémy-Ruyer et al., 2014). From the first observation,
we conclude that the DMR decreases by a factor of at least 2 within a galaxy. At medium to high over-all depletion (i.e. at $F^* = 1$ or 0.5), the DMR does not change from the MW to the LMC to the SMC. However, at low over-all depletion (i.e. at $F^* = 0$), the DMR is constant from the MW to the LMC but decreases from the LMC to the SMC. This suggests that in diffuse, low-depletion gas, the DMR stops being constant at a higher metallicity than in more dense, higher-depletion gas.

2.4.3 The solid-phase stoichiometry of silicon and iron

As shown in the previous section, the GDR is not constant throughout the DNM of each galaxy. We now use depletion measurements to show that throughout each galaxy’s DNM, the dust stoichiometry, or its relative bulk composition, also varies. Using Equation 2.7, we have computed the solid-phase abundance of Si and Fe towards each sightline for which gas-phase column density measurements are available. These solid-phase abundances are shown in Figure 2.11, along with solid-phase abundances corresponding to the observed range of Si and Fe depletions in the MW (Jenkins, 2009). The solid-phase Fe abundance is approximately constant across each galaxy, while the solid-phase Si abundance changes from the least- to the most-depleted sightlines by a factor of about 2.

In all three galaxies, the Fe:Si abundance ratio in dust ranges from about 2:1 along the least-depleted sightlines to about 1:1 along the most-depleted sightlines. Since we are merely measuring the bulk dust composition, we cannot use these ratios to determine the composition of each dust subspecies.
Figure 2.11: We show the solid-phase Fe abundance as a function of the solid-phase Si abundance. Data points from the SMC (blue) and LMC (red) are derived from reference abundances for the appropriate galaxy and gas-phase abundances using Equation 2.7, and data point error bars include uncertainties in both quantities. The MW region (black) is derived from solar abundances and MW depletions (Jenkins, 2009) using Equation 2.8. The dashed grey lines mark levels of constant stoichiometric Fe to Si ratio. Within each galaxy, the over-all depletion level increases from left to right.
Nevertheless, the constant Fe abundance and variable Si abundance suggest that the process by which most of the Fe forms into dust is different from the process by which at least half of the Si forms into dust. This suggests that the Fe-rich dust component is either particularly resilient, if most of the abundance variations are due to dust destruction, has a faster growth rate, if most of the abundance variations are due to ISM dust growth, or some combination of the two. While this last fact has been known for MW dust for quite some time (see, e.g. Savage and Sembach, 1996), we can now also confirm that it holds in other galaxies.

The least-depleted sightlines in the SMC may have a greater Fe:Si ratio than the MW or LMC. Draine and Hensley (2012) argue that in the SMC, but not in the MW or LMC, a large fraction of solid phase Fe may be in the form of resilient pure iron or iron oxide nanoparticles. An elevated Fe:Si ratio is consistent with such a scenario. We note, however, that our measurements are also consistent within the uncertainties with there being no change in the Fe:Si ratio from galaxy to galaxy.

2.5 Discussion

2.5.1 The ISM metallicity in the Magellanic Clouds

Studies of field star abundances in the MCs (e.g. Carrera et al. 2008; Cioni 2009) have found mild metallicity gradients as a function of galactocentric distance. The metallicities of stars of similar ages but different galactocentric radii tend to be the same, suggesting that these gradients are due to star formation occurring at different times in different locations. If the observed
Figure 2.12: Bars show the distribution of measured gas-phase P (dark color) and Zn (light color) abundances relative to each element’s solar abundance; vertical lines show the typically assumed metallicities of the LMC and SMC. P and Zn are relatively volatile elements. Their abundance at minimum depletion is a proxy for the ISM metallicity. Abundances greater than the mean MC metallicities (vertical lines) would indicate small-scale metallicity enhancements. We see no evidence for localized metal enrichment along our sightlines.
gradients were instead due to ISM inhomogeneities, stars that formed at the same time in different locations would have different metallicities.

We can use the abundances of our more volatile elements (P and Zn) to estimate the amount of localized metal enrichment towards some of our sightlines. At the lowest depletion levels, the gas-phase abundances of P and Zn should approach their total ISM abundances. An undepleted metal-enriched sightline would have a (local) metallicity greater than its corresponding galactic mean. Figure 2.12 shows the distribution of P and Zn abundances in the MCs relative to the solar abundance. While there are six apparently P-enriched and one apparently Zn-enriched sightlines across the pair of galaxies, this can be explained as the result of measurement uncertainty. Sightlines with very little depletion tend to have low, and as a result uncertain, total column densities. We do not find evidence for significant localized metal enrichment.

Since even the relatively volatile elements in this study can be significantly depleted, we cannot exclude the possibility that some of our sightlines are metal-poor. Our maximum measured gas-phase P and Zn abundances are consistent with the typically assumed MC metallicities of 1/2 and 1/5 times the solar metallicity for the LMC and SMC, respectively.

2.5.2 Previous depletion studies of the Magellanic Clouds

Depletion studies of the MCs have been either medium-sized (< 20 depletion measurements) surveys of single elements or multi-element case studies of single sightlines. All of the targets in the multi-element case studies of the MCs are part of our FUSE sample, and have been included in our analyses as described in...
Figure 2.13: Fe (from this work) and Ti (Welty and Crowther, 2010) depletions in the LMC (red) and SMC (blue). For comparison, the linear depletion relation for Fe and Ti in the MW from Jenkins (2009) is shown in black.
Section 2.2.3.

Welty and Crowther (2010) presented an optical survey of titanium (Ti) towards approximately twenty stars in either MC. Figure 2.13 shows a comparison of our Fe depletions and their Ti depletions for the sightlines which are included in both surveys. LMC and SMC sightlines are shown in red and blue. The black line represents the typical correlation of Fe and Ti depletions in the MW (Jenkins, 2009). Across both galaxies, all but two of the targets are above this line, meaning that at fixed Fe depletion, MW sightlines tend to contain a smaller fraction of gas-phase Ti than MC sightlines.

2.5.3 The evolution of gas-phase abundances with metallicity

Gas-phase abundance variations between pencil beam observations within a single galaxy can be succinctly summarized by the per-sightline depletion strength $F^*$ of the linear depletion relations of Section 2.3.4. Because these within-galaxy variations are quite large, with depletion-driven gas-phase abundance differences between sightlines of up to of order a decade, galaxy-to-galaxy comparisons should be not of individual sightlines but of galaxy-wide depletion relations. We will use the intrinsic depletion zero points and slopes of the linear depletion relations to summarize each galaxy’s depletion relation. While we do not have a quantitative "depletion-relation-relation" to describe variations between ensembles of pencil beam observations of different galaxies, we can use the changes we see from the MW to the LMC to the SMC as a qualitative depletion-relation sequence, at least to metallicities above that of the SMC. Starting from the MW and moving towards lower metallicity,
Figure 2.14: Blue and red data points are abundance measurements for the SMC and LMC from our COS sample. The black line is based on a fit to gas-phase abundances in the DNM of the MW (Jenkins, 2009). In the top panel, the red (LMC) and blue (SMC) lines are the MW line shifted to each galaxy’s metallicity. In the bottom panel, red and blue lines are the LMC and SMC’s linear depletion relations (see Sec.2.3.4). Since all of the LMC and SMC points in the top panel are above their corresponding lines, gas-phase abundances in the MCs differ from those of the MW by more than just the relative abundance differences.
intrinsic depletion zero points decrease in magnitude, while depletion slopes remain approximately unchanged. The intrinsic depletion zero points of P and Zn, whose magnitude is already consistent with zero, do not change.

Comparing depletion relations between galaxies takes a (generally) prohibitive amount of information. Computing an abundance requires absorption-derived hydrogen columns, computing an intrinsic depletion requires galaxy-specific reference abundances (see Sec.2.3.3), and computing a depletion relation requires a representative sample of intrinsic depletions. In a more typical case, one instead has to work with a metallicity instead of a reference abundance for each element and less than ten sightlines per galaxy. This was true of depletion studies of the MCs, remains true of depletion studies of other local galaxies (e.g. Welsh and Lallement, 2013; James et al., 2014), and is, in a sense, intrinsically true of DLA and sub-DLA studies.

A common exploratory technique in depletion studies of small samples involves making a comparison between a new measurement and some typical MW values for the abundance of a volatile element and the abundance ratio between the same volatile element and a refractory element. If one assumes that the MW depletion relation applies in the new measurement’s galaxy, one can estimate each element’s depletion and reference abundance. This type of exploratory analysis, if applied to the LMC or SMC, would be incorrect. We show an example of this type of exploratory analysis in the top panel of Figure 2.14. The lines in this panel are the MW depletion relation shifted to the metallicity of the MW (black), LMC (red), and SMC (blue). The diagonal portion of each line corresponds to a depletion strength ($F^*$) range of 0 (top
right) to 1 (bottom left), and includes what Savage and Sembach (1996) refer to as "warm disk" and "cool disk" depletion patterns. The vertical line extending upwards from $F^* = 0$ corresponds to the "diffuse halo" depletion pattern range from the same work. These metallicity-shifted MW depletion relations are inconsistent with our observations.

In the bottom panel of Figure 2.14, the lines are our MC depletion relations from 2.3.4. Examining these lines gives us a qualitative visual version of the earlier statement that intrinsic depletion zero points become smaller with decreasing metallicity. On a volatile abundance versus refractory-to-volatile ratio plot, a galaxy’s intrinsic depletion zero point corresponds to the top right end of that galaxy’s representative line. Because, at least in these three galaxies, the intrinsic depletion zero point becomes less negative with decreasing metallicity, the top right end of each galaxy’s line is shifted up and to the left as the metallicity decreases from solar (the MW) to 1/2 solar (the LMC) to 1/5 solar (the SMC). The fraction of metals in dust decreases with decreasing metallicity.

### 2.5.4 The Magellanic Clouds and damped Lyman-$\alpha$ systems

DLAs are reservoirs of neutral gas with H I column densities greater than $2 \times 10^{20} \text{ cm}^{-2}$. For a review of DLA properties, see Wolfe, Gawiser, and Prochaska (2005). Metal abundances in DLAs range from approximately solar to less than 1/100 of solar, making the DLA population a valuable resource for understanding cosmic chemical evolution. The conversion between observed and intrinsic abundances is a long standing problem in DLA studies, since
Figure 2.15: A comparison between abundances relative to solar in DLAs (data points, Vladilo et al. 2011, Rafelski et al. 2012) and the diffuse neutral media of the MW, LMC, and SMC (solid black, red, and blue lines, MW values from Jenkins 2009, LMC and SMC values from Section 2.3.4 of this work).
one observes a single sightline and needs to deconvolve the effects of metallicity, abundance variations (especially $\alpha$-enrichment), and depletion (Pettini, Boksenberg, and Hunstead, 1990; Sembach et al., 1995; Kulkarni, Fall, and Truran, 1997; Prochaska and Wolfe, 2002; Meiring et al., 2006; Rafelski et al., 2012; Vladilo et al., 2011; De Cia et al., 2013).

The depletion part of this deconvolution problem is usually approached using some variation of the metallicity-scaled MW technique described in the previous section (see, e.g. Rafelski et al., 2012; De Cia et al., 2013). Now that we have depletion relations from multiple galaxies over a range of metallicities, we are no longer limited to just the MW. While we do not have a quantitative model for the evolution of galaxy-wide depletion relations, we do have the previous section’s qualitative picture. Figure 2.15 compares the measured Fe-to-Zn and Si-to-Zn ratios and Zn abundances in DLAs with the corresponding ratios and abundances derived from the depletion relations of the MW, LMC and SMC. We first examine DLAs that have more positive Zn abundances or more negative refractory-to-volatile ratios than the SMC. The evolution of the Si-to-Zn ratio with the Zn abundance in our galaxy sample and in this DLA subsample appears to be the same. The upper envelope of the Fe-to-Zn ratio is perhaps slightly less negative in this subsample of DLAs than in our galaxies, but the separation of the upper and lower envelopes along the direction of intra-galaxy dust evolution (i.e. parallel to the galaxy lines) is the same as the extent of the galaxy lines. If we interpret a single DLA to be a pencil-beam-sized region in a larger system that can contain a variety of neutral medium conditions, the chemical evolution of the neutral ISM in these systems appears
to be quite similar to that of the neutral ISM in the MCs or MW.

Interpreting the measurements with sub-SMC Zn abundances is more difficult. Applying a metallicity-scaled version of the MW depletion relation does not give us an adequate description of gas-phase abundances in the MCs, so metallicity-scaling the SMC depletion relation may not necessarily give us an adequate description of gas-phase abundances in low-metallicity DLAs. The shape of the upper and lower envelopes of the DLA abundances and abundance ratios in Figure 2.15 broadly suggests that the concurrent metallicity and dust-to-metals ratio evolution that applies from the MW to the SMC continues to apply to even lower metallicities. By applying the previous paragraph’s interpretation of a DLA as a single sightline through some system and assuming that the metallicity and dust-to-metals ratio of these systems evolves in a consistent way, one could come up with a more quantitative version of this statement. We leave this exercise for the future.

2.5.5 Gas-to-dust ratios in the Magellanic Clouds

In Section 2.4.2, we computed GDRs for the DNM of the Magellanic Clouds from depletions. These GDRs are summarized in Figure 2.10. The DNM of each MC contains (spatially separate) gas with a range of overall depletion levels. In the figure, this level increases from left to right, as the amount of dust per amount of gas increases. The GDRs of the least depleted sightlines in the LMC and SMC DNM are 455-565 and 1540-2065; the GDRs of the most depleted sightlines are 190-245 and 480-595. We have compared these GDRs with values from the literature and found no significant discrepancies.
<table>
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<th>Location</th>
<th>GDR</th>
<th>Method</th>
<th>Reference</th>
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<td>Ext</td>
<td>Tumlinson et al. (2002)</td>
</tr>
<tr>
<td>SMC Wing</td>
<td>480-720</td>
<td>Ext</td>
<td>Gordon et al. (2003)</td>
</tr>
<tr>
<td>SMC Bar</td>
<td>850-1275</td>
<td>Ext</td>
<td>Gordon et al. (2003)</td>
</tr>
<tr>
<td>SMC DNM</td>
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<td>Em</td>
<td>Bot et al. (2004)</td>
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<td>SMC, global average</td>
<td>700</td>
<td>Em</td>
<td>Leroy et al. (2007)</td>
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<td>SMC Tail</td>
<td>850-1550</td>
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<td>SMC, CO-detected regions</td>
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<td>Em</td>
<td>Leroy et al. (2011)</td>
</tr>
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<td>This work</td>
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<td>Tumlinson et al. (2002)</td>
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<td>Em</td>
<td>Gordon et al. (2014)</td>
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<tr>
<td>LMC DNM</td>
<td>185-585</td>
<td>Dep</td>
<td>This work</td>
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</table>

Table 2.6: GDR measurements in the LMC and SMC. Some of the sources give GDRs as factors of the MW GDR. These relative GDRs were converted to absolute values by assuming an MW GDR of 100-150. These works used three types of methods for determining dust amounts. Extinction (Ext) and emission (Em) based methods measure dust optical depths, which are then converted to amounts of dust using dust opacities. Depletion (Dep) based methods measure gas phase abundances, which are subtracted from intrinsic abundances to get solid phase abundances.
The literature values are given in Table 2.6. All of their uncertainties have some overlap with the our GDR ranges. This does not mean that our GDR for any single depletion level is accurate. All of the values in the table other than ours are averages over different DNM conditions or, in some cases, multiple ISM phases. An average over a (possibly) wide range of GDRs with unknown proportions of mass at each GDR does not contain enough information to draw that sort of conclusion. The decrease in GDR from averages over more diffuse regions to averages over denser regions is heartening, though not conclusive.

2.6 Summary

In order to study the gas and dust content of the LMC and SMC, we have obtained and analyzed 16 HST COS NUV spectra and analyzed 85 archival FUSE FUV spectra towards the Large and Small Magellanic Clouds. From these spectra, we have measured P II, Zn II, Si II, Cr II, and Fe II column densities. We have combined these measurements with H I and H2 column densities and photospheric abundances of LMC and SMC stars from the literature to compute intrinsic elemental depletions, solid-phase elemental abundances, and GDRs. We see large variations in gas-phase abundances, depletions, solid-phase abundances, and GDRs from sightline to sightline within each galaxy. The depletion variations can be accurately described using a linear depletion relation of the type defined for the MW by Jenkins (2009), but with different linear coefficients.

We find that the ISM properties of the LMC are, up to metallicity, quite
similar to those of the MW while the ISM properties of the SMC have some significant differences. When we compare gas-phase abundances in the LMC and SMC with gas-phase abundances in damped Lyman-\(\alpha\) systems, we find a considerable amount of overlap. Within this overlap region, the gas-phase abundance ranges of the MCs and DLAs are very similar. Regardless of whether this similarity is meaningful, we caution against assuming that MW depletion patterns apply to low-metallicity systems.

Below, we list a number of more specific results.

1. The minimum Si depletion in the SMC is consistent with zero while the Fe depletion along the same sightline is substantial, suggesting that the composition of some dust in the MW and SMC differs.

2. The volatile elements P and Zn have non-zero depletions along most of our sightlines through both MCs. The maximum P and Zn depletions in the MW, LMC, and SMC are the same to within the uncertainties.

3. Si, Cr, and Fe are systematically less depleted in the SMC than in the LMC or MW.

4. We find GDR ranges of 190-565 in the LMC and 480-2100 in the SMC. These ranges are broadly consistent with GDR values from the literature.

5. The GDRs of pencil-beam-sized parcels of neutral medium vary by a factor of 2 in the MW and LMC and by a factor of 5 in the SMC. The GDR variations within each galaxy suggest some combination of dust evolution in the neutral medium and rapid cycling of interstellar matter between the neutral medium and dense molecular clouds.
2.7 Appendix

2.7.1 Analyzing a spectrum

The purpose of our model of a spectrum is to measure the total column density $N_{MC}^{X}$ of each species $X_{\ell}$ in the observation-appropriate Magellanic Cloud. We marginalize over, meaning integrate over the posterior probability distribution of, every other model parameter. The other important high-level quantities are the (ISM absorption-free) continuum flux as a function of wavelength $c(\lambda)$ and the distribution of $N_{\ell}^{X}$ as a function of Doppler velocity $N_{\ell}^{X}(v)$. To convert these quantities to observables, we first use the $N_{\ell}^{X}(v)$ to compute a transmittance function $T(\lambda)$. Then, we convolve the product of the continuum and transmittance with an instrumental line-spread function (LSF) $L(\lambda, \lambda')$ to get a model flux $f(\lambda)$. This model flux is the mean of a multivariate normal (MVN) distribution, from which we assume the data $y(\lambda)$ have been drawn. The covariance matrix $\Sigma$ of this MVN distribution is the sum of a diagonal measurement uncertainty matrix $\Sigma_{\text{meas}}$ and a not necessarily diagonal continuum uncertainty matrix $\Sigma_{\text{cont}}$.

We fit for the ISM absorption-free continuum emission using Gaussian process (GP) regression and prediction (Rasmussen and Williams, 2006). The regression and prediction were done using the GP code george (Ambikasaran et al., 2015). Our main motivation for using a GP rather than, for instance, splines is that the posterior predictive distribution of a GP conditioned on observations can be used to exactly compute the predicted values’ covariant uncertainties. This covariant continuum uncertainty is an important part of
our model’s error budget, particularly for high SNR measurements.

We run the GP regression on a subset of the data that we find, by visual inspection, to be free of ISM absorption, then compute the predicted mean and covariance matrix of the full dataset. This subset comes as close to the ISM absorption as possible in order to minimize the size of the prediction region. For the GP kernel, we use the sum of a square exponential kernel, a quadratic kernel, and the measurement uncertainties of the ISM-free subset. We fix the lengthscale of the square exponential kernel to be 6 Å and fit for the rest of the kernel parameters.

The dashed line in each panel of Figure 2.4 is an example of a continuum fit. The uncertainty of the full spectrum model, which includes the continuum uncertainty, is shown as a gray region in this figure.

Instead of explicitly modeling the transmittance $T(\lambda)$, we instead model the species’ column density distributions $N_{X_\ell}(v)$ as a function of Doppler velocity and use a deterministic non-linear transformation to convert that to $T(\lambda)$. The column density distributions are split into spatio-kinematic groups $S_j$, which are velocity ranges that we a priori assign to the MW, an I/HVC, or a MC, and the $S_j$ are further split into components $t = 1, \ldots, T_{S_j}$. Each component has a central velocity $\hat{v}_{S_j}^{t}$, a width $b_{S_j}^{t}$, and, for each species $X_\ell$, a fraction $\alpha_{S_j t}^{X_\ell}$ of the group-level column density of $X_\ell$. The column density of species $X_\ell$ in component $t$ is then $\alpha_{S_j t}^{X_\ell} \times N_{S_j t}^{X_\ell}$; note that the sum of the $\alpha$ for a single species over all of the components of a group are equal to 1.

The column density distribution of a species is the sum of the group level distributions, which are in turn the sum of the component level distributions.
The column density distribution of a single component is

\[ N_{S_{ij}}^{X_i}(v) = \frac{\sqrt{2}}{\sqrt{\pi}b_{S_{ij}}^{X_i}} \alpha_{S_{ij}}^{X_i} \exp \left( -\left( \frac{v - \sigma_{S_{ij}}^{X_i}}{b_{S_{ij}}^{X_i}} \right)^2 \right) \]  

(2.11)

and the full column density distribution of a single element is

\[ N^X_i(v) = \sum_{j=1}^{J} \sum_{t=1}^{T_j} N_{S_{ij}}^{X_i}(v). \]  

(2.12)

We use this two-level formalism because we believe that the groups are physically meaningful while the components may or may not be. The groups are physically meaningful because they correspond to different galaxies with reasonably well-separated systemic velocities. We believe that column density that has been assigned to a given group most likely actually arises in the corresponding galaxy. The components are not necessarily meaningful because, firstly, our instrumental LSFs are broader than the expected “individual” components, secondly, components that are distinct in velocity are not necessarily distinct spatially, and thirdly, the fragmentation of a continuous density into discrete subcomponents is almost always not unique. One consequence of the third point, particularly when the first point applies, is that we cannot even define a unique number of components. This is especially true when our observations are a product of the transmission function, which is a non-linear transformation and superposition of the column density distributions, with the uncertain continuum. Instead of trying to choose a fixed number of unphysical components, we marginalize over it. This means that the dimension of our parameter space is not constant.
We generate samples from the posterior probability over this variable-dimensional parameter space, using the Reversible-Jump Markov Chain Monte Carlo (RJMCMC) algorithm (Green, 1995). RJMCMC is a type of MCMC that can be applied to variable-dimensional parameter spaces. It works by considering each fixed-dimensional parameter space as a subspace of some larger, overarching parameter space. One then defines different Markovian steps for moving around within each fixed-dimensional subspace and between ‘adjacent’ fixed-dimensional subspaces. Further details of this framework are beyond the scope of this appendix and can be found in (Green, 1995). We use these samples to build posterior probability distributions for each species’ column density in the LMC or SMC and the model flux at each wavelength. The 16-th and 84-th percentiles of the column density posterior probability distributions are shown as error bars in Figure 2.5. The 5-th, 16-th, 84-th, and 95-th percentiles of the model flux marginals are shown as shaded regions in Figure 2.4. These marginals include measurement uncertainty, continuum uncertainty, and the possibility of observationally similar but physically different velocity component structures.

2.7.2 Cloudy parameters

Here, we provide the complete list of input parameters needed to reproduce the photoionization calculations described in section 2.3.2. These calculations were done using version 13.02 of the Cloudy photoionization code (Ferland et al., 2013). All of the models are of a constant-density cloud illuminated by a star $10^{16}$ cm from the cloud surface. We compute models with cloud volume
densities of 0.1, 1, 10, and 100 cm$^{-3}$. The cloud composition is given by the ‘abundances ism’ command, scaled to the appropriate metallicity (0.5 for the LMC, 0.2 for the SMC) using the ‘metals grains’ command. We run each cloud model for a B0-type and an O2-type illuminating star of the appropriate metallicity using stellar atmosphere models from Lanz and Hubeny (2003).

In addition to the illuminating star, the incident radiation field includes the cosmic microwave background and the local MW radiation field (‘table ism’) scaled by a factor of 4 in the LMC (Bernard et al., 2008) and 10 in the SMC (Sandstrom et al., 2010). We include the local cosmic ray background using the ‘cosmic rays background’ command.

### 2.7.3 Elemental abundance meta-analysis

In this appendix, we describe a multilevel model for the mean elemental abundance $\mu$ of an element from a collection of possibly biased studies with some repeated observations. A description of multilevel models and their application to meta-analysis problems can be found in Chapter 5 of Gelman et al. (2013). We can split the model into four blocks – population level, study level, individual star level, and study-star level.
The population level includes the mean abundance $\mu$, the intrinsic star-to-star variance $\sigma_{\text{star}}$, and the between-study variance $\sigma_{\text{study}}$:

\[ \mu \sim \text{Normal} \left( \mu = \mu_\odot + Z_{MC}, \sigma^2 = 0.5^2 \right) \]  
(2.13)

\[ \sigma_{\text{star}} \sim \text{Exponential} \left( \lambda = 5 \right) \]  
(2.14)

\[ \sigma_{\text{study}} \sim \text{Exponential} \left( \lambda = 5 \right) , \]  
(2.15)

where $\mu_\odot$ is the solar abundance of the relevant element, $Z_{MC}$ is the metallicity of the relevant Magellanic Cloud, and the notation “$x \sim \text{Distribution}$”, as in $\mu \sim \text{Normal}$, means that the specified distribution is our prior for $x$. The study and star levels include the bias terms $\Delta_{\text{study}, j}$, for study-wide effects, and $\Delta_{\text{star}, k}$, for star-to-star variations:

\[ \Delta_{\text{study}, j} \sim \text{Normal} \left( \mu = 0, \sigma^2 = \sigma_{\text{study}}^2 \right) \]  
(2.16)

\[ \Delta_{\text{star}, k} \sim \text{Normal} \left( \mu = 0, \sigma^2 = \sigma_{\text{star}}^2 \right) \]  
(2.17)

The study-star level consists of observations $y_{j,k}$ and observational precisions $\tau_{j,k}$:

\[ \tau_{j,k} \sim \text{Gamma} \left( \alpha = \alpha_{\text{study}, j}, \beta = \beta_{\text{study}, j} \right) \]  
(2.18)

\[ y_{j,k} \sim \text{Normal} \left( \mu = \mu + \Delta_{\text{study}, j} + \Delta_{\text{star}, k}, \sigma^2 = 1/\tau_{j,k} \right) \]  
(2.19)

\[ \alpha_{\text{study}, j} \equiv \left( \frac{\mu_{\tau_{\text{study}, j}}}{\sigma_{\tau_{\text{study}, j}}} \right)^2 ; \beta_{\text{study}, j} \equiv \frac{\mu_{\tau_{\text{study}, j}}}{\sigma_{\tau_{\text{study}, j}}^2} , \]  
(2.20)

where $\mu_{\tau_{\text{study}, j}}$ is the typical precision of the measurements in study $j$ and $\sigma_{\tau_{\text{study}, j}}$. 

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is the dispersion in the typical precision.

We implemented this model using PyMC (Patil, Huard, and Fonnesbeck, 2010) and generated samples from the posterior probability distribution using the No-U Turn Sampler. We ran each element’s MCMC chain for 500 burn-in steps and 5000 kept steps starting from the maximum a posteriori value, which, by visual inspection, appeared to be a long-enough burn-in phase for convergence.
Chapter 3

Analytic marginalization of absorption line continua

1Absorption line spectroscopy is a powerful way of measuring properties of stars and the interstellar medium. Absorption spectra are often analyzed manually, an approach that limits reproducibility and which cannot practically be applied to modern datasets consisting of thousands or even millions of spectra. Simultaneous probabilistic modeling of absorption features and continuum shape is a promising approach for automating this analysis. Existing implementations of this approach use numerical methods such as Markov chain Monte Carlo (MCMC) to marginalize over the continuum parameters. Numerical marginalization over large numbers of continuum parameters is too slow to be convenient for exploratory analysis, can increase the dimensionality of an inference problem beyond the capacity of simple MCMC samplers, and is in general impractical for the analysis of large datasets. When continua are parameterized as linear functions such as polynomials or splines, it is possible to reduce continuum parameter marginalization to an integral over a

1Adapted from a paper submitted to The Astronomical Journal (Tchernyshyov, 2019).
multivariate normal distribution, which has a known closed form. In addition to speeding up probabilistic modeling, analytic marginalization makes it trivial to marginalize over continuum parameterizations and to combine continuum description marginalization with optimization for absorption line parameters. These new possibilities allow automatic, probabilistically justified continuum placement in analyses of large spectroscopic datasets. We compare the accuracy to within which absorption line parameters can be recovered using different continuum placement methods and find that marginalization is in many cases an improvement over other methods. We implement analytic marginalization over linear continuum parameters in the open-source package amlc.

3.1 Introduction

Absorption lines contain information on the composition and properties of interstellar matter (ISM) and stellar atmospheres. To extract this information, it is necessary to decompose the spectrum into absorption features and the intrinsic flux, typically referred to as the continuum, produced by the illuminating background source towards which the absorption is seen. The most common way of doing this separation has been manually finding regions in a spectrum that do not contain absorption features, fitting a function to these regions, and using this function to interpolate over the absorption features. Given the longevity and popularity of this approach, it is clear that it can produce acceptable results. It does, however, have two important weaknesses. The first is that every spectrum must be examined and interacted with by a
human. This cannot efficiently be done for datasets containing thousands or even millions of spectra. The second is that it is unlikely that the absorption parameter estimator this procedure implicitly defines uses data efficiently. There is variance between analyses done by different humans as well as between analyses done by the same human at different times. If there is a subset of analysts whose estimates are the most accurate and precise, then the estimates of the rest are using the available data inefficiently.

An alternative approach is to infer absorption line and continuum parameters simultaneously. To improve the accuracy of the inferred absorption line parameters, it can be useful to marginalize over, rather than fit for, the continuum parameters. This has been done in packages meant for the analysis of absorption lines from both the ISM (BayesVP, Liang, Kravtsov, and Agertz 2018) and stellar atmospheres (Starfish, Czekala et al. 2015, and sick, Casey 2016). In these packages, continuum parameter marginalization is done numerically, using Markov chain Monte Carlo (MCMC). As the authors of two of these packages point out, including large numbers of continuum parameters in MCMC sampling leads to long convergence and autocorrelation times. To keep the number of continuum parameters low, these packages either do not support (BayesVP) or advise against (sick) including continuum parameters when simultaneously analyzing multiple spectral segments.

Even when there are few continuum parameters, using MCMC to analyze a modern spectroscopic dataset consisting of thousands or even millions of spectra will be computationally demanding. Probablistic analyses of comparable numbers of photometric observations (e.g. Green et al., 2015; Gordon
et al., 2016) require months or years of computation time. A single spectrum contains orders of magnitude more data points than a single set of photometric observations, which comes with an at least linearly proportional increase in required computation time.

In the packages discussed above and in much of the absorption line analysis literature, the continuum is assumed to be a low order polynomial or spline. While these are non-linear functions of wavelength, they are linear functions of the polynomial or spline coefficients. This linearity means that if some additional assumptions hold, it is possible to marginalize over these coefficients analytically.

Analytic marginalization has several advantages over numerical marginalization. First, it can speed up MCMC-based inference for absorption line parameters by reducing the dimensionality of the problem. Second, the ability to evaluate the continuum parameter-marginalized likelihood function and its gradient makes it possible to do optimization, rather than sampling, for the absorption parameters while still keeping the robustness provided by marginalizing over continuum parameters. Finally, it makes marginalization over different possible continuum parameterizations computationally trivial—simply sum together continuum-marginalized likelihoods that assume different parameterizations. Marginalization over parameterizations allows an even greater degree of automation and systematization of absorption line inference.

The assumptions required for this particular form of analytic marginalization are: that the continuum can be expressed as a linear function (not
necessarily a polynomial or spline); that the priors on the parameters of this linear function are either improper uniform or (multivariate) normal; and that residuals from the model are normally distributed. If these assumptions hold, then, given a model for the absorption, the posterior probability distribution function of the continuum parameters is itself a multivariate normal distribution. The result of marginalizing over the continuum parameters is simply an update to the covariance matrix of the model residuals. Conceptually, when a set of absorption line parameters is specified, the continuum parameters can be treated as additive, rather than multiplicative, linear nuisance parameters. An explanation of marginalization over additive linear nuisance parameters in an astronomical context is given in Luger, Foreman-Mackey, and Hogg (2017). This approach to marginalizing over multiplicative linear nuisance parameters has already been used for several astronomical applications, for example for analyzing sparsely sampled radial velocity measurements (Price-Whelan et al., 2017).

Models for absorption line spectra have features, such as the presence of a line spread function (LSF), which should be accounted for to more efficiently compute marginalized likelihoods and likelihood gradients. In this work, we derive expressions for these quantities that account for these features. This derivation is given in Section 3.2. We have created a package, amlc\(^2\), for evaluating these expressions. The package is described in Appendix 3.6. The performance of continuum parameter and parameterization marginalization is explored in Section 3.3. We discuss strengths and weaknesses of this method in Section 3.4 and conclude in Section 3.5.

\(^2\text{amlc is available at https://github.com/ktchrn/amlc.}\)
3.2 Assumptions and formalism

We assume the following model for a spectrum $y$ given parameters $\theta$, $m$, and $b$:

$$y(\theta) = L \left( d(\theta) \odot \left( \mu_m(\theta) + \sum_{i=1}^{P} a_{m,i} m_i \right) + \mu_b(\theta) + \sum_{i=1}^{Q} a_{b,i} b_i \right) + \epsilon. \quad (3.1)$$

The background source emits a continuum, which is expressed as the sum of a possibly non-linear term, $\mu_m(\theta)$, and a linear combination of basis elements $a_{m,i}$ with coefficients $m_i$. Intervening matter absorbs part of this continuum with transmittance function $d(\theta)$. The absorption happens independently at each wavelength. This is indicated by the elementwise product $\odot$ between the transmittance and continuum. Foregrounds, such as sky lines or instrumental artifacts are, like the continuum, expressed as the sum of a possibly non-linear term, $\mu_b(\theta)$, and a linear combination of basis elements $a_{b,i}$ with coefficients $b_i$. The resulting spectrum is convolved with an LSF $L$ and observed. $\epsilon$ are the residuals between the observed $y$ and the LSF-convolved spectrum and are assumed to be normally distributed with mean zero and covariance matrix $K$. The length of the observed spectrum is $M$, the length of the pre-LSF model spectrum is $N$, the number of continuum basis elements is $P$, and the number of foreground basis elements is $Q$.

Collecting the multiplicative (continuum) and additive (foreground) basis
elements $a_{m,i}$ and $a_{b,i}$ into matrices $A_m$ and $A_b$ and converting the transitory vector $d(\theta)$ into the diagonal matrix $D_\theta \equiv \text{diag}(d(\theta))$,

$$y = L (\mu_b(\theta) + A_b b + D_\theta (\mu_m(\theta) + A_m m)) + \epsilon$$  \hspace{1cm} (3.2)$$

$$\equiv L (\mu_b(\theta) + D_\theta \mu_m(\theta) + B c) + \epsilon.$$  \hspace{1cm} (3.3)

In the second expression, $B$ and $c$ are defined as:

$$B = \begin{bmatrix} D_\theta A_m & A_b \end{bmatrix} \quad c = \begin{bmatrix} m \\ b \end{bmatrix}.$$  \hspace{1cm} (3.4)

We consider two possible priors for the nuisance parameter vector $c$, a multivariate normal distribution with mean zero and covariance matrix $\Lambda$ and an improper uniform distribution:

$$p_n(c) = \mathcal{N}(0, \Lambda) \text{ (normal)} \quad \text{and} \quad p_u(c) = \prod_{i=1}^{p+q} Z_i^{-1} \text{ (uniform)},$$  \hspace{1cm} (3.5)

where $Z_i$ can be any positive real number.

### 3.2.1 Conditional probability of the nuisance parameters

For both priors, the conditional distribution of $c$ at fixed $\theta$ is proportional to a multivariate normal distribution. The mean $\hat{c}$ of this normal distribution is

$$\hat{c}_{n/u} = C_{n/u}^{-1} B^T L^T K^{-1} r,$$  \hspace{1cm} (3.6)

where $r$ is the vector of residuals

$$r = y - L (\mu_b(\theta) + D_\theta \mu_m(\theta)).$$  \hspace{1cm} (3.7)
and $C_{n/u}$ is

$$C_n = \Lambda^{-1} + B^T L^T K^{-1} L B,$$  \hspace{1cm} (3.8)

if the prior on $c$ is normal, and

$$C_u = B^T L^T K^{-1} L B$$ \hspace{1cm} (3.9)

if the prior on $c$ is uniform. The covariance matrix of the conditional distribution of $c$ is $C^{-1}_{n/u}$.

The conditional distribution of $c$ can be used for visualization and predictive checks. The mean of the conditional distribution is also its mode, so $LB\hat{c}$ is the best-fit model for $y$ at a given value of $\theta$. Samples drawn from the conditional distribution of $c$ can be used to visualize the effect and extent of nuisance parameter variation.

### 3.2.2 Marginal likelihood

Assuming the normal prior $p_n(c)$, marginalizing over $c$ following e.g. Luger, Foreman-Mackey, and Hogg (2017) or Rasmussen and Williams (2006) gives

$$p_n(y|\theta, L, B, K, \Lambda) = \int_{-\infty}^{+\infty} p(y|c, \theta, L, B, K, \Lambda) p_n(c) \, dc$$ \hspace{1cm} (3.10)

$$= (2\pi)^{-\frac{M}{2}} \det(K)^{-\frac{1}{2}} \det(\Lambda)^{-\frac{1}{2}} \det(C_n)^{-\frac{1}{2}}$$

$$\times \exp \left[ -\frac{1}{2} r^T K^{-1} (r - \hat{r}_n) \right],$$ \hspace{1cm} (3.11)
where

\[ \hat{r}_{n/u} = LB\hat{c}_{n/u}. \]  

(3.12)

If we instead assume the improper prior \( p_u(c) \),

\[
p_u(y|\theta, L, B, K) = \int_{-\infty}^{+\infty} p(y|c, \theta, L, B, K)p_u(c) \, dc
\]

(3.13)

\[
= \left( \prod_{i=1}^{P+Q} Z_i^{-1} \right)^{-1} (2\pi)^{-\frac{M-(P+Q)}{2}} \det(K)^{-\frac{1}{2}} \det(C_u)^{-\frac{1}{2}} \times \exp \left[ -\frac{1}{2} r^T K^{-1} (r - \hat{r}_u) \right].
\]

(3.14)

The marginal likelihood \( p_u \) will be proper if \( C_u \) is positive definite, which will be the case when \( LB \) is full rank and \( M \geq P + Q \). The marginal likelihood \( p_n \) is always proper because \( C_n \) is always positive definite. \( C_n \) is always positive definite because \( \Lambda^{-1} \) is always positive definite and \( B^T L^T K^{-1} LB \) is always at least positive semi-definite.

### 3.2.3 Gradients

We give expressions for the gradients of \( \log(p_n) \) and \( \log(p_u) \) with respect to \( d(\theta), \mu_b(\theta), \) and \( \mu_m(\theta) \). The gradient of \( \log(p) \) with respect to the parameters \( \theta \) can be obtained by evaluating each of these gradients, computing the Jacobians of \( d(\theta), \mu_b(\theta), \) and \( \mu_m(\theta) \) with respect to \( \theta \), and applying the chain rule.
The gradient of log\( (p) \) with respect to \( d(\theta) \) is
\[
\nabla \log(p)(d(\cdot)) = \left( L^T K^{-1} (r - \hat{r}_{n/u}) \right) \odot (B'\hat{c} + \mu_m)
\]
\[
- \frac{1}{2} \left( \left( C_{n/u}^{-1} B' T \right) \odot \left( B^T L^T K^{-1} L \right) \right)
\]
\[
+ \left( C_{n/u}^{-1} B^T L^T K^{-1} L \right) \odot B'^T \right) 1,
\]  
(3.15)

where \( 1 \) is a column vector of ones of length \( P + Q \). \( B' \) is the sum of derivatives of \( B \) with respect to each element of \( d(\theta) \):
\[
B' = \sum_{i=1}^{N} \frac{\partial B}{\partial d_i(\theta)}
\]  
(3.16)
\[
= \sum_{i=1}^{N} \begin{bmatrix} J_{ii} A_m & 0 \times A_b \end{bmatrix}
\]  
(3.17)
\[
= \begin{bmatrix} A_m & 0 \end{bmatrix},
\]  
(3.18)

where \( J_{ii} \) is a square matrix whose \((i,i)\)-th entry is 1 and whose other entries are all 0. The first row of Equation 3.15 is the gradient of the argument of the exponentials in Equations 3.10 and 3.13. The second row is the gradient of \( \log(\det(C_{n/u})) \).

The gradient of log\( (p) \) with respect to \( \mu_m(\theta) \) is
\[
\nabla \log(p)(\mu_m(\theta)) = D_\theta L^T K^{-1} (r - \hat{r}_{n/u})
\]  
(3.19)

and the gradient of log\( (p) \) with respect to \( \mu_b(\theta) \) is
\[
\nabla \log(p)(\mu_b(\theta)) = L^T K^{-1} (r - \hat{r}_{n/u}).
\]  
(3.20)
3.3 Practical test cases

Does marginalization over continuum parameters, analytic or numerical, have benefits beyond having a clear probabilistic justification? We consider two metrics: how marginalizing over, instead of fitting for, continuum parameters and parameterizations affects the error to within which absorption line parameters can be measured; and how marginalizing analytically, instead of numerically, affects the speed of MCMC-based inference.

For the error metric, we consider two possible cases: one in which the continuum parameterization is known and one in which it is necessary to choose a continuum parameterization from a set of possibilities. The suggested method is marginalizing over continuum parameters, in the first case, and marginalizing over continuum parameters and parameterizations, in the second. When the parameterization is known, all methods we consider are equally effective at high signal-to-noise ratios (SNRs) but marginalization is consistently more robust at low SNRs. When the parameterization is not known, marginalization over parameterizations has the lowest over-all error rate among the methods we consider. Furthermore, its error rate is close to that of parameter marginalization given the correct parameterization. These two cases are examined in Sections 3.3.1 and 3.3.2.

To assess the relative speed of analytic and numerical marginalization, we examine how two metrics change as the complexity of an inference problem increases: the number of iterations required for MCMC to converge and the number of independent samples generated per unit time. The basic problem is analyzing a single line on a continuum whose parameterization is known.
To build up more complicated problems, we add more spectral segments each of which has its own continuum and contains another absorption line. All of these absorption lines share widths and central velocities but have independent column densities. Problems with this structure arise when analyzing multiple lines from a single species or from multiple species that can be assumed to share a common component structure. The convergence speedup from using analytic marginalization is dramatic, reaching a full order of magnitude difference in the number of required iterations with as few as three spectral segments. Analytic marginalization yields more independent samples per unit time when there are multiple spectral segments with high-order continua. For example, when there are six spectral segments with 3rd order continua, analytic marginalization is three times faster than numerical marginalization. When there are few spectral segments, analytic marginalization is slightly slower or of comparable speed to numerical marginalization. These metrics are examined in Section 3.3.3.

### 3.3.1 Marginalization over parameters

Here, we consider the problem of measuring the column density of a single well-resolved, unsaturated absorption line superimposed on a continuum whose parameterization is known but whose parameters are not known. To do this, we generate spectra containing an absorption line with fixed absorption parameters but with varying continuum parameterizations, continuum parameters, and SNRs. The continuum parameterizations we consider are polynomials of order 0, 1, and 2 and the continuum-level SNRs we use are
Figure 3.1: Accuracy and precision of different methods of measuring the column density of a single line superimposed on a continuum with known parameterization. The accuracy/precision is defined in terms of the root mean square error (RMSE) of the logarithm of the column density measurements. The signal-to-noise ratios (SNRs) of the artificially generated spectra used for this test are shown on the x-axis of each panel. The panels correspond to different continuum parameterizations, from left to right: 0th order polynomial, 1st order polynomial, 2nd order polynomial. The line colors indicate different measurement methods, which are listed in the figure legend. These methods are explained in detail in Section 3.3.1.
between 5 and 25. We generate 1000 spectra at each combination of parameterization and SNR and measure the column density of the absorption line in each spectrum. From the recovered column densities, we compute the root mean square error (RMSE) of the base ten logarithm of the column density ($\log_{10} N$). We use the logarithm of the column density because its RMSE scale-free. In particular, physical constants such as oscillator strengths cancel in the $\log_{10} N$ RMSE calculation.

We measure the column density using four methods: (1) supply the correct continuum parameters and only fit for the absorption line parameters; (2) simultaneously fit for continuum and absorption line parameters; (3) analytically marginalize over continuum parameters while fitting for absorption line parameters; and (4) use the absorption line parameters recovered using method (1) to define a line-free spectral region, fit continuum parameters just to this region, and with those continuum parameters fit for the absorption line parameters. The first method provides a lower limit on the RMSE of $\log_{10} N$ as a function of SNR. The second and third methods are two possible ways of automatically modeling the continuum. The fourth method approximates the actions of a human manually analyzing a spectrum. We assume the human can correctly estimate the continuum by eye, correctly estimate the best-fit absorption line profile by eye given this continuum, and use this profile to determine which part of the spectrum is not affected by the line.

The RMSEs obtained using these methods are shown in Figure 3.1. Above an SNR of 10-15, all methods where the continuum is not a priori known yield equal results. At and below that SNR range, marginalization has a
Figure 3.2: Accuracy and precision of different methods of measuring the column density of a single line superimposed on a continuum with unknown parameterization. The accuracy/precision is defined in terms of the root mean square error (RMSE) of the logarithm of the column density measurements. The signal-to-noise ratios (SNRs) of the artificially generated spectra used for this test are shown on the x-axis of each panel. The panels correspond to different true continuum parameterizations, from left to right: 0th order polynomial, 1st order polynomial, 2nd order polynomial. The line colors indicate different measurement methods, which are listed in the figure legend. These methods are explained in detail in Section 3.3.2.

lower RMSE than both simultaneous fitting and the human-like analysis. This advantage becomes greater as the continuum parameterization becomes more complex.

3.3.2 Marginalization over parameterizations

Next, we consider a problem where there is still a single well-resolved and unsaturated absorption line but where it is only known that the continuum belongs to a family of possible continuum parameterizations. As in the previous section, we consider three possible continuum parameterizations: 0th, 1st, and 2nd order polynomials. The approach, simulating spectra, measuring $\log_{10} N$ for each simulated spectrum, and computing the RMSE of $\log_{10} N$, is
also the same. However, we consider a different range in continuum-level SNR: 10 to 100.

We measure the column density using four methods: (1) supply the correct parameterization and marginalize over its parameters; (2) assume the most complicated of the three parameterizations and marginalize over its parameters; (3) use an iterated likelihood ratio test to choose a parameterization and fit for its parameters; (4) marginalize over parameterizations as well as parameters. Method (1) establishes a reference minimum RMSE for this test case. Method (2) is a conservative assumption that can be made when the family of possible parameterizations is nested—a polynomial of order $n$ with leading coefficient 0 is a polynomial of order $n - 1$. Methods (3) and (4) are different ways of automatically accounting for the different possible parameterizations, in one case (3) by selecting a parameterization and in the other (4) by averaging over the possible parameterizations. The likelihood function that we maximize when using method (4) is the weighted sum of the continuum-marginalized likelihoods of the three continuum models. The weights in this sum are the prior probabilities of each of the models; we assume all three are equally likely.

The RMSEs of the four methods are shown in Figure 3.2. We compare the methods using three criteria: their robustness to decreasing the SNR and increasing the number of parameters relative to the number of observations; the value of their RMSE at fixed SNR; and the SNR they require to obtain the same RMSE. We consider a method to be robust if its RMSE scales consistently with SNR and true continuum order rather than rapidly increasing
at some critical value. The reference, conservative, and parameterization-marginalization methods are robust for SNRs between 10 and 100 while the parameterization-selection method is not. Its RMSE blows up below an SNR of 10 for spectra with 1st order continua and at all SNRs considered for 2nd order continua. While parameterization selection performs as well as the other methods on high SNR spectra, its lack of robustness means that it is not as generally applicable as the other methods.

In terms of RMSE, the parameterization-marginalized estimator is nearly as good as the reference estimator. The ratio RMSE_m/RMSE_r of the parameterization-marginalized RMSE, RMSE_m, to the reference RMSE, RMSE_r, is 1, 1.04, and 1.1 for spectra with 0th, 1st, and 2nd order continua. For spectra with 0th or 1st order continua, the conservative estimator is significantly worse than the reference estimator. RMSE_c/RMSE_r is 1.5, 1.5, and 1, respectively, where RMSE_c is the RMSE of the conservative estimator. These ratios are approximately constant across the entire considered SNR range. When analyzing an already acquired set of observations in which a variety of continuum parameterizations are present, using the parameterization-marginalization estimator rather than the conservative estimator will, on average, yield higher accuracy and precision.

It is also useful to compare the SNRs the conservative and parameterization-marginalization estimators require to achieve the same RMSE. For spectra with 0th, 1st, and 2nd continua, the ratio of the required SNRs SNR_c/SNR_m is 1.6, 1.5, and 0.9. These ratios are, again, consistent across the entire considered SNR range. Assuming that SNR is proportional to the square root of
observing time, as is the case for Poisson noise-limited data, these SNR ratios can be converted to required observing time ratios. Reaching the RMSE of the parameterization-marginalized estimator with the conservative estimator takes 1.26, 1.22, and 0.95 times as much observing time. When designing an observing strategy to meet a column density RMSE requirement, using the parameterization-marginalized estimator rather than the conservative estimator can save observing time given a fixed sample or increase the size of a sample given a fixed amount of observing time.

3.3.3 MCMC efficiency

In ISM absorption spectra, it is common to have multiple lines in a spectrum with shared parameters. These lines can be from the same species, e.g. the Lyman series, or from different species, e.g. from Mg $\text{I}$, Zn $\text{II}$, and Cr $\text{II}$ which have overlapping lines in the near ultraviolet. When these lines are in different parts of a spectrum, each part needs its own continuum parameters. This is a case in which analytic marginalization can potentially be more efficient than MCMC marginalization.

We compare how quickly MCMC done using each of the two methods converges and how efficient MCMC done using each method is post-convergence. Which comparison is more informative for choosing a method to use will depend on the purpose of the MCMC run. If the goal of an MCMC run is to estimate some value at low-to-moderate precision, the rate of convergence will be the more important factor. If the goal is instead to estimate some value at high precision, the burn-in period will usually be a small fraction of the
Figure 3.3: Convergence rate of MCMC with analytic and numerical continuum parameter marginalization for absorption line analysis problems with different complexities. The convergence diagnostic (y-axis) is the Rubin-Gelman statistic, an estimate of how much smaller the Monte Carlo error of an MCMC-based parameter estimate can get. Each line shows the evolution of this convergence diagnostic as a function of the number of MCMC steps taken (x-axis). Line styles indicate whether continuum parameters are marginalized over analytically (solid) or included in MCMC (dashed). Line colors and markers indicate the number of spectral regions being analyzed simultaneously; each region has its own set of continuum parameters. The Rubin-Gelman statistic and the problem setup are discussed in more detail in Section 3.3.3.
Figure 3.4: Relative efficiency of MCMC with analytic and numerical continuum parameter marginalization for absorption line analysis problems with different complexities. The relative efficiency is the ratio of the number of independent samples, $n_{\text{ind}}$, generated in the same amount of time by the two marginalization approaches; $n_{\text{ind}}^{(m)}$ uses the analytically marginalized likelihood, $n_{\text{ind}}^{(u)}$ uses the un marginalized likelihood. The larger the relative efficiency, the more independent samples generated by analytic marginalization. Line colors and markers correspond to different continuum parameterizations: 1st order polynomial (black squares), 2nd order polynomial (blue circles), 3rd order polynomial (orange triangles). Line styles indicate whether a non-trivial LSF is used in the analysis. The relative efficiency is shown as a function of the number of spectral regions being analyzed simultaneously; each spectral region has its own set of continuum parameters. The relative efficiency and the problem setup are discussed in more detail in Section 3.3.3.
total chain and post-convergency efficiency will be more important.

We consider a case where there are \( N \) absorption lines with shared central velocities and widths and independent column densities. Each absorption line is in a different spectral region. The continuum in each spectral region is a polynomial of order \( M \). The marginalized likelihood has \( 2 + N \) absorption line parameters. The un marginalized likelihood has \( 2 + N \) absorption line parameters and \( N \times M \) continuum parameters. We use the emcee implementation of the Goodman and Weare affine-invariant MCMC ensemble sampler to generate draws from the posterior corresponding to each of these likelihoods. We use the minimum number of “walkers,” which is twice the number of parameters.

We use the Rubin-Gelman statistic \( \hat{R} \) (Gelman and Rubin, 1992) to assess convergence. The Rubin-Gelman statistic compares the variance between and within different MCMC instances. If the instances have all converged, these two variances should be approximately equal. We run ten MCMC instances for 12800 (per-walker) steps and compute the Rubin-Gelman statistic from the second half of sub-chains of length \( 2^p \times 100 \) for \( p = 0, 1, \ldots, 7 \). \( \hat{R} \) is computed separately for each parameter. Following common usage, we consider convergence to be reached when the \( \hat{R} \) of all parameters is less than 1.1. We run this test for 1, 2, and 3 regions and absorption lines assuming a continuum of order 1. The value of the \( \hat{R} \) as a function of (total) number of steps is shown in Figure 3.3. When there is a single region and line, the MCMC marginalization chain takes twice as many steps as the analytic marginalization chain to converge; when there are two regions, it takes eight times as many steps;
when there are three, the MCMC marginalization chain has not converged by
the maximum chain length of 12800 while the analytic marginalization chain
converges within 1600 steps.

We use the number of independent samples per unit time to assess effi-
ciency. We run MCMC with the marginalized likelihood for 2000 burn-in steps
and 8000 converged steps and record the average time per sample, $t_s$. Because
MCMC with the unmarginalized likelihood takes many steps to converge, we
use draws from the converged part of the marginalized likelihood chain as a
starting point; these draws only have values for the absorption line param-
ters. At each set of absorption line parameters, we sample a set of continuum
parameters from the conditional distribution discussed in Section 3.2.1. From
this starting point, we run MCMC with the unmarginalized likelihood for
4000 burn-in steps and 36000 converged steps and record the average time per
sample. We then compute the average integrated autocorrelation times $\tau_f$ of
the walkers in both chains. The number of independent samples per unit time
is $n_i = (\tau_f t_s)^{-1}$.

We compute $n_i$ for a number of regions $N = 1, 2, \ldots, 6$, continua of poly-
nomial order $M = 1, 2, \text{and } 3$, and either a trivial LSF or a banded LSF. The
ratio $n_{ind}^{(m)} / n_{ind}^{(u)}$ for each of these cases is shown in Figure 3.4. When this ra-
tio is greater than 1, running MCMC with the marginalized likelihood for a
fixed amount of time will produce more independent samples than running
MCMC with the unmarginalized likelihood for the same amount of time. The
greater the number of regions and the order of the continuum, the greater the
efficiency advantage of the marginalized likelihood over the unmarginalized
likelihood. This advantage will not depend on the number of datapoints in each spectral region so long as the LSF is trivial or banded, since in these cases the evaluation time of both likelihoods grows linearly with dataset length (see Section 3.6.3).

3.4 Discussion

3.4.1 Assumptions and consequences

The explicit assumptions of the analytic marginalization method are that the continuum is a linear function, that the prior on the coefficients is the improper uniform or multivariate normal distribution, that residuals between the data and model are normally distributed, and that the covariance matrix of the residuals does not depend on the continuum. It is obvious that these assumptions do not hold strictly for any dataset. For example, both possible priors require that there not be constraints on the coefficients even though no background source produces negative flux. A less trivial example is data in the low photon count regime, which are better described by a Poisson distribution than a Gaussian distribution. This is particularly important when the uncertainties on the measurements are themselves highly uncertain and should be explicitly modeled. In that case, the uncertainties will depend on the Poisson intensity function, which explicitly depends on the continuum. Analytic marginalization of the kind described in this work should not be applied to low SNR X-ray or UV spectra.

An implicit assumption of the method is that the absorption model is realistic. For analytic marginalization to be useful, it must be possible for
the absorption model to correctly describe the actually present absorption features. For example, if a region of a spectrum contains two clearly distinct absorption lines but the model only allows for a single line, the presence of the un-modeled line will bias the continuum model. In short, improvements in continuum modeling cannot solve problems of absorption model misspecification.

The continuum models envisaged in this work will usually be effective descriptions rather than (often non-linear) physical descriptions. Most continua that vary over longer wavelength scales than the width of absorption lines in question can be approximated in this way. Examples of background sources with slowly varying continua include quasars and (particularly rapidly rotating) hot stars. With flexible linear models such as splines, it is even possible to describe more complicated pseudo-continua such as stellar wind lines. For even more complicated pseudo-continua such as those of cool stars (Zasowski et al., 2015, e.g.), it is necessary to use a non-linear model. Marginalizable linear models can still be useful even in this case as a way of introducing small corrections for pseudo-continuum features that are not perfectly described by the non-linear model.

3.4.2 Applications of analytic marginalization

The test cases in Section 3.3 showed that marginalization over continuum parameters and parameterizations is more precise, accurate, and robust than the alternatives. Considered purely as a replacement for numerical marginalization, analytic marginalization is just a potentially more computationally
efficient way of implementing an existing inference approach. However, it also allows two qualitatively new approaches: continuum model averaging and absorption parameter optimization with a continuum-marginalized likelihood function.

The test case in Section 3.3.2 combines both of these approaches—optimizing an absorption parameter likelihood function where the parameterization and parameters of the continuum have been marginalized over. Analytic marginalization makes this possible in two ways: availability of closed form likelihoods and availability of gradients of closed form likelihoods. Optimization with continuum-marginalized likelihoods is useful for analyzing large surveys. Analyses of absorption lines in tens of thousands of spectra (Zhu and Ménard, 2013; Zasowski et al., 2015, e.g.) cannot practically be done with MCMC. With analytic marginalization, it is possible to at least marginalize over continuum parameters. The results of the test cases suggest that this approach could mean a non-trivial improvement in the accuracy and precision of absorption line measurements.

In cases where MCMC is possible, combining continuum parameterization marginalization with a probabilistic specification of absorption component structure would allow absorption line analysis with human intervention only at the level of specifying priors and candidate continuum parameterizations. Component structure specification can be done using trans-dimensional inference, in which the dimensionality of parameter space (in this case the number of sets of absorption line parameters) is itself a parameter of the
model. This way of doing absorption line analysis has two potential advantages. First, marginalizing over the velocity structure of the absorption as well as the continuum should automatically include effects such as unresolved saturated structure in parameter uncertainties. Second, because inference approach is almost completely automatic, it allows blinding, which improves reproducibility.

### 3.5 Conclusion

Absorption lines are an important source of information about stars and the ISM. As larger spectroscopic datasets become available and as reproducibility becomes more standard in astronomy, it becomes necessary to move beyond ad-hoc analysis methods, particularly ones in which a human directly interacts with data. In multiple recent works, there have been attempts to partially automate continuum placement by including and marginalizing over continuum parameters in probabilistic spectral models. Marginalizing over continuum parameters has, in these works, been hypothesized to also improve the accuracy of the recovered absorption line parameters. Despite these advantages, this approach has so far not become popular, in part due to the computational expense of numerically marginalizing over these additional parameters.

In this work, we have shown that it is possible in many cases to replace this numerical marginalization with analytic marginalization (Section 3.2). Analytic marginalization speeds up MCMC-based analyses in problems with many continuum parameters (Section 3.3.3). The continuum parameter-marginalized likelihood can also be used for optimization over absorption
line parameters. This approach combines the speed of optimization with the advantages of continuum marginalization. Analytic marginalization over continuum parameters makes it trivial to also marginalize over continuum parameterizations. As with parameter marginalization, parameterization marginalization can be combined with optimization over absorption line parameters. Parameterization marginalization further reduces the amount of direct human interference in the analysis of individual spectra and will be especially useful in analyses of datasets containing spectra with different continuum shapes.

We have also confirmed that marginalization over continuum parameters and parameterizations indeed improves the accuracy of absorption line parameter measurements. The advantage of parameter marginalization is only significant at low SNRs (Section 3.3.1). On the other hand, parameterization marginalization is significantly more accurate than alternative methods of deciding on a continuum parameterization at all SNRs (Section 3.3.2).

We have released an open-source Python package, amlc, which can be used to evaluate continuum parameter-marginalized likelihoods and related quantities. Features of this package are described in Appendix 3.6. It is meant to be used as a drop-in replacement for likelihood functions in existing absorption spectrum analysis tools.

3.6 Appendix

In this Appendix, we describe how amlc is implemented (Section 3.6.1), list some of its capabilities (Section 3.6.2), and show how the computation time of different calculations grows with dataset and continuum model size (Section 3.6.3).
3.6.3)

3.6.1 Implementation

We have implemented amlc as a pure-Python package with numpy and scipy as dependencies. amlc does not contain functionality for building LSFs or computing transmittances from absorption parameters and is not intended to be a stand-alone analysis tool. It is meant to be used as a drop-in likelihood function replacement in analysis packages or scripts.

3.6.2 Package functionality

This package was designed for a use case where the log marginal likelihood and its gradient are evaluated at many different values of the \(\theta\)-dependent parameters (see Section 3.2) while the \(\theta\)-independent parameters are held constant. The core feature of the package is the MarginalizedLikelihood class. A MarginalizedLikelihood instance stores \(\theta\)-independent parts of the model and pre-computes quantities that are re-used during repeated marginalized likelihood evaluations. In particular, it stores the data covariance matrix \(K\); the \(c\) prior covariance matrix \(\mathbf{C}\) and its explicit inverse, if applicable; and the LSF mapping \(\mathbf{L}\) and its transpose.

Both covariance matrices can be diagonal or fully general. The package includes the CovarianceMatrix class, which defines a consistent interface for calculations, and two subclasses, DiagonalCovarianceMatrix and GeneralCovarianceMatrix. DiagonalCovarianceMatrix wraps the simple,
one-dimensional determinant and inverse calculations possible with a co-
variance matrix consisting purely of variances and does the book-keeping
required to produce output with the correct shape. GeneralCovarianceMatrix
uses the Cholesky decomposition of the supplied covariance matrix to calcu-
late its determinant and to left multiply matrices and vectors by its inverse.
Computing the Cholesky decomposition of a general covariance matrix of size
$M$ by $M$ takes $O(M^3)$ calculations, making it prohibitively computationally
expensive for large $M$.

The LSF mapping $L$ can be any object that implements the matrix multi-
plication interface, i.e. has a `matmul` or `__matmul__` method. For example, $L$
can be a dense matrix represented by a `numpy` array, a sparse matrix repre-
sented by a `scipy.sparse` matrix, or a convolution operator represented by
a `scipy.sparse.linalg.LinearOperator`. $L$ can also be the identity mapping
(indicated by `None`), in which case it is left out of any likelihood calculations.

### 3.6.3 Computation time as a function of dataset and basis size

The most time-consuming step in computing all of the quantities derived
in Section 3.2 is forming the matrix $C_{n/u}$. This step requires matrix-matrix
products, while most other steps only involve matrix-vector products. These
expensive products are $LB$ and $K^{-1}(LB)$. The amount of time required to
compute these products depends on the structure $L$ and $K$.

$L$ can be the identity matrix, a dense matrix, a sparse matrix, or a linear
mapping such as convolution. The fastest case is when $L$ is the identity matrix,
since then $LB$ does not need to be computed. The slowest case is when it is a dense matrix, in which case computation time grows as $O(MN(P + Q))$. When $L$ is a sparse matrix or linear mapping, the scaling depends on its exact structure. An LSF that varies with wavelength can be represented by a banded matrix, which will be sparse if the spectrum spans many resolution elements. If the bandwidth of $L$ is independent of the size of the dataset, the computation time of this product grows as $O(M(P + Q))$.

We consider covariance matrices $K$ that are either diagonal or general. If $K$ is diagonal, $K^{-1}(LB)$ requires exactly $M(P + Q)$ multiplications. When $K$ is a general covariance matrix, we decompose it into its Cholesky factors and left-multiply $LB$ by $K^{-1}$ by solving the linear problem $LB = KX$. The time needed to factor $K$ grows as $O(M^3)$ but only needs to be done once per set of observations. The time needed to solve the linear problem grows as $O(M^2(P + Q))$.

To empirically confirm these growth rates, we timed how long it takes to evaluate the log-likelihood and its gradient for a range of dataset sizes $M$ and basis sizes $P + Q$ and three $L$ and $K$ structure scenarios. The scenarios are: $L$ is the identity mapping, $K$ is diagonal; $L$ is a dense matrix, $K$ is general; and $L$ is a sparse, banded matrix and $K$ is diagonal. The first two scenarios are the fastest and slowest combination. The third scenario is more typical for a spectrum; the data uncertainty is diagonal and the LSF has finite extent. The evaluation time of the log-likelihood as a function of $M$ and $P + Q$ for these three scenarios is shown in Figures 3.5, 3.6, and 3.7. We do not show the evaluation time of the gradient because it behaves in the same way as the
evaluation time of the log-likelihood in all three scenarios; the most expensive step of the two calculations is the same.

The dependence of computation time on $M$ and $P + Q$ generally agrees with the predictions based on the two most time-consuming steps. At low $M$ and in particular at low $P + Q$, the computation time is either overhead-dominated or evenly split between the most time-consuming steps and other steps. When $M \gtrsim 10^5$, computation time increases faster than expected purely from the growth rate of the required number of operations (see e.g. the left panel of Figure 3.5). This excess increase in computation time is most likely due to changes in memory bandwidth, as the size of matrix rows and columns increases past the size of the highest-level CPU cache on the laptop used to run these tests.

To put these dataset sizes into context, a Sloan Digital Sky Survey (SDSS) BOSS or APOGEE spectrum is $\sim 10^3$ pixels long, a Hubble Space Telescope Cosmic Origins Spectrograph (HST-COS) spectrum is $\sim 10^4$ pixels long, and a spectrum from an echelle spectrograph such as the Ultraviolet and Visual Echelle Spectrograph on the Very Large Telescope or the Magellan Inamori Kyocera Echelle spectrograph is $\sim 10^5 - 10^6$ pixels long. The uncertainties associated with these spectra are usually assumed to be diagonal and the LSFs are acceptably described by sparse, banded matrices, so the computation times given in Figure 3.5 and 3.7 should apply.
Figure 3.5: Computation time of the marginal log-likelihood (Equations 3.10 and 3.13) when the data covariance matrix $K$ is diagonal and $L$ is the identity mapping as a function of dataset size $M$ (left panel) and basis size $P + Q$ (right panel). Values with the same marker shape were computed at the same dataset size $M$. Values with the same marker color were computed at the same dataset size $P + Q$. Polynomials of the form given in the bottom right corner of each panel are shown as dashed gray lines.

Figure 3.6: Computation time of the marginal log-likelihood when the data covariance matrix $K$ is not diagonal and $L$ is a dense matrix. See caption of Figure 3.5 for a description of figure elements.
Figure 3.7: Computation time of the marginal log-likelihood when the data covariance matrix \( K \) is diagonal and \( L \) is a sparse, banded matrix. See caption of Figure 3.5 for a description of figure elements.
Chapter 4

Kinetic Tomography I: A Method for Mapping the Milky Way’s Interstellar Medium in Four Dimensions

1We have developed a method for deriving the distribution of the Milky Way’s interstellar medium as a function of longitude, latitude, distance and line-of-sight velocity. This method takes as input maps of reddening as a function of longitude, latitude, and distance and maps of line emission as a function of longitude, latitude, and line-of-sight velocity. We have applied this method to datasets covering much of the Galactic plane. The output of this method correctly reproduces the line-of-sight velocities of high-mass star forming regions with known distances from Reid et al. (2014) and qualitatively agrees with results from the Milky Way kinematics literature. These maps will be useful for measuring flows of gas around the Milky Way’s spiral arms and into and out of giant molecular clouds.

1Adapted from a paper that originally appeared in The Astronomical Journal (Tchernyshyov and Peek, 2017).
4.1 Introduction

Many open problems in star formation, molecular cloud evolution, and galaxy-scale gas dynamics remain open because it has not been possible to measure the most useful quantities for resolving them – the 3D gas velocity vector and 3D gas density over an extended area of sky. A measurement of these fields would allow us to solve the continuity equation (Euler, 1757), and derive the rate at which density is changing across the Galaxy over a range of physical scales.

The formation of giant molecular clouds (GMCs), for instance, is in part a matter of collecting a large mass in a small volume. By looking for sites at which gas flows are converging, it may be possible to find currently forming GMCs. Conversely, one could look for diverging flows to detect and characterize the feedback-driven disruption of GMCs. With sufficient spatial and velocity resolution, it would be possible to distinguish between the many theories of exactly how the necessary mass is accumulated and converted to cold, molecular gas. These theories make different predictions for the properties of the required converging flows. For example, some theories assume the converging flows consist mostly of neutral hydrogen (HI) and invoke different sorts of instabilities at the collision interface of the flows to explain how this gas is rapidly converted to cold molecular hydrogen (H$_2$) (e.g. Heitsch et al., 2006; Clark et al., 2012; Carroll-Nellenback, Frank, and Heitsch, 2014). Other theories assume that GMCs form from the collision and agglomeration of smaller molecular cloudlets (e.g. Roberts and Stewart, 1987; Dobbs, 2008;
One could directly distinguish between these two possible modes of GMC formation by determining whether gas that is converging on forming GMCs is predominantly neutral or molecular. Without the ability to measure the velocity field as a function of all three spatial dimensions, it is difficult to even determine where converging flows are present.

The origin of the converging flows invoked above is also a matter of active interest. In some theories, the self-gravity of a modest overdensity can be sufficient to induce collapse (Kim and Ostriker, 2002; Vázquez-Semadeni et al., 2007; Dobbs, Pringle, and Burkert, 2012). Others invoke spatially coherent flows driven by feedback from star formation (Fujimoto et al., 2014) or perturbations in the Galactic potential such as spiral arms (Roberts, 1972; Bonnell et al., 2006). Strong, shocked flows driven by spiral arms have been seen in strongly tidally interacting two-arm spiral galaxies in the nearby universe (Visser, 1980a; Visser, 1980b; Shetty et al., 2007) using CO and H I observations. Unfortunately, the resolution in H I required to map these spiral shocks beyond very nearby galaxies with extreme two-armed spiral structure, is not observationally feasible (Visser, 1980a).

The nearest spiral galaxy is, of course, our own Milky Way. Studying the kinematics of the Milky Way replaces the problem of insufficient sensitivity and spatial resolution with the problem of confusion — from our vantage point, it is difficult to determine how the ISM is moving as a function of 3D position. In particular, it is essentially impossible to obtain the transverse velocity field of the ISM. Transverse velocities can only be derived from proper motions, which are difficult to measure for the diffuse and continuous ISM.
For many of the open problems we have outlined, even a measurement of the line-of-sight (radial) velocity as a function of 3D position (the 1-velocity field) would represent a significant step forward. While only having one component of the velocity field does make it difficult to empirically measure the rate of inflow and outflow of matter relative to any given structure, it should still be possible to empirically measure this rate statistically across a sample of structures.

No single observable can simultaneously measure the density and line-of-sight velocity at each location in the ISM, a construct we call the position-position-distance-velocity (PPDV) 4-cube. Instead, we have a number of observables of the ISM, each of which can be considered a (noisy and biased) projection of this PPDV 4-cube. We dub the process of reconstructing this PPDV 4-cube from some set of observations “Kinetic Tomography” (KT). There are a number of existing kinds of data we can use. The first are classical radio observations of the ISM in both diffuse tracers (e.g. HI) and denser tracers (e.g. CO). These are position-position-velocity (PPV) 3-cubes, a specific projection of the PPDV 4-cube, and have been classically used to infer the density of the ISM in 3-space assuming a Galactic rotation curve (e.g. Levine, Blitz, and Heiles, 2006, and references therein). Another observable is the position-position-distance (PPD) reddening 3-cubes generated by examining the photometry of large numbers of stars and performing inference on the intervening dusty ISM. There has been dramatic progress in this field (Marshall et al., 2006; Lallement et al., 2014; Green et al., 2015), which has been crucial for allowing this investigation. Interstellar absorption lines toward stars also
represent a projection of the PPDV 4-cube and can simultaneously contain distance, column density, and velocity information about the intervening matter (Welsh et al., 2010; Zasowski et al., 2015; Zasowski, 2015).

There have been some attempts to construct maps or point estimates of $v_{los}$ as a function of distance. Most such attempts have focused on individual spiral arms and used models of ISM flows around the spiral arms to directly invert PPV 3-cubes (e.g. Shane 1972; Foster and MacWilliams 2006). Reid et al. (2016) have developed a different approach, which combines probability distributions from the standard kinematic distance, various geometric hints, and possible associations of emitting gas with structures that have parallax-based distance measurements into a combined syncretic probability distribution for the distance. Neither of these approaches uses the information available in reddening-based PPD 3-cubes.

In the method we describe in this work, we use large-area CO and HI PPV 3-cubes and the Green et al. (2015) (henceforth GSF) PPD 3-cube to reconstruct the ISM PPDV 4-cube. We perform a restricted version of the full tomographic reconstruction in which we assume each parcel of gas in the PPD 3-cube is assigned a single central line-of-sight velocity with some line-of-sight velocity width. This can be considered an inversion of the usual kinematic distance method, in which a line-of-sight velocity is converted to a distance using a Galactic rotation curve. Here we map distance along a sightline to velocity and allow deviations from a rotation curve in order to better match the distribution of matter in the PPV 3-cube.

In this work, we describe our method, the map it produces, and our
evaluation of this map’s accuracy and precision. In Section 4.2, we describe the datasets we use to make and evaluate our PPDV map. In Section 4.3, we give a detailed explanation of the PPDV mapping technique and quantitatively demonstrate the accuracy of the technique’s results. In Section 4.4, we discuss the broader accuracy and applicability of the technique. We conclude in Section 4.5.

4.2 Data

4.2.1 HI and CO data

Radio emission lines of HI and CO trace the two dominant constituents of the Galactic ISM, atomic and molecular gas. Ionized phases of the ISM do not
contribute significantly to the column density and will therefore contribute negligibly to the extinction measured in GSF. 21-cm line emission from the hyperfine transition of HI is usually optically thin and its integral is an excellent tracer of HI column:

\[
N(\text{HI}) = 1.8 \times 10^{18} \text{ cm}^{-2} \int \frac{T_B \, dv}{K \, \text{km s}^{-1}}. \tag{4.1}
\]

When the 21-cm line becomes optically thick, Equation 4.1 will underestimate the HI column. However, this mostly happens in H$_2$-dominated regions (Goldsmith, Li, and Krčo, 2007).

We trace molecular gas using the 115 GHz 1-0 rotational transition of CO. The integral of this emission line can be converted to a H$_2$ column density using the conversion factor (Bolatto, Wolfire, and Leroy, 2013)

\[
X_{\text{CO}} = 2.0 \times 10^{20} \text{ cm}^{-2} \int \frac{T_B \, dv}{K \, \text{km s}^{-1}}. \tag{4.2}
\]

This conversion factor has a number of known weaknesses stemming from complex excitation and opacity effects and real variation in the relative population of CO and H$_2$ molecules. We will address the impacts of these weaknesses in §4.4.2.

For our CO data, we use the interpolated whole-Galaxy PPV 3-cube provided by Dame, Hartmann, and Thaddeus (2001). The 3-cube covers the full range in \( \ell \), \(-30^\circ\) to \(+30^\circ\) in \( b \), and \(-320 \text{ km s}^{-1}\) to \(+320 \text{ km s}^{-1}\) in \( V_{\text{LSR}} \) and has a velocity resolution of 1.3 km s\(^{-1}\). We find that the native resolution and PPV extent of these data are appropriate for our investigation and retain their exact pixelization for our other datasets.
The CO 3-cube contains single-pixel artifacts in both emission and absorption. To remove these artifacts, we apply a plus-shaped median smoothing kernel to each velocity channel. This kernel is three pixels wide along the $\ell$ and $b$ directions. This filtering procedure changes the total amount of CO emission by about 5% over the entire Galaxy.

For HI data, we use a combination of three large-area Galactic HI surveys. South of declination $0^\circ$, we use data from the 16$'$ resolution GASS survey (Kalberla et al., 2010); from declination $0^\circ$ to $38^\circ$ we use unpublished data from the 4$'$ resolution GALFA-HI survey (Peek et al., 2011) Data Release 2; North of $38^\circ$ we default to the 36$'$ resolution LAB Survey (Kalberla et al., 2005). We regrid these data onto the $7.5^\prime \times 7.5^\prime \times 1.3$ km s$^{-1}$ pixels of the Dame, Hartmann, and Thaddeus (2001) CO 3-cube. We note that each of these surveys has potential pitfalls. LAB is quite low resolution compared to the other data sets, meaning small scale Galactic features may be lost. GALFA-HI does not have stray radiation correction applied and so may overestimate columns in low column density regimes. Small artifacts exist in all of these databases but are typically most pronounced in high-latitude fields. The possibility of differences in the accuracy of the KT solution between regions in which we use different HI surveys is discussed in §4.3.3.

The HI and CO emission 3-cubes are converted to $N$(HI) and $N$(H$_2$) 3-cubes using Equations 4.1 and 4.2. These two column density 3-cubes are then added to make a single $N_{HI}$ data 3-cube.
4.2.2 Dust data

Our extinction 3-cube is derived from the GSF reddening data. GSF use PanSTARRS photometry of 800 million stars to infer the cumulative reddening along the line of sight in 6.8′ (NSIDE=512 HEALPix) pixels. The distance axis of the GSF 3-cube is in steps of half a distance modulus, from 63 pc to 63 kpc. We regrid these data onto the Dame, Hartmann, and Thaddeus (2001) ℓ-b grid and difference them in distance to find the reddening between each distance step. This differential reddening is then converted to an $N_H$ using the factor measured in Peek (2013),

$$N_H = E(B-V) \times 10^{21} \frac{\text{cm}^{-2}}{\text{mag}}.$$  \hspace{1cm} (4.3)

We use a single reddening to hydrogen column density conversion factor. This is, in principle, incorrect due to variations in both the relation between the amount of reddening and the amount of dust (e.g. Planck Collaboration et al. 2015) and the ratio of dust to gas (e.g. Savage and Sembach 1996; Jenkins 2009). We expect the latter to be the more important effect. The combination of HI and CO emission lines traces gas from at least three of the four cloud types in Savage and Sembach (1996), all of which have different depletion patterns and hence dust-to-gas ratios. This change in depletion pattern corresponds to a change in dust-to-gas ratio of about two, which while not negligible is also unlikely to be the dominant systematic uncertainty in our analysis. We discuss the impact of making this incorrect assumption in §4.4.2.
4.2.3 High-mass star forming region data

To check the accuracy of our method, we need measurements of the line-of-sight velocities and distances of clouds of gas. Reid et al. (2014) (henceforth Reid14) have measured the line-of-sight velocities, proper motions, and trigonometric parallaxes of water and methanol masers associated with 103 high-mass star forming regions (HMSFRs). Of these 103, 99 fall inside the footprint of the GSF reddening data. We adopt the line-of-sight velocities, velocity uncertainties, and parallaxes of these 99 HMSFRs as stated in Table 1 of Reid14.

4.3 Kinetic tomography

We have developed a procedure for deriving the distribution of interstellar matter in PPDV space from measurements of its distribution in PPD and PPV space. The technical term for deriving a multi-dimensional distribution from lower-dimensional measurements is tomographic reconstruction; in this context, lower-dimensional measurements are called projections. Tomographic reconstruction from two projections is, in general, not possible – there are many more independent variables than observational constraints. Our procedure for solving this specific case of the tomographic reconstruction problem uses simplifying assumptions about the structure of the ISM in PPDV space to reduce the number of independent variables.
For motivation, we first examine the assumptions behind a common technique for reconstructing a PPDV-space ISM distribution from PPV-space measurements alone. This is the widely known kinematic distance method, which maps line-of-sight velocities to distances based on an assumed rotation curve and Galactic geometry. While the kinematic distance method is usually presented as a way of converting a PPV-space distribution to a PPD-space, rather than PPDV-space, distribution, the two conversions are equivalent according to the kinematic distance method’s underlying assumptions. These assumptions can be combined into a single statement: (1) a location in PPD space can be assigned a single line-of-sight velocity (2) according to an assumed rotation curve and Galactic geometry. With these assumptions, it follows that knowing the PPD-space distribution of the ISM is equivalent to knowing its PPDV-space distribution.

We use PPD measurements in addition to PPV measurements, allowing us to relax these assumptions. Our version: (1) a parcel of interstellar matter in PPD space can be assigned a Gaussian distribution of line-of-sight velocities (2) whose center is within a fixed range of the line-of-sight velocity predicted by an assumed rotation curve and Galactic geometry. Here, a “parcel” of interstellar matter refers to the contents of a single PPD 3-cube voxel. That is to say, we aim to assign a central line-of-sight velocity $v_{\text{los}}$ and a line-of-sight Gaussian velocity width $\sigma_v$ to each voxel in the PPD 3-cube. From our assumptions, a description of the ISM in PPDV space consists of a description of its PPD-space distribution (the observed PPD 3-cube), a line-of-sight central velocity 3-cube in PPD space ($v_{\text{los}}(\ell, b, d)$), and a line-of-sight velocity width 3-cube in PPD.
space \( (\sigma_v(\ell, b, d)) \). Thus, we have reduced our original problem of finding a PPDV 4-cube which is consistent with our observed PPD and PPV 3-cubes to finding a \( v_{\text{los}}(\ell, b, d) \) and \( \sigma_v(\ell, b, d) \) pair consistent with our PPV observations.

### 4.3.1 Formalism

We are looking for a \( v_{\text{los}}(\ell, b, d) \) and \( \sigma_v(\ell, b, d) \) pair that, when combined with the observed PPD 3-cube, best matches the observed PPV 3-cube. This is an optimization problem. An optimization problem needs an objective function, and an objective function needs a quantity to compare to the data. In our case, that quantity is a model PPV 3-cube. To obtain a model PPV 3-cube, we produce a PPDV 4-cube and then integrate it along the distance axis.

Suppose that we have a matter density \( \rho(\ell, b, d) \) in PPD space and a \( v_{\text{los}}(\ell, b, d) \) and \( \sigma_v(\ell, b, d) \) pair. The matter density at a point \( (\ell, b, d, v) \) in PPDV space is

\[
\rho(\ell, b, d, v) = \frac{\rho(\ell, b, d)}{\sqrt{2\pi} \sigma_v(\ell, b, d)^2} \exp \left( -\frac{(v - v_{\text{los}}(\ell, b, d))^2}{2\sigma_v(\ell, b, d)^2} \right), \tag{4.4}
\]

and the matter density at a point \( (\ell, b, v) \) in PPV space is

\[
\rho(\ell, b, v) = \int_0^{d_{\text{max}}} \rho(\ell, b, d, v) \, dd, \tag{4.5}
\]

where \( d_{\text{max}} \) is the maximum distance to which \( \rho(\ell, b, d) \) is known.

These equations apply for continuous matter density and \( v_{\text{los}} \) fields. In our case, all quantities are defined on discrete grids. Instead of a PPD-space matter density \( \rho(\ell, b, d) \), for example, we have a PPD 3-cube whose entries are total masses of protons \( m(x, y, i) \) inside a voxel centered on \( \ell_x, b_y, \) and \( d_i \).
To move from the continuous case to the discrete case, we assume that \( v_{\text{los}}(\ell, b, d) \) and \( \sigma_v(\ell, b, d) \) are constant across a voxel and work with integrated quantities instead of densities. Equation 4.4 becomes

\[
m(x, y, i, j) = m(x, y, i) \times \int_{v_j - \Delta v}^{v_j + \Delta v} \frac{1}{\sqrt{2\pi}\sigma_v(x, y, j)^2} \exp \left( -\frac{(v - v_{\text{los}}(x, y, j))^2}{2\sigma_v(x, y, j)^2} \right) \, dv,
\]

where \( 2\Delta v \) is the length of a voxel along the velocity axis. Equation 4.5 becomes

\[
m(x, y, j) = \sum_i m(x, y, i, j).
\]

A cartoon representation of this procedure is shown in the top panel of Figure 4.2. In the cartoon, \( v_{\text{los}}(x, y, i) \) is assumed to be set by a rotation curve; the resulting \( m(x, y, j) \) does not match the cartoon PPV data. This mismatch is also generally true of the actual data. Assuming a rotation curve and propagating it through produces a model PPV 3-cube which is clearly inconsistent with the observed PPV 3-cube.

We quantify the discrepancy between a model PPV 3-cube, \( m(x, y, j) \), and the observed PPV 3-cube, \( PPV(x, y, j) \), with the objective function

\[
L_u(v_{\text{los}}(x, y, i), \sigma_v(x, y, i)) = \frac{1}{2} \sum_{x, y, j} (PPV(x, y, j) - m(x, y, j))^2,
\]

the sum of square differences between the model and the observations. This is the unregularized objective function; hence the subscript \( u \) in \( L_u \).

We optimize \( L_u \) by varying the entries of \( v_{\text{los}}(x, y, i) \) and \( \sigma_v(x, y, i) \). We
restrict \( \sigma_v(x, y, i) \) to be between 1 and 15 km sec\(^{-1}\). The lower bound on \( \sigma_v(x, y, i) \) is set to be slightly smaller than \( 2 \Delta v \), which in this case is 1.4 km sec\(^{-1}\), as there is very little difference between pixel-convolved Gaussians with standard deviations smaller than \( \Delta v \). We restrict \( v_{\text{los}}(x, y, i) \) to be within 45 km sec\(^{-1}\) of the line-of-sight velocity at \( \ell_x, b_y \), and \( d_i \) corresponding to the IAU-recommended 220 km sec\(^{-1}\) flat rotation curve and an 8.5 kpc separation between the Sun and the Galactic center. The middle panel of Figure 4.2 shows a cartoon solution to the the \( L_u \) optimization problem. Qualitative features of the cartoon such as the close match between the model and observed PPV 3-cubes, the magnitudes of deviations from the rotation curve, and the spatial coherence of deviations from the rotation curve are also typical of the actual solution to the unregularized problem.

This solution is not necessarily unique. While we have reduced the number of parameters in the problem by making assumptions about the structure of the ISM in PPDV space, there are still situations in which different \( v_{\text{los}}(x, y, i) \) 3-cubes produce equivalent \( m(x, y, j) \) 3-cubes. For example, if \( m(x_0, y_0, i_0) = m(x_0, y_0, i_1) \), then \( v_{\text{los}}(x_0, y_0, i_0) \) and \( v_{\text{los}}(x_0, y_0, i_1) \) are interchangeable.

To deal with this problem, we introduce external information. The \( \ell \) and \( b \) extent of the voxels in the 3-cubes and 4-cubes are often smaller than coherent structures such as molecular clouds. We may therefore expect voxels that share an \( \ell \) or \( b \) boundary to have similar line-of-sight velocities. We encode this expectation into a regularized objective function, \( L_r \), by adding a term penalizing large differences between the line-of-sight velocities of voxels with
shared $\ell$ or $b$ boundaries:

$$
\mathcal{L}_r (v_{\text{los}}(x, y, i), \sigma_v(x, y, i)) = \frac{1}{\sigma_u^2} \mathcal{L}_u (v_{\text{los}}(x, y, i), \sigma_v(x, y, i)) + \\
\frac{1}{2\sigma_r^2} \sum_{x,y} (v_{\text{los}}(x + 1, y, i) - v_{\text{los}}(x, y, i))^2 + \\
\frac{1}{2\sigma_r^2} \sum_{x,y} (v_{\text{los}}(x, y + 1, i) - v_{\text{los}}(x, y, i))^2,
$$

(4.9)

where $\sigma_u$ and $\sigma_r$ are parameters that set the relative strengths of the model-observation residuals and regularization terms in driving the solution. We set $\sigma_u$ to a value corresponding to 0.05 magnitudes of reddening. This is the standard deviation reported by GSF for the distribution of residuals between the GSF reddening 3-cube integrated along the distance axis and a Planck $\tau_{353\text{GHz}}$-based integrated reddening map. We set $\sigma_r$ to 5 km/s. This is approximately the value of the cloud-cloud dispersion found by Clemens (1985).

The bottom panel of Figure 4.2 shows a cartoon representation of a regularized solution. The regularization is represented by springs. As before, the qualitative features of the cartoon are realistic.

We evaluate the accuracy of the unregularized and regularized KT-derived $v_{\text{los}}$ 3-cubes in the next section. For clarity, we will refer to the discretized 3-cubes as $v_{\text{los}}(\ell, b, d)$.

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4.3.2 Checking the Kinetic Tomography solution

The Reid14 HMSFRs (see §4.2.3) are embedded in, born from, and, presumably, moving with dense molecular gas. The $v_{\text{los}}$ of an HMSFR should therefore be similar to the $v_{\text{los}}$ of the ISM at the HMSFR’s location in PPD space. We can use this property to check the accuracy of our KT-derived $v_{\text{los}}(\ell, b, d)$ 3-cubes by comparing the HMSFRs’ observed $v_{\text{los}}$ to the $v_{\text{los}}$ KT assigns to the HMSFRs’ $\ell$, $b$, and $d$ values. In this section, we make this comparison for the $v_{\text{los}}(\ell, b, d)$ fields associated with a radially-varying rotation curve from Clemens (1985), unregularized KT, and regularized KT.

We must propagate the uncertainty on the distance to an HMSFR when comparing the HMSFR’s observed $v_{\text{los}}$ to a $v_{\text{los}}(\ell, b, d)$ field. The typical uncertainty on the parallax of a Reid14 HMSFR is between 5 and 10% and is implicitly assumed to be Gaussian.

Following the discussion in Bovy, Hogg, and Rix (2009), we assume that this Gaussian parallax uncertainty propagates linearly to a Gaussian distance uncertainty.

We assume that the uncertainty on the assigned $v_{\text{los}}(\ell, b, d)$ value is also approximately Gaussian. Consider an HMSFR, $s$. To compute the mean $\mu_s$ and standard deviation $\sigma_s$ of this HMSFR’s distribution of possible $v_{\text{los}}(\ell, b, d)$ values, we start by drawing possible distance values $d_t$ from $p_s(d)$. Here, $p_s(d)$ is the distribution over possible distances to HMSFR $s$ and $t$ is an index over draws. For each draw, we extract $v_{\text{los}}(\ell = \ell_s, b = b_s, d = d_t)$ from $v_{\text{los}}(\ell, b, d)$. The mean and standard deviation of these extracted line-of-sight velocity values are $\mu_s$ and $\sigma_s$. 

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In Figure 4.3, we show a comparison of the HMSFRs’ observed $v_{\text{los}}$ values and the mean $v_{\text{los}}$ values extracted from line-of-sight velocity fields corresponding to the Clemens (1985) rotation curve, unregularized KT, and regularized KT. To highlight the peculiar motions of the HMSFRs, these values are shown with the line-of-sight velocity corresponding to a flat 220 km/sec rotation and a Sun-Galactic center separation of 8.5 kpc subtracted off. The similarity of a velocity field to the HMSFR observations is indicated by how close points derived from that velocity field tend to be to the one-to-one line in the appropriate panel of Figure 4.3. It should be clear from visual inspection that the radially-varying rotation curve does not accurately predict the velocities of the HMSFRs and that both versions of KT are clearly more accurate. There is also a significant, though possibly less visually obvious, improvement from unregularized to regularized KT.

To get a quantitative estimate of this improvement, we can compute the reduced $\chi^2$ values of the two sets of velocity estimates. The reduced $\chi^2$ value is given by the expression

$$\chi^2 = \frac{1}{\nu} \sum_{s} \left( \frac{v_{\text{los}} - \mu_s}{\sigma_s} \right)^2,$$  \hspace{1cm} (4.10)

where $\nu$ is the number of degrees of freedom in the problem and $S$ is the number of observations. If the uncertainties are Gaussian and correctly estimated, the reduced $\chi^2$ value should be approximately equal to 1. If we assume the regularization parameter counts against the number of degrees of freedom, the reduced $\chi^2$ values of the unregularized and regularized KT solutions are 5 and 3, respectively.
The $\chi^2$ value of the regularized KT solution is driven by 5 catastrophic outliers. If we remove these outliers, the reduced $\chi^2$ values of the unregularized and regularized KT solutions drop to 4 and 1.3, respectively. We consider the advantage of regularized over unregularized KT to be sufficient to adopt the regularized KT solution as the KT solution, and will refer to it as such below.

At the positions of 94 of 99 HMSFRs, KT performs remarkably well.

4.3.3 Catastrophic outliers

In this section, we discuss the five HMSFRs where the KT-derived and directly observed $v_{\text{los}}$ values are clearly inconsistent. The distribution of standardized residuals of the HMSFR sample is shown in panel (a) of Figure 4.4; the five outlier HMSFRs are marked in red. The reason why these five HMSFRs, specifically, are outliers seems to be that they are located in a particularly complex and confused part of the Galaxy. From panels (b), (c), and (d) of the same Figure, one can see that all of the outliers are in the inner Galaxy and relatively close to the Galactic center, at $0^\circ < \ell < 35^\circ$ and $R_{\text{GC}} < 6$ kpc. We note that four of these five outliers are in the area of sky covered by the GASS Galactic HI survey. We doubt GASS is to blame as it has relatively mild systematic errors and is intermediate in spatial resolution among the three surveys we use. If we compare the distributions of all HMSFRs and outlier HMSFRs in $\ell$ and $R_{\text{GC}}$, it should be apparent that the distribution of outliers does not follow the distribution of all HMSFRs.

We can quantify this deviation by assuming that any HMSFR is equally likely to be one of the five outliers and computing the probability of finding
all five in a randomly chosen subsample of the same size as one of our two selections. Since a single HMSFR can not be present in a sample twice, the appropriate distribution to use for this calculation is the hypergeometric distribution, which assumes that the subsample is chosen without replacement. The probability of finding all five outliers in a random subsample the size of either of the two selections is, in both cases, much less than 1%.

The implication of this difference in distribution is that there is an actual enhancement in the rate at which KT produces incorrect solutions for sightlines that pass near the Galactic center. There are three main reasons why KT would be less accurate along a sightline at low $\ell$. Firstly, these sightlines pass through more matter, due to both the increase in ISM surface density at low $R_{\text{GC}}$ and the fact that geometrically, a sightline at low $\ell$ will pass through more of the far side of the Galaxy. Having more matter along a sightline increases the complexity of the problem — more parcels of ISM in PPD space have to be correctly associated with velocity components in PPV space. Secondly, due in part to the increase in ISM surface density with decreasing $R_{\text{GC}}$, the well-measured part of the PPD cube does not extend as far towards the inner Galaxy as it does towards the outer Galaxy (GSF). If the PPD cube is not accurate past some distance, then we are unlikely to obtain a correct solution past that distance. Thirdly, the Galactic bar can stir interstellar matter up, inducing a complicated velocity field with lots of structure on small spatial scales. Given that the distance extent of PPD voxels near the inner Galaxy is of order a kpc, we could simply have insufficient spatial resolution to map this bar-induced velocity field.
Two of these three reasons are caused by being at low $\ell$ while the other is caused by being in a specific $R_{GC}$ range. To try to differentiate between the two possible causes, we can repeat the quantitative exercise described above with the $R_{GC}$ selection as the subsample and the $\ell$ selection, rather than the full set of 99 HMSFRs, as the population. The probability of finding all five outliers in a random 21-element subsample of the 31-element $\ell$ selection is about 11%. This probability is low but not unreasonable; we cannot differentiate between the two causes in this way.

4.4 Discussion

4.4.1 Qualitative features of the solution

We have established that KT is, quantitatively-speaking, correct at the locations of 94 dense, star-forming knots of interstellar matter and we have found a heuristic explanation for why KT is quite incorrect at the locations of 5 other dense, star-forming knots of interstellar matter. Given the lack of other published $v_{los}(\ell, b, d)$ measurements, we cannot quantitatively establish that our $v_{los}(\ell, b, d)$ 3-cube is also correct away from these 99 locations. There is, however, the previously published two-dimensional peculiar velocity map of Brand and Blitz (1993).

A two-dimensional peculiar velocity field derived from the KT solution is shown in Figure 4.5. This peculiar velocity field is derived by subtracting the line-of-sight velocity field corresponding to a flat rotation curve from the $v_{los}(\ell, b, d)$ 3-cube and taking the mass-weighted average of this peculiar velocity 3-cube along the $b$ axis over the range $-2.5^\circ \leq b \leq +2.5^\circ$. The
peculiar velocity field of Brand and Blitz (1993) is shown in Figure 10 of their paper. Qualitatively, the two peculiar velocity fields are quite similar. The locations, extents, and signs of regions of coherent peculiar velocity are, for the most part, the same in both maps. There are, however, some differences in the magnitudes of peculiar velocities in these regions.

We can also qualitatively compare the typical scale of coherent velocity fluctuations in our two-dimensional peculiar velocity field to measurements of this scale from the literature. Much of the power in the peculiar velocity field of disc gas (e.g. Clemens 1985) and disc stars (e.g. Bovy et al. 2015) is found on scales of about 2 kpc. This is consistent, at least by eye, with the typical extent of a coherent peculiar velocity fluctuation in our two-dimensional peculiar velocity field.

Figure 4.5 also shows the line-of-sight velocities at the $\ell$, $b$, and $d$ of HMSFRs according to our $v_{\text{los}}(\ell, b, d)$ 3-cube and the actual observations. All of the HMSFRs are in $b$ range we averaged over to produce our two-dimensional peculiar velocity field, but there are clear differences between the observed HMSFR line-of-sight velocities and the two-dimensional velocity field. If we assume the two-dimensional velocity field is, for the most part, correct, then these differences imply peculiar velocity fluctuations on spatial scales of order the typical height off the plane of an HMSFR, or 10-100 pc. The same differences, in most cases, are also seen in the velocities assigned based on our $v_{\text{los}}(\ell, b, d)$ 3-cube. Combining these facts, we can heuristically conclude that we are more-or-less correctly detecting peculiar velocity fluctuations on both large, multi-kpc scales and small, 100 pc scales.
4.4.2 Unmet assumptions and their potential consequences

Our treatment of the data, our parametrization of the 4-dimensional structure of the ISM, and our regularization scheme are all based on assumptions that are not always met. We convert our distributions of reddening, H I emission, and CO emission to distributions of absolute matter content in PPV and PPD space assuming there is a single, linear function relating the amount of each tracer to an amount of matter. Due to variations in the dust-to-gas and CO-to-\text{H}_2 ratios and radiative transfer effects such as self-absorption, these functions are neither uniquely defined nor linear. We have implicitly assumed that the PPD and PPV 3-cubes are projections of the same part of the same PPDV 4-cube. This is not the case — the PPV 3-cube is an integral of the PPDV 4-cube to an effectively infinite distance while the most distant well-measured voxels in the PPD 3-cube are only \( \sim 10 \text{ kpc} \) away from the Sun (GSF). Our parametrization of the 4-dimensional structure of the ISM assumes that the ISM’s velocity distribution within a PPD voxel can be described by a mean, which is close to the value of the Galactic rotation curve at the voxel’s center, and a dispersion. This will not be true for a voxel that contains a shock or is large compared to the spatial scale of velocity fluctuations; because our distance resolution is constant in log space, this effect will apply to all voxels beyond some distance. Our regularization scheme assumes that the velocity distributions of voxels with shared \( \ell \) or \( b \) boundaries will be similar. This will once again not be true of voxels that cross shocks or are sufficiently large.

Despite the fact that its underlying assumptions do not hold over some of the solution domain, KT produces a \( v_{\text{los}}(\ell, b, d) \) solution that quantitatively
agrees with independent \( v_{\text{los}}(\ell, b, d) \) observations (see §4.3.2). We can resolve this conflict by concluding that (1) the assumptions, as stated, are too strict or by arguing that (2) the particular set of \( v_{\text{los}}(\ell, b, d) \) observations are not representative of the ISM as a whole.

The fact that all of the poorly-reproduced HMSFRs lie in the inner Galaxy (see §4.3.3), where our assumptions tend to not be met more often and more egregiously than in the outer Galaxy, lends credence to the resolution (1). Perhaps KT is robust to some level of its assumptions not being met and this level is only exceeded in some parts of the inner Galaxy. As an example of the extent to which the inner Galaxy does not meet our assumptions, consider the fact that the maximum distance from the Sun to which the PPD 3-cube is accurate to in the inner Galaxy is approximately 5 kpc GSF while the PPV 3-cube is integrated out to the far edge of the Galaxy.

Resolution (2), that the comparison observations are atypical, seems unlikely considering the qualitative structure of the solution (see §4.4.1) but cannot yet be ruled out empirically. The comparison observations are of HMSFRs, which by definition will be associated with large overdensities of molecular gas. It is possible that the check we have performed in §4.3.2 only applies to dense molecular gas. For example, KT could merely be finding the most massive object along a sightline through the PPD 3-cube and associating it with the most massive objective in the corresponding sightline through the PPV 3-cube. This would usually correctly assign a distance and velocity to something like a GMC but would fail for less concentrated neutral gas. However, it would be difficult to reconcile the clear and non-trivial larger-scale
velocity structure seen in the previous section with a scenario in which the KT solution is only correct at extreme overdensities.

To get a more quantitative and broadly applicable understanding of when KT works and fails, we would need either a less density-biased set of independent \( v_{\text{los}}(\ell, b, d) \) measurements or a set of artificial injection tests. These artificial injection tests would consist of numerical experiments in which we artificially observe a model galaxy’s ISM, reconstruct the \( v_{\text{los}} \) field from these artificial observations using KT, and compare the reconstructed and input model \( v_{\text{los}} \) fields. To the best of our knowledge, there are no currently available catalogs of these sorts of less density-biased measurements, ruling out option one. The steps involved in artificial injection tests, particularly simulating galaxies at sufficiently high resolution and producing artificial observations in a way that includes the non-trivial systematics in the actual observations, are complicated enough to put option two beyond the scope of this work.

Both of these options are plausible directions for future work. The 1.527 \( \mu \text{m} \) diffuse interstellar band (DIB), for instance, has been mapped over much of the northern sky by the APOGEE survey (Zasowski et al., 2015). Observations of this DIB towards APOGEE stars with known distances could potentially be used to build catalogs or even maps of \( v_{\text{los}}(\ell, b, d) \) using an independent dataset. Artificial injection tests are conceptually straightforward, though they do require a substantial investment of time and computational resources. While neither option is easy, we would argue that some combination of the two will be necessary before the KT-derived \( v_{\text{los}} \) 3-cube can be trusted away from the HMSFRs of Reid14.
4.5 Conclusion

In this work we developed a method for measuring the radial velocity of parcels of the interstellar medium of a measured distance, which we dubbed Kinetic Tomography. We argued that this method is important as a tool for measuring converging and diverging flows around our Galaxy as well as for detecting large scale deviations from assumed rotation curves. The method takes as inputs the three-dimensional distribution of dust in our Galaxy measured from stellar photometry and the emission spectra from Galactic CO and H I. We developed a technique that assigns each 3D parcel of ISM from the dust map a line-of-sight velocity and line-of-sight velocity width, in order to best reproduce the observed CO and H I data. We found that we can improve the fidelity of our solution by implementing Tikhonov regularization, effectively coupling the line-of-sight velocity of adjacent pixels.

As a test of our method we compare our results to independent measurements of HMSFRs from Reid14, which contain both distances and line-of-sight velocity information. We find that of the 99 HMSFRs in the area of sky we study, 94 are consistent with our results and 5 are outliers, all of which lie near Galactic center. This consistency indicates our map is an accurate representation of the velocity field of the ISM, at least in denser regions consistent with HMSFRs. We also find qualitative consistency with the peculiar velocity maps of Brand and Blitz (1993).

Here we conclude that KT can be a very powerful tool for the study of the velocity structure of the Galactic ISM. In future work, we will investigate what KT can tell us about the Galactic rotation curve, streaming motions within the
Galactic disk, and the vertical structure of Galactic flows.
Figure 4.2: Diagrams explaining the inverse kinematic distance methods, unregularized Kinetic Tomography, and regularized Kinetic Tomography. In each diagram, we show a map of residuals from a flat rotation curve (left quarter-circle), mock PPD and PPV data along a single sightline \((x_0, y_0)\) (narrow vertical and horizontal panels), and the mean \(v_{\text{los}}(x_0, y_0, i, j)\) and standard deviation \(\sigma_v(x_0, y_0, i, j)\) of the velocity along that sightline. The \(\ell, b, \) distance, and \(v_{\text{los}}\) axes are indexed by \(x, y, i,\) and \(j\); note that the residual map shows only a single latitude. The results of applying a fixed inverse kinematic distance method, unregularized Kinematic Tomography, and regularized Kinetic Tomography are shown in black, purple, and pink. Regularization is indicated in the bottom schematic with spring symbols. Our regularization method minimizes the velocity difference between voxels that are connected by spring symbols.
Figure 4.3: The three panels show the residuals from flat rotation of the Reid et al. (2014) HMSFR line-of-sight velocity observations on the y-axis and residuals from flat rotation of the values of the Clemens (1985) rotation curve (left panel), the unregularized kinetic tomography solution (middle panel), and the regularized kinetic tomography solution (right panel) at the positions of the HMSFRs on the x-axis. In each panel, the one-to-one line is indicated in gray.
Figure 4.4: (a) The distribution of residuals per standard deviation (standardized residuals) between the observed and KT-derived line-of-sight velocities of HMSFRs (filled histogram), with an appropriately-scaled standard normal distribution for reference (empty histogram). We consider HMSFRs with $|\Delta v/\sigma| > 3$ to be outliers. In all three panels, outliers are denoted in red and non-outliers are denoted in gray. (b) The distribution of the HMSFRs’ Galactic longitudes. HMSFRs with $\ell < 35^\circ$ are outlined with a dashed black line. (c) The distribution of the HMSFRs’ Galactocentric radii. HMSFRs with $\ell < 35^\circ$ are outlined with a dashed black line. (d) The locations of the HMSFRs in heliocentric Cartesian coordinates, where $X_{HC}$ increases towards $\ell = 0^\circ$ and $Y_{HC}$ increases towards $\ell = 90^\circ$. 
Figure 4.5: Colors show the difference between an observed or estimated $v_{\text{los}}$ and the value predicted from a flat rotation curve. The background is an average of the kinetic tomography-derived velocity field over $-2.5\,\text{deg} \leq b \leq +2.5\,\text{deg}$. The color of the inner part of each circle is the $v_{\text{los}}$ of an HMSFR. The color of the outer ring of each circle is the value of the kinetic tomography-derived velocity field at the position (including $b$) of the HMSFR.
Chapter 5

Kinetic Tomography. II. A second method for mapping the velocity field of the Milky Way Interstellar Medium and a comparison with spiral structure models

In this work, we derive a spatially resolved map of the line-of-sight velocity of the interstellar medium and use it, along with a second map of line-of-sight velocity from Paper I of this series, to determine the nature of gaseous spiral structure in the Milky Way. This map is derived from measurements of the 1.527 μm diffuse interstellar band (DIB) in stellar spectra from the APOGEE survey and covers the nearest 4-5 kpc of the Northern Galactic plane. We cross-check this new DIB-based line-of-sight velocity map with the map derived in Paper I and find that they agree. We then compare these maps with line-of-sight velocity maps derived from simulations of quasi-stationary density wave

1Adapted from a paper that originally appeared in The Astronomical Journal (Tchernyshyov, Peek, and Zasowski, 2018).
spiral structure and dynamic, or material, spiral structure in a Milky Way-like galaxy. While none of the maps derived from these simulations is an exact match to the measured velocity field of the Milky Way, the measurements are more consistent with simulations of dynamic spiral structure. In the dynamic spiral structure simulation that best matches the measurements, the Perseus spiral arm is being disrupted.

5.1 Introduction

There are two main models for how a differentially rotating galaxy can have long-lived spiral structure. The first is the stationary density wave model (SDW; Lin and Shu, 1964; Shu, 2016). In the SDW model, spiral arms are global oscillatory modes of a stellar or gaseous disc. The group velocity of a wave does not have equal the velocity of the oscillating matter, so the arms can propagate without winding up. The second model for long-lived spiral structure is known as the dynamic, the transient and recurrent, or the material spiral structure model (Sellwood and Carlberg, 1984). Here, we will use the term “dynamic” to describe these models. In the dynamic spiral structure model, the pattern is corotating with the matter. Individual spiral arms form through a process such as swing amplification, wind up, and dissipate over one to a few Galactic rotation periods (Sellwood and Carlberg, 1984; Grand, Kawata, and Cropper, 2012; Baba, Saitoh, and Wada, 2013; D’Onghia, Vogelsberger, and Hernquist, 2013). If the arm formation process is efficient, these dissipating arms are rapidly replaced, meaning that although individual spiral arms are short-lived, spiral structure in general is long-lived. It is not
known whether the type of spiral structure in most spiral galaxies is SDW or dynamic. Evidence has been found for both models, sometimes in the same galaxies; see Shu (2016) for examples of evidence in support of the SDW model and Dobbs and Baba (2014) in support of the dynamic model. In this paper, we focus on the spiral structure of the Milky Way.

Since the 1950s, the consensus has been that the Milky Way has spiral arms in gas, star formation, and young stars (Morgan, Sharpless, and Osterbrock, 1952; van de Hulst, Muller, and Oort, 1954) The gaseous spiral arms are detected as contiguous features in $\ell - v$ diagrams and have been seen in HI-traced neutral gas (van de Hulst, Muller, and Oort, 1954) and CO-traced molecular gas (Cohen et al., 1980). Arms traced by young stars (e.g. Morgan, Sharpless, and Osterbrock, 1952; Xu et al., 2018) and star formation regions (e.g., Reid et al., 2014) are detected as contiguous overdensities in space. Emission from the gaseous arms can be detected out to large distances, including the far side of the Galaxy (Dame and Thaddeus, 2011), but their positions in space can only be inferred using indirect methods such as the kinematic distance method. The situation is reversed for the star forming arms – their positions in space are known directly, allowing measurements of arm properties such as pitch angles to be made, but the necessary observations are not available at large distances from the Sun. The measurable distribution of stars and star formation in $\ell$, $b$, and $d$ and of gas in $\ell$, $b$, and $v_d$ can fit into the context of either model of spiral structure and cannot decisively distinguish between them. In this work, we investigate what can be determined about the Milky Way’s spiral structure from the velocity field of its interstellar medium.
These two theories of spiral structure make different predictions for large-scale streaming motions, i.e. spatially coherent deviations from simple rotation. Spiral structure induces, and is produced by, streaming motions. These streaming motions should be particularly clear in the velocity field of interstellar matter, which is collisional and hence dynamically cold. In the SDW model, interstellar matter flows through a spiral arm or, equivalently, the overdensity of ISM that is an arm moves through the disc of the galaxy (Roberts, 1969). An SDW arm is simultaneously accumulating matter from one side and losing it from the other in a flow that spans the entire length of the arm. In the dynamic model, gas converges on a spiral arm that is growing and is sheared or blown away (e.g., by stellar and supernova feedback) from a spiral arm that is winding up and dispersing (Baba et al., 2016). This convergence is thought to happen due to a combination of orbit crowding and the gravitational influence of the stellar component of the spiral arm. The SDW model predicts a global flow through each arm; the dynamic model predicts local flows converging or diverging from each arm. This distinction is why the velocity field of the ISM is a powerful discriminator.

To have a quantity that can be directly compared to a gas velocity field measurement, we have collected ten simulations of spiral structure in Milky Way-like galaxies. Five of these are SDW simulations and five are dynamic simulations. These simulations were tuned by their authors to match certain observations of the Milky Way but are not considered to be perfect matches. Our primary observable, the line-of-sight velocity of interestellar matter as a
function of position in the Galaxy (which we call $v_d(x, y)$), was not directly used to tune any of the simulations and so can be considered a prediction.

We construct empirical maps of the Milky Way’s $v_d(x, y)$ field and compare them with predictions for $v_d(x, y)$ from the simulations. The maps are made using a collection of techniques we call “Kinetic Tomography” (KT). In Tchernyshyov and Peek (2017, henceforth TP17), we developed a method for combining measurements of HI and CO emission in $(\ell, b, v_d)$ space with the three-dimensional $(\ell, b, d)$ reddening map of Green et al. (2015) to produce a map of $v_d(\ell, b, d)$. We will call this method “gas and dust KT” (G&D KT) and the resulting map the G&D KT map. In TP17, we validated the G&D KT map in regions containing very dense gas. To discriminate between theories of spiral structure, we also need to be sure that the $v_d$ map is correct in more diffuse regions.

The main observational contribution of this work is a second map of the Milky Way ISM velocity field, which we will compare to the G&D KT map and simulations of spiral structure. This map is based on ISM absorption lines in spectra of stars with known distances. An ISM absorption line provides the sightline-integrated distribution of its carrier species with respect to $v_d$. By taking differences between the optical depth profiles of the ISM along approximately the same sightline but with different terminal distances (i.e., different stellar distances), we can get a measurement of the average $v_d$ of the ISM between the endpoints of those sightlines. With enough background stars, a more sophisticated version of this procedure can be used to make a continuous map of $v_d$. The absorption line we use is the 1.527 $\mu$m diffuse
interstellar band (DIB) (Geballe et al., 2011; Zasowski et al., 2015, henceforth Z+15) in stellar spectra from the APOGEE survey (Section 5.2.1; Majewski et al., 2017). APOGEE covers much of the Northern Galactic plane and, because it is a near infrared survey, can obtain high resolution, high signal-to-noise ratio spectra of distant, highly reddened stars. In the first half of this paper, we analyze DIB absorption in APOGEE spectra to produce a map of the local (i.e., non-integrated) line-of-sight velocity using a procedure we will call DIB KT.

The rest of the paper is organized as follows: In Section 5.2, we describe the datasets we use. In Section 5.3, we explain our map-making procedure, and in Section 5.4, we list and describe the simulations to which we compare our $v_d$ maps. In Section 5.5, we check the DIB KT map against the G&D KT map. In Section 5.6, we compare the DIB KT and G&D KT maps with $v_d$ maps from simulations and argue that the Milky Way has dynamic, rather than SDW, spiral structure. Finally, in Section 5.7, we conclude. Throughout this work, we assume a Sun-Galactic center separation of 8.5 kpc, a Galactic rotation rate of 220 km s$^{-1}$, and a motion of the Sun relative to the local standard of rest (LSR) of 12 km/s towards the Galactic center, 9 km/s in the direction of Galactic rotation at the Sun, and 7 km/s towards the North Galactic pole.

## 5.2 Data

The new map of $v_d(x, y)$ is based on an analysis of absorption by the 1.527 μm DIB in APOGEE spectral residuals. We describe the APOGEE data and our procedure for selecting and reducing a subsample of the full APOGEE dataset.
Figure 5.1: (Left) The equivalent width of the DIB feature towards stars in our subsample of the APOGEE survey. The Galactic center is to the right and the direction of Galactic rotation at the position of the Sun is upwards. (Middle) The first moment $v_{d,\text{int}}$ of the DIB feature towards stars in our dataset. The velocity $v_{d,\text{int}}$ is the DIB density-weighted average of the (local, un-integrated) velocity $v_d$ along the line of sight. (Right) The $v_{d,\text{int}}$ field of a uniform interstellar medium undergoing flat 220 km/s rotation. The measured and computed $v_{d,\text{int}}$ are both in the heliocentric rest frame.
in Section 5.2.1, the characteristics of the 1.527 μm DIB that make it useful for this sort of analysis in Section 5.2.2, and our procedure for obtaining distances to stars in our sample in Section 5.2.3. In Sections 5.2.4 and 5.2.5, we describe two prior measurements of the ISM velocity field. The first of these is the G&D KT $v_d(\ell, b, d)$ map derived from HI and CO emission and dust reddening derived in TP17 (Section 5.2.4). The second is collection of measurements of the velocities and parallax distances of high mass star formation regions (HMSFRs; Section 5.2.5).

### 5.2.1 APOGEE Spectra

We measure the 1.527 μm DIB profiles in spectra from the Apache Point Observatory Galactic Evolution Experiment (APOGEE; Majewski et al., 2017), part of the Sloan Digital Sky Survey III (SDSS-III; Eisenstein et al., 2011) and SDSS-IV (Blanton et al., 2017). This dataset comprises high-resolution $H$-band spectra and derived radial velocities (RVs), stellar parameters, and chemical abundances for $\sim$263,000 stars in the Milky Way (MW) and Local Group, released as part of SDSS Data Release 14 (Abolfathi et al., 2018). See Zasowski et al. (2013) and Zasowski et al. (2017) for details of the APOGEE targeting selection, Nidever et al. (2015) for a description of the custom data reduction and RV pipeline, García Pérez et al. (2016) for details about APOGEE Stellar Parameters and Chemical Abundances Pipeline (ASPCAP), and Holtzman et al. (2015, 2018 in press) for details about the data calibration and released data products.

The DIB analysis in Z+15 used the synthetic spectra fits of ASPCAP to
remove the stellar absorption lines from APOGEE spectra and isolate the interstellar absorption features (§5.2.2). In this analysis, we instead adopt stellar spectral models generated by the Cannon (Ness et al., 2015; Casey et al., 2016), which we found to produce cleaner spectral residuals at lower SNR for a wide range of stellar types.

To train our data-driven model, we selected stars with high-quality spectra and reliable stellar parameters, requiring SNR $\geq 100$, valid calibrated $T_{\text{eff}}$ and $\log g$ values, and that the METALS_BAD, ALPHAFE_BAD, and STARBAD flags not be set. We also required that the stars have Galactic latitudes $|b| \geq 60^\circ$, that the spectra have been observed with the Sloan Foundation 2.5-meter telescope rather than the NMSU 1-meter telescope to ensure consistency with the rest of the sample, and that the stars not have a significant DIB detection in the DIB feature catalog of Z+15. The $|b|$ limits and quality criteria ensure that our spectral training set does not contain DIB signatures or significant noise that would be carried into the test set’s spectral models. Even though the interstellar and stellar absorption lines are theoretically independent and come from physically distinct sources, some correlation at the pixel level is expected due to the selection-induced correlation between, e.g., DIB strength and stellar temperature; stars need to be more luminous, and hence cooler, to be seen at large distances and behind large amounts of interstellar material. Thus, eliminating as much DIB contamination as possible from the training set is critical to creating the cleanest residual profiles for this analysis.

The criteria above yielded a training set of 8900 stellar spectra. We trained a four-label Cannon model ($T_{\text{eff}}$, $\log g$, $[\text{M/H}]$, and $[\alpha/\text{M}]$) on these spectra
using the “Annie’s Lasso” version of the Cannon\(^2\). We then applied this model to all midplane DR14 spectra (with \(|b| \leq 1^\circ|\)) and generated best-fit spectra for each sightline, in addition to the computed stellar labels. The ratio of each observed spectrum with its Cannon-derived counterpart is the residual spectrum in which we identify DIB absorption. Of the full \(|b| < 1^\circ|\) sample, we keep the 17546 stars for which this instance of the Cannon finds non-null values for all four stellar parameters.

5.2.2 The 1.527 μm Diffuse Interstellar Band

The 1.527 μm DIB was discovered by Geballe et al. (2011) in heavily-reddened sightlines towards the Galactic Center. It is the strongest DIB in APOGEE’s 1.5 – 1.7 μm wavelength range. Z+15 measured this feature along ∼60,000 APOGEE sightlines throughout the Northern sky, deriving its empirical rest wavelength (\(\lambda_{0,\text{vac}} = 1.5274\) μm) and the relationship between its equivalent width (\(W_{\text{DIB}}\)) and dust reddening. Cox et al. (2014) studied this feature towards a small sample of early-type stars with a range of foreground extinction, and Elyajouri et al. (2016) extracted and characterized profiles of this DIB from spectra of ∼6700 early-type stars in the APOGEE dataset.

Three characteristics of the 1.527 μm DIB make it particularly useful for an analysis of the ISM velocity field throughout the Galactic plane. Because its rest wavelength is in the near infrared, where the impact of dust extinction is much weaker than at optical wavelengths (\(A(H)/A(V) \approx 0.17\); e.g., Schlafly and Finkbeiner, 2011), the DIB can be measured towards stars behind dense

\(^2\)https://github.com/andycasey/AnniesLasso
molecular gas and/or very long columns of diffuse ISM. This property enables us to detect the DIB and map the ISM velocity field out to large distances from the Sun. The equivalent width of the DIB is a near-linear tracer of $A(V)$ at interstellar extinctions typical of even the dusty inner Galactic disc and bulge (Z+15). Elyajouri, Cox, and Lallement (2017) find that this linear relationship cannot be applied in clouds with volume density $n_H \gtrsim 10^5$ cm$^{-3}$ such as the Barnard 68 Bok globule. Fortunately, clouds this dense comprise only a small fraction of the volume of the interstellar medium, which permits us to take advantage of the more typical linear behavior for the large-scale mapping performed here. Finally, the intrinsic profile of the 1.527 $\mu$m DIB is symmetric and consistent. If the band were asymmetric, this asymmetry would need to be modeled and the degree of asymmetry would be degenerate with the actual value of the velocity field. This degeneracy is not present when the DIB is symmetric.

To demonstrate that the 1.527 $\mu$m DIB contains meaningful and non-trivial information about the ISM velocity field, we show the equivalent width and first moment of the DIB feature towards all of the stars in our sample in Figure 5.1. For comparison, we also show the integrated velocity field one would expect from a flat 220 km/s rotation curve and a uniform-density ISM. There are clear differences between the measured and expected sightline-integrated velocities.
5.2.3 Stellar distances

Our analysis requires an estimate of the distance to each star in the sample. We use a combination of spectrophotometric distances from the APOGEE DR14 red clump catalog (Bovy et al., 2014) and the DR14 distance Value Added Catalogs (Santiago et al., 2016; Wang et al., 2016, and Holtzman et al, in prep) and parallaxes from Gaia DR2 (Gaia Collaboration et al., 2016; Gaia Collaboration et al., 2018). We collected parallaxes for all APOGEE sources in our sample using the Gaia DR2-2MASS precomputed crossmatch table (Salgado et al., 2017; Marrese et al., 2019).

We combined spectrophotometric distances with parallaxes using a simplified version of the approach described in McMillan et al. (2018). The spectrophotometric distance $d_{sp}$ and its (assumed Gaussian) uncertainty $\sigma_{sp}$ can be thought of as providing a prior for the “true” distance $d$ and the parallax $\varpi$, and its uncertainty $\sigma_{\varpi}$ can be thought of as providing a likelihood for $\varpi$ given $d$. The posterior probability distribution for $d$ is then given by the expression

$$p(d | d_{sp}, \sigma_{sp}, \varpi, \sigma_{\varpi}) \propto \mathcal{N}(1/d; \varpi + \delta, \sigma_{\varpi}^2) \times \mathcal{N}(d; d_{sp}, \sigma_{sp}^2),$$

(5.1)

where $\delta = 0.029$ mas is the parallax zero point offset given in Luri et al. (2018) and $\mathcal{N}(d; d_{sp}, \sigma_{sp}^2)$ is a normal distribution with mean $d_{sp}$ and variance $\sigma_{sp}^2$ evaluated at a point $d$. McMillan et al. (2018) include stellar parameters, which are covariant with the spectrophotometric distance, in this expression. As we do not have the necessary probability density functions for any of the distance catalogs we use, we assume $d_{sp}$ and $\sigma_{sp}$ provide a sufficient description of the distance probability density function.
There can be multiplicative shifts between the calibrations of distance estimates from different sources. To infer the value of these shifts between the Gaia DR2 distances and the Bovy et al. (2014, RC), Santiago et al. (2016, BPG), Wang et al. (2016, NAOC), and Holtzman et al (in prep, NMSU) spectrophotometric distances, we modify Equation 5.1 to include a shift term $a \equiv d / d_{\omega}$ and an excess variance term $\sigma_{\text{ext}}$:

$$p(d_i | d_{sp,i}, \sigma_{sp,i}, \omega_i, \sigma_{\omega,i}, a, \sigma_{\text{ext}}) \propto \mathcal{N}(1/d_i; \omega_i + \delta, \sigma_{\omega,i}^2) \times \mathcal{N}(d_i; ad_{sp,i}, \sigma_{sp,i}^2 + \sigma_{\text{ext}}^2).$$

(5.2)

The shift and excess variance terms are assumed to be the same for all spectrophotometric distances determined using a given method. The per-star variables are given a subscript $i$ to indicate that they vary from star to star.

To avoid complications from unmodeled systematics, we only use stars with parallax signal-to-noise ratios $\omega / \sigma_\omega > 25$ and with nominal parallax and spectrophotometric distances that are less than 2 kpc. We evaluate Equation 5.2 for each star in this subset from a given method over a grid with $d_i$ ranging from 0 to 10 kpc in steps of 0.1 kpc, $a$ ranging from 0.8 to 1.2 in steps of 0.002, and $\sigma_{\text{ext}}$ ranging from 0 to 0.5 kpc in steps of 0.01 kpc. We then integrate over each $d_i$ and over $\sigma_{\text{ext}}$ to get a probability density function for $a$.

The expected value and standard deviation of $a$ for each method is shown in Figure 5.2. The RC shift has a greater uncertainty than the shifts for the other methods because few stars in the RC catalog are within 2 kpc of the Sun. Because they are mutually consistent, we use the NMSU and RC distances. We combine the NMSU and RC catalogs with the DR2 parallaxes using the
following procedure:

- If a star has an RC distance and a parallax, shift the RC distance using $a_{RC}$ and combine the result with the parallax using Equation 5.1. (3277 stars)

- If a star has an RC distance but no parallax, shift the RC distance using $a_{RC}$. (53 stars)

- If a star has an NMSU distance and a parallax but no RC distance, shift the NMSU distance using $a_{NMSU}$ and combine the result with the parallax using Equation 5.1. (13226 stars)

- If a star has an NMSU distance but no parallax or RC distance, shift the NMSU distance using $a_{NMSU}$. (990 stars)

The shifts used are the expected values shown as points in Figure 5.2.

5.2.4 The Tchernyshyov et al. $v_d(\ell, b, d)$ map

In TP17, we presented a method for mapping the ISM velocity field using measurements of dust reddening and CO and HI emission. This method was based on matching the amount of dust in voxels of a 3D dust map (Green et al., 2015) with velocity components in a 3D gas emission cube under certain restrictions on the shape of the resulting velocity field. We will be using the ISM velocity map produced in that work (the gas and dust, or G&D, KT map) to check the DIB-derived velocity map. The two maps were produced using entirely different datasets and methods and should therefore have different
systematics, meaning that features of the velocity field that are the same in both maps are most likely real.

The G&G KT map is 3D and in spherical coordinates while the DIB KT is 2D and in Cartesian coordinates. We project and regrid the G&G KT map onto the DIB KT coordinate frame using ISM density-weighted averaging.

5.2.5 The Reid et al. high mass star formation regions

R+14 published complete 6D phase space information – on-sky positions, parallax distances, line-of-sight velocities, and proper motions – for 103 high mass star forming regions (HMSFRs). In TP17, we used these HMSFRs to test the accuracy of the G&G KT map. In this work, we will use them to delineate the locus of dense gas and enhanced star formation in the Perseus and Local
spiral arms.

5.3 Kinetic Tomography with the 1.5 μm DIB

We generate a map of \( v_d(x, y) \) by modeling differences between the DIB spectra (the residual spectra of Section 5.2.1) of pairs of stars with small angular and line-of-sight distance separations. These DIB difference spectra are an approximation to the derivative of the DIB carrier optical depth distribution \( \tau_{\text{DIB}}(\ell, b, d, v_d) \) with respect to distance, \( \frac{d\tau_{\text{DIB}}}{dd} \). \( v_d(\ell, b, d) \) is the first moment of \( \frac{d\tau_{\text{DIB}}}{dd} \). The key assumption of our method is that \( \frac{d\tau_{\text{DIB}}}{dd} \) has a fixed profile, though not necessarily a fixed amplitude, over small regions of space. We assume this profile is a Gaussian function in \( v_d \). Our method consists of two parts: assigning pairs of sightlines to pixels in the Galactic \( (x, y) \) plane (Section 5.3.1) and inferring each pixel’s \( \frac{d\tau_{\text{DIB}}}{dd} \) profile (Sections 5.3.2 through 5.3.6).

5.3.1 Pixel assignment

Assigning pairs of sightlines to pixels also consists of two parts. First, we find pairs of stars whose angular separation \( \delta \) is less than some threshold \( \delta_{\text{max}} \). The smaller a pair’s \( \delta \), the more likely it is that that pair’s DIB difference spectrum consists mostly of DIB absorption from ISM between the stars rather than from differences in the spatial distribution of the foreground ISM. The smaller the adopted \( \delta_{\text{max}} \) is, the purer the DIB difference spectra will be; the greater \( \delta_{\text{max}} \) is, the more accepted pairs there will be.

We then divide the Galactic plane into square pixels in \( x - y \) and assign
the pairs with $\delta \leq \delta_{\text{max}}$ to at most one pixel. A pair of stars is assigned to a given pixel if the probability $p(> 0.5 \times \text{path} \in \text{pixel}) \equiv p_{\text{pair, pix}}$ is greater than a threshold $p_{\text{min}}$. To compute this probability for a given pair of stars, we generate realizations of the path between the stars according to the stars’ distances and distance uncertainties. For each realization, we compute the fraction of the path that falls within each pixel. We then combine the realizations by computing $p_{\text{pair, pix}}$, the fraction of the realizations in which more than half of the path falls within each pixel. If there is a pixel for which $p_{\text{pair, pix}} > p_{\text{min}}$, the stellar pair is assigned to that pixel. If there is no such pixel, the pair is not used.

This pixel assignment procedure depends on three parameters: the maximum angular separation $\delta_{\text{max}}$, the pixel sidelength $\Delta x \equiv \Delta y$, and the minimum probability $p_{\text{min}}$. For our final $v_d(x, y)$ map, we set $\delta_{\text{max}} = 0.3^\circ$, $\Delta x = \frac{10}{21}$ kpc, and $p_{\text{min}} = 0.5$. These parameter choices represent a tradeoff between the purity of the DIB difference spectra and pixel assignments and the number of DIB difference spectra available for analysis. As we will show in Section 5.5, varying these parameters over a reasonable range does not significantly change the resulting $v_d(x, y)$ map.

### 5.3.2 Likelihood function

Once the stellar pairs have been assigned, we use Bayesian inference to determine $v_d$ for each pixel. This inference involves four separate models:

- A pixel-level model (Section 5.3.3), which is used to determine $v_d$ for each map pixel.
• A model that uses (non-difference) DIB spectra towards nearby stars to determine the distribution of DIB widths (Section 5.3.4). The width of the DIB is not constant but some widths are more common than others. Including this information as a prior improves the precision and accuracy of the pixel-level solution.

• A model that uses all pairs of sightlines that have been assigned to any pixel to determine the distribution of DIB difference spectrum uncertainties (Section 5.3.5). As with the DIB width, the noise level of the spectra is not constant but also not uniformly distributed.

• A model for determining whether a DIB difference spectrum is an outlier (Section 5.3.6). Some spectra contain extraneous features, such as imperfectly modeled stellar lines, which degrade the quality of the \( v_d \) modeling. Removing these spectra increases the precision and accuracy of the pixel-level solution.

In principle, these models could be combined into a large single model. To simplify computation, we have kept them separate.

All four models are based on the same likelihood function. Given a pair of DIB spectra \( f_1(v) \) and \( f_2(v) \), we assume the corresponding DIB difference spectrum \( y \equiv f_1(v) - f_2(v) \) can be described as the sum of a Gaussian function \( a \times f(v; v_d, \sigma_v^2) \) with amplitude \( a \), center \( v_d \), and standard deviation \( \sigma_v \); a constant offset \( b \); and independent Gaussian noise with standard deviation \( \sigma_y \). We include the constant term \( b \) because the DIB-free region of the DIB spectrum can be slightly offset from zero due to imperfect modeling of the
stellar spectrum. The likelihood function for $y$ given these assumptions is

$$p(y \equiv \{y_1, y_2, \ldots, y_N\}|a, v_d, \sigma_v, b, \sigma_y)$$

$$= \prod_{i=1}^{N} \mathcal{N}(y_i; a \times f(v_i; v_d, \sigma_v^2) + b, \sigma_y^2),$$

(5.3)

where $\mathcal{N}(y_i; a \times f(v_i; v_d, \sigma_v^2) + b, \sigma_y^2)$ is a normal distribution with mean $a \times f(v_i; v_d, \sigma_v^2) + b$ and standard deviation $\sigma_y$ evaluated at the velocity of the $i$th pixel $v_i$.

### 5.3.3 Pixel-level model

In the pixel-level model for $v_d$, we assume that all DIB difference spectra that have been assigned to the same pixel have the same $v_d$ and $\sigma_v$ but that each DIB difference spectrum has its own amplitude $a$, offset $b$, and noise level $\sigma_y$. Our priors on $a$ and $b$ are Gaussian distributions with mean 0 and standard deviations $\sigma_a = 0.5$ and $\sigma_b = 0.01$. This prior on $a$ is essentially uninformative because the maximum amplitude of a DIB difference spectrum in our sample is approximately 0.25. The prior on $b$ is based on a by-eye estimate of the typical continuum offset. For most $y$, changing $\sigma_b$ from 0.01 to 1 does not appreciably change the posterior probability distribution for $v_d$.

Our prior on the uncertainty of $y$ is parametrized in terms of the precision $\tau_y \equiv 1/\sigma_y^2$ rather than the standard deviation $\sigma_y$. The prior on $\tau_y$ is a truncated gamma distribution with range 1 to 20000, shape parameter $\alpha = 1.47$, and rate parameter $\beta = 0.95$. We use a truncated, rather than full, gamma distribution because we marginalize over $\tau_y$ using numerical integration on a fixed (and finite) grid. The shape and rate parameters of the prior on $\tau_y$ are set in Section 154.
5.3.5. The likelihood of the \( M \) DIB difference spectra \( y_1, y_2, \ldots, y_M \) that have been assigned to a single pixel, given the pixel-level parameters, is

\[
p(y_1, y_2, \ldots, y_M | v_d, \sigma_v, \sigma_a, \sigma_b, \alpha, \beta) = \prod_{j=1}^{M} p(y_j | v_d, \sigma_v, \sigma_a, \sigma_b, \alpha, \beta)
\]

\[
= \prod_{j=1}^{M} \left( \int_{1}^{2/0.01^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p(y_j | a_j, b_j, v_d, \sigma_v, \sigma_{y,j}) \right)
\times p(a_j | \sigma_a) p(b_j | \sigma_b) p(1/\sigma_{y,j}^2 | \alpha, \beta) \, da_j \, db_j \, d(1/\sigma_{y,j}^2).
\]

The integrals over the amplitudes \( a_j \) and offsets \( b_j \) have an analytic solution, which we give in Appendix 5.8. The integral over \( \sigma_{y,j} \) is done numerically.

The prior for \( v_d \) is a uniform distribution between \( v_{\text{min}} = v_{d,\text{rot}}(x, y) - 40 \, \text{km s}^{-1} \) and \( v_{\text{max}} = v_{d,\text{rot}}(x, y) + 40 \, \text{km s}^{-1} \), where \( v_{d,\text{rot}}(x, y) \) is the line-of-sight velocity corresponding to rotation according to our fiducial rotation curve at the center of each pixel. The prior for \( \sigma_v \) is a truncated log-normal distribution with range 10 to 50 km s\(^{-1}\), mean parameter \( m = 3.44 \) and standard deviation parameter \( s = 0.17 \). These parameters are set in Section 5.3.4. The posterior probability for \( v_d \) in the pixel-level model is then

\[
p(v_d | y_1, y_2, \ldots, y_M, \sigma_a, \sigma_b, \alpha, \beta, m, s) \propto \int_{10 \, \text{km/s}}^{50 \, \text{km/s}} \left( \prod_{j=1}^{M} p(y_j | v_d, \sigma_v, \sigma_a, \sigma_b, \alpha, \beta) \right)
\times p(\sigma_v | m, s) p(v_d | v_{\text{min}}, v_{\text{max}}) \, d\sigma_v.
\]

The integral over \( \sigma_v \) is done numerically.
5.3.4 Setting the $\sigma_v$ prior

We set the parameters of the prior on $\sigma_v$ by modeling the distribution of widths of DIB absorption towards stars within 1 kpc of the Sun. The pathlength between the Sun and each of these stars is comparable to the typical pathlength between the stars in pairs assigned to a pixel. The width and amplitude of the total DIB absorption towards these stars should therefore be comparable to the absorption in a DIB difference spectrum $y$. We set the $\sigma_v$ prior parameters using these (non-difference) DIB spectra, rather than DIB difference spectra, for two reasons. First, the non-difference spectra will usually have a higher signal-to-noise ratio than the difference spectra. Second, we know that the DIB absorption towards a nearby star comes from the path between the Sun and that star, while the absorption in a DIB difference spectrum may, despite our assumptions, be partially corrupted by a mismatch between the foreground DIB absorption towards the corresponding pair of stars.

The model for these nearby stars uses the same likelihood function as the pixel-level model (Section 5.3.3) but has some different priors and a different model structure. The prior on the Gaussian amplitude $a$ has the same standard deviation as in the pixel-level model but is now a half-normal distribution rather than a normal distribution because the sign of the DIB absorption should be positive. The prior on the offset $b$ is still a normal distribution but has a smaller standard deviation, $\sigma_b = 0.01/\sqrt{2}$, because the standard deviation on the baseline of a single DIB spectrum should be a factor of $\sqrt{2}$ smaller than the standard deviation on the baseline of the difference of two DIB spectra. The prior on $\sigma_y$ is a gamma distribution over $1/\sigma_y^2$ with
parameters $\alpha'$ and $\beta'$, which are allowed to vary. We do not use the same $\sigma_y$ prior as for the pixel-level model because the noise properties of single DIB spectra towards nearby stars will be different from the noise properties of DIB difference spectra of stars from a wider range of distances. The prior on $v_d$ is defined as before, $v_{d,\text{rot}} \pm 40 \text{ km s}^{-1}$, but $v_{d,\text{rot}}$ is evaluated at the location of the star rather than at the center of a pixel. The prior on $\sigma_v$ is a log-normal distribution with mean parameter $m$ and standard deviation parameter $s$, which are allowed to vary. Unlike in the pixel-level model, each sightline has its own $v_d$ and $\sigma_v$ which are marginalized over separately for each star rather than in a tied way for a collection of stars.

The posterior probability distribution for $m$ and $s$ in this model is

$$p(m,s|y_1, y_2, \ldots, y_M, \sigma_a, \sigma_b) \propto p(m,s) \times$$

$$\int_{\alpha_{\min}}^{\alpha_{\max}} \int_{\beta_{\min}}^{\beta_{\max}} \prod_{j=1}^{M} \left( \int_{\sigma_v_{\min}}^{\sigma_v_{\max}} \int_{v_{\min}}^{v_{\max}} p(y_j|v_d, \sigma_v, \sigma_a, \sigma_b, \alpha, \beta) \right)$$

$$\times p(\sigma_v|m,s) p(v_d) \, dv_d \, d\sigma_v \, p(\alpha, \beta) \, d\beta \, d\alpha.$$

(5.6)

where the $y_j$ are now just DIB spectra rather than DIB difference spectra. Priors on $m$, $s$, $\alpha$, and $\beta$ are uniform distributions between $-\infty$ and $\ln 70$, 0 and 10, 0 and $+\infty$, and 0 and $+\infty$. The integrals over $v_d$ and $\sigma_v$ are done numerically on a fixed grid. We draw samples from the distribution over $m$ and $s$ and integrate over $\alpha$ and $\beta$ using the emcee implementation of the affine-invariant ensemble sampler for Markov chain Monte Carlo (Foreman-Mackey et al., 2013). The means and standard deviations of the distributions of $m$ and $s$ are $3.44 \pm 0.02$ and $0.17 \pm 0.02$. 

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We have repeated this procedure using all stars within successively smaller volumes around the Sun: \(d < 0.9, 0.8, 0.7, 0.6, \text{ and } 0.5 \text{ kpc.} \) For all cases except 0.5 kpc, the mean values of \(m\) and \(s\) are the same as that of \(d < 1 \text{ kpc}\) to within the standard error on the mean of each parameter. For the 0.5 kpc case, there are not enough observations to provide much of a constraint on \(m\) or \(s\). The standard deviations of the \(m\) and \(s\) distributions are over 50 and over 5, respectively. We use the mean values of the 1 kpc \(m\) and \(s\) distributions for the prior on \(\sigma_v\) in the pixel-level model (Section 5.3.3).

### 5.3.5 Setting the \(\sigma_y\) prior

We apply a similar procedure to all of the DIB difference spectra to set the parameters of the prior on \(\sigma_y\). We assume that anything that is not captured by our usual model for a DIB difference spectrum, a single Gaussian superimposed on a constant baseline, is noise. As in the procedure for determining the prior on \(\sigma_v\), we assume each DIB difference spectrum has its own \(v_d\) and \(\sigma_v\). Our prior on each \(v_d\) is once again \(v_{d,\text{rot}} \pm 40 \text{ km s}^{-1}\), where we evaluate \(v_{d,\text{rot}}\) at the center of the 0.5 × 0.5 kpc pixel to which the stellar pair in question has been assigned. The priors on \(a\), \(b\), and \(\sigma_v\) are the same as in the pixel-level model (Section 5.3.3).
With these priors and model structure, the posterior probability distribution for $\alpha$ and $\beta$ is

$$p(m, s | y_1, y_2, \ldots, y_M, \sigma_a, \sigma_b) \propto p(\alpha, \beta) \times$$

$$\prod_{j=1}^{M} \int_{v_{\min}}^{v_{\max}} \int_{\sigma_{v_{\min}}}^{\sigma_{v_{\max}}} p(y_j | v_d, \sigma_v, \sigma_a, \sigma_b, \alpha, \beta)$$

$$\times p(\sigma_v | m, s) p(v_d) \, dv_d \, d\sigma_v \right).$$

(5.7)

The priors on $\alpha$ and $\beta$ are uniform distributions between 0 and $+\infty$. The marginalization over $v_d$ and $\sigma_v$ is done numerically on a fixed grid. We draw samples from the posterior probability distribution for $\alpha$ and $\beta$ once again using the affine-invariant ensemble sampler implemented in emcee. The means and standard deviations of these distributions are $1.47 \pm 0.04$ and $0.95 \pm 0.03$. We use these mean values as the parameters of the $\sigma_y$ prior in the pixel-level model (Section 5.3.3).

5.3.6 Deciding if a difference spectrum is an outlier

Many of the DIB spectra contain spurious absorption and emission features. These features are the result of imperfect modeling of stellar, telluric, and sky emission lines but are mistaken to be (possibly quite strong) DIB absorption by our simple model. Including DIB difference spectra with these sorts of features in pixel-level inference without expanding the model to include them will degrade the quality of the $v_d(x, y)$ map. While we do not have a model for these features, we do have a way of identifying these contaminated DIB difference spectra.
Figure 5.3: Priors on $v_d$ (left), $\sigma_v$ (center), and $\frac{1}{\sigma^2}$ (right). Priors used to make the $v_d(x,y)$ map are shown in solid orange. For $v_d$ and $\sigma_v$, flat priors used for deciding whether a given DIB difference spectrum is an outlier (Section 5.3.6) are shown in dashed blue. The center of the $v_d$ prior varies depending on location in the Galaxy, but the width remains constant.

Figure 5.4: Bottom panel: distribution of $p$(informative). Top panels, from left to right: examples of DIB difference spectra with $0 \leq p$(informative) $< 1/4$, $1/4 \leq p$(informative) $< 1/2$, $1/2 \leq p$(informative) $< 3/4$, and $3/4 \leq p$(informative) $\leq 1$. 
Stellar, telluric, and sky lines tend to be narrower than DIB absorption and, unlike DIB absorption, can be centered at unphysical velocities in the DIB velocity frame. The Gaussian parameters that best describe these contaminants are disfavored (in the case of $\sigma_v$) or outright excluded (in the case of $v_d$) by our informative priors. A contaminated spectrum should therefore be better described by a Gaussian + baseline model with a flat prior on $\sigma_v$ and a broad, flat prior on $v_d$ than by a model with our informative priors. We show these informative priors on $v_d$, $\sigma_v$, and $\sigma_y$ and flat priors over the same range on $v_d$ and $\sigma_v$ in Figure 5.3.

To determine whether a given DIB difference spectrum is better described by a model with informative priors or flat priors on the Gaussian parameters, we marginalize over all parameters with the two sets of priors to get two marginal likelihoods, $p(y)_{\text{inf}}$ and $p(y)_{\text{flat}}$, for each model. The probability that the model with informative priors is a better description of the DIB difference spectrum is then

$$p(\text{informative}) = \frac{p(y)_{\text{inf}}}{p(y)_{\text{inf}} + p(y)_{\text{flat}}},$$

(5.8)

where we have implicitly assumed that the informative prior and flat prior models are equally likely a priori. We show the distribution of $p(\text{informative})$ among all DIB difference spectra that were assigned to any pixel in Figure 5.4 along with some example DIB difference spectra from four different $p(\text{informative})$ ranges. We assume all DIB difference spectra with $p(\text{informative}) > 0.5$ are uncontaminated. These are the spectra we use to derive the $v_d(x, y)$ map (Section 5.5) using the pixel-level model described in Section 5.3.3.
5.4 Comparison simulations

To help interpret the G&D KT and DIB KT $v_d(x, y)$ maps, we compare them with $v_d(x, y)$ maps derived from simulations of gas flow in disc galaxies with spiral structure. These simulations fall into two broad classes — those with a fixed background potential, corresponding to the SDW model, and those with a dynamically evolving background potential, corresponding to the dynamic model.

Both classes of simulation follow the flow of ISM in a gravitational potential that is set mostly by dark matter and stars. In the first class, the evolution of the stellar distribution is described analytically. For example, the stellar distribution can be described as a linear spiral density wave or as a stable bar-induced spiral. In the second class, the stellar distribution evolves in the same gravitational potential as the gas. We consider five SDW simulations (Section 5.4.1) and five dynamic spiral structure simulations (Section 5.4.2).

From each simulation, we compute a flat rotation-subtracted $v_d(x, y)$ map. These $v_d(x, y)$ maps are initially computed at the native resolution of each simulation and then degraded to the resolution of the KT maps using surface density-weighted averaging. We obtain the rotation rate by taking the mean of the (galactocentric) azimuthal velocity of the simulated ISM in an annulus centered on the (simulated) galactic center. The annulus extends 0.5 kpc inward and outward from the galactocentric radius of the observer. We use a flat rotation curve with a rotation rate appropriate for the location of the observer to match what we have done for the KT-derived $v_d(x, y)$ maps. Computing a radially varying rotation curve from the simulated velocity field
would be trivial but would erase features from the simulated $v_d(x, y)$ maps that could potentially be present in the KT-derived $v_d(x, y)$ maps.

### 5.4.1 Stationary density wave simulations

All five of the SDW simulations include spiral arm-like perturbations, but they differ in the number of arms, the properties of the arms, the presence of a bar, and the properties of the bar. Four of the simulations come from Pettitt et al. (2014) and one comes from Li et al. (2016). For each set of simulations, we describe below the shape of the perturbing potential, the included physics, and the solution method used for evolving the equations of hydrodynamics.

#### 5.4.1.1 Pettitt et al. (2014)

Pettitt et al. (2014) made a suite of simulations in an attempt to reproduce the Galactic CO $\ell - v$ diagram. Here, we examine the four simulations shown in their Figure 25. We will refer to these four simulations as P-SDW1 through P-SDW4. These simulations are available at http://hdl.handle.net/10871/15057; we received useful advice on orienting them from the authors (Pettitt 2017, private communication communication). The axisymmetric part of the potential consists of bulge, halo, and disc terms with amplitudes tuned to reproduce the Sofue (2012) rotation curve.

There are four different perturbing potentials, combining two- and four-armed logarithmic spiral perturbations with bars of two different strengths. P-SDW1 and P-SDW2 have two-armed spiral perturbations while P-SDW3 and P-SDW4 have four-armed spiral perturbations. The amplitude of these
spiral potential perturbations is approximately 200 km$^2$ s$^{-2}$ (Dobbs, Bonnell, and Pringle, 2006). The pitch angles of the four spirals are 15° (P-SDW1 and P-SDW4), 12.5° (P-SDW2), and 10° (P-SDW3). P-SDW1, P-SDW3, and P-SDW4 have pattern speeds of 20 km s$^{-1}$ kpc$^{-1}$ and P-SDW2 has a pattern speed of 15 km s$^{-1}$ kpc$^{-1}$, placing the corotation radii of all four models at approximately 11 and 12 kpc, respectively.

The pattern speeds of the bars in the simulations are 50 km s$^{-1}$ kpc$^{-1}$ for P-SDW1 and P-SDW3 and 60 km s$^{-1}$ kpc$^{-1}$ for P-SDW2 and P-SDW4. The outer Linblad resonances (OLR) of these bars are at radii of approximately 7.5 and 6 kpc, respectively. At and outside the radius of the observer, $\approx 8$ kpc, the dynamics of the gas are determined mostly by the spiral arms rather than by the bar.

While the general purpose of the work was to reproduce spiral features in the $\ell - v$ diagram, it was found that no one simulation was perfect; each of these four simulations reproduces some, but not all, of the known $\ell - v$ diagram features. The simulations should therefore be thought of as Milky Way-like rather than as best fits to the Milky Way data.

The simulations are computed in 3D and include compressible, inviscid gas hydrodynamics with an adiabatic equation of state, simplified H$_2$ and CO chemistry, and ISM heating and cooling. They do not include star formation feedback or gas self-gravity. The equations of motion are solved using smoothed particle hydrodynamics. ISM state variables such as temperature and chemical composition are tracked and evolved independently for each particle.
5.4.1.2 Li et al. 2016

Li et al. (2016) were aiming to reproduce features from l-v diagrams, in particular inner-Galaxy features such as Bania’s Clump 2 and the details of the molecular ring (Scutum-Centaurus arm). This simulation was tailored to match the R+14 spiral arms and so can be expected to be a more accurate estimate of the density and velocity field of the Milky Way than any of the Pettitt et al. (2014) simulations. We will refer to this simulation as L-SDW. We received a snapshot of the simulation shown in Figure 2 of Li et al. (2016) directly from the first author (Li 2017, private communication). Their potential is built from a bulge model from Portail et al. (2015), a nuclear bulge component, four logarithmic spiral arms based on the star formation-traced arms defined in R+14, and a long bar component. The imposed spiral arm potential has an amplitude of 800 km$^2$ s$^{-2}$, a pitch angle of 12.5$^\circ$, and a pattern speed of 23 km s$^{-1}$ kpc$^{-1}$, placing the corotation radius of the spiral pattern at approximately 8 kpc. This is the only simulation we consider in which the Perseus arm-analog in the vicinity of the observer is clearly outside the spiral corotation radius.

The pattern speed of the bar in this simulation is 33 km s$^{-1}$ kpc$^{-1}$. This bar’s OLR is approximately 10.5 kpc from the Galactic center, right around the location of the Perseus arm near the Sun. The velocity field in this area appears quite regular and aligned with the spiral structure, suggesting that the spiral potential dominates the dynamics. The 4:1 resonance of the bar, which is approximately 8.5 kpc from the Galactic center, has a stronger effect and is partially responsible for this simulation’s Local arm analog. Li et al. (2016)
explore the effect of removing different parts of the perturbing potential. When they remove the spiral perturbation, the Scutum, Sagittarius, and Perseus arm analogs disappear but the Local arm analog remains and has approximately the same location and peak density as in the fiducial simulation.

This simulation is computed in 2D and includes compressible, inviscid gas hydrodynamics with an isothermal equation of state. It does not include star formation, gas self-gravity, chemistry, or heating and/or cooling. The equations of motion are solved using a finite volume method on a fixed Cartesian grid.

5.4.2 **Dynamic spiral structure simulations**

In addition to the five stationary density wave simulations with fixed potentials, we also consider five dynamic spiral structure simulations with live, evolving potentials. In these simulations, the stellar spiral and bar perturbations form spontaneously from an initially cylindrically symmetric configuration. These spiral perturbations are not stable. Over the course of a simulation, a given arm will form, persist for some time, and then dissipate. The presence of spiral structure, however, is stable: individual arms may form and dissipate, and the number of arms may change, but at any given time, there will be morphologically obvious spiral structure. Characteristics of this spiral structure such as the average number of arms, their amplitude above the baseline, and their typical lifetime are set by the disc-to-halo mass ratio (Sellwood and Carlberg, 1984). We describe the initial conditions and included physics in more detail below. In all cases, the simulations are 3D,
the live stellar component is simulated using N-body techniques, and the gas component is simulated using smoothed particle hydrodynamics.

### 5.4.2.1 Kawata et al. 2014

The Kawata et al. (2014) simulation is meant to have Milky Way-like stellar, gaseous, and dark matter masses. We received a snapshot of this simulation directly from the first author (Kawata 2017, private communication). This particular snapshot was chosen because it has a spiral arm and bar that roughly line up with the Perseus arm and Galactic bar. This snapshot occurs 925 million years into the simulation, when the Perseus-like arm is still growing. This simulation is not meant to reproduce specific features of the Milky Way in detail. We will refer to this simulation as K-D.

The dark matter halo is assumed to be static and there is no bulge component. The simulation includes metal enrichment, ISM heating and cooling, self-gravity, density threshold-based star formation, stellar (wind) feedback, and supernova feedback. This is the only simulation we consider that includes star formation and feedback. Supernova-driven features appear in the simulation’s equivalent of the Perseus arm, though we do not compare features between the simulations and observations at that level of detail.

### 5.4.2.2 Pettitt et al. 2015

The Pettitt et al. (2015) simulations were made in order to accurately reproduce the Milky Way CO $\ell - v$ diagram, particularly away from the nuclear region. Runs with seven different initial and static mass distributions were performed. Among all snapshots of these seven simulations, the four best matches to
the observed CO $\ell - v$ diagram were chosen. These best matches are shown in Figure 10 of Pettitt et al. (2015). We received the snapshot files directly from the first author (Pettitt, private communication). We will refer to these simulations as P-D1 through P-D4.

As stated in Pettitt et al. (2015), the best matches come from simulations with a static dark matter halo and a live stellar bulge and disc. The simulations include the same basic H$_2$ and CO chemistry and ISM cooling and heating as the Pettitt et al. (2014) simulations. They do not include gas self-gravity or star formation.

5.5 Results

The primary result of this work, a planar map of $v_d(x, y)$ derived from DIB absorption, is shown in the bottom right panel of Figure 5.5. The DIB KT map and planar version of the G&D KT map are available at 10.7910/DVN/UPJM6D. We compare the DIB KT map with the $v_d(x, y)$ maps derived from simulations of spiral structure in Section 5.6. In the current section, we demonstrate that the DIB KT $v_d(x, y)$ map does not strongly depend on the parameters of the map-making method (Section 5.5.1) and compare the DIB KT and G&D KT $v_d(x, y)$ maps (Section 5.5.2).

5.5.1 Parameter choices

Once star pairs have been assigned to pixels, DIB KT is essentially self-calibrating. We describe this self-calibration in detail in Sections 5.3.4, 5.3.5, and 5.3.6. The procedure for assigning star pairs to pixels depends on three
Figure 5.5: Flat rotation-subtracted ISM velocity fields measured using Kinetic Tomography (G&D KT and DIB KT) and predicted by simulations (all other panels). Colors indicate the rotation-subtracted line-of-sight velocities. In the simulation panels, black contours indicate locations where the ISM surface density is in the top decile of surface densities in the simulation domain. In the KT panels, black dots indicate the locations of high mass star formation regions from Reid et al. (2014).
parameters for which we do not have a self-calibration scheme. These are the pixel sidelength \( \Delta x \), the maximum angular separation between stars in a pair \( \delta_{\text{max}} \), and the minimum value \( p_{\text{min}} \) of \( p_{\text{pair, pix}} \) required for a pair to be assigned to a pixel.

One way to test our choice for \( \Delta x \) is to compare the uncertainties on the DIB-derived \( v_d(x, y) \) map to the sub-pixel variance of the simulated \( v_d(x, y) \) maps at different pixel sizes. The sub-pixel variance is the variance of the distribution of velocities in a pixel. As pixel size increases, the uncertainties decrease and the sub-pixel variances increase. Assigning a single velocity to a pixel is an approximation whose accuracy can be described by the sub-pixel variance. When the \( v_d \) uncertainty is smaller than the sub-pixel variance, the \( v_d \) estimate error is dominated by the limitations of the approximation.

Figure 5.6 compares the median uncertainty of the DIB-derived \( v_d(x, y) \) map to the median amount of sub-pixel variation in two of the simulations we consider, the Li et al. (2016) spiral density wave (L-SDW) and the fourth Pettitt et al. (2015) spiral density wave (P-SDW4) simulations. Because the L-SDW simulation has the strongest velocity contrasts among the simulations we consider, it also has the greatest amount of sub-pixel variation. The P-SDW4 simulation has the weakest velocity contrasts and therefore has the smallest amount of sub-pixel variation. If we want to be able to confirm or rule out the P-SDW4 simulation, we should pick a pixel size such that the typical uncertainty is not significantly greater than the typical amount of sub-pixel variation. Conversely, it is not useful to pick a pixel size for which the typical uncertainty is significantly smaller than the typical amount of
sub-pixel variation.

A second way to motivate a choice for $\Delta x$ is to compute the area of the $v_d(x, y)$ map as a function of pixel size. Decreasing the size of the pixels reduces the number of usable star pairs, since it requires pairs of stars to have more precise distances and smaller separations in order to be assigned to a pixel. This in turn tends to reduce the area over which there are pixels with a sufficient number of pairs of stars to measure $v_d$. We show how the area depends on the pixel size in Figure 5.6.

$A$ $\Delta x$ of $\frac{10}{22}$, $\frac{10}{21}$, or $\frac{10}{20}$ kpc would be reasonable according to both of these metrics. We use a $\Delta x$ of $\frac{10}{21}$ kpc. In Figure 5.7, we show $v_d(x, y)$ maps derived assuming five different pixel sizes. While the area of the maps decreases as the pixel size gets smaller, there is no substantive change in the features of the velocity field. In the same Figure, we also show how the $v_d(x, y)$ map changes as a result of varying $\delta_{\text{max}}$ and $p_{\text{min}}$. As with $\Delta x$, there is no substantive change except for a decrease in the area covered by the map.

### 5.5.2 Comparing DIB KT and G&D KT

We can check the DIB KT map by comparing it to the G&D KT map. Both KT techniques measure the same quantity, $v_d(x, y)$, but use completely different dataset and techniques. One simple way to compare the two maps is to directly compare the velocities they assign to pixels where they overlap. This comparison is shown in Figure 5.8. While there are points where the maps do not agree by an amount that is greater than what we would estimate is the uncertainty on either measurement, the two maps agree on average — the
Figure 5.6: **Left panel:** Median RMS of $v_d$ as a function of pixel size for two simulations and the DIB KT map. For the simulations, the RMS is the standard deviation of the distribution of velocities in each pixel. For the DIB KT map, the RMS is the standard deviation of the posterior probability distribution of $v_d$ in each pixel. **Right panel:** The area of the DIB KT map as a function of the pixel size.

In addition to being pointwise consistent on average, the maps contain the same qualitative velocity features. We highlight four major features in the KT maps in Figure 5.5: a receding (red) region in the 1st quadrant, an approaching (blue) region in the near part of the 2nd quadrant, a receding or zero velocity region in the far part of the 2nd quadrant, and a receding or zero velocity region in the 3rd quadrant. The locations and shapes of these features are almost identical in the two maps. The main differences between shapes of velocity features are in the 1st quadrant, where we expect the G&D KT map to be less accurate than in the outer galaxy. The Green et al. (2015) dust map, which is the source of distance information in G&D KT, is accurate to greater distances in the lower-average-density outer Galaxy than in the
Figure 5.7: The effect of varying one map-making parameter at a time on the DIB KT velocity map. In each row, the map made using the adopted parameters is indicated with a box. **Top:** Map pixel size in kpc. **Middle:** Maximum angular separation between stars in a sightline pair. **Bottom:** Minimum $p_{\text{pair,pix}}$ required for a sightline pair to be assigned to a pixel. See Section 5.3.1 for an in-depth description of these parameters and their role in DIB KT.
Figure 5.8: The rotation-subtracted velocities assigned to each pixel by G&D KT (x-axis) and DIB KT (y-axis). The black line is the best-fit linear relation, the gray filled area is the 95% confidence interval for the linear relation, and the orange line is a one-to-one relation.
higher-average-density inner Galaxy. The gas emission cubes, which are the source of velocity information in G&D KT, are more confused in the inner Galaxy than the outer Galaxy since gas at a given velocity can be located at two very different distances. These possible issues are explored in more detail in Section 4.2 of TP17. We conclude that the two KT maps are mutually consistent.

5.6 Discussion

5.6.1 A comparison between the KT maps and spiral structure simulations

As can be seen in Figure 5.5, none of the simulations provide an exact match to our inferred velocity field. The two simulations which come closest to reproducing the KT velocity field are P-D1 and P-SDW3. We will argue below that the differences between P-D1 and KT are reasonable and not unexpected in the dynamical spiral structure model while the differences between P-SDW3 and KT are insurmountable in the SDW model. Furthermore, we will argue that these differences have to be present in any stationary density wave ISM velocity field. KT is strongly inconsistent with the SDW model but can be consistent with a dynamic spiral structure model in which the Perseus arm near the Sun is in the process of dissipating.

The simplest way to quantitatively compare two maps is to compare their values point by point. We do this point by point comparison by computing the Spearman correlation coefficient between each of the KT-derived \( v_d(x, y) \) maps and each of the simulated \( v_d(x, y) \) maps. These coefficients are shown...
Figure 5.9: Spearman correlation coefficients computed between the pixel-wise values of $v_d(x, y)$ from G&D and DIB KT and from spiral structure simulations.

in Figure 5.9. An identical pair of maps would have a correlation coefficient of 1. A map and its opposite, i.e. the result of multiplying each $v_d$ value by -1, would have a correlation coefficient of -1. The two simulated maps that most closely resemble the DIB and G&D KT maps according to this metric are P-D1, a dynamic spiral structure simulation from Pettitt et al. (2015), and P-SDW3, a spiral density wave simulation from Pettitt et al. (2014).

Point by point comparisons such as this correlation coefficient ignore spatial structure and can be confused by small spatial shifts. To better understand the similarity and dissimilarity of maps, we look at features of the map that could be driving these coefficients. Major features in the KT maps include: an approaching region in the near part of second quadrant, a receding region in the first quadrant, and minimal streaming in the third quadrant. P-D1 and P-SDW3 contain all of these features. P-D2 and P-D4 have negative correlation coefficients because they have an approaching region in the near part of the
second quadrant and an approaching region in the 3rd quadrant. Simulations such as L-SDW and K-D agree in some parts (near part of the second and first quadrants, respectively) but disagree in others and so get correlation coefficients near 0. This qualitative comparison is thus consistent with the Spearman correlation analysis.

The P-D1 and P-SDW3 simulations cannot both be correct or close to correct, since they are based on different assumptions about the nature of spiral structure. To get a better sense of which is correct, we examine broader, less realization-specific predictions for the velocity fields of dynamic spiral structure and SDW spiral structure. These sorts of predictions are more likely to actually apply to the KT velocity field and can be more constraining than any realization-specific detail. We also examine the location of dense gas relative to velocity field features. The dense gas, i.e. the actual gaseous spiral arms, are a natural reference point when trying to compare observations with simulations. According to these more general predictions and additional information from dense gas, the KT $v_d$ maps favor the dynamic spiral structure simulation over the SDW simulation.

SDW models predict that a gaseous spiral arm is fed by diffuse gas flowing into the arm from one side. Inside the corotation radius of the spiral pattern, this gas flow should be mostly outward into the trailing edge of the spiral arm. Outside the corotation radius, the gas flow should be mostly inward into the leading edge of the spiral arm. The dense gas should be located downstream from this strong radial flow and should have a relatively small peculiar velocity in the Galactocentric radial direction.
These diffuse, mostly radial flows should be consistent over the extent of the spiral arm and should be particularly obvious in regions of the outer Galaxy where $v_d \approx v_R$ due to the viewing angle. These flows can clearly be seen in all of the SDW simulations and are clearest in the L-SDW simulation, where at $d_\odot \cos \ell \approx -4$ kpc, there is a 1.5 kpc by 8 kpc region of consistently negative $v_d$. The presence of such a region is a basic and fundamental prediction of the SDW model — without this flow, there would be no gaseous arm.

There is no such region of consistent inflow or outflow in the outer Galaxy portion of either KT map. The lack of this region of consistent flow cannot be the result of assuming an incorrect Solar motion relative to the local standard of rest. Adjusting the Solar motion changes the velocity field in a way that varies only with position on the sky, while the changes that would need to be made to the KT maps in order to introduce a consistent radial flow require a correction that varies with distance.

The velocity field around the Perseus arm HMSFRs in the 2nd quadrant is hard to reconcile with the SDW prediction that dense gas should be downstream from a rapid radial flow. If the Perseus arm is inside corotation, there should be gas flowing outward towards the HMSFRs from the near side of the arm. If it is instead outside corotation, there should be gas flowing inward towards the HMSFRs from the far side of the arm. Instead, these HMSFRs are entrained in a strong inward flow. There is no region that could be “feeding” the Perseus arm in the 2nd quadrant.

These two observations – a lack of consistent radial flow across the 2nd
and 3rd quadrants and the velocity field in the vicinity of the HMSFRs – are
based on large portions of both KT maps and directly contradict qualitative
predictions of the SDW model. The simulations we compare the KT map with
are somewhat idealized. In particular, most of the simulations do not include
feedback and do not produce certain expected instabilities (e.g. Dobbs and
Bonnell, 2006). However, the effect of any missing physical processes would
need to be strong enough to destroy large-scale properties of gaseous SDW
spiral arms. The SDW model with this missing physics included would need
to be qualitatively different from the relatively simple SDW model.

The dynamic spiral structure model does not have as many broad predic-
tions as the SDW model. For example, there is no expectation of coherent
flow over long spatial scales. This is one reason for the greater diversity of
$v_d$ fields in the dynamic spiral structure simulations relative to those in the
SDW simulations. The two main qualitative predictions of the dynamic spiral
structure model are that dense gas in growing spiral arms should be located
at the center of converging flows and that spiral arms should, at some point,
dissipate (Baba et al., 2016). When a spiral arm is in the dissipation phase, the
gas in that arm should be located in diverging parts of the velocity field.

Based on the divergence of the velocity field at the location of dense gas,
which we show in Figure 5.10, the Perseus-like arm in the P-D1 simulation is
in the dissipation phase. In the P-D2 and P-D3 simulations, the Perseus-like
arms are located at sites of convergence while in the P-D4 simulation, there
is no analog to the Perseus arm. The fact that the Perseus-like arms are at a
site of convergence in P-D2 and P-D3 can be seen directly from the $v_d$ maps,
in which the Perseus-like arms are located at places where gas is converging along the line of sight. Since the KT maps are mostly consistent with the P-D1 simulation but are not consistent with the P-D2, P-D3, or P-D4 simulations, we can conclude that the Milky Way has dynamic spiral structure and that the nearby section of the Perseus arm is in the process of dissipating.

It is true that the P-D1 simulation is not a perfect match for KT. For example, in the P-D1 simulation, the region beyond the dense gas of the Perseus arm is flowing outward while in the KT map, this region has \( v_d \approx 0 \) km/s. This and other small differences are not required by the dynamic spiral structure model and are instead realization-specific. The outward flow outside the Perseus arm in the P-D1 simulation is gas converging on the Outer arm, which in the simulation is closer to the Sun than appears to be the case in the actual Milky Way. The spacing between arms is not a fundamental prediction of the dynamic spiral structure model, as can be seen from the range of separations between arms in P-D1 through P-D4. The velocity field we find using KT requires degrees of freedom in the velocity field that are not available in the SDW model but are available in the dynamic model. Small, non-qualitative differences such as those between the P-D1 simulation and the KT maps are preferable to the broad and qualitative differences between the SDW model and the KT maps.

Our findings that the gaseous spiral arms in the outer galaxy are likely dynamic, and that the Perseus are is in a dissipating phase, are consistent with several recent analyses of stellar velocities based on \textit{Gaia} DR1 and DR2.
Quillen et al. (2018) analyzed overdensities and boundaries between overdensities in the stellar velocity distribution seen in Gaia DR2 to determine the pattern speeds of nearby spiral arms. Based on this analysis, the spiral arms near the Sun are all corotating or nearly corotating with the disc, which is inconsistent with the SDW model but predicted by the dynamic model. Hunt et al. (2018) show that ridges in the same stellar velocity distribution resemble predictions from the dynamic model. An analysis of Cepheid velocities based on Gaia DR1 data by Baba et al. (2018) found that the Perseus arm is likely to be a dynamic arm in the dissipation phase.

One potential counterargument to a dynamical model for the Milky Way’s gaseous spiral structure is the “tidiness” of the HMSFR locations. As R+14 have shown, one can assign most of the known HMSFRs to spiral arms whose pitch angles and lengths seem more consistent with the SDW model than the dynamical model. In Figure 5.11, we compare the location of dense gas in each of the simulations with the locations of the HMSFRs. Based on this naive, by-eye comparison, we would argue that the distribution of HMSFRs is not so different from many of the arrangements of dense gas in dynamic simulations. This interpretation can, for example, provide a simple explanation for the “gap” in the Perseus arm at roughly $\ell = 180^\circ$ — the HMSFRs in the second quadrant and the HMSFRs in the third quadrant actually belong to two different spiral arms. There is not a perfect mapping between dense gas and HMSFRs and distance uncertainties tend to elongate structures along the line of sight. Despite these caveats, we believe this comparison is sufficient to establish that the distribution of known HMSFRs
does not rule out the possibility that the outer Milky Way has flocculent spiral arms with high pitch angles, and thus is consistent with dynamic spiral structure.

5.7 Conclusion

In this work, we have been able to distinguish between different theories of spiral structure for the Milky Way using maps of the Milky Way ISM velocity field. In particular

- In a process called Kinetic Tomography, we have constructed a map of Milky Way’s ISM velocity field using observations of a diffuse interstellar band ISM absorption line toward distant disc stars that is consistent with previous maps.

- The ISM velocity fields predicted by spiral density wave theory and dynamic spiral structure theory are significantly different, particularly in the neighborhood of spiral arms.

- We find that one simulation of each spiral structure theory has rough quantitative agreement with the maps of the Milky Way velocity field.

- The spatial structure of the differences between the maps and predictions is difficult to explain within density wave theory but reasonable within dynamic spiral structure theory.

- Of the two theories considered in this work, only dynamic spiral structure theory can account for the complexity of the Milky Way’s velocity
Figure 5.10: The divergence, $\nabla \cdot \mathbf{v}$, of the ISM velocity field of in dense regions in the spiral structure simulations. The divergence is indicated by the color scale. The regions shown are in the top surface density decile in their simulations. The simulations are, going first from left to right and then from top to bottom: P-D1 through P-D4, P-SDW1 through P-SDW 4, K-D, and L-SDW. Note that this figure, unlike the similarly structured Figures 5.5, 5.7, and 5.11, only shows the second quadrant of the Galactic plane.
Figure 5.11: The location of ISM in the top surface density decile in each simulation is shown in black. The locations of the Reid et al. (2014) high mass star formation regions are shown in orange.
field and the divergence of the velocity field detected at the Perseus Arm.

This work has shown that measuring the velocity field of the dynamically cold interstellar medium can provide a unique and powerful tool for distinguishing between theories of how our Milky Way is structured. The theories we have considered here all assume that the structure of the Milky Way depends only on internal processes. This assumption is at odds with the hypothesis that the Milky Way has recently been significantly perturbed by the passage of the Sagittarius dwarf galaxy through the Galactic disc (Purcell et al., 2011; Antoja et al., 2018; Binney and Schönrich, 2018; Poggio et al., 2018; Kawata et al., 2018; Laporte et al., 2018; Bland-Hawthorn et al., 2019). This encounter would be a plausible explanation for the Galactic warp and certain wave-like motions of stars perpendicular to the plane. Hydrodynamical simulations of this passage that are informed by the latest observations (e.g. the Antoja et al. 2018 phase space spiral) could allow a more accurate interpretation of the observed ISM velocity field. Comparing the KT velocity fields with these simulations may help constrain the time at which the encounter occurred — since the ISM is collisional, motions excited by the passage itself should damp out over about a dynamical time (Chakrabarti and Blitz, 2009; Chakrabarti et al., 2011).

There are a number of upcoming programs that will continue to enhance our view of the velocity field of the ISM. APOGEE-II (Zasowski et al., 2017) will explore the southern hemisphere in DIBs, and the DECaPS program (Schlafly et al., 2018), designed to fill in the fourth quadrant of the Green et al.
(2015) 3D dust map, will allow us to construct all-sky G&D maps. These maps will allow us to study the complete Scutum-Centaurus arm in the inner galaxy, home of much of Milky Way’s star formation. SDSS-V, expected to begin observations in 2020, will observe many millions of giants across the Milky Way disc at APOGEE resolution, and has a subprogram devoted to measuring DIBs and dust toward stars within 4 kpc of the Sun. This will give us both better reach to study velocity fields across the entire Milky Way, and a much more detailed picture locally.

5.8 Appendix

The integrals over profile amplitude $a$ and continuum offset $b$ in Equation 5.4 can be evaluated analytically when the values of the other parameters are held fixed. Given a profile shape $f(v_d, \sigma_v^2)$, an uncertainty $\sigma_y^2$, and prior variances $\sigma_a^2$ and $\sigma_b^2$ for $a$ and $b$, inferring $a$ and $b$ is a regularized linear problem. Following e.g. Luger, Foreman-Mackey, and Hogg (2017), the integral with limits $-\infty$ and $+\infty$ for both $a$ and $b$ evaluates to

$$p \left( y | f, \sigma_y^2, \sigma_a^2, \sigma_b^2 \right) = \mathcal{N}(y; 0, \sigma_y^2 I + AA^T)$$

$$= \frac{1}{(2\pi)^{N/2} \det(\sigma_y^2 I + AA^T)}$$

$$\times \exp \left[ -\frac{1}{2} y^T (\sigma_y^2 I + AA^T)^{-1} y \right]$$

(5.9) (5.10)

Here, $I$ is the identity matrix, $A$ is the design matrix for the problem, $\Lambda$ is a 2-by-2 diagonal matrix with diagonal entries $\sigma_a^2$ and $\sigma_b^2$, and $N$ is the length of
The first column of \( A \) consists of the elements of \( \mathbf{f} \) and the second column consists of ones.

An explicit form for the determinant term can be obtained by invoking the generalized matrix determinant lemma. We give the expression in terms of the inverse variances \( \tau_y, \tau_a, \) and \( \tau_b \) for notational convenience:

\[
\det\left(\sigma_y^2 I + A \Lambda A^T\right) = \det\left(\Lambda^{-1} + \tau_y A^T A\right) \det(\tau_y I) \det(\Lambda)
\]

\[
\quad = \frac{1}{\tau_a \tau_b \tau_y} \left(\left(\tau_a + \tau_y \sum_i f_i^2\right) \left(\tau_b + N \tau_y\right) - \left(\tau_y \sum_i f_i\right)^2\right),
\]

where all sums are from \( i = 1 \) to \( N \). The explicit form of the argument of the exponential is unwieldy and inconvenient to use. In terms of the regularized least-squares solution \( \hat{x} \) to this linear problem and the corresponding least-squares prediction \( A \hat{x} \equiv \hat{y} \), the argument is:

\[
y^T \left(\sigma_y^2 I + A \Lambda A^T\right)^{-1} y = \tau_y y^T I y - \tau_y y^T I \hat{y}
\]

\[
\quad = \tau_y \left(\sum_i y_i^2 - \sum_i y_i \hat{y}_i\right).
\]

The intermediate steps use the Woodbury identity and the definition of the regularized least-squares estimator.

When the integral over \( b \) is still taken from \(-\infty\) to \(+\infty\) but the integral over \( a \) is taken from 0 to \(+\infty\), as is done in the model we use to derive a prior on the DIB profile’s width (Section 5.3.4), the result is the product of the expression
given in Equation 5.9 and a number between 0 and 1. To arrive at this result, we marginalize over $a$ and $b$ separately instead of simultaneously. This can be done in our case because the prior on $a$ and $b$ assumes they are independent. Marginalizing over $b$ gives

$$p \left( y \mid f, a, \sigma_y^2, \sigma_a^2, \sigma_b^2 \right) = \mathcal{N} \left( y \mid fa, \sigma_y^2 I + \sigma_b 11^T \right)$$

$$\equiv \mathcal{N} \left( y \mid fa, C_b \right)$$

where $1$ is an $N$-by-$1$ vector of ones. Integrating this expression over $a$ from $-\infty$ to $+\infty$ gives

$$p \left( y \mid f, \sigma_y^2, \sigma_a^2, \sigma_b^2 \right) = \mathcal{N} \left( y \mid fa + \sigma_b 11^T \right)$$

$$\equiv \mathcal{N} \left( y \mid fa, \sigma_y^2 I + \sigma_a^2 11^T \right),$$

which is equal to Equation 5.9.

If we instead integrate over $a$ from $0$ to $+\infty$, the only term that changes in Equation 12 of Luger, Foreman-Mackey, and Hogg (2017) is the integral itself. Using their variables $h$ and $\Sigma$,

$$\int_0^{+\infty} \exp \left[ (a-h)\Sigma^{-1}(a-h) \right] \, da = 2\pi \Sigma \times \frac{1}{2} \left( 1 - \text{erf} \left[ \frac{-h}{\sqrt{2}\Sigma} \right] \right).$$

The quantity $\Sigma$, which Luger, Foreman-Mackey, and Hogg (2017) define in terms of its inverse in their Equation 9, evaluates to

$$\Sigma^{-1} = \tau_a + \tau_y \sum_i f_i^2 - \frac{\left( \tau_y \sum_i f_i \right)^2}{\tau_b + N \tau_y}.$$
The quantity $h$, which is defined in their Equation 10, evaluates to

$$h = \sum \left( \tau_y \sum_i y_i f_i - \frac{\tau_y^2 (\sum_i y_i) (\sum_i f_i)}{\tau_b + N\tau_y} \right).$$  \hfill (5.21)

Multiplying Equation 5.9 by $\frac{1}{2} \left( 1 - \text{erf} \left[ \frac{-h}{\sqrt{2\tau}} \right] \right)$ gives the marginal likelihood of $y$ when the DIB profile amplitude is constrained to be positive.
Chapter 6

Conclusions and Future Directions

This thesis describes efforts to understand two aspects of the ISM: its chemistry at sub-solar metallicities and the interplay between gas dynamics and spiral structure. Key results, their place in current scientific context, and my plans for further research in each of these areas are described below.

6.1 Chemistry of the ISM at sub-solar metallicities

The main quantitative result of Chapter 2 is that dust-to-metals ratios in neutral and molecular gas in the Large and Small Magellanic Clouds and Milky Way are, in most conditions, similar. Qualitatively, this means that the Magellanic Clouds form and retain interstellar dust with approximately the same efficiency as the Milky Way. A secondary result is that along sightlines with the lowest dust-to-gas ratios in the Small Magellanic Cloud, the dust-to-metals ratio is lower than in the Large Magellanic Cloud or Milky Way. These results confirm the conclusions of studies based on gas and dust emission, which find that dust-to-metals ratios start to fall below that of the Milky Way.
at approximately $Z/5$, the metallicity of the Small Magellanic Cloud.

The work described in this chapter was, at the time, the largest set of measurements of depletions in low metallicity galaxies. Since its publication, there have been dedicated observational programs to study depletions in the Small (Jenkins and Wallerstein, 2017) and Large Magellanic Clouds (the METAL survey: Roman-Duval et al. 2019). These surveys acquired new spectra in order to measure a greater number of the constituents of dust and to confirm, using higher resolution or signal-to-noise ratio data, the results described in Chapter 2.

I continue to be involved in the study of dust propertites in the Magellanic Clouds as a member of the METAL survey team. I am also conducting an archival study of the chemistry of carbon monoxide (CO) in diffuse molecular gas in the Magellanic Clouds. This study will expand the number of CO measurements in this regime from five (André et al., 2004) to 35 and will cover a greater range of H$_2$ column densities and fractions. These measurements will improve our understanding of molecular cloud structure at sub-solar metallicities, an understanding which is vital for calibrating the metallicity dependence of the CO-to-H$_2$ conversion factor.

### 6.2 Gas dynamics and spiral structure in the Milky Way

The main observational result of Chapters 4 and 5 are the first measurements of the motions of dense and diffuse interstellar matter as a function of position in the Milky Way. These measurements provide a previously unavailable view
of our Galaxy. The main astronomical result of these chapters is that the Milky Way is better described by transient spiral structure models than by stationary density wave spiral structure models.

Measurements of the ISM velocity field are part of the wider study of the Milky Way’s ISM. Careful application of established techniques (Reid et al., 2014) and the development of new ones (Green et al., 2015; Zucker, Battersby, and Goodman, 2015; Rezaei Kh. et al., 2018; Zucker et al., 2018; Lallement et al., 2019) is producing more detailed views of how the ISM is distributed in the three spatial dimensions. These works provide input data and tests for velocity mapping and their interpretation benefits from the additional context provided by the velocity maps.

Measurements of the ISM velocity field are also useful for studies of the structure and dynamics of the Milky Way. The combination of line-of-sight velocities from large spectroscopic surveys and parallax and proper motions measurements from the Gaia mission has produced detailed measurements of the stellar velocity field. These measurements are being used to study the assembly history of the Milky Way and the properties of the Milky Way’s bar and spiral structure. The velocity fields of the stars and ISM provide complementary information for these studies.

A new direction in spatially resolved ISM dynamics that I have started to pursue is the assembly and evolution of molecular clouds. There is not yet a consensus on the time scales on which molecular clouds form and collapse, the conditions that initiate their formation, and the prevalence and importance of cloud-cloud collisions. Measurements of the motions of molecular clouds
and the diffuse gas surrounding them as a function of three dimensional position would provide a currently unavailable view of these processes. To this end, I am involved in a study of the motion of diffuse interstellar matter around the nearby California molecular cloud. If successful, this study will help distinguish between different models of how molecular clouds form and grow.
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Vita

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