Modeling the Constituents of the Early Universe

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Modeling the Constituents of the Early Universe

A dissertation presented

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Modeling the Constituents of the Early Universe

Abstract

Understanding how baryons assembled into the first stars and galaxies given the underlying dark matter distribution in the early Universe remains one of the key challenges in the field of cosmology. Given the great distances and extreme faintness of the oldest celestial objects, direct observation of the high redshift Universe remains difficult. Due to the biased, small number statistics, various other avenues have been sought out and paved to construct a coherent picture of the large-scale structure of the Universe at these early times. This thesis explores several of these avenues in a series of studies aimed at characterizing the first galaxies and the star-forming molecular gas that drives their evolution in the early Universe.

We model the effects of strong gravitational lensing and find that by magnifying sources that would otherwise be too faint to detect and lifting them over the instrumental detection threshold, lensing allows us to probe the luminosity function (LF) below current survey limits and constrain the low-luminosity cut-off of the Schechter LF. Using the most recent dust estimates and $z \sim 4-8$ LF measurements, we then model the LF evolution at higher redshifts by employing abundance matching techniques and derive the redshift evolution of the star formation rate density along with the associated cosmic reionization history.

To model the molecular interstellar medium (ISM), we employ the large velocity gradient (LVG) method, a radiative transfer technique used to quantitatively analyze
CO spectral line energy distributions (SLEDs). In particular, we probe the average state of the molecular gas in HDF 850.1, a $z \sim 5.2$ submillimetre source, as well as a series of local starburst, Seyfert, and ultraluminous infrared galaxies. We identify characteristic properties of the local and high-redshift ISM, including the kinetic temperature, gas density, and column density in each case, and derive the gas masses of the various CO-emitting sources along with the corresponding CO-to-H$_2$ conversion factors.

Furthermore, we develop a theoretical framework to estimate the intensity mapping signal and power spectrum of any CO rotational line emitted at high redshifts, particularly during the epoch of reionization. By linking the characteristic properties of emitting molecular clouds to the global properties of the host halos, we model the spatially averaged brightness temperature of all the CO transitions and find the predicted signals to be within reach of existing instruments. We further apply our formalism to compute the cumulative CO emission from star-forming galaxies throughout cosmic time.

Lastly, we explore the emergence of planetary systems around carbon-enhanced metal-poor (CEMP) stars, possible relics of the early Universe residing in the halo of our galaxy. We determine the maximum distance from the host CEMP star at which carbon-rich planetesimal formation is possible and characterize the potential planetary transits across these chemically anomalous stars.

We conclude by exploring the possibility of probing the stellar black hole population using astrometric observations provided by missions such as Gaia. We predict that nearly $3 \times 10^5$ astrometric binaries hosting black holes should be discovered during Gaia’s five year mission. The invisible companions of astrometrically observed metal-poor, low-mass stars may be stellar remnants from the dawn of the Universe, offering to shed light on
the formation of the first stellar black holes in the early stages of galaxy assembly.
Contents

Abstract iii

Acknowledgments xii

Dedication xiii

1 Introduction 1

1.1 Early Galaxies . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 2
  1.1.1 Theoretical Perspective . . . . . . . . . . . . . . . . . . . . . . . . . . 2
  1.1.2 High-Redshift Observations . . . . . . . . . . . . . . . . . . . . . . . 5
  1.1.3 Stellar Archaeology . . . . . . . . . . . . . . . . . . . . . . . . . . . . 7

1.2 Cool Molecular Gas . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 9
  1.2.1 Tracing the Molecular ISM . . . . . . . . . . . . . . . . . . . . . . . . 10
  1.2.2 Modeling CO Excitation . . . . . . . . . . . . . . . . . . . . . . . . . . 12
  1.2.3 Observational Studies . . . . . . . . . . . . . . . . . . . . . . . . . . . 14

I High Redshift Galaxies 17

2 Constraining the Minimum Luminosity of High Redshift Galaxies through Gravitational Lensing 18

  2.1 Abstract . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 19
  2.2 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 20
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3 The Lensing Model</td>
<td>24</td>
</tr>
<tr>
<td>2.4 Results</td>
<td>32</td>
</tr>
<tr>
<td>2.5 Discussion</td>
<td>43</td>
</tr>
<tr>
<td>2.6 Acknowledgements</td>
<td>44</td>
</tr>
<tr>
<td>3.1 Abstract</td>
<td>45</td>
</tr>
<tr>
<td>3.2 Introduction</td>
<td>46</td>
</tr>
<tr>
<td>3.3 The Formalism</td>
<td>50</td>
</tr>
<tr>
<td>3.3.1 The Observed Star-Formation Rate Functions</td>
<td>50</td>
</tr>
<tr>
<td>3.3.2 Method to derive the average $SFR - M_h$ relation</td>
<td>53</td>
</tr>
<tr>
<td>3.3.3 Modeling the SFR Functions</td>
<td>55</td>
</tr>
<tr>
<td>3.4 Results</td>
<td>56</td>
</tr>
<tr>
<td>3.4.1 The Constant $SFR - M_h$ Relation</td>
<td>56</td>
</tr>
<tr>
<td>3.4.2 The Modeled SFR Functions at $z = 4 - 8$</td>
<td>59</td>
</tr>
<tr>
<td>3.4.3 A Prediction for the UV LF at $z = 9 - 10$</td>
<td>61</td>
</tr>
<tr>
<td>3.4.4 Extrapolation to $z \sim 20$ and Predictions for JWST</td>
<td>63</td>
</tr>
<tr>
<td>3.4.5 Contribution of Galaxies to Cosmic Reionization</td>
<td>67</td>
</tr>
<tr>
<td>3.5 Summary</td>
<td>71</td>
</tr>
<tr>
<td>3.6 Acknowledgements</td>
<td>73</td>
</tr>
<tr>
<td>II The Molecular Interstellar Medium</td>
<td>74</td>
</tr>
<tr>
<td>4 The Ratio of CO to Total Gas Mass in High-Redshift Galaxies</td>
<td>75</td>
</tr>
<tr>
<td>4.1 Abstract</td>
<td>75</td>
</tr>
<tr>
<td>4.2 Introduction</td>
<td>76</td>
</tr>
<tr>
<td>4.3 Large Velocity Gradient Model</td>
<td>79</td>
</tr>
</tbody>
</table>
CONTENTS

5.5.7  IC 694 & NGC 3690  . . . . . . . . . . . . . . . . . . . . . . 145
5.5.8  Arp 220  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 146
5.5.9  NGC 6240  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 147
5.5.10 Mrk 231  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 148
5.6  Summary  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 149
5.7  Acknowledgements  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 152

6  Predicting the Intensity Mapping Signal for multi-J CO lines  154
   6.1  Abstract  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 154
   6.2  Introduction  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 155
   6.3  Modeling the CO Emission  . . . . . . . . . . . . . . . . . . . . . . . . . . 159
       6.3.1  CO Brightness Temperature  . . . . . . . . . . . . . . . . . . . . . 159
       6.3.2  The Star Formation Model  . . . . . . . . . . . . . . . . . . . . . . 162
       6.3.3  Theoretical Models for LVG Parameters  . . . . . . . . . . . . . . 164
           6.3.3.1  Gas Kinetic Temperature  . . . . . . . . . . . . . . . . . . 165
           6.3.3.2  Cloud volume density  . . . . . . . . . . . . . . . . . . . 166
           6.3.3.3  Velocity Gradient  . . . . . . . . . . . . . . . . . . . . 172
           6.3.3.4  CO-to-H$_2$ Abundance Ratio  . . . . . . . . . . . . . . . 172
           6.3.3.5  CO Column Density, including photodissociation  . . . . 172
       6.3.4  Model CO SLEDs  . . . . . . . . . . . . . . . . . . . . . . . . . . . . 176
   6.4  Results  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 179
       6.4.1  Predicted CO Fluxes and Spatially Averaged CO Brightness Tem-  179
            perature  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
       6.4.2  CO Power Spectrum  . . . . . . . . . . . . . . . . . . . . . . . . . . 186
   6.5  Discussion  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 190
   6.6  Acknowledgements  . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 195

7  Spectral Distortion of the CMB by the Cumulative CO Emission from
### CONTENTS

**Galaxies throughout Cosmic History** 196

7.1 Abstract ................................................................. 196
7.2 Introduction ............................................................ 197
7.3 The Formalism .......................................................... 201
7.4 Results ................................................................. 204
7.5 Discussion ............................................................. 209
7.6 Acknowledgements ..................................................... 211

### III Early Planetary Systems 212

**8 CEMP Stars: Possible Hosts to Carbon Planets in the Early Universe** 213

8.1 Abstract ................................................................. 213
8.2 Introduction ............................................................ 214
8.3 Star-forming Environment of CEMP Stars ......................... 217
8.4 Orbital Radii of Potential Carbon Planets ......................... 220
8.5 Mass-Radius Relationship for Carbon Planets ..................... 229
8.6 Transit Properties ..................................................... 234
8.7 Discussion ............................................................. 240
8.8 Acknowledgments ..................................................... 244

**9 EPILOGUE** 246

9.1 Abstract ................................................................. 246
9.2 Introduction ............................................................ 247
9.3 The Model ............................................................. 249
  9.3.1 Black holes with stellar companions .......................... 250
  9.3.2 Visible binary companions .................................... 252
  9.3.3 Accessible range of periods ................................. 253
Acknowledgments

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“When I see Your heavens, the work of Your fingers, the moon and stars that You have established, what is man that You should remember him?....” (Psalms 8:4-5)
Chapter 1

Introduction

The early Universe, still shrouded in mystery, has captivated the human imagination for millennia. Questions of “Where do we come from? Where are we going? What are we?” have evolved to take on the more empirically-driven form of “Did our Universe have a beginning, or is it infinitely old? Will it come to an end some time in the future? What is the Universe made of?” Advances in technology over the last several decades have opened the door to critically exploring the story of genesis through direct observation. The cosmic microwave background (CMB) offers the first glimpse of the Universe when it was merely 400,000 years old, marking the beginning of the cosmic dark ages when neutral hydrogen filled most of the Universe. Deep images from the Hubble Space Telescope (HST) provide the next snapshot, nearly one billion years later, revealing a Universe filled with a highly ionized intergalactic medium (IGM) and teeming with star-forming galaxies, many with stellar masses exceeding $10^{10} \, M_\odot$.

These observations, among others, have led cosmologists to construct a picture of cosmic history in which the Universe starts out simple, primarily homogeneous
CHAPTER 1. INTRODUCTION

and isotropic, with small spatial fluctuations in the energy density and gravitational potential. These fluctuations then grow over time due to gravitational instability and eventually lead to the formation of the large-scale structure observed in the present Universe. While cosmic geometry, the mass-energy content of the Universe, and the initial density fluctuation spectrum have all been constrained to high accuracy, our understanding of galaxy formation is still far from complete. Three main epochs have been identified in the star formation history of the Universe: a steady rise in the cosmic star formation rate density (SFRD) from $z \sim 10$ to 6 (Bouwens et al. 2011a; Coe et al. 2013), followed by the epoch of galaxy assembly from $z \sim 1$ to 3 during which the SFRD peaks and nearly half of the stars in the present Universe form (Shapley 2011; Reddy et al. 2008), and ending with an order of magnitude decline in the SFRD from $z \sim 1$ to the present (Lilly et al. 1996; Madau et al. 1996).

To explain this observed star formation history and decipher how baryonic matter assembled into the observed Universe given the underlying dark matter distribution, we rely on studies that probe two main components of the universe: (i) the products of the galaxy formation process, i.e. stars, star formation, and ionized gas, and (ii) the fuel driving the process, mainly the cool molecular gas in galaxies.

1.1 Early Galaxies

1.1.1 Theoretical Perspective

On the theory side, a “galaxy” is defined as a gravitationally-bound system of stars embedded in a dark matter halo that is capable of sustaining star formation over
cosmological time periods. This definition therefore requires the system to have \((a)\) sufficient mass to be stable against feedback from its own stars and neighboring halos; \((b)\) a virialized dark matter halo able to accrete baryons; and \((c)\) an efficient mechanism to cool the baryonic gas, allowing it to condense and fragment to form protostars (Loeb & Furlanetto 2013).

In the current theoretical framework, the existence of such systems only becomes possible after the emergence of the first generation of stars at \(z \sim 20 - 30\) which ends the cosmic dark ages and initiates the gradual enrichment of the Universe with metals (Stark 2016). These stars, known as Population III stars, form inside "minihalos" cooled by molecular hydrogen (\(H_2\)), and proceed to exert extremely strong feedback on their host halo’s gas, photoevaporating the diffuse gas in the region and blasting out the rest of the halo’s gas with their explosive deaths via supernovae. The background of Lyman-Werner photons produced by these first generation stars further photodissociates the \(H_2\) and gradually raises the critical virial temperature for cold gas formation to a value that effectively chokes off Population III star formation in minihalos. At this point in cosmic history, star formation is believed to have shifted to halos with virial temperatures \(T_{\text{vir}} > 10^4\) K where atomic hydrogen can take over as the main cooling agent. With potential wells deep enough to retain photoheated gas, these systems can maintain reasonable star formation rates without completely disrupting their gas supplies. This second generation of halos therefore gives birth to the first galaxies, which are predicted to form at \(z \sim 10 - 15\), roughly 500 million years after the Big Bang.

Over the next billion years, these early galaxies are expected to have rapidly accreted gas and built up stellar mass while releasing Lyman continuum radiation that ionized their intergalactic surroundings. These bubbles of ionized hydrogen grew over time and
CHAPTER 1. INTRODUCTION

gradually came to overlap around overdensities in the matter distribution, leading to the cosmic reionization of hydrogen. High redshift star-forming galaxies have thus long been considered the primary candidates responsible for the reionization of intergalactic hydrogen by $z \approx 6$. In order for this to be the case, recent calculations demonstrate that there must exist an abundant population of faint star-forming galaxies below the sensitivity limit of current $z > 6$ surveys. In particular, galaxies with luminosities as faint as $M_{UV} = -10$ to -13, corresponding to 4-7 magnitudes below the current HST detection limits, are necessary to achieve the observed reionization (Robertson et al. 2013; Bouwens et al. 2015a). Furthermore, the high redshift galaxy population must be fairly efficient ionizing agents, with ionizing photon escape fractions of $f_{esc} = 10$-20%. Though significantly higher than the typical value found in luminous $z \approx 3$ galaxies, such large escape fractions may be possible, especially given the population of runaway massive stars whose ionizing flux will be much more likely to escape the host galaxy (Conroy & Kratter 2012). Alternatively, more extreme ionizing radiation fields would close the “missing photons” gap, supplying the critical ionizing photon production rate for IGM reionization by $z > 6$ galaxies.

The large angular-scale patterns in the CMB polarization maps provide further constraints on the epoch of reionization and the primary source of ionizing photons. Due to Thomson scattering by free electrons in the reionized IGM, CMB photons are left polarized with damped temperature fluctuations. Recent measurements of the resulting Thomson scattering optical depth by the Planck Collaboration et al. (2016c) yield an integrated CMB optical depth of $\tau = 0.058 \pm 0.012$. Current models have found these measurements to be consistent with a scenario where the bulk of reionization occurs at $6 < z < 9$, with early star-forming galaxies dominating the reionization process and
leaving an IGM that is nearly 50% neutral by $z = 7$ (Bouwens et al. 2015a; Robertson et al. 2015).

1.1.2 High-Redshift Observations

Over the course of the last decade, the cosmic frontier has been pushed back to a redshift of $z \approx 10$, allowing the first direct tests of the theoretical picture presented above. These advances are mostly due to the deep imaging campaigns carried out by the Wide Field Camera 3 (WFC3) onboard HST. With its unprecedented near-infrared sensitivity, WFC3 has identified thousands of galaxies within the first billion years after the Big Bang, providing a census of star formation activity and insight into the physical nature of these early star-forming galaxies in the redshift range $6 < z < 10$.

One of the most fundamental and important observables for galaxy studies in the early Universe is the luminosity function (LF), which provides the volume density of galaxies as a function of their luminosity. Constraints on the abundance of star-forming systems in this time interval are provided most thoroughly by the ultraviolet (UV) LF of UV continuum dropout galaxies, which is generally parametrized by a Schechter function (Schechter 1976),

$$\frac{dn}{dL} = \phi(L) = \left( \frac{\phi^*}{L^*} \right) \left( \frac{L}{L^*} \right)^{\alpha} e^{-L/L^*}$$

(1.1)

where $\phi^*$ is the characteristic volume density, $L^*$ is the characteristic luminosity, and $\alpha$ is the faint-end slope. This function provides a good fit for populations that demonstrate an exponential cutoff above the characteristic luminosity $L^*$, while following a near power-law slope $\alpha$ at the faint end of the spectrum. When considering high-redshift sources, the Schechter function is often expressed in terms of the absolute magnitude
CHAPTER 1. INTRODUCTION

instead,

\[ \phi(M) = \frac{\ln 10}{2.5} \phi^* (10^{0.4(M^* - M)}) a + 1 \exp [-10^{0.4(M^* - M)}] \]  

(1.2)

where \( M^* \) is the characteristic absolute magnitude and \( M \) is typically the absolute magnitude corresponding to the luminosity at a rest-frame wavelength of 1500 Å.

With the expanding dataset of detected high redshift sources, measurements of the UV LF have gradually improved. The most recent \( z > 4 \) LF s are derived from HST imaging that provide samples of 4,000-6,000 \( z \simeq 4 \) galaxies, 2,000-3,000 \( z \simeq 5 \) galaxies, 700-900 \( z \simeq 6 \) galaxies, 300-500 \( z \simeq 7 \) galaxies, and 100-200 \( z \simeq 8 \) galaxies (Finkelstein et al. 2015; Bouwens et al. 2015b). These HST samples, which allow the UV LF to be characterized over a large dynamic range (\( \Delta M_{UV} \simeq 6 \) at \( z \simeq 6 \)), are complemented by ground-based imaging surveys that constrain the volume density of galaxies as bright as \( M_{UV} \simeq -23 \) (Bowler et al. 2014, 2015). Current measurements all suggest a rapid decline in the abundance of UV-luminous galaxies at \( z > 4 \), with a volume density at \( M_{UV} = -21 \) that drops by a factor of 15-20 between \( z \simeq 4 \) and \( z \simeq 8 \) (Finkelstein et al. 2015; Bouwens et al. 2015b). This evolution is less dramatic for galaxies that are ten times less luminous (\( M_{UV} = -18.5 \)), in which case, the volume density only decreases by a factor of 2 to 3 over the same redshift range (Finkelstein et al. 2015; Bouwens et al. 2015b). These findings suggest that at earlier times, low-luminosity galaxies are the dominant contributors to the integrated UV luminosity density.

Less agreement presides over measurements of higher redshift UV luminosity functions. Roughly 20 candidates have thus far been identified at \( z \simeq 9 - 11 \) in deep WFC3/IR imaging of the Hubble Deep Field (HUDF) and CANDELS fields (Oesch et al. 2010, 2012a, 2013, 2014, 2016; Ellis et al. 2013; McLure et al. 2013; Bouwens et al.
2015b, 2016). To push beyond the current Hubble detection limit, initiatives such as the Hubble Frontier Fields (HFF) program take advantage of the strong gravitational lensing power of massive galaxy clusters to magnify distant background galaxies, enhancing the detectability of high redshift sources that are intrinsically fainter than the observational threshold. Several such gravitationally lensed systems have already been identified in the HFF and CLASH surveys, augmenting the sample of high redshift galaxies (Zheng et al. 2012; Coe et al. 2013; Bouwens et al. 2014a; Zitrin et al. 2014; Ishigaki et al. 2015; McLeod et al. 2015). Yet, given the small number statistics, quantifying the evolution of the UV LF at these high redshifts remains difficult. Several studies have found that the volume density of UV-luminous galaxies accelerates in its decline at $z > 8$ (Oesch et al. 2012a, 2013, 2014; Bouwens et al. 2014a, 2015b), consistent with predictions from some hydrodynamic simulations and semi-analytic models (Finlator et al. 2011b; Dayal et al. 2013; Tacchella et al. 2013; Sun & Furlanetto 2016). Others report an evolution over $8 < z < 10$ that continues at the same rate suggested by $4 < z < 8$ galaxies (Coe et al. 2013; Ellis et al. 2013; McLeod et al. 2015, 2016). Future parallel observations with HST’s BoRG campaign and RELICS initiative promise to provide further insight and better constrain the evolution of these high redshift objects residing in the early Universe.

1.1.3 Stellar Archaeology

While traditional far-field cosmology tries to shed light on the first billion years after the Big Bang via high redshift observations, “near-field” cosmology strives to constrain the early Universe by studying the chemical abundance patterns in the most metal-poor
stars in the local Universe. In contrast to their high-mass counterparts who rapidly burn through their fuel and die as supernovae in a relatively short time frame, low-mass stars, 
$M \lesssim 0.8 \, M_\odot$, live for some $\sim 10(M/M_\odot)^{-3}$ Gyr before ending up as white dwarfs. They therefore contain detailed information about the history of their host systems and can be used to study the conditions that existed at the beginning of star and galaxy formation (Frebel & Norris 2015).

Identifying these early galaxy fossils relies on the assumption that the most metal-poor stars that exist today are also the oldest stars. Given the lack of elements heavier than lithium in the Universe before the formation of the first stars, the chemical abundance profile of a star stands as the main proxy for determining its age (Frebel & Norris 2015). Moreover, the stellar composition yields valuable information on the star’s formation era, the extent of chemical enrichment within its natal cloud, and ultimately, the cosmic chemical evolution following the Big Bang. Extensive efforts have thus been devoted to searching for “very metal poor” (VMP) stars in the Milky Way and its satellite dwarf galaxies, stars defined by $[\text{Fe/H}] \leq -2.0$ where $[\text{Fe/H}]$ refers to the star’s iron abundance relative to that of the Sun (Beers & Christlieb 2005).

Surveys of these VMP candidates have revealed that approximately 20% of stars that fall into this category exhibit large overabundances of carbon, with $[\text{C/Fe}] \geq +0.7$. The fraction of sources with such large carbon-to-iron ratios, known as CEMP (carbon enhanced metal poor) stars, increases to 30% for stars with $[\text{Fe/H}] < -3.0$ and 75% for $[\text{Fe/H}] < -4.0$ (Beers & Christlieb 2005; Norris et al. 2013; Frebel & Norris 2015). This discovery seems particularly odd when compared to the fact that no more than a few percent of disk stars with near-solar metallicities exhibit such large carbon overabundances (Norris et al. 1997a). Though no census has been reached in
understanding their origin, the dominating hypothesis posits that these CEMP stars are second-generation, Population II stars, born from an interstellar medium polluted with the nucleosynthetic products of Population III supernovae. In the case of a ‘faint’ supernova explosion, only the outer layers, rich in lighter elements, are ejected while the innermost layers, rich in iron, fall back on the remnant and are not recycled in the ISM (Umeda & Nomoto 2003, 2005). These peculiar metal-deficient objects are thus promising probes of the formation of the first stars and will be furthered considered in terms of their potential to host early planetary systems in the last section of this thesis.

1.2 Cool Molecular Gas

Detailed studies of star formation in nearby galaxies suggest that the cool gas content of the Universe is a critical parameter in galaxy evolution, providing the raw material from which stars form. In particular, star formation is found to be closely linked to the molecular gas content, while showing little relation to the atomic neutral gas content in a given galaxy (Bigiel et al. 2008). This observation is corroborated at high redshifts by the lack of evolution of the cosmic HI mass density over the same redshift range where the SFRD grows by more than an order of magnitude (Prochaska & Wolfe 2009). This suggests that the other phases of the ISM cannot form stars directly unless they cool sufficiently to form cold and dense molecular gas, leaving the molecular gas phase as the most relevant to the study of galaxy formation and evolution.

Furthermore, studies show that once molecular gas forms and becomes self-gravitating, star formation proceeds to first order according to a star formation law via local processes inherent to the giant molecular cloud (GMC) (Kennicutt 1998b; Bigiel
et al. 2008; Leroy et al. 2008; Krumholz et al. 2009; Genzel et al. 2010). Therefore, if this universal star formation law were to hold out to high redshifts, the cosmic star formation rate density would just be a reflection of the molecular gas density history of the Universe.

1.2.1 Tracing the Molecular ISM

Molecular hydrogen, H$_2$, which dominates the molecular gas component of the Universe, is unfortunately not directly observable in emission. Given the lack of a permanent dipole moment, the lowest energy transitions of H$_2$ are strongly forbidden, with spontaneous decay lifetimes of $\sim 100$ years (Bolatto et al. 2013). More importantly, the two lowest para and ortho transitions have upper level energies $E/k \approx 510$ K and 1015 K which are significantly higher than temperatures in GMCs and are thus very difficult to excite. Consequently, H$_2$ remains practically invisible in the ISM and observers have to instead rely on tracer molecules to detect and quantify molecular gas in galaxies.

Carbon monoxide, CO, has become the commonly used tracer molecule of the ISM, serving as the most abundant molecule after H$_2$. With its weak permanent dipole moment and a ground rotational transition with a low excitation energy $E/k \approx 5.53$ K, CO is easily excited even in cold molecular clouds (Bolatto et al. 2013). Its $J = 1 \rightarrow 0$ transition also falls in a relatively transparent atmospheric window, leading astronomers to employ emission in the CO(1-0) line to measure molecular gas masses. The standard approach assumes a basic linear relationship between the observed CO luminosity and the H$_2$ gas mass,

$$M_{H_2} = \alpha_{CO} L_{CO(1-0)}$$  (1.3)
CHAPTER 1. INTRODUCTION

where $M_{H_2}$ is in units of solar mass and the luminosity $L'_{CO(1-0)}$ is expressed in K km s$^{-1}$ pc$^2$. $\alpha_{CO}$ is therefore a mass-to-light ratio, commonly referred to as the “CO-to-H$_2$ conversion factor.” For the GMCs in our Galaxy, this linear relation has been derived with $\alpha_{CO} \sim 4.6 M_\odot (K \text{ km s}^{-1} \text{ pc}^2)^{-1}$ using three independent methods: (a) correlation of optical/infrared extinction with CO column densities in interstellar dark clouds (Dickman 1978); (b) correlation of $\gamma$-ray flux with the CO line flux for the Galactic molecular ring (Bloemen et al. 1986; Strong et al. 1988); and (c) the observed relations between virial mass and CO line luminosity for Galactic GMCs (Solomon et al. 1987).

The characteristic value of $\alpha_{CO}$ is observed to drop to $\alpha_{CO} \sim 0.8 M_\odot (K \text{ km s}^{-1} \text{ pc}^2)^{-1}$ in nearby nuclear starburst galaxies and ultraluminous infrared galaxies (ULIRGs) (Downes & Solomon 1998), implying more CO emission per unit molecular mass. Downes & Solomon (1998) suggest most of the CO emission in these starburst and ULIRG systems comes from an overall warm, pervasive molecular inter-cloud medium, in which case, the line luminosity is determined by the total dynamical mass (gas plus stars). Others hypothesize that this lower $\alpha_{CO}$ value may reflect different molecular gas heating processes in these systems, with cosmic rays and turbulence dominating over photons (Papadopoulos et al. 2012b).

With the recent explosion in the number and type of galaxies detected in molecular line emission at $z > 1$, calibrating this conversion factor for the high redshift universe has become paramount to the study of the star-forming ISM at the earliest epochs. The standard practice in the field has been to estimate the molecular gas masses of high redshift sources by applying the local starburst value to CO observations of quasars and submillimeter galaxies (SMGs), and the Galactic value ($\alpha_{CO} \sim 4.6 M_\odot (K \text{ km s}^{-1} \text{ pc}^2)^{-1}$) to ‘main-sequence’ color-selected galaxies (CSGs) (Tacconi et al. 2008; Daddi et al. 2011).
CHAPTER 1. INTRODUCTION

2010). There is mounting evidence, however, that there may be a continuum of values of $\alpha_{CO}$ and that this conversion factor is likely a function of local ISM conditions such as pressure, gas dynamics, and metallicity (Papadopoulos et al. 2012b). Galaxies that harbor more compact gas reservoirs and hyper-star forming environments (SFR $\sim$ 1000 $M_\odot$/yr) are found to have the most extreme gas excitation and correspondingly, the lowest mass-to-luminosity ratios. Alongside the star formation rate and SFR surface density, the host galaxy’s metallicity appears to play a central role in determining $\alpha_{CO}$ as well. There is increasing evidence that in metal-poor environments, the lack of dust shielding dramatically reduces the CO content while leaving the H$_2$-rich cloud envelopes intact, resulting in much higher conversion factors (Leroy et al. 2011; Schruba et al. 2012; Sandstrom et al. 2013). Calibrating the conversion factor for these various source populations at high redshift remains an active field of research.

1.2.2 Modeling CO Excitation

Radiative transfer techniques are often employed to model the spectral line energy distribution (SLED) of a given molecule and derive the physical conditions within the emitting molecular cloud. In the large velocity gradient (LVG) method, an iterative escape probability formalism is used to compute how the various levels of the CO molecule are populated through collisional excitation with H$_2$ for a given kinetic temperature $T_{kin}$, H$_2$ density, CO abundance [CO]/[H$_2$], and velocity gradient $dv/dr$ (Sobolev 1960; Castor 1970; Lucy 1971). (The same modeling can be applied to any molecule.) The velocity gradient introduced in this model is a means of quantifying the number of emission photons that can eventually leave the cloud, given the optically thick
CHAPTER 1. INTRODUCTION

nature of the CO emission (at least in the low-J transitions). The assumption that such a gradient exists is justified by observations of interstellar molecular line widths which range from a few up to a few tens of kilometers per second, far in excess of plausible thermal velocities in the clouds (Goldreich & Kwan 1974). This suggests that the observed velocity differences in the molecular medium arise from large-scale turbulence which enables CO photons to leave their parental clouds.

Once the population fractions in each level are calculated, the optical depths for each transition as well as the resulting line intensities can be computed. Therefore, given a measurement of the line emission ladder for a given molecule, constraints may be placed on the temperature and density of the gas and mass estimates can be derived from the column density.

In the case where the cloud is exposed to a radiation field, PDR (photon-dominated region) and XDR (X-ray dominated region) models are employed to determine the gas conditions. These models take into account elaborate chemical networks and the cooling, heating, and chemical processes that are entirely dictated by the radiation field to derive the temperature and density distribution of the H$_2$ molecules (Wolfire et al. 2010; Meijerink & Spaans 2005; Meijerink et al. 2007). Once these quantities are determined, a code similar to LVG is then used to compute the rotational line intensities emitted by the given molecule. However, since most PDR/XDR models are based on one-dimensional infinite slabs, gas mass estimates can not be derived for these unconfined volumes.
CHAPTER 1. INTRODUCTION

1.2.3 Observational Studies

With the explosion in the number and type of galaxies detected in molecular emission at \( z > 1 \), the last few years have seen unprecedented progress in the study of cool molecular gas in the early Universe. The physical conditions of the gas in some of the brightest high redshift systems have been investigated using the detailed multi-transition, multi-species observations provided by centimeter and (sub)millimeter telescopes. Emerging from these high-redshift CO excitation analyses is the general result that different source populations at high \( z \) show distinctly different excitation patterns (Carilli & Walter 2013).

Of all objects detected at high redshifts, quasars show the most extreme molecular gas excitation (Weiss et al. 2007; Riechers et al. 2009). Their CO emission ladders can be modeled with simple models characterized by one gas component, i.e. one temperature and density, out to the highest J transitions, with typical temperatures of \( T_{\text{kin}} \approx 40 - 60 \) K and gas densities of \( \log (n_{H_2} [\text{cm}^{-3}]) = 3.6 - 4.3 \) (Riechers et al. 2006, 2011b). This finding suggests that the molecular gas emission in quasars originates from a very compact gas reservoir in the center of the system, an interpretation which has been confirmed in the few cases where the CO emission could be resolved (Walter et al. 2004; Riechers et al. 2008a,b, 2011b). The resulting star formation rate densities are thus typically high \( \sim 10^3 \text{ M}_\odot \text{ yr}^{-1} \text{kpc}^{-2} \) and the molecular gas masses are on the order of \( \sim 10^{10} (\alpha_{\text{CO}}/0.8) \text{ M}_\odot \) with short gas consumption times \( \sim 10^7 \) yr (Walter et al. 2009).

Surveys at submm wavelengths have identified another population of galaxies known as submillimeter galaxies (SMGs). These extreme starburst galaxies (SFR \( > 10^3 \text{ M}_\odot/\text{yr} \)) are also found to have compact, but large, molecular gas reservoirs, suggesting they may
be the result of mergers in which the gas settled into the center of the two colliding
galaxies and led to a starburst (Tacconi et al. 2006, 2008). Relative to quasars, the
average excitation of the molecular gas in SMGs is not as extreme, a fact that may be
attributed to the fact that star formation in some SMGs occurs on more extended scales
than quasars (Weiss et al. 2007). The typical temperatures and gas densities in SMGs is
$T_{\text{kin}} \sim 30 - 50 \ K$ and $\log (n_{H_2} [\text{cm}^{-3}]) = 2.7 - 3.5$, respectively. Furthermore, observations
of CO emission reveal an excess in the CO(1-0) line and a more spatially extended
emission in the ground transition than the higher energy transitions (Ivison et al. 2011;
Riechers et al. 2011a). These findings indicate that a two-component gas model is
necessary to account for the observed excitation and that neglecting this additional
component would lead to an underestimation of the total gas mass.

More recently, progress has been made in excitation measurements for more normal
star-forming galaxies at high redshift. These galaxies, selected via their optical or
near-infrared colors, are referred to as “color-selected star-forming galaxies”, CSGs,
and have a volume density more than an order of magnitude larger than SMGs. CSGs
contain molecular gas reservoirs that are more extended, $\sim 10 \ \text{kpc}$ in size, but similar in
mass to their SMG counterparts (Daddi et al. 2010; Tacconi et al. 2010, 2013). However,
studies have found that gas fractions are very high in these galaxies, comparable to or
larger than the corresponding stellar mass, with 50-65% of the baryons in the galaxies’
half-light radius in the form of gas. With intrinsic star formation rates of $\sim 100 \ M_{\odot} \text{yr}$,
CSGs are forming stars at $\sim 10$ times lower rates than quasars and SMGs (Daddi et al.
2008). The combination of these factors leads to the less extreme gas excitation observed
in these high-redshift objects, though measurements only exist up to the $J = 3 \rightarrow 2$ line
(Dannerbauer et al. 2009). Follow-up observations of higher-order CO transitions will be
CHAPTER 1. INTRODUCTION

necessary to further characterize these CSGs.
Part I

High Redshift Galaxies
Chapter 2

Constraining the Minimum Luminosity of High Redshift Galaxies through Gravitational Lensing

This thesis chapter originally appeared in the literature as

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CHAPTER 2. CONSTRAINING MINIMUM LUMINOSITY THROUGH LENSING

2.1 Abstract

We simulate the effects of gravitational lensing on the source count of high redshift galaxies as projected to be observed by the Hubble Frontier Fields program and the James Webb Space Telescope (JWST) in the near future. Taking the mass density profile of the lensing object to be the singular isothermal sphere (SIS) or the Navarro-Frenk-White (NFW) profile, we model a lens residing at a redshift of \( z_L = 0.5 \) and explore the radial dependence of the resulting magnification bias and its variability with the velocity dispersion of the lens, the photometric sensitivity of the instrument, the redshift of the background source population, and the intrinsic maximum absolute magnitude \( (M_{\text{max}}) \) of the sources. We find that gravitational lensing enhances the number of galaxies with redshifts \( z \gtrsim 13 \) detected in the angular region \( \theta_E/2 \leq \theta \leq 2\theta_E \) (where \( \theta_E \) is the Einstein angle) by a factor of \( \sim 3 \) and \( \sim 1.5 \) in the HUDF \( (df/d\nu_0 \sim 9 \text{ nJy}) \) and medium-deep JWST surveys \( (df/d\nu_0 \sim 6 \text{ nJy}) \). Furthermore, we find that even in cases where a negative magnification bias reduces the observed number count of background sources, the lensing effect improves the sensitivity of the count to the intrinsic faint-magnitude cut-off of the Schechter luminosity function. In a field centered on a strong lensing cluster, observations of \( z \gtrsim 6 \) and \( z \gtrsim 13 \) galaxies with JWST can be used to infer this cut-off magnitude for values as faint as \( M_{\text{max}} \sim -14.4 \) and \( -16.1 \) mag \( (L_{\text{min}} \approx 2.5 \times 10^{26} \text{ and } 1.2 \times 10^{27} \text{ erg s}^{-1} \text{ Hz}^{-1}) \) respectively, within the range bracketed by existing theoretical models. Gravitational lensing may therefore offer an effective way of constraining the low-luminosity cut-off of high-redshift galaxies.
CHAPTER 2. CONSTRAINING MINIMUM LUMINOSITY THROUGH LENSING

2.2 Introduction

The characterization of the earliest galaxies in the universe remains one of the most important frontiers of observational cosmology, and also one of the most challenging (Loeb & Furlanetto 2013). High-redshift searches carried out with the *Hubble Space Telescope* (HST) have recently provided significant insights to the mass assembly and buildup of the earliest galaxies ($z \gtrsim 6$) and the contribution of star formation to cosmic reionization (Bunker et al. 2004; Yan & Windhorst 2004b; Bouwens et al. 2010; Ellis et al. 2013). However, because of their great distances and extreme faintness, as well as the high sky background, high redshift galaxies remain difficult to detect. Furthermore, those sources which are bright enough to be studied individually are drawn from the bright tail of the luminosity function (LF) of high redshift galaxies and are therefore not necessarily representative of the bulk of the population (Bayliss et al. 2010). Gravitational lensing by galaxy clusters has been highlighted as an efficient way of improving this situation, providing an opportunity to observe the high-redshift universe in unprecedented detail (Bradley et al. 2008; Zheng et al. 2012).

Light rays propagating through the inhomogeneous gravitational field of the Universe are often deflected by intervening clumps of matter, which cause most sources to appear slightly displaced and distorted in comparison with the way they would otherwise appear in a perfectly homogeneous and isotropic universe (Schneider & Falco 1992; Bartelmann & Schneider 2001; Treu 2010). When the light from a distant galaxy is deflected by foreground mass concentrations such as galaxies, groups, and galaxy clusters, its angular size and brightness are increased and multiple images of the same source may form. This phenomenon, referred to as *strong gravitational lensing*, leads to a magnification bias that
can have a significant effect on the observability of a population of galaxies. Magnified sources, that would otherwise be too faint for detection without a huge investment of observing time, can be found, and unresolved substructure and morphological details in these intrinsically faint galaxies can be studied (Smail et al. 1997; Pettini et al. 2000; Ellis et al. 2001). The light magnification produced by nature’s ”cosmic telescopescan be exploited in the study of high-redshift galaxies which have greater probability of falling in alignment with, and therefore being lensed by, a foreground galaxy (Barkana & Loeb 2000). Zackrisson et al. (2012) explored the prospect of detecting a hypothetical population of population III galaxies via gravitational lensing by a particular galaxy cluster (MACS J0717.5 + 3745) as the lens. Indeed, several highly magnified galaxy candidates at up to redshift $z \sim 10$ have already been discovered behind massive clusters Bayliss et al. (2010); Bradley et al. (2008); Zheng et al. (2012); Richard et al. (2006); Stark et al. (2007); Richard et al. (2008); Bouwens et al. (2009b); Coe et al. (2013).

The Hubble Frontier Fields program$^1$ is expected to lead to many more such discoveries. With its six deep fields centered on strong lensing galaxy clusters in parallel with six deep “blank fields”, the Hubble Frontier Fields will reveal previously inaccessible populations of $z = 5-10$ galaxies that are 10-50 times intrinsically fainter than any presently known. In the coming decade, the planned James Webb Space Telescope (JWST)$^2$ promises to go even further by placing new constraints on the stellar initial mass function at high redshift, on the luminosity function of the first galaxies, and on the progress of the early stages of reionization with observations of galaxies at $z \gtrsim 10$ (Gardner et al. 2006; Windhorst et al. 2006; Haiman et al. 2008).

$^1$http://www.stsci.edu/hst/campaigns/frontier-fields/

$^2$http://www.stsci.edu/jwst/
CHAPTER 2. CONSTRAINING MINIMUM LUMINOSITY THROUGH LENSING

While lenses magnify the observed flux and lift sources which are intrinsically too faint to be observed over the detection threshold, they simultaneously increase the solid angle within which sources are observed and thus reduce their number density and measured surface brightness in the sky (Refregier & Loeb 1997). Zemcov et al. (2013) recently reported measuring a deficit of surface brightness within the central region of several massive galaxy clusters with the SPIRE instrument, and used the deficit to constrain the surface brightness of the cosmic infrared background. The outcome of this trade-off between depth and area depends on a variety of factors, such as the photometric sensitivity of the detecting device and the slope of the luminosity function of background sources. Given a photometric sensitivity capable of detecting faint sources even in the absence of any light amplification, the lensing effect leads to a negative magnification bias, reducing the apparent surface density behind lensing clusters. If, however, the fainter sources cannot be observed unless magnified, then whether the magnification bias leads to a surplus or deficit of observed sources depends on the effective slope of their luminosity function (Turner et al. 1984). At fainter magnitudes where the effective slope, \( \alpha \), is shallow, there may not be enough faint sources in the lensed population to compensate for the increase in total surface area. However, in cases where \( \alpha \gtrsim 2 \), the gain in depth due to apparent brightening may outweigh the loss in area; gravitational lensing will thus increase the apparent surface density behind the lensing object, boosting up the number of detected sources relative to that which would otherwise be observed in an unlensed field (Bouwens et al. 2009b; Broadhurst et al. 1995).

The observed number counts of galaxies residing at redshifts greater than some \( z' \) may also be sensitive to the intrinsic faint-magnitude cut-off chosen for the extrapolation of the galaxy LF. Theoretical and numerical investigations have established that a halo
CHAPTER 2. CONSTRAINING MINIMUM LUMINOSITY THROUGH LENSING

at \( z \lesssim 10 \) irradiated by a UV field comparable to the one required for reionization needs a mass \( M_h \gtrsim (0.6 - 1.7) \times 10^8 \, \text{M}_\odot \), with a corresponding temperature \( T_{\text{vir}} \gtrsim (1 - 2) \times 10^4 \) K at \( z = 7 \), in order to cool and form stars (Haiman et al. 1996; Tegmark et al. 1997; Muñoz & Loeb 2011). Such claims have motivated models with cut-offs for the absolute magnitude of the smallest halo capable of forming stars as faint as \( M_{\text{AB}} \approx -10 \) Wyithe & Loeb (2006); Trenti et al. (2010). Gravitational lensing may provide an effective way to constrain the value of this minimum luminosity given the fact that the lensed number count of high-redshift galaxies remains sensitive to this intrinsic low-luminosity cut-off at much fainter values compared to the observed number count in a blank field.

In this paper, we predict the lensing rate of high-redshift objects that will be observed with both HST Frontier Fields in the upcoming months, and JWST within the next decade. In section 2.3 we consider two different axially symmetric lens models: a singular isothermal sphere and a NFW profile (Navarro et al. 1997) lens for comparison, examining their respective effects on the number count of the background lensed galaxy population. In addition to considering lensing clusters, we also consider galaxy-group lensing and compute the lensing rates expected in each case given the velocity dispersion of the lensing object. We present our numerical results in section 2.4 and show the transition from a positive to a negative magnification bias as a function of the minimum intrinsic luminosity, the photometric sensitivity, and the angular distance from the given lens. We conclude in section 2.5 with a discussion of our findings and their implications for observations with the HST Frontier Fields and JWST in the near future. Throughout this paper, we adopt \( \Omega_m = 0.3 \) and \( \Omega_\Lambda = 0.7 \) as the present-day density parameters of matter and vacuum, respectively and take \( H_0 = 100h \, \text{km s}^{-1} \, \text{Mpc}^{-1} \) as the Hubble constant with \( h = 0.7 \). We express all magnitudes in the AB system.

23
2.3 The Lensing Model

The ray-tracing equation that relates the position of a source, \( \tilde{\eta} \), to the impact parameter of a light ray in the lens plane, \( \tilde{\xi} \), is given in angular coordinates by

\[
\tilde{\beta} = \tilde{\theta} - \tilde{\alpha}(\tilde{\theta})
\]  

(2.1)

where \( \tilde{\beta} = \tilde{\eta}/D_s \), \( \tilde{\theta} = \tilde{\xi}/D_l \), and \( \tilde{\alpha} \) is the reduced deflection angle due to a lens with surface mass density \( \Sigma \),

\[
\tilde{\alpha}(\tilde{\theta}) = \frac{4G D_{ls} D_l}{c^2 D_s} \int \frac{(\tilde{\theta} - \tilde{\theta}')\Sigma(\tilde{\theta}')}{|\tilde{\theta} - \tilde{\theta}'|^2} d^2\theta' .
\]  

(2.2)

\( D_{l,s,ls} \) are the angular-diameter distances between observer and lens, observer and source, and lens and source, respectively. In the standard ΛCDM cosmology, the angular-diameter distance \( D_A(z) \) of a source at redshift \( z \) is defined as

\[
D_A(z) = \frac{c}{H_0} \frac{1}{(1 + z)} \int_0^z \frac{dz'}{E(z')}
\]  

(2.3)

where

\[
E(z) = \sqrt{\Omega_m (1 + z)^3 + \Omega_\Lambda} .
\]  

(2.4)

For a circularly-symmetric mass distribution, \( \Sigma(\tilde{\theta}) = \Sigma(|\tilde{\theta}|) \); the dimensionless surface mass density, also referred to as the convergence, is then given by

\[
\kappa(x) = \frac{\Sigma(x)}{\Sigma_{cr}} \quad \text{with} \quad \Sigma_{cr} = \frac{c^2 D_s}{4\pi G D_l D_{ls}}
\]  

(2.5)

where we have introduced the dimensionless impact parameter \( \tilde{x} = \tilde{\theta}/\theta_0 \) with an arbitrary angular scale \( \theta_0 \). The corresponding dimensionless mass \( m(x) \) within a circle of angular radius \( x \) is then

\[
m(x) = 2 \int_0^x dx' x' \kappa(x')
\]  

(2.6)
and the magnification factor in terms of these dimensionless quantities takes the following form,

\[ \mu(x) = \frac{1}{(1 - \frac{\kappa(x)}{x^2})(1 + \frac{\kappa(x)}{x^2} - 2\kappa(x))} \tag{2.7} \]

A simple model for the matter distribution in a gravitational lens is a Singular Isothermal Sphere (SIS) (Schneider & Falco 1992) with a surface mass density of

\[ \Sigma_{\text{SIS}}(\xi) = \frac{\sigma_v^2}{2G\xi} \tag{2.8} \]

where \( \sigma_v \) is the line-of-sight velocity dispersion of the lens. In this case, the reduced deflection angle, commonly referred to as the Einstein angle for the SIS lens and denoted as \( \theta_E \), is independent of the impact parameter,

\[ \theta_E = 4\pi \frac{\sigma_v^2 D_{ls}}{c^2 D_s} \tag{2.9} \]

and the lens equation reduces to

\[ \bar{\beta} = \bar{\theta} - \bar{\alpha}(\bar{\theta}) = \bar{\theta} - \frac{\bar{\theta}}{\left|\bar{\theta}\right|} \theta_E \tag{2.10} \]

where negative angles refer to positions on the opposite side of the lens center. The lensing effect causes the image of the source to be displaced, magnified, and sometimes split (Refregier & Loeb 1997). When \( |\beta| < \theta_E \), the lens equation has two solutions, \( \theta_{\pm} = \beta \pm \theta_E \), and multiple images are obtained. Conversely, if the source lies outside the Einstein ring, i.e. \( |\beta| > \theta_E \), only one image is present at \( \theta = \theta_+ = \beta + \theta_E \). The corresponding magnification factor due to a SIS lens is given by

\[ \mu_{\text{SIS}}(\theta) = \left(1 - \frac{\theta_E}{|\theta|}\right)^{-1} \tag{2.11} \]

where negative values of \( \mu \) correspond to inverted images. For large values of \( \theta \), \( \mu \approx 1 \) and the source is weakly affected by the lensing potential, while for \( \theta = \theta_E \), the
CHAPTER 2. CONSTRAINING MINIMUM LUMINOSITY THROUGH LENSING

magnification diverges, corresponding to the formation of an Einstein ring. In practice, the maximum magnification is limited by the finite extent of the lensed source (Peacock 1982). Since we are considering primarily the lensing effect on compact, high-redshift galaxies (Oesch et al. 2010), we ignore the angular size of the sources and model the background as a collection of point sources.

Although the SIS model is useful in providing a good first-order approximation to the projected mass distribution of known early-type galaxies and cluster lenses (Tyson & Fischer 1995; Narayan & Bartelmann 1996; Treu & Koopmans 2002; Koopmans & Treu 2003; Rusin et al. 2003), it is not an entirely realistic model. In particular, Meneghetti et al. (2007) finds that the contributions of ellipticity, asymmetries, and substructures amount to \( \sim 40\% \), \( \sim 10\% \), and \( \sim 30\% \) of the total strong lensing cross section respectively. However, since we do not want to restrict our attention to specific cases and we expect the qualitative trends to remain the same, we use the SIS model and compare our results with those obtained by assuming a Navarro-Frenk-White (NFW) mass density profile (Navarro et al. 1997) which is shallower than isothermal near the center and steeper in the outer regions,

\[
\rho(x) = \frac{\rho_{\text{cr}} \delta_{\text{NFW}}}{x(1 + x)^2}, \quad x = \frac{r}{r_{\text{vir}}} = \frac{c}{\theta_{\text{vir}}}
\]  

(2.12)

where \( \rho_{\text{cr}} \) is the critical density at the epoch of the halo virialization. \( \delta_{\text{NFW}} \) is related to \( c \), the halo concentration parameter, by

\[
\delta_{\text{NFW}} = \frac{200}{3} \frac{c^3}{\ln(1 + c) - c/(1 + c)}
\]  

(2.13)

where \( c \) can be calculated using the virial mass through a fit to simulations (Bullock et al. 2001)

\[
c(M, z) = \frac{9}{(1 + z)} \left( \frac{M}{M'} \right)^{-0.13}
\]  

(2.14)
with \( M' = 1.5 \times 10^{13} h^{-1} M_\odot \). The virial radius of a halo at redshift \( z \) depends on the halo mass as,

\[
r_{\text{vir}} = 0.784 \left( \frac{\Omega_m}{\Omega_m(z)} \frac{\Delta_c}{18 \pi^2} \right)^{-1/3} \left( \frac{M}{10^8 M_\odot} \right)^{1/3} \left( \frac{1+z}{10} \right)^{-1} h^{-2/3} \text{kpc}.
\]  

(2.15)

In a universe with \( \Omega_m + \Omega_\Lambda = 1 \), the virial overdensity at the collapse redshift has the fitting formula (Bryan & Norman 1998)

\[
\Delta_c = 18 \pi^2 + 82d - 39d^2
\]  

(2.16)

with \( d = \Omega_m(z)+1 \) and

\[
\Omega_m(z) = \frac{\Omega_m(1+z)^3}{\Omega_m(1+z)^3 + \Omega_\Lambda}.
\]  

(2.17)

The lens equations for the NFW profile (Bartelmann 1996), use the dimensionless surface mass density is

\[
\kappa_{\text{NFW}}(x) = \frac{2 \rho_c \delta_{\text{NFW}} r_{\text{vir}}}{c \Sigma_{\text{cr}}} \frac{f(x)}{x^2-1}
\]  

(2.18)

with

\[
f(x) = \begin{cases} 
1 - \frac{2}{\sqrt{x^2-1}} \arctan \sqrt{\frac{x-1}{x+1}}, & x > 1 \\
1 - \frac{2}{\sqrt{1-x^2}} \arctan \sqrt{\frac{1-x}{x+1}}, & x < 1 \\
0, & x = 1.
\end{cases}
\]

The ray-tracing equation takes the form

\[
\beta = \theta - \left( \frac{\theta_{\text{vir}}}{c} \right)^2 \frac{m_{\text{NFW}}(c \theta / \theta_{\text{vir}})}{\theta}
\]  

(2.19)

where the dimensionless mass in this case is

\[
m_{\text{NFW}}(x) = \frac{4 \rho_c \delta_{\text{NFW}} r_{\text{vir}}}{c \Sigma_{\text{cr}}} g(x) \quad \text{with} \quad g(x) = \ln \frac{x}{2} + 1 - f(x)
\]  

(2.20)
Figure 2.1: Left: Source position, $\beta$, as a function of image position, $\theta$ for SIS (solid) and NFW (dashed) lenses at redshift $z_L = 0.5$ with halo mass $M = 10^{14.9} \, M_\odot$, ($\sigma_v = 1000 \, \text{km s}^{-1}$) and a source redshift of $z_s = 8$. A horizontal line of fixed source position $\beta$ may intersect each respective curve at multiple positions $\theta$, signaling the formation of multiple images. For the NFW lens, three images will form if $|\beta| \leq \beta_{cr}$, where $\beta_{cr} = -\beta(\theta_{cr})$ and $\theta_{cr} > 0$ is determined by $(d\beta/d\theta)|_{\theta=\theta_{cr}} = 0$. For the SIS lens, two images will form if $|\beta| < \theta_{E}$. Right: Magnification as a function of angular separation $\theta$ from the cluster center assuming SIS (solid) and NFW (dashed) profiles with $z_L = 0.5$ and $z_s = 8$. 
and \( \theta_{\text{vir}} = r_{\text{vir}}/D_l \). As can be seen in Figure 2.1, an NFW profile lens will form three distinct images if \( |\beta| \leq \beta_{\text{cr}} \), where \( \beta_{\text{cr}} = -\beta(\theta_{\text{cr}}) \) and \( \theta_{\text{cr}} > 0 \) is determined by \( (d\beta/d\theta)_{\theta=\theta_{\text{cr}}} = 0 \); for all \( |\beta| \geq \beta_{\text{cr}} \), a single image is formed.

The equations for \( \kappa_{\text{NFW}}(x) \) and \( m_{\text{NFW}}(x) \), used in conjunction with eq. (2.7), yield the corresponding magnification factor for a NFW profile lens. The two spikes in \( \mu_{\text{NFW}}(\theta) \) seen in Figure 2.1 represent the tangential and radial critical curves where the magnification is formally infinite. The critical curves of the NFW lens are closer to the lens center than for the SIS lens and the image magnification decreases, approaching unity, more slowly away from the critical curves.

To model the background galaxy population, we use the Schechter luminosity function,

\[
\phi(z, M) dM = 0.4 \ln 10 \, \phi^*(z) \, 10^{0.4(M^*(z)-M)} \, e^{-10^{0.4(M^*(z)-M)}}
\]  

(2.21)

where the parameters are the comoving number density of galaxies \( \phi^* \), the characteristic absolute AB magnitude \( M^* \), and the faint-end slope \( \alpha \). (Note that we denote absolute AB magnitude in this paper as \( M_l \).) The evolution of \( \phi^* \) and \( M^* \) as functions of redshift in the interval \( z \geq 4 \) are taken as the central values of the fitting formulae provided in Bouwens et al. (2011b),

\[
\phi^*(z) = (1.14 \pm 0.20) \times 10^{-3} 10^{(0.003 \pm 0.055)(z-3.8)} \, \text{Mpc}^{-3},
\]  

(2.22)

\[
M^*(z) = (-21.02 \pm 0.09) + (0.33 \pm 0.06)(z - 3.8).
\]  

(2.23)

Bouwens et al. (2011b) also provides a fitting formula describing the evolution of \( \alpha \) as a function of redshift,

\[
\alpha(z) = (-1.73 \pm 0.05) + (-0.01 \pm 0.04)(z - 3.8).
\]  

(2.24)
Recent studies have investigated the form of the \( z = 8 \) luminosity function by combining the faint-end results in Bouwens et al. (2011b) with improved constraints at the bright end (Bradley et al. 2012; Oesch et al. 2012b; McLure et al. 2013; Schenker et al. 2013). There is very good agreement between the new results, with all studies converging on a steep faint-end slope of \( \alpha \simeq -2.0 \). We therefore adopt the expression for \( \alpha(z) \) in eq. (2.24) for all redshifts \( z < 8 \) and use a faint-end slope of \( \alpha = -2.02 \) for all higher redshifts, assuming that the slope remains unchanged for redshifts \( z \geq 8 \) (McLure et al. 2013). This faint-end slope, along with the formulae describing the evolution of the LF, represent an extrapolation of the present LF results \( (z \sim 7-8) \) to even higher redshifts; the fall-off in UV luminosity at \( z > 8 \) is still debated in the literature (Coe et al. 2013; McLure et al. 2013). The results in this paper may therefore change as the evolution of the LF parameters \( \phi^*, M^* \), and \( \alpha \) as functions of redshift are modified in light of new observations.

In the absence of a lensing object \( (\mu = 1) \), the number of sources with redshift in the range \( z_i < z < z_f \) seen in an angular region \( [\theta_i, \theta_f] \) about the optical axis is simply the number which falls in the angular region with an absolute magnitude less than the limiting absolute magnitude. This limiting magnitude is set either by the maximum intrinsic absolute magnitude associated with a star-forming halo, \( M_{\text{max}} \), or, by what we denote as \( M_{\text{det}} \), the absolute magnitude that a source at redshift \( z \) must have to be above \( df/d\nu_0 \), the flux threshold set by the detector. This number is thus obtained by integrating the comoving number density \( \phi(z, M) dM \) given by eq. (2.21) over the appropriate volume and magnitude range,

\[
N_{\text{unlensed}}(\theta_i, \theta_f, z_i, z_f) = 2\pi \int_{\theta_i}^{\theta_f} d\theta' \theta' \frac{dN_{\text{unlensed}}}{d\Omega}(z_i, z_f)
\]  (2.25)
where

\[
\frac{dN_{\text{lensed}}}{d\Omega}(z_i, z_f) = \frac{c}{H_0} \int_{z_i}^{z_f} \frac{dz}{E(z)} D_s^2(z) \int_{-\infty}^{\text{Min}[M_{\text{max}}, M_{\text{det}}(z) \mid M]} dM \phi(z, M).
\]

(2.26)

and \(D_{\text{com}}\) is the comoving angular diameter distance, \(D_{\text{com}}(z) = D_A(1 + z)\). In the presence of a lens, the magnification due to gravitational lensing has two effects on background point sources: their surface number density is diluted by a factor of \(\mu\),

\[
n_{\text{obs}}(\theta) = n(z, \theta) / \mu
\]

(2.27)

and their luminosities are simultaneously magnified by the same factor,

\[
L_{\text{obs}}(\theta) = \mu(z, \theta)L \rightarrow M_{\text{obs}} = M + 2.5 \log \mu(z, \theta).
\]

(2.28)

Furthermore, in the case of strong lensing, multiple images will often be produced by SIS and NFW profile lenses depending on the source position, \(\beta\). When \(\beta < \theta_E\), an SIS lens will form two images with a splitting angle of \(\Delta \theta_{\text{SIS}} = 2\theta_E\). Similarly, an NFW profile lens will form three distinct images if \(\beta \leq \beta_{\text{cr}}\); however, only two of those images will lie in the region \(|\theta| \geq \theta_E/2\) (Figure 2.1), the region of interest in the following section. In general, the splitting angle \(\Delta \theta\) between these two outside images is insensitive to the value of \(\beta\) and is approximately given by Li & Ostriker (2002)

\[
\Delta \theta_{\text{NFW}} \approx \Delta \theta(\beta = 0) = 2\theta_0, \text{for } |\beta| < \beta_{\text{cr}}
\]

(2.29)

where \(\theta_0\) is the positive root of \(\beta(\theta) = 0\). Consequently, the total number of sources detected in a lensed field takes the following modified form,

\[
N_{\text{lensed}}(\theta_f, z_i, z_f) = 2\pi \int_{\theta_E/2}^{\Delta \theta/2} d\theta' \theta' \frac{dN_{\text{lensed}}}{d\Omega}(\theta', z_i, z_f)
\]

\[
+ 2\pi \int_{-\Delta \theta/2}^{-\theta_E/2} d\theta' \theta' \max \left[ 0, \frac{dN_{\text{lensed}}}{d\Omega}(\theta', z_i, z_f) - \frac{dN_{\text{lensed}}}{d\Omega}(|\theta' - \Delta \theta|, z_i, z_f) \right]
\]

\[
+ 2\pi \int_{\theta_E/2}^{\theta_f} d\theta' \theta' \frac{dN_{\text{lensed}}}{d\Omega}(\theta', z_i, z_f)
\]

(2.30)
CHAPTER 2. CONSTRAINING MINIMUM LUMINOSITY THROUGH LENSING

where

\[
\frac{dN}{d\Omega}^{\text{lensed}}(\theta', z_i, z_f) = \frac{c}{H_0} \int_{z_i}^{z_f} \frac{dz}{E(z)} D_s^{2, \text{com}}(z) \frac{1}{\mu^2(z, \theta')} \int_{-\infty}^{\min[M_{\text{max}}, M_{\text{det}}(z) + 2.5 \log \mu(z, \theta')]} dM \phi(z, M). \tag{2.31}
\]

### 2.4 Results

We now apply the general relations discussed above to lensing of background sources by a lens positioned at a redshift \(z_L = 0.5\). This redshift is chosen to be consistent with the average redshift of the galaxy clusters centered in the six deep fields of the HST Frontier Fields program. In all the calculations presented below, we take \(z_f = 16\) as the upper bound on the redshift range. Beyond this redshift, \(z_f > 16\), the results remain the same (within a precision of one part in ten-thousand); the numerical results drop by \(\lesssim 4\%\) if instead we assume the first galaxies formed at \(z_f = 13\). Although we focus on the lensing effect due to galaxy clusters (\(\sigma_v \approx 1000 \text{ km/s}\)), we also include the results obtained when considering lensing by galaxy groups (\(\sigma_v \approx 500 \text{ km/s}\)). We restrict our attention to the flux thresholds set by the WFC3 aboard the HST and the NIRCam imager of JWST.

The Frontier Fields program achieves AB \(\approx 28.7-29\) mag optical (ACS) and NIR (WFC3) imaging, corresponding to flux limits of \(df/d\nu_0 \sim 9-12\) nJy for a 5\(\sigma\) detection of a point source after \(\sim 10^5\) s. Medium-deep (\(m_{\text{lim}} \approx 29.4\) mag) and ultra-deep (\(m_{\text{lim}} \approx 31.4\) mag) JWST surveys, (corresponding to a 5\(\sigma\) detection of a point source after 10\(^4\) and 3.6\(\times\)10\(^5\) s of exposure respectively), will detect fluxes as low as \(\sim 6\) and 1 nJy, respectively.

The radial dependence of the number of background sources with redshifts \(z \geq 13\) detected by HST and JWST behind a SIS lens at \(z_L = 0.5\) is depicted in the left panels of Figures 2.2 - 2.4. At large distances from the lens center (\(\theta/\theta_E \gg 1\)), the
CHAPTER 2. CONSTRAINING MINIMUM LUMINOSITY THROUGH LENSING

Figure 2.2: Predictions for observations by HST ($df/dv_0 \sim 9$ nJy) of sources at redshifts $z \gtrsim 13$ behind a SIS cluster lens with $\sigma_v \approx 1000$ km s$^{-1}$ at $z_L = 0.5$. Left Panel: Radial dependence of the number of sources detected in concentric annular cells Right panel: Cumulative number of detected sources, starting from an angular radius $\theta_E/2$ and extending outward to an angular radius $\theta$. The solid and dashed lines correspond to the lensed and unlensed numbers respectively. The dotted line in the right panel corresponds to $N'$, the cumulative number of magnified sources that were lifted over the detection threshold of the given instrument; this represents the component of $N_{lensed}$ that would remain undetected without the aid of lensing. The top panel assumes a maximum intrinsic absolute AB magnitude of -18.2 mag while the bottom panel assumes $M_{max} = -10$ mag.
Figure 2.3: Predictions for observations in JWST’s medium-deep ($df/dv_0 \sim 6$ nJy) field of sources at redshifts $z \gtrsim 13$ behind a SIS cluster lens with $\sigma_v \approx 1000$ km s$^{-1}$ at $z_L = 0.5$. 
Left Panel: Radial dependence of the number of sources detected in concentric annular cells. 
Right panel: Cumulative number of detected sources, starting from an angular radius $\theta_E/2$ and extending outward to an angular radius $\theta$. The solid and dashed lines correspond to the lensed and unlensed numbers respectively. The dotted line in the right panel corresponds to $N'$, the cumulative number of magnified sources that were lifted over the detection threshold of the given instrument due to lensing by an SIS profile lens; this represents the component of $N_{lensed}$ that would remain undetected without the aid of lensing. The top panel assumes a maximum intrinsic absolute AB magnitude of -18.2 mag while the bottom panel assumes $M_{max} = -10$ mag.
Figure 2.4: Predictions for observations in JWST’s ultra-deep ($df/d
\nu_0 \sim 1$ nJy) field of sources at redshifts $z \gtrsim 13$ behind a SIS cluster lens with $\sigma_v \approx 1000 \text{ km s}^{-1}$ at $z_L = 0.5$.

Left Panel: Radial dependence of the number of sources detected in concentric annular cells. Right panel: Cumulative number of detected sources, starting from an angular radius $\theta_E/2$ and extending outward to an angular radius $\theta$. The solid and dashed lines correspond to the lensed and unlensed numbers respectively. The dotted line in the right panel corresponds to $N'$, the cumulative number of magnified sources that were lifted over the detection threshold of the given instrument due to lensing by an SIS profile lens; this represents the component of $N_{lensed}$ that would remain undetected without the aid of lensing. The top panel assumes a maximum intrinsic absolute AB magnitude of -18.2 mag while the bottom panel assumes $M_{max} = -10$ mag.
magnification factor approaches unity and the number of detected sources per annular ring converges to the constant number that would be observed in the absence of a lens (dotted line). For an image at $|\theta| < \theta_E/2$, $|\mu|$ is smaller than unity, and the source luminosity is demagnified relative to the unlensed luminosity while the surface number density is amplified by the same factor. As $\theta$ approaches the Einstein angle, the magnification diverges, allowing small sources perfectly aligned with the lens center to form an "Einstein ring" and otherwise, causing the number density of observed sources to plummet. (This phenomenon corresponds to the sharp drop in $dN/d\Omega$ at $\theta/\theta_E = 1$). At image distances larger than the Einstein angle, $\mu$ converges back to unity, resulting in magnified luminosities and diluted number densities that gradually reduce to their unlensed values. The overall magnification bias depends on which of the two magnification effects wins out: under circumstances where the number of magnified sources lifted over the detection threshold outweighs the simultaneous dilution of the number density of sources in the sky, there is a positive magnification bias and $(dN/d\Omega)_{\text{lensed}} > (dN/d\Omega)_{\text{unlensed}}$. Conversely, when the reduction in number density dominates over luminosity magnifications, a negative magnification bias results and $(dN/d\Omega)_{\text{lensed}} < (dN/d\Omega)_{\text{unlensed}}$ in those regions.

The plots of $dN/d\Omega$ and $N(\theta_E/2 < \theta)$ (the cumulative number of sources observed starting from an angular radius of $\theta_E/2$ and extending outward to an angular radius $\theta$) in Figures 2.2 - 2.4 highlight the sensitivity of the magnification bias to the different model parameters. The expected magnification bias effect on the source counts observed around a lensing cluster depends strongly on the flux threshold of the instrument used for the survey and its strength relative to the characteristic magnitude of the galaxy sample. If the instrumental detection threshold places the observer in the exponential drop-off
region of the luminosity function of a galaxy sample, \((M_{\text{det}}(z, f_{\text{min}}) < M^*(z))\), lensing will significantly increase the number of observed sources when it pushes the detection threshold to fainter values of \(M\), resulting in a positive magnification bias. This is the case with detections of \(z \geq 13\) galaxies in HST and medium-deep JWST surveys. On the other hand, in an ultra-deep JWST survey, where the instrumental limiting magnitude is fainter than the characteristic magnitude, (placing the observer in the power-law region of the Schechter function), pushing the threshold to fainter magnitudes does not result in the inclusion of a substantial population of otherwise undetectable sources; the diluting effect of lensing therefore wins out and a deficit in the total source count is consistently observed (Figure 2.4). Source counts of lower redshift galaxy populations in HUDF and medium-deep JWST surveys suffer from this negative magnification bias as well.

However, note that even in these instances where gravitational lensing reduces the total source count, a significant fraction of the sources that are observed in the lensed field belong to a population of galaxies that, without lensing, lie below the survey limit (dotted lines in right panels of Figures 2.2 - 2.4). By lifting these galaxies over the instrumental detection threshold, lensing may help constrain another model parameter, \(M_{\text{max}}\), the maximum intrinsic absolute magnitude of the background galaxy population.

Figures 2.5 - 2.6 depict the expected source count integrated over the range of angular distances \(\theta \in [\theta_E/2, 2\theta_E]\) from the lens center, as a function of the \(M_{\text{max}}\), assuming a SIS (solid) and NFW (dashed) profile. Images in this region fall far enough away from the lens that their detectability is not compromised by the brightness of the foreground lens, yet close enough that the magnification bias introduced by \(\mu(\theta)\) has a noticeable effect on the source count. These plots demonstrate that the degree to which the number count varies as a function of \(M_{\text{max}}\) at the fainter end of the considered range
Figure 2.5: Expected number of sources with redshift $z \gtrsim 8$ integrated over the region $\theta_E/2 \leq \theta \leq 2\theta_E$ as a function of the maximum intrinsic absolute magnitude, $M_{AB,\text{max}}$, of the background sources. The solid and dashed lines respectively show the expected numbers due to lensing by a SIS and NFW-profile lens respectively. The dash-dot line represents the expected numbers in the unlensed case. The dotted line represents the number of sources in the lensed field that have been lifted over the given instrumental detection threshold due to lensing by an SIS profile lens. The top, center, and bottom panels show the expected results given a flux threshold of 9 (HST), 6 (JWST medium-deep), and 1 nJy (JWST ultra-deep) in the case where galaxy groups (left panel) and clusters (right panel) are used as lenses with corresponding Einstein angles 0.095', and 0.38'.
Figure 2.6: Expected number of sources with redshift $z \geq 13$ integrated over the region $\theta_E/2 \leq \theta \leq 2\theta_E$ as a function of the maximum intrinsic absolute magnitude, $M_{AB,max}$, of the background sources. The solid and dashed lines respectively show the expected numbers due to lensing by a SIS and NFW-profile lens, respectively. The dash-dot line represents the expected numbers in the unlensed case. The dotted line represents the number of sources in the lensed field that have been lifted over the given instrumental detection threshold due to lensing by an SIS profile lens. The top, center, and bottom panels show the expected results given a flux threshold of 9 nJy (HST), 6 nJy (JWST medium-deep), and 1 nJy (JWST ultra-deep) in the case where galaxy groups (left panel) and clusters (right panel) are used as lenses with corresponding Einstein angles 0.095', and 0.38'.
relies significantly on the presence of a magnification bias. In the case of a blank field, the number count of sources detected by an instrument grows insensitive to $M_{\text{max}}$ if this faint-magnitude cut-off is fainter than $M_{\text{det}}$; since sources with magnitudes fainter than $M_{\text{det}}$ cannot be observed without the aid of gravitational lensing, the unlensed number count, $N_{\text{unlensed}}$, plateaus for values of $M_{\text{max}} \gtrsim M_{\text{det}}$ and the presence of these faint galaxies remains unverifiable. Therefore, an instrument with a flux threshold of $\sim 9$ nJy, such as HST, cannot confirm the existence of sources at redshifts $z \gtrsim 8$ and $z \gtrsim 13$ with absolute magnitudes fainter than -18.1 and -18.9 mag, respectively. Similarly, the medium-deep JWST survey loses sensitivity to sources fainter than -17.7 ($z \geq 8$) and -18.5 mag ($z \geq 13$) while the ultra-deep survey will not detect sources fainter than -15.7 ($z \geq 8$) and -16.5 mag ($z \geq 13$) when observations are made in a blank field.

This sensitivity to the intrinsic faint-magnitude cut-off significantly improves when considering $N_{\text{lensed}}$, the number of high-redshift sources one expects to observe behind a lensing group or cluster. Although the gain in depth does not balance the dilution of sources in most instances, particularly when observing sources at redshifts $z < 13$ with HST and JWST, it permits the detection of sources fainter than $M_{\text{det}}$ and thus allows the lensed number count to remain sensitive to $M_{\text{max}}$, down to values much fainter than was the case for the unlensed number count. In particular, the number count of $z \gtrsim 8$ galaxies lensed by a foreground cluster modeled as a SIS lens, can be used to infer the intrinsic faint-magnitude cut-off of the Schecter function up to values as faint as $M_{\text{max}} \sim -17.8$, -17.3, and -15.0 mag ($L_{\text{min}} \sim 5.8 \times 10^{27}$, $3.6 \times 10^{27}$, and $4.4 \times 10^{26}$ erg s$^{-1}$Hz$^{-1}$) in the HUDF, medium-deep, and ultra-deep JWST surveys, respectively (Figure 2.5, right panel). Similarly, observations of $z \gtrsim 13$ galaxies in ultra-deep JWST surveys can yield an estimate of $M_{\text{max}}$ for values as faint as -16.1 mag ($L_{\text{min}} \sim 1.2 \times 10^{27}$) (Figure 2.6, right panel).
CHAPTER 2. CONSTRAINING MINIMUM LUMINOSITY THROUGH LENSING

panel). Modeling the cluster as a NFW lens instead results in the same constraints on $M_{\text{max}}$ and changes the magnitude of $N_{\text{lensed}}$ by at most ~20% compared to the numbers obtained for the SIS lens.

Given that the number of galaxies in a field of observation follows a Poisson distribution and that the sample size is large (which is expected in fields centered on strong lensing galaxy clusters), the 1-$\sigma$ confidence interval around the measured count translates into a range of inferred $L_{\text{min}}$ values. Using the appropriate plots in Figures 2.5 and 2.6, one can therefore identify the most likely value of $M_{\text{max}}$ to within the Poisson uncertainty of the observed number count, $\sqrt{N_{\text{obs}}}$. An observed number count with an error bar that lies outside the model, (i.e. $N_{\text{obs}} + \sqrt{N_{\text{obs}}}$ exceeds the maximum number count accommodated by the model), will subsequently yield only a lower bound on the intrinsic faint-magnitude cut-off. Figure 2.7 compares the constraint on $M_{\text{max}}$ that may be obtained by observing galaxy populations within a given range of redshifts with HST and JWST in blank versus lensed fields. When observing $z \geq 6$ galaxies, the intrinsic maximum magnitude can be inferred up to values as faint as -14.4 mag ($2.5 \times 10^{26}$ erg s$^{-1}$Hz$^{-1}$) with JWST.

In addition to constraining the value of $L_{\text{min}}$, Figures 2.5 and 2.6 also demonstrate the instances in which gravitational lensing improves the detection of high redshift sources as well as the magnitude of the bias in each case. Gravitational lensing by a group or cluster modeled as an SIS lens reduces the number of detected sources with redshift $z \gtrsim 8$ by a factor of ~2-3 in HST and JWST observations. However, even though the total source count is reduced in these cases, the majority of the sources that are observed in the lensed field are galaxies that, without lensing, would remain undetectable. In particular, nearly ~73-76% of the $z \geq 8$ galaxies observed in HUDF
Figure 2.7: The lower bound on $M_{\text{max}}$ obtained with and without the lensing effect. The dashed lines represent $M_{\text{det}}(z', f_{\text{min}})$, the absolute AB magnitude of the faintest galaxy at redshift $z \geq z'$ that can be detected in the HUDF (black), JWST medium-deep (red), and JWST ultra-deep (blue) surveys. Without the aid of lensing, these detection thresholds set the lower bound on the intrinsic maximum absolute magnitude of the Schecter luminosity function. The solid lines represent the tightest constraint on $M_{\text{max}}$ that can be obtained using the lensed number count of galaxies in each of the respective surveys (solid lines in Figures 2.5 and 2.6).
and JWST surveys have been lifted over the respective instrumental detection thresholds (dotted lines). At higher redshifts, the magnification bias transitions from negative to positive and enhances the number of $z \gtrsim 13$ sources detected behind a lensing group or cluster by a factor of $\sim 3$ and $1.5$ in HUDF and JWST medium-field surveys, respectively. Of these observed sources, nearly $\sim 96-98\%$ of them lie below the survey limit and would thus remain undetected without the aid of gravitational lensing.

2.5 Discussion

In this paper, we studied the effects of gravitational lensing on the source count of high redshift objects as observed by both the HST Frontier Fields and JWST. Although lensing magnifies the background sources, effectively lowering the flux threshold above which they can be detected, it simultaneously dilutes the apparent number density of sources on the sky. We found that the details of whether the number counts of distant background sources seen through a foreground gravitational lens are enhanced or reduced depends on several parameters characterizing the system. Using the axially symmetric SIS and NFW mass density profiles to model a lens residing at a redshift $z_L = 0.5$, we explored how the magnification bias varied with the velocity dispersion of the lens ($\sigma_v$), the angular distance from the lens ($\theta$), the photometric sensitivity of the instrument ($df/d\nu_0$), the redshift of the background source population, and the intrinsic faint-magnitude cut-off characterizing the population ($M_{max}$). We found that when observing sources at redshifts $z \gtrsim 8$, lensing by a group or cluster will reduce the number of detected sources by a factor of $\sim 2-3$ in both HST and JWST observations. The magnification bias transitions from negative to positive only when considering higher
CHAPTER 2. CONSTRAINING MINIMUM LUMINOSITY THROUGH LENSING

redshift galaxies; in particular, the bias will enhance the number of sources at redshifts $z \gtrsim 13$ behind a lensing group or cluster by a factor of $\sim 3$ and 1.5 in HUDF and JWST medium-deep surveys, respectively.

Although the gain in depth does not balance the simultaneous dilution of sources in most instances, it permits the detection of sources fainter than $M_{\text{det}}$ and thus allows the lensed number count to remain sensitive to $M_{\text{max}}$, down to values much fainter than was the case for the unlensed number count. In particular, the number count of $z \gtrsim 8$ galaxies lensed by a foreground cluster, can be used to infer the intrinsic maximum magnitude of the Schecter function up to values as faint as $M_{\text{max}} \sim -17.8$ and -15 mag ($L_{\text{min}} \sim 5.8\times10^{27}$ and $4.4\times10^{26}$ erg s$^{-1}$Hz$^{-1}$) in the HUDF and ultra-deep JWST surveys, respectively, within the range bracketed by existing theoretical models (Muñoz & Loeb 2011; Wyithe & Loeb 2006). Similarly, observations of $z \gtrsim 13$ galaxies in ultra-deep JWST surveys can yield an estimate of $M_{\text{max}}$ for values as faint as -16.1 mag ($L_{\text{min}} \sim 1.2\times10^{27}$ erg s$^{-1}$Hz$^{-1}$).

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Chapter 3

An Empirical Model for the Galaxy Luminosity and Star Formation Rate Function at High Redshift

This thesis chapter originally appeared in the literature as


3.1 Abstract

Using the most recent measurements of the ultraviolet (UV) luminosity functions (LFs) and dust estimates of early galaxies, we derive updated dust-corrected star-formation
rate functions (SFRFs) at $z \sim 4-8$, which we model to predict the evolution to higher redshifts, $z > 8$. We employ abundance matching techniques to calibrate a relation between galaxy star formation rate (SFR) and host halo mass $M_h$ by mapping the shape of the observed SFRFs at $z \sim 4-8$ to that of the halo mass function. The resulting scaling law remains roughly constant over this redshift range. We apply the average $SFR - M_h$ relation to reproduce the observed SFR functions at $4 \lesssim z \lesssim 8$ and also derive the expected UV LFs at higher redshifts. At $z \sim 9$ and $z \sim 10$ these model LFs are in excellent agreement with current observed estimates. Our predicted number densities and UV LFs at $z > 10$ indicate that JWST will be able to detect galaxies out to $z \sim 15$ with an extensive treasury sized program. We also derive the redshift evolution of the star formation rate density and associated reionization history by galaxies. Models which integrate down to the current HUDF12/XDF detection limit ($M_{UV} \sim -17.7$ mag) result in a SFRD that declines as $(1 + z)^{-10.4 \pm 0.3}$ at high redshift and fail to reproduce the observed CMB electron scattering optical depth, $\tau \approx 0.066$, to within $1\sigma$. On the other hand, we find that the inclusion of galaxies with SFRs well below the current detection limit ($M_{UV} < -5.7$ mag) leads to a fully reionized universe by $z \sim 6.5$ and an optical depth of $\tau \approx 0.054$, consistent with the recently derived Planck value at the $1\sigma$ level.

3.2 Introduction

The sensitive, near-infrared imaging capabilities of the Hubble Space Telescope (HST) have significantly expanded our understanding of galaxy evolution through cosmic time. Efforts to identify galaxies through photometric selections and follow-up spectroscopy have progressively extended the observational frontier to higher and higher redshifts,
CHAPTER 3. GALAXY LUMINOSITY AND SFR FUNCTION

resulting in robust galaxy samples in the range $z \sim 4$-8 (e.g. Madau et al. 1996; Steidel et al. 1999; Bouwens et al. 2004, 2010, 2011b, 2014b; Dickinson et al. 2004; Yan & Windhorst 2004a; Bunker et al. 2010; Finkelstein et al. 2010, 2012b,a, 2015; McLure et al. 2010, 2013; Oesch et al. 2010, 2012b; Schenker et al. 2012, 2013; Bradley et al. 2014; Schmidt et al. 2014). With the Wide Field Camera 3 (WFC3/IR) on board the HST, the current frontier for identifying high-redshift galaxies now lies at $z \sim 11$, a mere half a billion years after the Big Bang, and new surveys are now building up the sample sizes of $z \gtrsim 9$ galaxies (e.g. Bouwens et al. 2011a; Ellis et al. 2013; Zheng et al. 2012; Coe et al. 2013; McLure et al. 2013; Oesch et al. 2013, 2014; Bouwens et al. 2014a; Oesch et al. 2012a; McLeod et al. 2015; Ishigaki et al. 2015).

However, due to the small number statistics, our understanding of galaxies beyond $z \sim 8$ is still very limited and obtaining accurate constraints on the evolution of the galaxy rest-frame ultraviolet luminosity function (hereafter referred to as the luminosity function, or UV LF) in the early universe remains challenging. Typically parameterized by a Schechter function with a power-law slope at faint luminosities and an exponentially declining form at the bright end, the luminosity function provides a measure of the relative space density of galaxies over a wide range of luminosities at a particular redshift (Schechter 1976). Since the UV 1500 Å light probes recent star formation activity, the integral of the dust-corrected (intrinsic) luminosity function can then be used to derive the cosmic star formation rate density (SFRD) and estimate the galaxy population’s contribution to cosmic reionization, a process that appears to have been completed by $z \sim 6$ (Finkelstein et al. 2012b; Loeb & Furlanetto 2013; Robertson et al. 2013; Bouwens et al. 2015b). Given the scarce number of $z \sim 9$-10 galaxy candidate detections, a reliable determination of the SFRD at these redshifts remains difficult, with conclusions
CHAPTER 3. GALAXY LUMINOSITY AND SFR FUNCTION

from separate analyses disagreeing on the SFRD evolutionary trends (Coe et al. 2013; Ellis et al. 2013; Oesch et al. 2013, 2014). Furthermore, with the identification of galaxies at these redshifts, we are approaching the limit of HST’s detection capabilities. Sources beyond $z \sim 11$ will continue to remain largely inaccessible until the advent of the James Webb Space Telescope (JWST), whose scheduled launch in 2018 promises to yield revolutionary insights into early galaxy formation at $z > 10$ (Gardner et al. 2006).

The analysis and extrapolation of the UV luminosity function evolution towards higher ($z \approx 8$) redshifts has been the focus of several past studies, in the form of both hydrodynamical simulations (e.g. Nagamine et al. 2010; Finlator et al. 2011a; Salvaterra et al. 2011; Jaacks et al. 2012; Dayal et al. 2013; O’Shea et al. 2015) and semi-analytical models (e.g. Trenti et al. 2010; Muñoz 2012; Tacchella et al. 2013; Cai et al. 2014; Dayal et al. 2014; Behroozi & Silk 2015). Successfully reproducing the statistical properties of the observed Lyman-break galaxy (LBG) population at $z = 6-9$, simulations predict a large number of undetected, low-mass galaxies that may have significantly contributed to the reionization of the Universe at $z \geq 6$. Semi-empirical models which tie the evolution of galaxy luminosity to the dark matter properties of the host halos reach similar conclusions, predicting a steepening faint-end slope of the LF with redshift and a sharp decline in the cosmic star formation rate above $z = 8$ (Mason et al. 2015; Trac et al. 2015).

In this paper, we take advantage of the recent progress in the observed galaxy statistics at redshifts $z \sim 4-8$ to evolve the luminosity function, along with its derived properties, towards higher redshifts by establishing a link between the galaxy star formation rate (SFR) and its host halo mass via abundance matching techniques (Vale & Ostriker 2004, 2006; Conroy & Wechsler 2009). Since galaxy formation is governed
CHAPTER 3. GALAXY LUMINOSITY AND SFR FUNCTION

by the inflow of baryonic matter into the gravitational potential wells of dark matter halos where it cools and initiates star formation, the properties of galaxies are invariably linked to the characteristics of their host halos. We thus seek to derive a scaling relation between dark matter halo mass, $M_h$ and galaxy SFR at each redshift by assuming that there is a one-to-one, monotonic correspondence between these two properties. We anchor our model to the observed luminosity functions at $z \sim 4-8$ corrected for dust-extinction, mapping their shape to that of the halo mass function at the respective redshifts. Finding that the SFR-$M_h$ scaling law remains roughly constant across this redshift range, we apply the average relation, $SFR_{av}(M_h)$, to reproduce the observed $z \sim 9-10$ luminosity functions and then further explore how the UV LF, and the corresponding SFRD, evolve at higher redshifts, $z \sim 11-20$.

We describe the details of our approach and the theoretical framework used to derive the shape and amplitude of the galaxy UV LF in section 3.3. Our predictions for the evolving LF, the resulting SFRD, and the contribution of these galaxy populations to cosmic reionization at high redshifts are presented in section 3.4. We conclude in section 3.5 with a summary of our findings and their implications for future surveys with JWST. We adopt a flat, $\Lambda$CDM cosmology with $\Omega_m = 0.3$, $\Omega_\Lambda = 0.7$, $\Omega_b = 0.045$, $H_0 = 70$ km s$^{-1}$Mpc$^{-1}$, i.e. $h = 0.7$, $\sigma_8 = 0.82$, and $n_s = 0.95$, consistent with the most recent measurements from Planck (Planck Collaboration et al. 2016b). All magnitudes in this work are in the AB scale (Oke & Gunn 1983).
3.3 The Formalism

The goal of this paper is to derive an empirical prediction of the evolution of UV LFs at $z > 8$ tied to the evolution of dark matter haloes. We do so by first calibrating a $SFR - M_h$ relation at $z \sim 4 - 8$, which we then evolve to $z > 8$. Our formalism is described in the following sections.

3.3.1 The Observed Star-Formation Rate Functions

One important limitation of the UV LFs in probing the galaxy build-up in the early universe is dust extinction, which significantly affects the UV luminosities of galaxies. Thanks to deep multi-wavelength photometry with HST, it has become clear that dust extinction evolves with redshift, becoming significantly less important at earlier cosmic times (Bouwens et al. 2009a; Castellano et al. 2012; Finkelstein et al. 2012b; Dunlop et al. 2013; Bouwens et al. 2014b; Rogers et al. 2014). Thus, the UV LF at high redshift evolves due to two effects: (i) evolution in dust extinction, and (ii) SFR build-up of the underlying galaxy population. Any model of the UV LFs therefore has to disentangle these two effects.

Alternatively, we can directly make use of the SFR functions (SFRF), $\phi(SFR, z)$. These provide the number density of galaxies with a given SFR, and are thus corrected for dust extinction. Following Smit et al. (2012), we derive the observed SFR functions based on the most recent UV LFs at $z > 4$ taken from Bouwens et al. (2015b), which we correct for dust extinction using the observed UV continuum slopes $\beta$ and their relation with UV extinction (Meurer et al. 1999). The UV continuum slopes are modeled as a
function of luminosity using the most recent relations from Bouwens et al. (2014b). For more details on this approach see Smit et al. (2012).

The dust correction effectively shifts the LF to higher luminosities and slightly lowers the volume densities due to the renormalization of the magnitude bins. The dust-corrected, intrinsic UV luminosities are then converted to SFRs using the following empirical relation (Kennicutt 1998a),

\[
\frac{\text{SFR}}{M_\odot \text{yr}^{-1}} = 1.25 \times 10^{-28} \frac{L_{\text{UV,corr}}}{\text{erg s}^{-1}\text{Hz}^{-1}}
\] (3.1)

and the resulting SFR functions are represented with the typical Schechter parameterization,

\[
\phi(\text{SFR}) \, d\text{SFR} = \phi^* \left( \frac{\text{SFR}}{\text{SFR}^*} \right)^\alpha \exp \left( -\frac{\text{SFR}}{\text{SFR}^*} \right) \frac{d\text{SFR}}{\text{SFR}^*}.
\] (3.2)

The Schechter parameters for the \(z \sim 4-8\) SFR functions are directly related to the Schechter function parameters of the UV LF and the slope of the \(L_{\text{UV}} - \beta\) relation (see sections 2.1 and 2.2 in Smit et al. 2012). Using the most recent UV LFs and UV continuum slope measurements, we thus update the previous SFR functions of Smit et al. (2012). The resulting Schechter function parameters are listed in Table 3.1. They are also shown in Figure 3.1, where we compare our results with the previous

<table>
<thead>
<tr>
<th>(&lt;z&gt;)</th>
<th>(\log_{10} \phi^*_{\text{Mpc}^{-3}})</th>
<th>(\log_{10} \frac{\text{SFR}^*}{M_\odot \text{yr}^{-1}})</th>
<th>(\alpha)</th>
</tr>
</thead>
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<tr>
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<td>1.61±0.06</td>
<td>-1.53±0.03</td>
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<td>1.75±0.09</td>
<td>-1.59±0.08</td>
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<tr>
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<td>-1.62±0.08</td>
</tr>
<tr>
<td>6.8</td>
<td>-3.67±0.23</td>
<td>1.54±0.20</td>
<td>-1.76±0.12</td>
</tr>
<tr>
<td>7.9</td>
<td>-3.79±0.31</td>
<td>1.31±0.36</td>
<td>-1.79±0.18</td>
</tr>
</tbody>
</table>
Figure 3.1: The evolution of the star-formation rate function, $\Phi_{\text{SFR}}$, across redshift $z = 4 - 8$. The points correspond to the dust-corrected stepwise UV LFs from Bouwens et al. (2015b), which were corrected for dust extinction based on the UV continuum slope distributions measured in Bouwens et al. (2014b). The solid lines show the corresponding Schechter parameters for the SFRFs. These can be compared to the dashed lines from Smit et al. (2012), which were derived using the same procedure, but based on now-outdated UV LFs and $\beta$ distributions (covering only $z = 4 - 7$). The combination of less evolution in the characteristic luminosity found in newer UV LF results as well as the consistently redder UV continuum slopes, result in significantly higher SFRFs compared to the previous analysis, in particular at higher redshift.
analysis of Smit et al. (2012). As can be seen, the combination of less evolution in the characteristic luminosity found in newer UV LF results, as well as the consistently redder UV continuum slopes found in updated measurements, result in significantly higher SFRFs compared to the previous analysis, in particular at higher redshift.

We perform the same analysis also for $z \sim 9 - 10$ galaxy SFR functions. These are much more uncertain, given the very large uncertainties in the UV LFs at these redshifts. Also, note that based on the evolution of the UV continuum slope distribution at lower redshift (Bouwens et al. 2012b, 2014b; Dunlop et al. 2013; Finkelstein et al. 2012b; Wilkins et al. 2011), the dust correction is expected to be negligible at redshifts $z > 8$; the $z \sim 9$ and 10 SFR function parameters are thus directly related to the uncorrected UV LFs at those redshifts.

### 3.3.2 Method to derive the average $SFR - M_h$ relation

Adopting the approach presented in Vale & Ostriker (2004), we use the observed, dust-corrected $z \sim 4-8$ luminosity functions, i.e. SFR functions, to derive an empirical relation between the galaxy SFR and its host halo mass. In this abundance matching method, the SFR-$M_h$ relation is calculated by setting the SFR of a galaxy hosted in a halo of mass $M_h$ to be such that the number of galaxies with a star formation rate greater than SFR equals the number of halos with mass greater than $M_h$ at a given epoch:

$$\int_{M_h}^{\infty} n(M_h', z) dM_h' = \int_{SFR}^{\infty} \phi(SFR', z) dSFR', \quad (3.3)$$
where the $\phi(SFR, z)$ are the observed SFR function derived in the previous section and $n(M_h, z)$ is the Sheth-Tormen halo mass function (Sheth & Tormen 1999),

$$n(M_h, z) dM = A \left(1 + \frac{1}{\nu^2}q^2\right) \sqrt{\frac{2}{\pi}} \frac{d\nu}{dM} \frac{d\nu}{dM} e^{-\nu^2/2}$$ \hspace{1cm} (3.4)

with $\nu = \sqrt{a\delta_c/[D(z)\sigma(M)]}$, $a = 0.707$, $A = 0.322$ and $q = 0.3$; $\sigma(M)$ is the variance on the mass scale $M$ (assuming the linear theory density power spectrum) while $D(z)$ is the growth favor and $\delta_c$ is the linear threshold for spherical collapse, which in a flat universe is $\delta_c = 1.686$.

The abundance matching technique, as prescribed in eq. (3.3), presupposes that the SFR is a monotonic function of the halo mass. This is supported by the observed trend that the clustering strength of galaxies at high redshift increases with their UV luminosity, similar to that of the clustering strength of halos increasing with mass (Lee et al. 2009). Hence, a scaling relation that assumes the SFR of a galaxy is a monotonically increasing function of the mass of its host halo is a reasonable starting point. Furthermore, our model assumes a one-to-one correspondence between galaxies and host halos. This neglects the substructure expected to exist within a halo, comprised mainly of halos that formed at earlier epochs and merged to become subhaloes of more massive hosts (Bullock et al. 2002; Wechsler et al. 2000). To include the contribution of this subhalo population and the galaxies they are potentially hosting, we modified the left-hand side of eq. (3.3) to integrate over the total mass function, i.e. the sum of the regular Sheth-Tormen halo mass function and the unevolved subhalo mass function taken from Vale & Ostriker (2004). We found that because values for the subhalo mass function are generally lower than those of the halo mass function, the inclusion of this additional substructure has a negligible effect on the resulting scaling law; the subhaloes’
CHAPTER 3. GALAXY LUMINOSITY AND SFR FUNCTION

contribution to the expression is most important at the low-mass end, and even there, its inclusion changes the results by \( \lesssim 10\% \). Therefore, for the sake of simplicity, we neglect multiple halo occupation and assume that each dark-matter halo hosts a single galaxy.

3.3.3 Modeling the SFR Functions

Once the average relation between the SFR and the halo mass are known, we can model the SFR functions assuming a realistic dispersion around the average relation. We model the probability density for a halo of mass \( M_h \) to host a galaxy with a star formation rate \( SFR \) to obey a log-normal distribution (Giavalisco & Dickinson 2001; Yang et al. 2003; Muñoz & Loeb 2011),

\[
P(SFR|M_h)dSFR = \frac{1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{\log_{10}(SFR/SFR_{av}(M_h))^2}{2\sigma^2} \right) d\log_{10}SFR \tag{3.5}
\]

where \( SFR_{av}(M_h) \) is the mean SFR-\( M_h \) relation derived by averaging the \( SFR(M_h, z) \) relations obtained for \( 4 \leq z \leq 8 \) over the specified range of redshifts at fixed halo mass. The variance, \( \sigma^2 \), represents the scatter in SFR at a fixed \( M_h \) that arises from the stochastic nature of star formation activity. Halos of similar masses can have a range of large-scale environments, merger histories, and central concentrations (Lee et al. 2009). These conditions, along with interactions with nearby systems can result in different rates of gas accretion and star formation in galaxies. To account for this variance in the SFR-\( M_h \) relation, we adopt a constant intrinsic scatter of 0.5 dex. This choice is motivated by the 0.5 dex scatter in stellar mass at constant SFR found by González et al. (2011), a result further confirmed by Wyithe et al. (2014) as providing the best statistical fit to observations of the SFR-\( M_h \) relation.

The SFR function, \( \phi(SFR) \), can then be obtained by integrating over the
probability-weighted number densities of all halos that can achieve the star formation rate SFR within the allowed scatter:

$$\phi(SFR, z) = \int dM_h n(M_h, z) P(SFR|M_h)$$

$$= \frac{1}{\sigma \sqrt{2\pi} SFR} \int dM_h n(M_h, z) e^{-\frac{\log_{10}(SFR/SFR_{av}(M_h))^2}{2\sigma^2}}.$$ (3.6)

Note that in the limit of the variance $\sigma^2 \to 0$, the log-normal probability distribution becomes a delta function and the equation is reduced to the simpler form,

$$\phi(SFR, z) = n(M_h, z) \left| \frac{dSFR_{av}(M_h)}{dM_h} \right|^{-1}. \quad (3.7)$$

### 3.4 Results

#### 3.4.1 The Constant $SFR - M_h$ Relation

The curves in the top panel of Figure 3.2 depict the SFR-$M_h$ relations inferred from the observed LF functions at redshifts $4 \leq z \leq 8$ via the abundance matching technique discussed in Section 3.3. The scaling law remains roughly constant within 0.2 dex across this redshift range and is fairly well fit by a double power law with a turnover at a characteristic halo mass of $M_h^* \approx 2 \times 10^{11} M_\odot$. Averaging the relations over $z \sim 4$-8 at a fixed halo mass, we obtain a mean scaling law, $SFR_{av}(M_h)$ (solid black curve), characterized by a power-law slope $\beta \sim 0.9$ at the high-mass end, i.e. $M_h \gtrsim M_h^*$, and $\beta \sim 1.5$ at the faint end where $M_h$ falls below the characteristic mass.

These results are consistent with the models presented in Trenti et al. (2010) where the $L - M_h$ relation is calibrated at $z \sim 6$ and a $L \sim M_h^\beta$ relation is derived with $\beta \sim 1.3$-1.6 at the low-mass end. This steepening of the SFR-$M_h$ relation towards lower
CHAPTER 3. GALAXY LUMINOSITY AND SFR FUNCTION

Figure 3.2: Top panel: the relation between galaxy SFR and dark matter halo mass, $SFR(M_h, z)$, derived at $z \sim 4$-8 via abundance matching of the dust-corrected SFR functions to the halo mass function. For comparison, we show the $SFR - M$ relation at redshift $z = 8$ obtained by abundance matching the observed (uncorrected) UV LF function to the halo mass function at $z = 8$ (dotted black line). The solid black curve represents the mean SFR-$M_h$ scaling law, $SFR_{av}(M_h)$, obtained by averaging the (dust-corrected) relations over the redshift range at a fixed halo mass. The uncertainty in our model calibration of $SFR_{av}(M_h)$ (shaded region), was derived by varying the $z \sim 4$-8 SFR function parameters within their respective 1σ confidence regions. Bottom panel: ratio of the mean scaling law to the SFR-$M_h$ relations derived at each redshift. The vertical axis represents the factor by which the average relation over/underestimates the $z \sim 4$-8 scaling laws over the halo-mass range of interest.
masses may be due to the increased importance of feedback mechanisms in the star formation activity, such as supernovae and stellar winds (Giavalisco & Dickinson 2001). Meanwhile, the overall flattening of $SFR(M_h)$ at these redshifts compared to the local universe, where $SFR \propto M_h^\alpha$ is mainly a consequence of the steepening faint-end slope of the observed LF at these redshifts, where $\alpha < -1.5$ (Cooray & Milosavljević 2005).

The uncertainty in our model calibration of $SFR_{av}(M_h)$, represented by the shaded region in Figure 3.2, is derived by varying the $z \sim 4$ SFR function parameters within their respective 1σ confidence regions and rederiving the average SFR-$M_h$ relation. As can be seen, the dashed curves defining the SFR-$M_h$ relation at each redshift fall well within the boundaries of the uncertainty in the average scaling law, with the exception of the $z \sim 4$ relation at the high-mass end. The bottom panel of Figure 3.2 illustrates the accuracy with which the mean scaling law approximates SFR as a function of halo mass at different redshifts. Overall, the $SFR_{av}(M_h)$ relation provides a reasonable representation of the $SFR(M_h, z)$ relations at all redshifts, with departures of less than 0.2 dex within the halo mass range of interest. With the exception of the $z \sim 4$ relation, the $SFR(M_h, z)$ are all very similar (within 0.5 dex) at $M_h > 10^{12}$ $M_\odot$. At the low-mass end, the $z \sim 5$-$6$ and $z \sim 7$-$8$ scaling laws are over- and under-estimated respectively by less than a factor of two, while the SFR at $z \sim 4$ is overestimated over the full halo-mass range by approximately the same factor. We therefore expect the mean relation to yield accurate estimates of the SFR function at these redshifts and, assuming that the SFR-$M_h$ relationship continues to remain roughly unchanged for $z > 8$, at higher redshifts as well.
CHAPTER 3. GALAXY LUMINOSITY AND SFR FUNCTION

3.4.2 The Modeled SFR Functions at $z = 4 - 8$

Applying $SFR_{av}(M_h)$, we derive the expected SFR functions at redshifts $z \gtrsim 4$ assuming only evolution of the underlying dark-matter halo mass function. The results of our LF model are shown in Figure 3.3, both for the case where an intrinsic scatter of $\sigma \sim 0.5$ dex is assumed (solid colored curves) and in the limiting case where the variance is set to zero (dashed curves). Plotted alongside these results are the dust-corrected data points and the Schechter LFs with the observed best-fit parameters reported in Table 3.1 (gray curves). We find that including an intrinsic scatter increases the number density and yields SFR functions that are more consistent with observation, particularly at the luminous end where the increase in $\phi(SFR)$ due to scatter is most apparent. This boost in number density with the introduction of scatter can be attributed to the shape of the halo mass function. Even though $SFR(M_h)$ is log-normally distributed around the mean, $SFR_{av}(M_h)$, and the SFR scatter can thus go in either direction, the net change in the LF will always be dominated by low-mass halos entering into the galaxy sample by scattering into a SFR higher than its mean value, leading to a larger estimate of $\phi(SFR)$.

With the exception of $z \sim 4$, our predicted SFR functions accurately reproduce the observed ones and provide very good fits to the data points at the luminous end when intrinsic scatter is accounted for. At $z \sim 4$ our model predicts a SFRF which lies significantly above the observed data points by factors of 2-10×. This is likely due to a combination of two effects: (i) As also argued by Smit et al. (2012), the bright end of the observed $z \sim 4$ SFRF is likely underestimated due to heavily obscured galaxies, which are missed in UV-selected Lyman break galaxy samples; and (ii) quiescent galaxies start
Figure 3.3: Comparison of the predicted SFRFs at $z \sim 4 - 8$ assuming an intrinsic scatter $\sigma = 0.5$ dex (eq. (3.6); solid colored curves) with those obtained by setting the variance equal to zero (eq. (3.7); dashed curves). Our model SFRFs are overplotted with the data points at each respective redshift, along with the Schechter functions found to best approximate these measurements (gray curves; parameters recorded in Table 3.1). The data points represent the intrinsic UV luminosities, corrected for dust extinction and converted to SFRs using eq. (3.1); the SFR functions are thus the intrinsic, dust-corrected LFs at these redshifts. The shaded areas in each panel correspond to the $1\sigma$ confidence regions for our model LFs (when intrinsic scatter is accounted for).
to appear in the Universe at $z \sim 4$ in significant numbers (e.g. Straatman et al. 2014). Since our model does not include any prescription to quench star formation in galaxies, this is likely another reason why the model appears to be inadequate at $z \sim 4$. We conclude that our model should only be used at $z > 4$, where it provides a very good representation of the observed SFRFs.

### 3.4.3 A Prediction for the UV LF at $z = 9 - 10$

Building on the successful calibration of the SFR-$M_h$ relation at $z \sim 5 - 8$, we use our model to predict the galaxy UV luminosity function at $z \sim 9 - 10$. This represents the most distant galaxies in reach with HST, and recent observations have started to provide the first LF estimates at these redshifts. However, the sample sizes are still very small resulting in highly uncertain LF parameters (see e.g. Oesch et al. 2013).

We derive the model UV LFs at $z = 9$ and 10 by converting the SFR-$M_h$ relation calibrated in the previous section to a $L_{UV} - M_h$ relation using the standard Kennicutt (1998a) SFR-$L_{UV}$ relations. As can be seen in Figure 3.4, our model provides an excellent fit to the current, albeit scarce, data. In particular, our model explains the somewhat puzzling absence of $z \sim 10$ galaxy candidates between $M_{UV} = -18.5$ and $-20.5$ in current datasets. Incoming observations of the Hubble Frontier Field initiative will allow us to test this model further at $z \sim 9 - 10$ in the future.
Figure 3.4: Comparison of the predicted LFs assuming an intrinsic scatter $\sigma = 0.5$ dex (eq. (3.6); solid colored curves) with those obtained by setting the variance equal to zero (eq. (3.7); dashed curves). Since at $z \sim 9$ and 10, the dust extinction is expected to be negligible, the curves represent the observed, uncorrected LFs. We include determinations of the $z \sim 9$ and $z \sim 10$ UV LFs from Oesch et al. (2013), Oesch et al. (2014), and Bouwens et al. (2016). Arrows signify upper bounds on the number density at a given absolute UV magnitude, $M_{UV}$. The shaded area in each panel represents the 1$\sigma$ confidence region for the model LF when intrinsic scatter is accounted for. Our model UV LFs are in excellent agreement with the current observed estimates at these redshifts (albeit the latter are still based on small samples).
CHAPTER 3. GALAXY LUMINOSITY AND SFR FUNCTION

3.4.4 Extrapolation to $z \sim 20$ and Predictions for JWST

Motivated by the good agreement obtained by applying an unevolving SFR-$M_h$ relation to reproduce the observed LFs at $5 \lesssim z \lesssim 10$, we extend our approach to even higher redshifts for JWST predictions. The predicted LFs for redshifts $z > 10$, again assuming a constant intrinsic scatter of $\sigma = 0.5$ dex, are shown in Figure 3.5. These model LFs, which are well-fitted by Schechter functions across the redshift range $4 \lesssim z \lesssim 20$, significantly evolve with redshift. The drop in number density from $z \sim 4$ to 20 is reflected in the evolution of the characteristic number density, $\phi^*$, which decrease as $d \log \phi^*/dz \sim -0.3$. We also find a gradual steepening of the faint-end slope ($d\alpha/dz \sim -0.08$) and a shifting of the characteristic luminosity towards fainter values for increasing redshift ($dM^*_{UV}/dz \sim 0.4$). These trends in Schechter parameters are quite consistent with results from previous studies and extrapolations of observed $z \lesssim 10$ LFs, except that our model $M^*$ evolves more significantly than found in observations (e.g., Trenti et al. 2010; Bouwens et al. 2011b, 2012b; McLure et al. 2013; Finkelstein et al. 2015).

The shaded region in Figure 3.5 corresponds to the comoving volume and magnitude range accessible with a 200 arcmin$^2$ treasury sized ultra-deep JWST survey ($m_{lim} \simeq 31.5$ mag). According to our model predictions, the limiting redshift for galaxy observations with a very deep JWST survey is $z \sim 15$ (see also Windhorst et al. 2006). At higher redshifts, where the surface density drops below $\sim 10^{-6}$ Mpc$^{-3}$, wider, deeper surveys would be required to observe the luminosity function of these rare, faint objects.

Figure 3.6 shows the model predictions for the redshift evolution of the SFR density, obtained by integrating the SFR functions down to different SFR limits, ranging from
Figure 3.5: Predicted LFs for $z > 10$ based on our empirical model. The shaded region indicates the observable magnitude and volume within reach of a 200 arcmin$^2$ JWST treasury sized ultra-deep survey ($m_{lim} \approx 31.5$ mag). This indicates that the limiting redshift range observable with JWST may be $z \sim 15$ for unlensed galaxies.
CHAPTER 3. GALAXY LUMINOSITY AND SFR FUNCTION

\( SFR_{\text{min}} \sim 10^{-5} \, M_\odot/\text{yr} \) to 0.7 \( M_\odot/\text{yr} \). A minimum SFR of 0.7 \( M_\odot/\text{yr} \) corresponds to \( M_{UV} \sim -17.7 \) mag, the magnitude of the faintest object observed in the HUDF12/XDF data; integrating down to this limit thus facilitates comparison with the most recent, dust-corrected measurements of the SFRD, which have been plotted alongside the predicted curves in Figure 3.6. While our model appears to overpredict the SFRD measured for \( z \lesssim 6 \) by \( \sim 0.2 \) to 0.3 dex, the estimates of the \( \dot{\rho}_* \) at higher redshifts agree quite well with observations. Furthermore, the evolution of the cosmic SFRD in our model is consistent with previous published results: the dust-corrected SFRD values evolve as \((1 + z)^{-4.3 \pm 0.1}\) at \( 3 < z < 8 \) before rapidly declining at higher redshifts where \( \dot{\rho}_* \propto (1 + z)^{-10.4 \pm 0.3} \) for \( 8 \leq z \leq 10 \). In addition to accurately reproducing the order of magnitude drop in SFRD from \( z < 8 \) to \( z < 10 \) that has been observationally inferred in several separate analyses (Oesch et al. 2013), our model finds that the SFRD continues to steeply decline towards higher redshift, predicting a cosmic SFRD of \( \log \dot{\rho}_* \sim -7.0 \pm 0.3 \) \( M_\odot \, \text{yr}^{-1} \, \text{Mpc}^{-3} \) at \( z \sim 16 \).

However, as will be shown and discussed in the following section, a star-formation rate density that declines as \((1 + z)^{-10.4}\) at high redshifts, as derived assuming a minimum SFR of 0.7 \( M_\odot/\text{yr} \), fails to reproduce the observed Planck optical depth. Furthermore, galaxies are expected to exist beyond the current, observed magnitude limit. Theoretical and numerical investigations indicate that a halo at \( z \leq 10 \) irradiated by a UV field comparable to the one required for reionization needs a minimum mass of \( M_h \sim 6 \times 10^7 \) \( M_\odot \) in order to cool and form stars (Haiman et al. 1996; Tegmark et al. 1997). We therefore explore the implications of this prediction by integrating the SFR density down to minimum SFRs as low as \( 10^{-(5.0 \pm 0.8)} \) \( M_\odot \, \text{yr}^{-1} \), the star formation rate corresponding to the minimum halo mass based on our average SFR-\( M_h \) relation. This leads to a more
Figure 3.6: The redshift evolution of the star formation rate density (SFRD) $\dot{\rho}_*\,\min$ derived by integrating the model SFR functions down to different star-formation limits, ranging from $SFR_{\min} \sim 10^{-5}$ to 0.7 $M_\odot$/yr. The shaded blue and red regions represents the 1σ uncertainty in the SFRD obtained when integrating down to $M_{UV} \sim -17.7$ mag (i.e., $SFR_{\min} \sim 0.7$ $M_\odot$/yr) and $M_{UV} \sim -5.7$ mag (i.e., $SFR_{\min} \sim 10^{-5}$ $M_\odot$/yr), respectively. Our model results (blue curve) can thus be compared with the (dust-corrected) measurements of the cosmic SFRD (blue circles) derived from this dataset. We find that the best-fit evolution of the SFRD at $8 \leq z \leq 10$ is $\dot{\rho}_* \propto (1+z)^{-10.4\pm0.3}$, significantly steeper than the lower redshift trends which fall as $(1+z)^{-4.3}$. 
moderate decline of the cosmic SFRD towards higher redshift. In this case, the best-fit evolution for $8 \leq z \leq 10$ is $\dot{\rho}_s \propto (1 + z)^{-7.3 \pm 0.5}$, with an estimated SFRD of $\sim 4 \times 10^{-5}$ $M_{\odot}$ yr$^{-1}$Mpc$^{-3}$ at $z \sim 16$, a mere $\sim 250$ million years after the Big Bang.

### 3.4.5 Contribution of Galaxies to Cosmic Reionization

If star-forming galaxies supply the bulk of the photons that drive the cosmic reionization process, then our redshift-evolving SFRD $\dot{\rho}_s(z)$ can be used to determine the reionization history of the universe. The ionized hydrogen fraction $Q(z)$ can be expressed as a time-dependent differential equation (Loeb & Furlanetto 2013),

$$\dot{Q} = \frac{\dot{n}_{\text{ion}}}{\langle n_H \rangle} - \frac{Q}{t_{\text{rec}}}$$

(3.8)

where $\langle n_H \rangle$ is the comoving number density of hydrogen atoms and $\dot{n}_{\text{ion}}$ is the comoving production rate of ionizing photons, $\dot{n}_{\text{ion}} = f_{\text{esc}} N_\gamma \dot{\rho}_s(z)$ where $N_\gamma$ is the number of ionizing photons per unit mass of stars and $f_{\text{esc}}$ is the average escape fraction from galaxies. The recombination time in the IGM is

$$t_{\text{rec}} = \left[ C \alpha_B(T)(1 + Y_p/4X_p)\langle n_H \rangle(1 + z)^3 \right]^{-1}$$

(3.9)

where $\alpha_B(T)$ is the case B recombination coefficient for hydrogen (we assume an IGM temperature of 10,000 K corresponding to $\alpha_B \approx 2.79 \times 10^{-79}$ Mpc$^3$yr$^{-1}$), $X_p = 0.75$ and $Y_p = 1 - X_p$ are the primordial hydrogen and helium mass-fractions respectively, and $C$ is the clumping factor that accounts for the effects of IGM inhomogeneity. Estimates of the contribution of star-forming galaxies to reionization therefore depend on assumptions about the stellar IMF, metallicity, escape fraction, and clumping factor.

In this paper, we take $N_\gamma$ equal to $7.65 \times 10^{60}$ $M_{\odot}^{-1}$, corresponding to a low-metallicity
Chabrier IMF (Behroozi & Silk 2015). The escape fraction is more difficult to constrain, especially at higher redshifts where the correction for intervening IGM absorption systems is high; while inferences at $z < 5$ suggest $f_{\text{esc}} < 10\%$, simulations suggest that $f_{\text{esc}}$ can be very large (Wise & Cen 2009; Wise et al. 2014; Hayes et al. 2011). For the sake of simplicity, we follow the approach in the previous literature and adopt a constant fiducial value of $f_{\text{esc}} = 0.2$ for all redshifts. The determination of the clumping factor is also uncertain, with estimates ranging from $C = 2$ to $C = 4$ at high redshifts (Pawlik et al. 2009; Finlator et al. 2012; Shull et al. 2012); we therefore assume $C = 3$ in our fiducial model (see also Oesch et al. 2009; Bouwens et al. 2012a; Finkelstein et al. 2015; Behroozi & Silk 2015; Bouwens et al. 2015a; Robertson et al. 2015).

For a given reionization history $Q(z)$, the electron scattering optical depth $\tau$ can also be calculated as a function of redshift,

$$\tau(z) = \int_0^z c \langle n_H \rangle \sigma_T (1 + Y_p/4X_p) Q(z') H(z')(1 + z')^2 dz'$$

where $c$ is the speed of light, $\sigma_T$ is the Thomson cross section, and $H(z)$ is the Hubble parameter. This optical depth can be inferred from observations of the cosmic microwave background, and for a while, the accepted value from the Wilkinson Microwave Anisotropy Probe (WMAP) 9-year dataset was $\tau = 0.088 \pm 0.014$, which, in the simplest model, corresponds to instantaneous reionization at $z_{\text{reion}} \approx 10.5 \pm 1.1$. In early 2015, a significantly lower value of $\tau = 0.066 \pm 0.016$ was reported (Planck Collaboration et al. 2016b), consistent with instantaneous reionization occurring at $z_{\text{reion}} \approx 8.8^{+1.2}_{-1.1}$. More recently, the value has again shifted up to $\tau = 0.078 \pm 0.019$, consistent with instantaneous reionization occurring at $z_{\text{reion}} \approx 9.9^{+1.8}_{-1.6}$ (Planck Collaboration et al. 2016a).

Figure 3.7 shows the expected reionization history of the universe (left panel) and
Figure 3.7: Left panel: The reionization history $Q(z)$ calculated by solving the differential equation given by eq. (3.8) assuming an ionizing photon escape fraction $f_{\text{esc}} = 0.2$, an IGM clumping factor of $C = 3$, and an average number of ionizing photons per unit mass of stars $N_\gamma = 7.65 \times 10^{60} \, M_\odot^{-1}$. The blue and red curves denote the reionization histories derived by using the cosmic SFRD $\dot{\rho}_s$ integrated down to $SFR_{\text{min}} = 0.7$ and $10^{-5.0\pm0.8} \, M_\odot/\text{yr}$ respectively (i.e. $M_{UV} < -17.7$ and $<-5.7$ mag; galaxies hosted by the minimum halo mass to cool and form stars). For these chosen parameters, 68% confidence limits on the redshift of half-reionization are $6.2 < z < 7.3$ when considering only the currently observed galaxy population, and $6.5 < z < 8.1$ with the inclusion of galaxies that expected to exist beyond this magnitude limit. Right panel: The corresponding Thomson electron scattering optical depths $\tau$ integrated over redshift from the present day, along with the Planck constraint $\tau = 0.066\pm0.016$ (gray area). The shaded regions correspond to the 68% confidence intervals, computed from the uncertainties in the cosmic SFRD $\dot{\rho}_s$ shown in Figure 3.6.
the corresponding optical depth (right panel) computed using the cosmic SFRD $\dot{\rho}_*$ we derived from our model UV LFs. We find that the currently observed galaxy population at magnitudes brighter than $M_{UV} \leq -17.7 \ (SFR \geq 0.7 \ M_\odot/yr$, blue curve) fully reionize the universe by redshift $z \sim 6$ and that the model corresponding to this magnitude limit predicts a Thomson optical depth of $\tau \simeq 0.048$. Integrating further down to $M_{UV} \leq -5.7 \ (SFR \geq 10^{-5} \ M_\odot/yr$, red curve) produces a model that reionizes the universe slightly earlier, at $z \sim 6.5$, with a predicted optical depth of $\tau \simeq 0.054$. The shaded regions corresponding to each of these curves represent the 68% confidence limits arising solely from the uncertainties in the normalization of the cosmic SFRD.

Our results for the reionization history are consistent with measurements from high-redshift quasar and gamma-ray burst spectra, as well as from Lyman alpha emission in high-$z$ galaxies which collectively indicate that reionization ended near $z \simeq 6$ (Bolton & Haehnelt 2007; Kuhlen & Faucher-Giguère 2012; Chornock et al. 2013; Treu et al. 2013; Schenker et al. 2014; McGreer et al. 2015). Furthermore, the model which includes the population of low-mass halos with SFRs as faint as $10^{-5} \ M_\odot/yr$ produces an optical depth that is consistent with the previous inferred value by Planck, $\tau = 0.066$ (Planck Collaboration et al. 2016b), at the 1$\sigma$ level. These findings, in line with previous analyses, indicate that a significant population of low-mass star-forming galaxies is necessary for cosmic reionization and strengthen the conclusion that the bulk of photons responsible for reionizing the early universe emerged from ultra-faint galaxies.

In order for our model to reproduce the most recent value of $\tau = 0.078$ inferred from CMB observations by Planck, the average $SFR - M_h$ relation used would have to allow for larger star formation rates at the low-mass end. One simple way to satisfy such conditions is to permit $SFR_{av}(M_h)$ to vary according to the average relation derived via
abundance matching for $M_h \gtrsim 10^{11} \, M_\odot$, but decline as a power law for $M_h \lesssim 10^{11} \, M_\odot$ with a slope of $\beta \sim 1.3$, shallower than the slope derived empirically in section 3.4.1 at the low mass end. In such a model, the corresponding optical depth would be $\tau \sim 0.076$, similar to the latest reduced measurement of $\tau = 0.078$. While the high-redshift LF functions derived assuming such a form for the average $SFR - M_h$ relation are in tension with current observations, future measurements taken with JWST will shed more light on how the LF functions evolve at these low SFRs.

We also note that the results for $Q(z)$ and $\tau(z)$ depend on the choices for the escape fraction $f_{esc}$, the number of ionizing photons per unit stellar mass $N_\gamma$, and the clumping factor $C$; if one assumes a smaller clumping factor, or a higher value for $f_{esc}$ or $N_\gamma$, the evolution of $Q(z)$ will be shifted towards higher redshifts and an optical depth closer to the one measured by Planck Collaboration et al. (2016a) will be obtained. Furthermore, the ionizing photons of Population III stars are expected to additionally increase the optical depth at high redshift (Sobral et al. 2015).

3.5 Summary

In this paper, we use the most recent $z \sim 4-8$ UV LFs and UV continuum slope measurements to derive an empirical prediction of the evolution of UV LFs at $z > 8$. Assuming a monotonic, one-to-one correspondence between the observed galaxy SFRs and the host halo masses, we map the shape of the observed $z \sim 4-8$ UV LFs to that of the halo mass function at the respective redshifts. We find that the resulting $SFR - M_h$ scaling law remains roughly constant over this redshift range and is fairly well fit by a double power law, $SFR \propto M_h^\beta$, with $\beta \sim 0.9$ at the high-mass end, i.e. $M_h \gtrsim 2 \times 10^{11} \, M_\odot$. 
CHAPTER 3. GALAXY LUMINOSITY AND SFR FUNCTION

and $\beta \sim 1.5$ at the low-mass end. We note that the unevolving nature of this relation with redshift is an empirical result, an explanation for which lies beyond the scope of this paper. Future work based on semi-analytic models and numerical simulations, as well as anticipated observations with Atacama Large Millimeter Array (ALMA), are expected to shed further light on this matter.

Applying this average $SFR - M_h$ relation with an intrinsic scatter of $\sigma \sim 0.5$, we accurately reproduce the observed SFR functions at $5 \lesssim z \lesssim 10$ (Figures 3.3 and 3.4) and extend our approach to predict the evolution of the UV LF at redshifts $z \sim 11-20$. We find an evolving characteristic number density $\phi^*$ which decreases as $d \log \phi^*/dz \sim -0.3$, a gradually steepening faint-end slope, $d\alpha/dz \sim -0.08$, and a shifting of the characteristic luminosity towards fainter values, $dM^*_\text{UV}/dz \sim 0.4$. Given the comoving volume and magnitude range of an ultra-deep JWST survey, our model predicts that observations of the LF up to $z \sim 15$ are within reach in the absence of gravitational lensing, while deeper and wider surveys would be necessary to observe higher redshift objects.

We also derive the evolution of the SFR density by integrating the SFRFs down to various SFR limits, ranging from $0.7 \text{ M}_\odot/\text{yr}$ (corresponding to the faintest object observed in HUDF12/XDF), to $10^{-5} \text{ M}_\odot/\text{yr}$ (corresponding to the minimum halo mass necessary to cool and form stars). The inclusion of galaxies with SFRs well below the current detection limit results in a more moderately declining cosmic SFRD with redshift and leads to a fully reionized universe by $z \sim 6.5$. Furthermore, the corresponding predicted optical depth in this model, $\tau \simeq 0.054$, is consistent with the reduced value of $\tau = 0.066 \pm 0.016$ inferred from CMB observations by Planck at the 1$\sigma$ level. These results strengthen the claim that a significant portion of the reionizing photons in the early universe were emitted by a population of low-mass, star-forming galaxies that have
3.6 Acknowledgements

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Part II

The Molecular Interstellar Medium
Chapter 4

The Ratio of CO to Total Gas Mass in High-Redshift Galaxies

This thesis chapter originally appeared in the literature as


4.1 Abstract

Walter et al. (2012) have recently identified the J=6-5, 5-4, and 2-1 CO rotational emission lines, and [CII] fine-structure emission line from the star-forming interstellar medium in the high-redshift submillimeter source HDF 850.1, at z = 5.183. We employ large velocity gradient (LVG) modeling to analyze the spectra of this source assuming the [CII] and CO emissions originate from (i) separate virialized regions, (ii) separate
unvirialized regions, (iii) uniformly mixed virialized regions, and (iv) uniformly mixed unvirialized regions. We present the best fit set of parameters, including for each case the ratio $\alpha$ between the total hydrogen/helium gas mass and the CO(1-0) line luminosity. We also present computations of the ratio of $H_2$ mass to $[\text{C}^\text{II}]$ line-luminosity for optically thin conditions, for a range of gas temperatures and densities, for direct conversion of $[\text{C}^\text{II}]$ line-luminosities to “CO-dark” $H_2$ masses. For HDF 850.1 we find that a model in which the CO and $C^+$ are uniformly mixed in gas that is shielded from UV radiation, requires a cosmic-ray or X-ray ionization rate of $\zeta \approx 3 \times 10^{-14} \text{ s}^{-1}$, plausibly consistent with the large star-formation rate ($\sim 10^3 \text{ M}_\odot \text{ yr}^{-1}$) observed in this source. Enforcing the cosmological constraint posed by the abundance of dark matter halos in the standard $\Lambda$CDM cosmology and taking into account other possible contributions to the total gas mass, we find that the two models in which the virialization condition is enforced can be ruled out at the $\gtrsim 2\sigma$ level while the model assuming mixed unvirialized regions is less likely. We conclude that modeling HDF 850.1’s ISM as a collection of unvirialized molecular clouds with distinct CO and $C^+$ layers, for which $\alpha = 1.2 \text{ M}_\odot \text{(K km s}^{-1} \text{ pc}^2)^{-1}$ for the CO to $H_2$ mass-to-luminosity ratio, (similar to the standard ULIRG value), is most consistent with the $\Lambda$CDM cosmology.

## 4.2 Introduction

Observations of high-redshift CO spectral line emissions have greatly increased our knowledge of galaxy assembly in the early Universe. At redshifts $z \sim 2$, this includes the discovery of turbulent star-forming disks with cold-gas mass fractions and star-formation rates significantly larger than in present day galaxies (Daddi et al. 2010; Genzel et al.
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

2012; Magnelli et al. 2012; Tacconi et al. 2010, 2013). The high star-formation rates are correlated with large gas masses and luminous CO emission lines (Kennicutt & Evans 2012) observable to very high redshifts. A prominent example is the luminous submillimeter and Hubble-Deep-Field source HDF 850.1, which is at a redshift of $z = 5.183$ as determined by recent detections of CO(6-5), CO(5-4), and CO(2-1) rotational line emissions, and also [Cii] fine-structure emission in this source (Walter et al. 2012). The high redshift of HDF 850.1 offers the opportunity of setting cosmological constraints on the conversion factor from CO line luminosities to gas masses, via the implied dark matter masses and the expected cosmic volume density of halos of a given mass. Such analysis is the subject of our paper.

CO emitting molecular clouds, which provide the raw material for star formation, are usually assumed to have undergone complete conversion from atomic to molecular hydrogen. However, since $\mathrm{H}_2$ has strongly forbidden rotational transitions and requires high temperatures ($\sim 500$ K) to excite its rotational lines, it is a poor tracer of cold ($\lesssim 100$ K) molecular gas. Determining $\mathrm{H}_2$ gas masses in the interstellar medium (ISM) of galaxies has therefore relied on tracer molecules. In particular, $^{12}\mathrm{CO}$ is the most commonly employed tracer of ISM clouds; aside from being the most abundant molecule after $\mathrm{H}_2$, CO has a weak dipole moment ($\mu_e = 0.11$ Debye) and its rotational levels are thus excited and thermalized by collisions with $\mathrm{H}_2$ at relatively low molecular hydrogen densities (Solomon & Vanden Bout 2005).

The molecular hydrogen gas mass is often obtained from the CO luminosity by adopting a mass-to-luminosity conversion factor $\alpha = M_{\mathrm{H}_2}/L'_{\mathrm{CO}(1-0)}$ between the $\mathrm{H}_2$ mass and the $J = 1-0$ 115 GHz CO rotational transition (Bolatto et al. 2013). The value for $\alpha$ has been empirically calibrated for the Milky Way Galaxy by three independent
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

techniques: (i) correlation of optical extinction with CO column densities in interstellar dark clouds (Dickman 1978); (ii) correlation of gamma-ray flux with the CO line flux in the Galactic molecular ring (Bloemen et al. 1986; Strong et al. 1988); and (iii) observed relations between the virial mass and CO line luminosity for Galactic GMCs (Solomon et al. 1987). These methods have all arrived at the conclusion that the conversion factor in our Galaxy is fairly constant. The standard Galactic value is $\alpha = 4.6 \, M_\odot / (K \, \text{km}^{-1} \, \text{pc}^2)$. Subsequent studies of CO emission from unvirialized regions in Ultra-Luminous Infrared Galaxies (ULIRGs) found a significantly smaller ratio. For such systems, $\alpha = 0.8 \, M_\odot / (K \, \text{km}^{-1} \, \text{pc}^2)$ (Downes & Solomon 1998). These values have been adopted by many (Sanders et al. 1988; Tinney et al. 1990; Wang et al. 1991; Walter et al. 2012) to convert CO J=1-0 line observations to total molecular gas masses, but without consideration of the dependence of $\alpha$ on the average molecular gas conditions found in the sources being considered. Since all current observational studies of $\alpha$ leave its range and dependence on the average density, temperature, and kinetic state of the molecular gas still largely unexplored, its applicability to other systems in the local or distant Universe is less certain (Papadopoulos et al. 2012a).

In this paper, we estimate the CO emitting gas masses in HDF 850.1 using the large-velocity-gradient (LVG) formalism to fit the observed emission line spectral energy distribution (SED) for a variety of model configurations, and for a comparison to the Galactic and ULIRG conversions. In section 4.3 we outline the details of the LVG approach, including an overview of the escape probability method and a derivation of the gas mass from the line intensity of the modeled source. In section 4.4, we present the best fit set of parameters that reproduce HDF 850.1’s detected lines and calculate the corresponding molecular gas mass, assuming the CO and [CII] emission lines originate
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

from (i) separate virialized regions, (ii) separate unvirialized regions, (iii) uniformly mixed virialized regions, and (iv) uniformly mixed unvirialized regions. The inferred gas masses enable us to set lower-limits on the dark-matter halo mass for HDF 850.1. In section 4.5 we compare the estimated halo-masses to the number of such objects expected at high redshift in ΛCDM cosmology, and show that models with lower values of α are favored. We conclude with a discussion of our findings and their implications in section 4.6.

4.3 Large Velocity Gradient Model

We start by describing our procedure for quantitatively analyzing the [C\textsc{ii}] and CO emission lines detected at the position of HDF 850.1 using the large velocity gradient (LVG) approximation. We consider a multi-level system with population densities of the ith level given by \(n_i\). The equations of statistical equilibrium can then be written as:

\[
n_i \sum_{j \neq i} R_{ij} = \sum_{j \neq i} n_j R_{ji}
\]

where \(l\) is the total number of levels included; since the set of \(l\) statistical equations is not independent, one equation may be replaced by the conservation equation

\[
n_{\text{tot}} = \sum_{j=0}^{l} n_j
\]

where \(n_{\text{tot}}\) is the number density of the given species in all levels. In our application, \(n_{\text{tot}} = n_{\text{CO}}\). Following the notation of Poelman & Spaans (2005), \(R_{ij}\) is given in terms of the Einstein coefficients, \(A_{ij}\) and \(B_{ij}\), and the collisional excitation \((i < j)\) and de-excitation
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

rates \((i > j)\) \(C_{ij}\):

\[
R_{ij} = \begin{cases} 
A_{ij} + B_{ij}\langle J_{ij}\rangle + C_{ij}, & (i > j) \\
B_{ij}\langle J_{ij}\rangle + C_{ij}, & (i < j)
\end{cases}
\]  

(4.3)

where \(\langle J_{ij}\rangle\) is the mean radiation intensity corresponding to the transition from level \(i\) to \(j\) averaged over the local line profile function \(\phi(\nu_{ij})\). The total collisional rates \(C_{ij}\) depend on the individual temperature-dependent rate coefficients and collision partners, usually \(H_2\) and \(H\) for CO rotational excitation.

The difficulty in solving this problem is that the mean intensity at any location in the source is a function of the emission and varying excitation state of the gas all over the rest of the source, and is thus a nonlocal quantity. To obtain a general solution of the coupled sets of equations describing radiative transfer and statistical equilibrium, we adopt the approach developed by Sobolev (1960) and extended by Castor (1970) and Lucy (1971) and assume the existence of a large velocity gradient in dense clouds. This assumption is justified given the interstellar molecular line widths which range from a few up to a few tens of kilometers per second, far in excess of plausible thermal velocities in the clouds (Goldreich & Kwan 1974). They suggest that these observed velocity differences arise from large-scale, systematic, velocity gradients across the cloud, a hypothesis that lies in accord with the constraints provided by observation and theory.

In the limit that the thermal velocity in the cloud is much smaller than the velocity gradient across the radius of the cloud, the value of \(\langle J_{ij}\rangle\) at any point in the cloud, when integrated over the line profile, depends only upon the local value of the source function and upon the probability that a photon emitted at that point will escape from the cloud.
without further interaction. Thus \( \langle J_{ij} \rangle \) becomes a purely local quantity, given by:

\[
\langle J_{ij} \rangle = (1 - \beta_{ij})S_{ij} + \beta_{ij}B(\nu_{ij}, T_B) \tag{4.4}
\]

where \( S_{ij} \) is the line source function,

\[
S_{ij} = \frac{2h\nu_{ij}^3}{c^2} \left( \frac{g_i n_j}{g_j n_i} - 1 \right)^{-1} \tag{4.5}
\]

assumed constant through the medium. In this expression \( g_i \) and \( g_j \) are the statistical weights of levels \( i \) and \( j \) respectively, \( \beta_{ij} \) is the “photon escape probability”, and \( B_{ij}(\nu_{ij}, T_B) \) is the background radiation with temperature \( T_B \). In our models we set \( T_B \) to the CMB temperature of 16.9 K at \( z = 5.183 \). We ignore contributions from warm dust (da Cunha et al. 2013).

For a spherical homogenous collapsing cloud, the probability that a photon emitted in the transition from level \( i \) to level \( j \) escapes the cloud is given by

\[
\beta_{ij} = \frac{1 - e^{-\tau_{ij}}}{\tau_{ij}} \tag{4.6}
\]

where \( \tau_{ij} \) is the optical depth in the line,

\[
\tau_{ij} = \frac{A_{ij} c^2}{8\pi \nu_{ij}^2} \frac{n_{\text{tot}}}{dv/dr} \frac{n_j g_i}{n_i} \frac{n_i g_j}{n_j} (1 - \frac{g_j n_i}{g_i n_j}). \tag{4.7}
\]

The equations of statistical equilibrium are therefore reduced to the simplified form

\[
\sum_{j \neq i}^l (n_i C_{ij} - n_j C_{ji}) + n_i \sum_{j \neq i}^l A_{ij} \beta_{ij} - \sum_{j \neq i}^l n_j A_{ji} \beta_{ji} = 0 \tag{4.8}
\]

and can be solved through an iterative process to give the fractional level populations \( n_i/n_{\text{tot}} \) (for a given choice of densities for the collision partners, usually \( \text{H}_2 \) but also \( \text{H} \), and kinetic temperature \( T_{\text{kin}} \)). Assuming the telescope beam contains a large number of these identical homogeneous collapsing clouds (e.g., Hailey-Dunsheath 2009), the
corresponding emergent intensity of an emission line integrated along a line of sight is then simply

\[ I_{ij} = \frac{h \nu_{ij}}{4\pi} \frac{n_i}{n_{tot}} A_{ij} \beta_{ij} N_{tot} = \frac{h \nu_{ij}}{4\pi} \frac{n_i}{n} A_{ij} \beta_{ij} \chi N \]  

(4.9)

where \( \chi \) is the abundance ratio, \( \chi \equiv n_{tot}/n \), where \( n \) is the total hydrogen gas volume density (cm\(^{-3}\)) and \( N \) is the hydrogen column density (cm\(^{-2}\)).

Given a series of observed lines with frequency \( \nu_{ij} \), one can identify a set of characterizing parameters that best reproduces the observed line ratios and intensity magnitudes; among these parameters are the cloud’s kinetic temperature (\( T_{kin} \)), velocity gradient (\( dv/dr \)), gas density \( n \) and collision partner (H and H\(_2\)) gas fractions, abundance ratio (\( \chi \)), and column density (\( N \)). For a spherical geometry, this column density can then be further related to the molecular gas mass of the cloud in the following way

\[ M = \pi R^2 \mu m N' \]  

(4.10)

where the factor \( \mu = 1.36 \) takes into account the helium contribution to the molecular weight and \( R = D_A \theta/2 \) is the effective radius of the cloud, with \( D_A \) being the angular diameter distance to the source and \( \theta \) the beam size of the line observations. \( N \) is defined in terms of the column density obtained from the LVG calculation, \( N' = N(1 + z)^4 \) where the \( (1 + z)^4 \) multiplicative factor reflects the decrease in surface brightness of a source at redshift \( z \) in an expanding universe.

In the case where the emitting molecular clouds are gravitationally bound, applying the virial theorem to a homogenous spherical body yields the following constraint (Goldsmith 2001),

\[ \frac{dv}{dr} \approx \sqrt{\frac{G \pi \mu m n}{15}} \approx a \sqrt{\frac{n}{(\text{cm}^{-3})}} \text{ km s}^{-1} \text{ pc}^{-1} \]  

(4.11)

where \( a = 7.77 \times 10^{-3} \) if \( n = n_{H_2} \) and \( a = 5.50 \times 10^{-3} \) if \( n = n_H \). The velocity gradient
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

is inversely proportional to the dynamical time scale. In models where the clouds are
assumed to be virialized, \( \frac{dv}{dr} \) and \( n \) are no longer independent input parameters of the
model, but rather vary according to eq. (4.11).

For the optically thick \(^{12}\)CO J=1-0 transition line (\( \beta \approx 1/\tau \)), carrying out the LVG
calculations with this additional virialization condition leads to a simple relation between
the gas mass and the CO(1-0) line luminosity,

\[
\alpha_{\text{CO}} = \frac{M_{\text{H}_2}}{L_{\text{CO(1-0)}}} = 8.6 \sqrt{\frac{n_{\text{H}_2}/(\text{cm}^{-3})}{T_{\text{exc}}/(\text{K})}} \text{ M}_\odot(\text{K km s}^{-1} \text{ pc}^2)^{-1}
\]

where the excitation temperature \( T_{\text{exc}} \approx T_{\text{kin}} \) when the emission line is thermalized. (In
this expression we assume complete conversion to \( \text{H}_2 \) so that the gas mass is the \( \text{H}_2 
\) mass.) Empirically, the Galactic value of this mass-to-luminosity ratio for virialized
objects bound by gravitational forces is \( \alpha = \frac{M_{\text{H}_2}}{L_{\text{CO(1-0)}}} = 4.6 \text{ M}_\odot(\text{K km s}^{-1} \text{ pc}^2)^{-1} 
\) (Solomon & Barrett 1991), corresponding to \( \sqrt{n_{\text{H}_2}}/T \sim 0.5 \text{ cm}^{-3/2} \text{K}^{-1} \).

4.4 Analysis of HDF 850.1

4.4.1 Properties of the Galaxy

HDF 850.1, the brightest submillimetre source in the Hubble Deep Field at a wavelength
of 850 micrometers, was discovered by Hughes et al. 1998. A full-frequency scan of
this source by Walter et al. (2012) using the IRAM (Institut de Radioastronomie
Millimetrique) Pleateau de Bure Interferometer and the National Radio Astronomy
Observatory (NRAO) Jansky Very Large Array has detected three CO lines, identified
as the CO(2-1) 230.5 GHz, CO(5-4) 576.4 GHz, and CO(6-5) 691.5 GHz rotational
transitions. [CII] 1900.1 GHz (158 μm), one of the main cooling lines of the star-forming in stellar medium, has also been detected (Table 4.1). These lines have placed HDF 850.1 in a galaxy over density at z = 5.183, a redshift higher than those of most of the hundreds of submillimetre-bright galaxies identified thus far.

Walter et al. (2012) used an LVG model to characterize the CO spectral energy distribution of HDF 850.1 and found that the observed CO line intensities could be fit with a molecular hydrogen density of $10^{3.2}$ cm$^{-3}$, a velocity gradient of 1.2 km s$^{-1}$pc$^{-1}$, and a kinetic temperature of 45 K. Then, assuming $\alpha = 0.8$ M$_{\odot}$ (K km s$^{-1}$pc$^2$)$^{-1}$ as for ULIRGs, they used the 1-0 line luminosity inferred from their LVG computation to infer that $M_{H_2} = 3.5 \times 10^{10}$ M$_{\odot}$. However, as Papadopoulos et al. (2012a) argue, adopting a uniform value of $\alpha$ for ULIRGs neglect its dependence on the density, temperature, and kinematic state of the gas; this may limit the applicability of computed conversion factors to other systems in the local or distant Universe.

Here, we broaden the LVG analysis carried out in Walter et al. 2012 and use the LVG-modeled column density to estimate the total gas mass of the source. We present several alternative models, each subject to a slightly different constraint. In particular,

<table>
<thead>
<tr>
<th>Line</th>
<th>$\nu_{\text{obs}}$ [GHz]</th>
<th>Integrated Flux Density [Jy km s$^{-1}$]</th>
<th>Luminosity [10$^{10}$ K km s$^{-1}$ pc$^2$]</th>
<th>Intensity [erg cm$^{-2}$ str$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO(2-1)</td>
<td>37.286</td>
<td>0.17±0.04</td>
<td>4.1±0.9</td>
<td>(2.16±0.51)$\times 10^{-9}$</td>
</tr>
<tr>
<td>CO(5-4)</td>
<td>93.202</td>
<td>0.5±0.1</td>
<td>1.9±0.4</td>
<td>(1.59±0.32)$\times 10^{-8}$</td>
</tr>
<tr>
<td>CO(6-5)</td>
<td>111.835</td>
<td>0.39±0.1</td>
<td>1.0±0.3</td>
<td>(1.49±0.82)$\times 10^{-8}$</td>
</tr>
<tr>
<td>[CII]</td>
<td>307.383</td>
<td>14.6±0.3</td>
<td>5.0±0.1</td>
<td>(1.5±0.03)$\times 10^{-6}$</td>
</tr>
</tbody>
</table>
we first consider the case where the CO and [C\text{II}] lines originate from different regions of the molecular cloud. This picture is consistent with the standard structure of PDRs in which there is a layer of almost totally ionized carbon at the outer edge, intermediate regions where the carbon is atomic, and internal regions where the carbon is locked into CO (Sternberg & Dalgarno 1995; Tielens & Hollenbach 1985; Wolfire et al. 2010). In this picture then, the hydrogen is fully molecular in the CO emitting regions. We then consider models in which the CO molecules and C\text{+} ions are uniformly mixed, such that the line emissions originate in gas at the same temperature and density. These models resemble conditions found in UV-opaque cosmic-ray dominated dark cores of interstellar molecular clouds where the chemistry is driven entirely by cosmic-ray ionization. For HDF850.1, the ionization rates could be significantly higher than in the Milky Way, leading to enhanced C\text{+} in the UV-shielded regions. In both instances, we perform our LVG computations assuming (a) virialized clouds for which the virialization condition (eq. (4.11)) has been imposed and (b) gravitationally-unbound clouds.

To carry out these computations, we use the Mark & Sternberg LVG radiative transfer code described in Davies et al. (2012). Energy levels, line frequencies and Einstein A coefficients are taken from the Cologne Database for Molecular Spectroscopy (CDMS). The excitation and deexcitation rates of the CO rotational levels that are induced by collisions with H\text{2} are taken from Yang et al. (2010) while the C\text{+} collisional rate coefficients come from Flower & Launay (1977) and Launay & Roueff (1977).
4.4.2 Separate CO, C$^+$ Virialized Regions

We first consider a model in which the CO and [CII] emission lines detected at the position of HDF 850.1 originate in separate regions of the molecular gas cloud, regions which are not necessarily at the same temperature and number density. For self-gravitating clouds in virial equilibrium, the velocity gradient is no longer an independent input parameter of the LVG model, but varies with $n_{H_2}$ according to eq. (4.11). To find the unique solution that yields the two observed line ratios, $I_{CO(6-5)}/I_{CO(2-1)}$ and $I_{CO(6-5)}/I_{CO(5-4)}$, we assume a canonical value of $\chi_{CO} = 10^{-4}$ for the relative CO to H$_2$ abundance and vary the remaining two parameters, temperature and molecular hydrogen density, over a large volume of the parameter space. We find, under this virialization constraint, that the observed CO lines are best fit with a kinetic temperature of 70 K and a molecular hydrogen number density of $10^{2.6}$ cm$^{-3}$ (with a corresponding velocity gradient of $\approx 0.16$ km s$^{-1}$ pc$^{-1}$). The column density that yields the correct line intensity magnitudes is $4.2 \times 10^{19}$ cm$^{-2}$, corresponding to a molecular hydrogen gas mass of $M_{H_2} \approx 2.13 \times 10^{11}$ M$_\odot$. The H$_2$ mass to CO luminosity conversion factor obtained in this model is $\alpha = 5.1$ M$_\odot$ (K km s$^{-1}$ pc$^2$)$^{-1}$, a value similar to the Galactic conversion factor observed for virialized molecular clouds in the Milky Way, suggesting that HDF 850.1 may have some properties in common with our Galaxy.

Reducing the relative CO to H$_2$ abundance by a factor of two, to $\chi_{CO} = 5 \times 10^{-5}$, results in a best fit solution with a molecular hydrogen gas mass of $M_{H_2} \approx 2.68 \times 10^{11}$ M$_\odot$, nearly 25% larger than the value obtained assuming $\chi_{CO} = 10^{-4}$. Ranges on the fit parameter consistent with the observational uncertainties are listed in Tables 4.2 and 4.3.
## Chapter 4. CO to Total Gas Mass in High-Z Galaxies

### Table 4.2. LVG Model: Best Fit Parameters

<table>
<thead>
<tr>
<th>Model Parameters†</th>
<th>Separate, virialized</th>
<th>Separate, unvirialized</th>
<th>Mixed, virialized</th>
<th>Mixed, unvirialized</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{\text{kin}}$</td>
<td>70 [K] [30,180]</td>
<td>100 [K] [30,200]</td>
<td>160 [K] [120,180]</td>
<td>180 [K] [140,260]</td>
</tr>
<tr>
<td>$dv/dr$</td>
<td>0.16 [km s$^{-1}$ pc$^{-1}$] [0.14,0.20]</td>
<td>1.6 [km s$^{-1}$ pc$^{-1}$] [0.14,0.28]</td>
<td>0.17 [km s$^{-1}$ pc$^{-1}$]</td>
<td>1.7 [km s$^{-1}$ pc$^{-1}$]</td>
</tr>
<tr>
<td>$\log_{10} n_{H_2}$</td>
<td>2.6 [cm$^{-3}$] [2.5,2.8]</td>
<td>3 [cm$^{-3}$] [3.3,2.2]</td>
<td>2.6 [cm$^{-3}$] [2.6,2.9]</td>
<td>2.9 [cm$^{-3}$] [2.8,3.1]</td>
</tr>
<tr>
<td>$\log_{10} n_H$</td>
<td>– [cm$^{-3}$]</td>
<td>– [cm$^{-3}$]</td>
<td>3 [cm$^{-3}$] [2.8,3.4]</td>
<td>3.4 [cm$^{-3}$] [3.3,3.5]</td>
</tr>
<tr>
<td>$\chi_{CO/H_2}$</td>
<td>$10^{-4}$</td>
<td>$10^{-4}$</td>
<td>$7 \times 10^{-6}$</td>
<td>$7 \times 10^{-6}$</td>
</tr>
<tr>
<td></td>
<td>– [cm$^{-3}$]</td>
<td>– [cm$^{-3}$]</td>
<td>$[5.9] \times 10^{-6}$</td>
<td>$[5.9] \times 10^{-6}$</td>
</tr>
<tr>
<td>$\chi_{CO/H}$</td>
<td>– [cm$^{-3}$]</td>
<td>– [cm$^{-3}$]</td>
<td>$9.3 \times 10^{-5}$</td>
<td>$9.3 \times 10^{-5}$</td>
</tr>
<tr>
<td></td>
<td>– [cm$^{-3}$]</td>
<td>– [cm$^{-3}$]</td>
<td>$[9.1,9.5] \times 10^{-5}$</td>
<td>$[9.1,9.5] \times 10^{-5}$</td>
</tr>
<tr>
<td>$N_{H_2}$</td>
<td>4.2 [10$^{19}$ cm$^{-2}$] [1.9,15]</td>
<td>1.0 [10$^{19}$ cm$^{-2}$] [0.5,5.4]</td>
<td>3.4 [10$^{19}$ cm$^{-2}$] [2.0,7.4]</td>
<td>1.0 [10$^{19}$ cm$^{-2}$] [0.6,1.5]</td>
</tr>
<tr>
<td>$N_H$</td>
<td>– [10$^{19}$ cm$^{-2}$]</td>
<td>– [10$^{19}$ cm$^{-2}$]</td>
<td>8.5 [10$^{19}$ cm$^{-2}$]</td>
<td>2.9 [10$^{19}$ cm$^{-2}$]</td>
</tr>
</tbody>
</table>

†For each model parameter, the top row represents the unique, best fit value obtained for the specified model. The bottom row provides the range of parameter values that yield results consistent with the observed line intensity ratios within the error bars of the observed data points (Walter et al. 2012).
Table 4.3. LVG Model: Results

<table>
<thead>
<tr>
<th>Properties</th>
<th>Separate, virialized</th>
<th>Separate, unvirialized</th>
<th>Mixed, virialized</th>
<th>Mixed, unvirialized</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_{H_2}$</td>
<td>$2.13 \times 10^{11}$</td>
<td>$5.16 \times 10^{10}$</td>
<td>$1.72 \times 10^{11}$</td>
<td>$5.20 \times 10^{10}$</td>
</tr>
<tr>
<td>[M(_\odot)]</td>
<td>[9.26,74.9] \times 10^{10}</td>
<td>[2.61,27.2] \times 10^{11}</td>
<td>[1.11,3.73] \times 10^{11}</td>
<td>[3.37,7.65] \times 10^{10}</td>
</tr>
<tr>
<td>$M_H$</td>
<td>–</td>
<td>–</td>
<td>$2.14 \times 10^{11}$</td>
<td>$7.33 \times 10^{10}$</td>
</tr>
<tr>
<td>[M(_\odot)]</td>
<td>–</td>
<td>–</td>
<td>[1.54,3.01] \times 10^{11}</td>
<td>[5.85,9.4] \times 10^{10}</td>
</tr>
<tr>
<td>$M_{\text{gas}}$</td>
<td>$2.13 \times 10^{11}$</td>
<td>$5.16 \times 10^{10}$</td>
<td>$3.86 \times 10^{11}$</td>
<td>$1.25 \times 10^{11}$</td>
</tr>
<tr>
<td>$L_{CO(1-0)}$</td>
<td>$3.95 \times 10^{10}$</td>
<td>$4.41 \times 10^{10}$</td>
<td>$2.49 \times 10^{10}$</td>
<td>$4.18 \times 10^{10}$</td>
</tr>
<tr>
<td>[K km s(^{-1}) pc(^2)]</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\alpha$(^\dagger)</td>
<td>5.1</td>
<td>1.2</td>
<td>9.8</td>
<td>5.1</td>
</tr>
<tr>
<td>[M(_\odot)(K km s(^{-1}) pc(^2))(^{-1})]</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(^\dagger\) $\alpha$ here is defined as the ratio of total gas mass to CO(1-0) luminosity, $\alpha = M_{\text{gas}}/L'_{CO(1-0)}$. In the models where the CO and [C\(\text{II}\)] lines are assumed to be originating from separate regions, $M_{\text{gas}} = M_{H_2}$ since estimates of the atomic hydrogen gas mass could not be obtained via the LVG calculations. In the models where the CO molecules and C\(^+\) ions are assumed to be uniformly mixed, the total gas mass is the sum of the molecular and the atomic gas masses, $M_{\text{gas}} = M_{H_2} + M_H$. 

88
4.4.3 Separate CO, C$^+$ Unvirialized Regions

We then consider a model in which the CO and [C$\text{II}$] emission lines are assumed to originate from separate regions of gravitationally-unbound molecular clouds. Since unvirialized clouds generally demonstrate a higher degree of turbulence relative to their virialized counterparts, we expect the velocity gradient in this model to be greater than the velocity gradient obtained for the virialized model, $(dv/dr)_{\text{virialized}} \approx 0.16$ km s$^{-1}$ pc$^{-1}$. We therefore fix the velocity gradient to be ten times the virialized value, $(dv/dr)_{\text{unvirialized}} = 1.6$ km s$^{-1}$ pc$^{-1}$, and, assuming a canonical value of $\chi_{\text{CO}} = 10^{-4}$, find the solution that yields the two observed line ratios by varying $T$ and $n_{\text{H}_2}$. We find, under these assumptions, that the CO SED is best fit with a molecular hydrogen density of $10^3$ cm$^{-3}$ and a kinetic temperature of 100 K. For this set of parameters, the beam-averaged H$_2$ column density is $N_{\text{H}_2} \approx 1.0 \times 10^{19}$ cm$^{-2}$, giving an associated molecular gas mass of $M_{\text{H}_2} \approx 5.16 \times 10^{10}$ M$_\odot$. This estimate of the gas mass is nearly 50% larger than that obtained by Walter et al. (2012) by applying the H$_2$ mass-to-CO luminosity relation with the typically adopted conversion factor for ULIRGs, $\alpha = 0.8$ M$_\odot$ (K km s$^{-1}$ pc$^2$)$^{-1}$. Given our inferred H$_2$ gas mass and predicted CO(1-0) line luminosity from our LVG fit, we find that $\alpha = 1.2$ M$_\odot$ (K km s$^{-1}$ pc$^2$)$^{-1}$, in this model.

The increase in molecular hydrogen density and the reduction in inferred mass (relative to the values obtained in the previous model where the virialization condition was imposed) arise from our assumption that the velocity gradient in this model is greater than the velocity gradient obtained in the virialized case. For a fixed $\chi$, the optical depth drops with increasing $dv/dr$ (eq. (4.7)); since $\beta$, the probability of an emitted photon escaping, correspondingly increases, the radiation is less “trapped” and a higher
density, \( n_{H_2} \), is required to produce the observed CO excitation lines. Furthermore, since 
\( I_{i,j} \propto \beta_{i,j} M \), a larger \( \beta \) implies that less mass is required to reproduce an observed set
of line intensities. Therefore, assuming \((dv/dr)_{unvirialized} = 10 (dv/dr)_{virialized}\) causes the
optical depth, and consequently, the inferred mass, to drop by a factor of nearly 4 in this
model.

### 4.4.4 Optically thin [CII]

In the two models above, where the CO and [CII] lines are assumed to be emitted
from separate regions of the molecular clouds, the single detected ionized carbon line is
insufficient in constraining the parameters of the LVG modeled [CII] region. We thus
consider the optically thin regime of the [CII] line (\( \beta \simeq 1 \)), such that

\[
I_{ij} \approx \frac{h\nu_{ij}}{4\pi} A_{ij} x_i \chi_{C^+} N_{H_2} \to \frac{M_{H_2}}{L_{[CII]_{ij}}} = \frac{\mu m_{H_2} (1 + z)^4}{h\nu_{ij} A_{ij} x_i \chi_{C^+}}
\]

(4.13)

where \( \chi_{C^+} \) is the \( C^+ \) to \( H_2 \) abundance ratio (fixed at a value of \( 10^{-4} \) in these
calculations) and \( x_i \) represents the fraction of ionized carbon molecules in the \( i \)th
energy level. Assuming that the fine-structure transition \( J=3/2 \to 1/2 \) is due solely to
spontaneous emission processes and collisions with ortho- and para-\( H_2 \), the equations of
statistical equilibrium reduce to a simplified form and can be solved to obtain \( x_{(J=3/2)} \) as
a function of temperature and \( H_2 \) number density. In Figure 4.1, we have plotted the
resulting mass-to-luminosity ratio, \( M_{H_2}/L_{[CII]} \), as a function of the kinetic temperature
for several different values of \( n_{H_2} \). Given the high [CII]/far-infrared luminosity ratio
of \( L_{[CII]}/L_{FIR} = (1.7 \pm 0.5) \times 10^{-3} \) in HDF 850.1 (Walter et al. 2012), it is reasonable
to assume the ionized carbon is emitting efficiently and to thus consider the high
temperature, large number density limit (\( T_{kin} \simeq 500 \) K, \( n_{H_2} \simeq 10^4 \) cm\(^{-3} \)). In this
Figure 4.1: Dependence of the density ratios, $n_{C^+}/n_{CO}$ (solid line) and $n_{H_2}/n_H$ (dashed line), on the H$_2$ ionization rate $\zeta$ at a fixed solar metallicity $Z'=1$, for our best-fit LVG parameters $T_{kin} = 160$ K and $n_{H_2} = 10^3$ cm$^{-3}$). As $\zeta$ increases, the abundance of C$^+$ relative to CO in the cosmic-ray dominated dark cores of interstellar clouds grows while that of H$_2$ to atomic hydrogen decreases. The desired value $n_{C^+}/n_{CO} \approx 13$ is obtained for $\zeta \approx 2.5 \times 10^{-14}$ s$^{-1}$, at which point $n_{H_2} \approx 0.4n_H$. 

\[ n_{H_2} = 10 \text{ cm}^{-3} \]
\[ n_{H_2} = 10^2 \text{ cm}^{-3} \]
\[ n_{H_2} = 10^3 \text{ cm}^{-3} \]
\[ n_{H_2} = 10^4 \text{ cm}^{-3} \]
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

limit, the mass-to-luminosity ratio is \( \approx 1.035 \, M_\odot (K \, km^{-1} \, pc^2)^{-1} \) and the corresponding molecular gas mass of the \( C^+ \) region, using the detected line intensity of the ionized carbon line \( L_{[CII]} = 1.1 \times 10^{10} \, L_\odot \), is found to be \( M_{H_2} \approx 5.2 \times 10^{10} \, M_\odot \).

4.4.5 Uniformly Mixed CO, \( C^+ \) Virialized Region

We next consider models in which the CO molecules and \( C^+ \) ions are mixed uniformly, such that the corresponding line emissions originate in gas at the same temperature, density, and velocity gradient. For these conditions, the chemistry is driven by cosmic-ray ionization and the density fractions \( n_i/n \) for CO and \( C^+ \) depend on a single parameter, the ratio of the cloud density to the cosmic-ray ionization rate \( \zeta \) (Boger & Sternberg 2005). For Galactic conditions with \( \zeta \sim 10^{-16} \, s^{-1} \), the \( C^+ \) to CO ratio is generally very small. However, in objects such as HDF 850.1 where the ionization rate may be much larger due to high star formation rates, this ratio may be enhanced significantly.

Assuming a virialized cloud with \( \chi_{CO} + \chi_{C^+} = 10^{-4} \), the unique LVG fit for the observed set of line intensity ratios, \( \{I_{[CII]}/I_{CO(2-1)}, I_{[CII]}/I_{CO(5-4)}, I_{[CII]}/I_{CO(6-5)}\} = \{7.08 \pm 1.67, 0.96 \pm 0.19, 1.03 \pm 0.2\} \times 10^2 \) (Walter et al. 2012), yields \( T_{kin} = 160 \, K, n = 10^3 \, cm^{-3} \) and a \( C^+ \) to CO abundance ratio of 13. To estimate the ionization rate required to produce this \( C^+ \)/CO abundance ratio, we employed the Boger & Sternberg (2005) chemical code that captures the \( C^+ \) – C – CO interconversion in a purely ionization-driven chemical medium.

For solar abundances of the heavy elements \( Z' = 1 \), a fairly reasonable assumption given the high star formation rate observed in HDF 850.1, the cosmic-ray ionization rate required to achieve this high \( C^+ \) to CO ratio in a cloud with temperature \( T = 160 \, K \) and
Figure 4.2: Dependence of the density ratios, \( n_{C^+}/n_{CO} \) (solid line) and \( n_{H_2}/n_H \) (dashed line), on the \( H_2 \) ionization rate \( \zeta \) at a fixed solar metallicity \( Z' = 1 \), for our best-fit LVG parameters \( T_{kin} = 160 \) K and \( n_{H_2} = 10^3 \) cm\(^{-3} \)). As \( \zeta \) increases, the abundance of \( C^+ \) relative to CO in the cosmic-ray dominated dark cores of interstellar clouds grows while that of \( H_2 \) to atomic hydrogen decreases. The desired value \( n_{C^+}/n_{CO} \approx 13 \) is obtained for \( \zeta \approx 2.5 \times 10^{-14} \) s\(^{-1} \), at which point \( n_{H_2} \approx 0.4n_H \).
density $n_{H_2}=10^3$ cm$^{-3}$ is of order $\zeta \simeq 2.5 \times 10^{-14}$ s$^{-1}$ (Figure 4.2). This is significantly enhanced compared to the Milky Way value, $\zeta \sim 10^{-16}$ s$^{-1}$, and is plausibly consistent with the fact that HDF 850.1 has a star-formation rate of 850 solar masses per year, a value which is larger than the measured Galactic SFR by a factor of $10^3$ (Walter et al. 2012).

Furthermore, for such a high cosmic-ray ionization rate of this magnitude, the hydrogen is primarily atomic for the implied LVG gas density. We find that the ratio of molecular hydrogen to atomic hydrogen in the interstellar clouds is $n_{H_2}/n_H \approx 0.4$ (Figure 4.2). We thus replace $H_2$ with $H$ as the dominant collision partner. Given the uncertain CO-H rotational excitation rates (see Shepler et al. 2007), we assume that the rate coefficients are equal to the rates for collisions with ortho-$H_2$ (Flower & Pineau Des Forêts 2010). We find that the observed CO and [CII] lines together are best fit with a temperature of 160 K, an atomic hydrogen number density of $n_H = 10^3$ cm$^{-3}$ (with a corresponding velocity gradient of 0.17 km s$^{-1}$ pc$^{-1}$), and an abundance ratio (relative to H) of $9.3 \times 10^{-5}$ and $7 \times 10^{-6}$ for C$^+$ and CO respectively. The column density that yields the correct line intensity magnitudes is $8.5 \times 10^{19}$ cm$^{-2}$, corresponding to an atomic hydrogen gas mass of $M_H \approx 2.14 \times 10^{11}$ M$_\odot$. The molecular hydrogen mass is then $M_{H_2} = 2(n_{H_2}/n_H)M_H \approx 1.72 \times 10^{11}$ M$_\odot$ and the total gas mass estimate is $M_{gas} \approx 3.86 \times 10^{11}$ M$_\odot$. The corresponding conversion factor in this model is $\alpha = 9.8$ M$_\odot$(K km s$^{-1}$ pc$^2$)$^{-1}$, where $\alpha$ is now defined as the total gas mass to CO luminosity ratio.

Reducing the fixed sum of abundance ratios (relative to H) of CO and C$^+$ by a factor of two, to $\chi_{CO} + \chi_{C^+} = 5 \times 10^{-5}$, results in a best fit solution with a total gas mass of $M_{gas} \approx 4.57 \times 10^{11}$ M$_\odot$, nearly 20% larger than the value obtained assuming $\chi_{CO} + \chi_{C^+} = 10^{-4}$.
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

4.4.6 Uniformly Mixed CO, C$^+$ Unvirialized Region

In the case where we assume gravitationally-unbound molecular clouds, we again find a best fit model with a C$^+$ to CO ratio of $\chi_{C^+}/\chi_{CO} \approx 13$, indicating that atomic hydrogen is the dominant collision partner in the LVG calculations. We thus calculate a three-dimensional grid of model CO and [CII] lines, varying $T_{\text{kin}}$, $n_H$, and the relative abundances $\chi_{[\text{CII}]}$ and $\chi_{CO}$, with the constraints that $\chi_{CO} + \chi_{C^+} = 10^{-4}$ and $(dv/dr)_{\text{unvirialized}} = 10(dv/dr)_{\text{virialized}} = 1.7 \text{ km s}^{-1} \text{ pc}^{-1}$. The observed set of CO and [CII] lines, assumed to have been emitted from the same region, are fit best with a temperature of 180 K, an atomic hydrogen number density of $10^{3.4} \text{ cm}^{-3}$ and an abundance ratio of $9.3 \times 10^{-5}$ and $7 \times 10^{-6}$ for C$^+$ and CO respectively. For this set of parameters, the beam-averaged H column density is well constrained to be $N_H \approx 2.9 \times 10^{19} \text{ cm}^{-2}$. This corresponds to an atomic and molecular gas mass of $M_H \approx 7.33 \times 10^{10} \text{ M}_\odot$ and $M_{H_2} \approx 5.20 \times 10^{10} \text{ M}_\odot$ respectively, yielding a total gas mass estimate of $M_{\text{gas}} \approx 1.25 \times 10^{11} \text{ M}_\odot$. The ratio of the total gas mass to the CO luminosity in this model is $\alpha = 5.1 \text{ M}_\odot(\text{K km s}^{-1} \text{ pc}^2)^{-1}$.

4.5 Cosmological Constraints

Our inferred gas masses enable us to set cosmological constraints. For a particular set of cosmological parameters, the number density of dark matter halos of a given mass can be inferred from the halo mass function. The Sheth-Tormen mass function, which is based on an ellipsoidal collapse model, expresses the comoving number density of halos
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

$n$ per logarithm of halo mass $M$ as,

$$n_{ST}(M) = \frac{dn}{d\log M} = A \sqrt{\frac{2a}{\pi}} \rho_m \frac{d\nu}{d\log M} (1 + \frac{1}{(av^2)^p}) e^{-av^2/2} \tag{4.14}$$

where a reasonably good fit to simulations can be obtained by setting $A = 0.322$, $a = 0.707$, and $p = 0.3$ (Sheth & Tormen 1999). Here, $\rho_m$ is the mean mass density of the universe and $\nu = \delta_{\text{crit}}(z)/\sigma(M)$ is the number of standard deviations away from zero that the critical collapse overdensity represents on mass scale $M$. Integrating this comoving number density over a halo mass range and volume element thus yields $N$, the expectation value of the total number of halos observed within solid angle $A$ with mass greater than some $M_h$ and redshift larger than some $z$,

$$N(z, M_h) = \frac{c}{H_0} A \int_z^\infty dz \frac{D_A(z)^2}{\sqrt{\Omega_m (1+z)^3 + \Omega_\Lambda}} \int_M^{M_h} d\log M \frac{dn}{d\log M} \tag{4.15}$$

where $H_0$ is the Hubble constant, $D_A$ is the angular diameter distance, and $\Omega_m$ and $\Omega_\Lambda$ are the present-day density parameters of matter and vacuum, respectively.

Under the assumption that the number of galaxies in the field of observation follows a Poisson distribution, the probability of observing at least one such object in the field is then $P = 1 - F(0, N)$ where $F(0, N)$ is the Poisson cumulative distribution function with a mean of $N$. Given the detection of HDF 850.1, we can say that out of the hundreds of submillimetre-bright galaxies identified so far, at least one has been detected in the Hubble Deep Field at a redshift $z > 5$ with a halo mass greater than or equal to the halo mass associated with this source. This observation, taken together with the theoretical number density predicted by the Sheth-Tormen mass function, implies that an atomic model that yields an expectation value $N$ can be ruled out at a confidence level of

$$F(0, N(5, M_{h,min})) \tag{4.16}$$
where the solid angle covered by the original SCUBA field in which HDF850.1 was discovered is $\simeq 9$ arcmin$^2$ (Hughes et al. 1998) and a $\Lambda$CDM cosmology is assumed with $H_0 = 70$ km s$^{-1}$ Mpc$^{-1}$, $\Omega_m = 0.73$, and $\Omega_{m} = 0.27$ (Komatsu et al. 2011). $M_{h,min}$, the minimum inferred halo mass for HDF 850.1, is related to the halo’s minimum baryonic mass component, a quantity derived in section 4.4 via the LVG technique, in the following way:

$$M_{h,min} = \frac{\Omega_{m}}{\Omega_{b}} M_{b,min} \quad (4.17)$$

where the baryonic and the total matter density parameters are $\Omega_{b} = 0.05$ and $\Omega_{m} = 0.27$ respectively. Each model’s estimate of the minimum baryonic mass associated with HDF 850.1 therefore corresponds to an estimate of $N(\tilde{\tau}, M_{h,min})$ and respectively yields the certainty with which the model can be discarded.

The confidence with which models can be ruled out on this basis is plotted as a function of the minimum baryonic mass estimated by the model (solid curve in Figure 4.3). To check the consistency of the four LVG models considered in section 4.4 with these results, dashed lines representing the masses derived from each model are included in the plot (upper left panel). Assuming the CO and [CII] molecules are uniformly mixed in virialized clouds results in a baryonic mass $M_{b,min} \sim 3.86 \times 10^{11}$ M$_{\odot}$. The probability of observing at least one such source, with a corresponding halo mass $M_{h} \geq 2.1 \times 10^{12}$ M$_{\odot}$, is $\sim 7 \times 10^{-2}$; this model can thus be ruled out at the 1.8$\sigma$ level (solid). The model which postulate separate virialized regions (dashed) can be ruled out with relatively less certainty, at the 1$\sigma$ level. On the other hand, modeling the CO and [CII] emission lines as originating from mixed (dotted) or separate (dash-dot) unvirialized regions, results in minimum baryonic masses which are consistent with the constraint posed by eq. (4.15). We expect to find $N \sim 1.5$ and 10 such halos, respectively, at a redshift $z \geq 5$. The
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

Figure 4.3: $N$ represents the expectation value of the number of halos one expects to find with mass $M_b \geq M_{b,min}/f_b$ at a redshift $z \geq 5$ within a solid angle of $A_{HDF} \approx 9$ arcmin$^2$. Assuming that the number of galaxies in a field of observation follows a Poisson distribution, the probability of observing at least one such object in the field with $M_b \geq M_{b,min}/f_b$ at a redshift $z \geq 5$ is $1 - F(0, N(z, M_{b,min}))$ where $F(0, N)$ is the Poisson cumulative distribution function with a mean of $N$. The confidence with which an LVG model can be ruled out as a function of the minimum baryonic mass derived from the model is therefore $P = F(0, N)$ (solid curve). **Upper left panel:** The vertical lines represent the mass values obtained for each of the four models presented in section 4.4: (a) separate and virialized (dashed), (b) separate and unvirialized (dash-dot), (c) mixed and virialized (solid), and (d) mixed and unvirialized regions (dotted). In models (a) and (b), $M_{b,min} = M_{H_2}$ while in models (c) and (d), $M_{b,min} = M_{H_2} + M_H$. **Upper right panel:** The minimum baryonic masses obtained for each model were doubled to account for neglected contributions to the total gas mass; models (a) and (c) can now be ruled out at the $2\sigma$ and $2.7\sigma$ levels respectively. **Lower left panel:** The vertical lines represent the mass values implied by the predicted CO(1-0) line luminosities from models (a) and (b) with a CO-to-H$_2$ conversion factor of $\alpha = 0.8$ and $4.6$ $M_\odot$ (K km s$^{-1}$ pc$^2$)$^{-1}$. If these minimum baryonic mass values are then doubled (**lower right panel**), both models can be ruled out at the $\sim 1.8\sigma$ level in the case where $\alpha = 4.6$ $M_\odot$ (K km s$^{-1}$ pc$^2$)$^{-1}$ is adopted as the conversion factor.
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

fact that the expected average number of observed sources for the latter model is much higher than the actual number of sources observed may be due to the incompleteness of the conducted survey and is therefore not grounds for ruling out this model.

The baryonic masses, obtained via the LVG method, represent conservative estimates of the total baryonic content associated with HDF 850.1. In particular, mass contributions from any ionized gas or stars residing in the galaxy are not taken into account, and in the models where a layered cloud structure is assumed, the atomic hydrogen mass component is left undetermined. Furthermore, ejection of baryons to the IGM through winds may result in a halo baryon mass fraction that is smaller than the cosmic ratio, $\Omega_b/\Omega_m$, used in this paper, resulting in a conservative estimate of the minimum halo mass. We therefore consider the effects on the predicted number of observed halos, $N(M_{b,\text{min}})$, if the minimum baryonic mass derived for each model is doubled, e.g. assuming a molecular-gas mass fraction of $\sim 1/2$ (Tacconi et al. 2013). Using these more accurate estimates of HDF 850.1’s baryonic mass, we find that the two models in which the virialization condition is enforced can be ruled out at the $\sim 2.7\sigma$ and $2\sigma$ level for the mixed and separate models, respectively (upper right panel).

For comparison, we also consider the gas masses implied by the CO(1-0) line luminosities predicted by the two models where distinct CO and C$^+$ layers are assumed (lower left panel). Adopting a CO-to-H$_2$ conversion factor of $\alpha = 0.8$ (K km s$^{-1}$ pc$^2$)$^{-1}$, we find that enforcing the cosmological constraint posed by the abundance of dark matter halos does not rule out either of the two models in which separate CO and C$^+$ regions were assumed, even if the minimum baryonic masses are doubled to account for neglected contributions to the total gas mass (lower right panel). If a conversion factor of $\alpha = 4.6$ (K km s$^{-1}$ pc$^2$)$^{-1}$ is used, both models can be ruled out at the $\sim 1\sigma$ level and
increasing these obtained masses by a factor of two drives up the sigma levels to \( \sim 1.8\sigma \) for both models.

### 4.6 Summary

In this paper, we employed the LVG method to explore alternate model configurations for the CO and C\(^+\) emission lines regions in the high-redshift source HDF 850.1. In particular, we considered emissions originating from (i) separate virialized regions, (ii) separate unvirialized regions, (iii) uniformly mixed virialized regions, and (iv) uniformly mixed unvirialized regions. For models (i) and (ii) where separate CO and C\(^+\) regions were assumed, the kinetic temperature, \( T_{\text{kin}} \), and the molecular hydrogen density, \( n_{H_2} \), were fit to reproduce the two observed line ratios, \( I_{\text{CO}(6-5)}/I_{\text{CO}(2-1)} \) and \( I_{\text{CO}(6-5)}/I_{\text{CO}(5-4)} \), for a fixed canonical value of the CO abundance (relative to H\(_2\)), \( \chi_{\text{CO}} = 10^{-4} \). The column density of molecular hydrogen, \( N_{H_2} \), was then fit to yield the correct line intensity magnitudes and the molecular gas mass was derived for each respective model. In models (iii) and (iv) where the CO molecules and C\(^+\) ions were assumed to be uniformly mixed with abundance ratios that satisfied the constraint, \( \chi_{\text{CO}} + \chi_{C^+} = 10^{-4} \), we found that a relatively high ionization rate of \( \zeta \simeq 2.5 \times 10^{-14} \text{ s}^{-1} \) is necessary to reproduce the set of observed line ratios, \( \{ I_{[\text{CII}]}/I_{\text{CO}(2-1)}, I_{[\text{CII}]}/I_{\text{CO}(5-4)}, I_{[\text{CII}]}/I_{\text{CO}(6-5)} \} \). Since the hydrogen in a cloud experiencing an ionization rate of this magnitude is primarily atomic, two additional parameters, \( n_H \) and \( N_H \), were introduced and the set of LVG parameters, \( \{ T_{\text{kin}}, n_{H_2}, n_H, \chi_{\text{CO}}, \chi_{C^+}, N_{H_2}, N_H \} \), were fit and used to obtain both a molecular and an atomic hydrogen gas mass for each model. The gas masses derived by employing the LVG technique thus represent conservative estimates of...
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

the minimum baryonic mass associated with HDF 850.1.

These estimates were then used, together with the Sheth-Tormen mass function for dark matter halos to calculate the average number of halos with mass \( M_h \geq M_{b,\text{min}} \) that each model predicts to find within the HDF survey volume. Given that at least one such source has been detected, we found that models (i) and (iii) can be ruled out at the 1\( \sigma \) and 1.8\( \sigma \) levels respectively. The confidence with which these models are ruled out increases if a less conservative estimate of the baryonic mass is taken; increasing the LVG-modeled gas masses by a factor of two to account for neglected contributions to the total baryonic mass, drives up these sigma levels to \( \sim 2\sigma \) and 2.7\( \sigma \) respectively. Furthermore, model (iv) can now be ruled out at the 1\( \sigma \) level as well. We are therefore led to the conclusion that HDF 850.1 is modeled best by a collection of unvirialized molecular clouds with distinct CO and C\(^+\) layers, as in PDR models. The LVG calculations for this model yield a kinetic temperature of 100 K, a velocity gradient of 1.6 km s\(^{-1}\) pc\(^{-1}\), a molecular hydrogen density of \( 10^3 \) cm\(^{-3}\), and a column density of \( 10^{19} \) cm\(^{-2}\). The corresponding molecular gas mass obtained using this LVG approach is \( M_{H_2} \approx 5.16 \times 10^{10} \) M\(_\odot\). For this preferred model we find that the CO-to-H\(_2\) luminosity to mass ratio is \( \alpha = 1.2 \) (K km s\(^{-1}\) pc\(^2\))\(^{-1}\), close to the value found for ULIRGs in the local universe.

4.7 Acknowledgements

We thank Dean Mark for his assistance with the LVG computations. This work was supported by the Raymond and Beverly Sackler Tel Aviv University-Harvard/ITC Astronomy Program. A.L. acknowledges support from the Sackler Professorship by
CHAPTER 4. CO TO TOTAL GAS MASS IN HIGH-Z GALAXIES

Special Appointment at Tel Aviv University. This work was also supported in part by NSF grant AST-0907890 and NASA grants NNX08AL496 and NNA09DB30A (for A.L.).
Chapter 5

High-J CO Sleds in Nearby Infrared Bright Galaxies Observed by Herschel/PACS

This thesis chapter originally appeared in the literature as

CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

5.1 Abstract

We report the detection of far-infrared (FIR) CO rotational emission from nearby active galactic nuclei (AGN) and starburst galaxies, as well as several merging systems and Ultra-Luminous Infrared Galaxies (ULIRGs). Using Herschel-PACS, we have detected transitions in the $J_{\text{upp}} = 14 - 20$ range ($\lambda \sim 130 - 185$ $\mu$m, $\nu \sim 1612 - 2300$ GHz) with upper limits on (and in two cases, detections of) CO line fluxes up to $J_{\text{upp}} = 30$. The PACS CO data obtained here provide the first well-sampled FIR extragalactic CO Spectral Line Energy Distributions (SLEDs) for this range, and will be an essential reference for future high redshift studies. We find a large variety in overall SLED shape, demonstrating the uncertainties in relying solely on high-J CO diagnostics to characterize the excitation source of a galaxy. Combining our data with low-J line intensities taken from the literature, we present a CO ratio-ratio diagram and discuss its potential diagnostic value in distinguishing excitation sources and physical properties of the molecular gas. We find that the position of a galaxy on such a diagram is less a signature of its excitation mechanism, but rather an indicator of the presence (or absence) of warm, dense molecular gas. We then quantitatively analyze the CO emission from a subset of the detected sources with Large Velocity Gradient (LVG) radiative transfer models to fit the CO SLEDs. Using both single-component and two-component LVG models to fit the kinetic temperature, velocity gradient, number density and column density of the gas, we derive the molecular gas mass and the corresponding CO-to-H$_2$ conversion factor, $\alpha_{\text{CO}}$, for each respective source. For the ULIRGs we find $\alpha$ values in the canonical range $0.4 - 5$ $M_\odot/(K \text{ km}^{-1}\text{pc}^2)$, while for the other objects, $\alpha$ varies between 0.2 and 14. Finally, we compare our best-fit LVG model results with those
obtained in previous studies of the same galaxies and comment on any differences.

5.2 Introduction

Molecular spectral line energy distributions (SLEDs) provide us with the opportunity to probe the average state of the molecular gas in galaxies and estimate the total and star-forming molecular gas masses in these sources. Carbon monoxide (CO), the most abundant molecule after molecular hydrogen, is the most commonly employed tracer of interstellar molecular gas. With the small gaps between its energy levels allowing for a fine sampling of density-temperature relations, CO has become an important tool in the study of the star formation energetics and the effects of AGN in nearby galaxies.

The lowest 3 rotational transitions of CO, which trace the cooler gas component, are relatively easily accessible with ground-based radio and submillimeter telescopes, and have been observed in many local galaxies. On the other hand, far-IR CO rotational lines, with $J_{upp} \geq 13$, arise from states 500 - 7000 K above ground and have critical densities of $10^6 \sim 10^8$ cm$^{-3}$ (Hailey-Dunsheath et al. 2012). These lines, which trace the warmer, denser molecular gas in the center of galaxies, are difficult to excite solely with star formation and can thus be used to test models that distinguish between AGN and starburst systems. However, until the advent of Herschel, the diagnostic use of these higher rotational levels was poorly developed since these lines were either difficult to observe or completely inaccessible from the ground.

The Herschel Space Observatory (Pilbratt et al. 2010) is uniquely suited to measure the submillimeter properties of nearby galaxies in a frequency range that
cannot be observed from the ground. This paper focuses on the data obtained with the Photodetector Array Camera and Spectrometer (PACS) (Poglitsch et al. 2010) on-board the Herschel Space Observatory, which provides observations in the 60 - 210 \( \mu\)m wavelength range, sampling the FIR CO emission of high-J transition lines between \( J_{\text{upp}} = 14 \) up to \( J_{\text{upp}} = 50 \).

Complementary CO observations are provided by the Spectral and Photometric Imaging Receiver (SPIRE) (Griffin et al. 2010) which consists of an imaging Fourier Transform Spectrometer (FTS) continuously covering the spectral range from 190 - 670 \( \mu\)m. The CO rotational ladders (from \( J_{\text{upp}} = 4 \) to \( J_{\text{upp}} = 13 \)) of several extragalactic sources have been studied with SPIRE-FTS within the last five years, including the nearby starbursts and AGNs NGC 253, M 82, IC 694, and NGC 3690 (Rosenberg et al. 2014a; Panuzzo et al. 2010; Rosenberg et al. 2014b), and the local ULIRGs Arp 220, NGC 6240, and Mrk 231 (Rangwala et al. 2011; Meijerink et al. 2013; van der Werf et al. 2010). In Hailey-Dunsheath et al. (2012) we have carried out a detailed analysis of the full CO SLED of the Seyfert 2 galaxy NGC 1068 using ground based and PACS observations, which was complemented by an analysis of the SPIRE data for this object by Spinoglio et al. (2012).

In this paper, we want to address the question of to what extent high-J CO transitions can be used to trace the excitation conditions in galactic nuclei, in particular the existence and physical properties of starburst-heated, AGN-heated or shock-heated gas. We therefore present the PACS \(^{12}\)CO line dataset for a sample of local sources including nearby starburst galaxies (NGC 253, M 83, M 82, IC 694, NGC 3690), Seyfert galaxies (NGC 4945, Circinus, NGC 1068, Cen A), (U)LIRGs (NGC 4418, Arp 220, NGC 6240, Mrk 231), and the nearby interacting system (Antennae). In section 5.3 we
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

describe the source sample and the Herschel-PACS observations of the FIR CO lines in these sources, as well as observations of the CO(18-17) and CO(20-19) line fluxes and upper limits of 19 ULIRGs of the Revised Bright Galaxy Sample (RBGS). In section 5.4 we discuss the potential use of line ratios as a diagnostic tool for distinguishing between different energy sources responsible for gas excitation, e.g. starbursts or AGN, and introduce the LVG radiative transfer modeling technique used to analyze the full CO SLEDs. In section 5.5 we present estimates of the physical parameters characterizing the molecular gas, obtained from single-component and two-component LVG fits to the data. We also derive the CO-to-H$_2$ conversion factors in these sources and compare our LVG results to those obtained in previous studies of these galaxies. We conclude with a summary of our findings and their implications in section 5.6.

5.3 Target Selection, Observations, and Data

Reduction

The *Herschel* data presented here are part of the guaranteed time key program SHINING (Survey with Herschel of the ISM in Nearby INfrared Galaxies, PI: E. Sturm), which studies the far-infrared properties of the ISM in starbursts, Seyfert galaxies and infrared luminous galaxies, as well as the OT1 and OT2 follow up programmes (PIs: S. Hailey-Dunsheath and J. Fischer) and the OT1 programme of R. Meijerink. The observations were made with the PACS spectrometer on board the Herschel Space Observatory.

To fully characterize the high-J CO emission associated with star formation,
AGN, and large-scale shocks in galaxies, we defined a sample of objects consisting of 4 starbursts (NGC 253, M 83, M 82, IC 694), 4 Seyferts (NGC 4945, Circinus, NGC 1068, Cen A), three ULIRGs (Arp 220, NGC 6240, Mrk 231), the highly obscured LIRG NGC 4418, and the nearby, well-studied interacting system NGC 4038/4039 (Antennae). The observations of IC 694 were complemented by observations of NGC 3690 (a mixed source with a low luminosity AGN). Together, these two objects are known as the merger system Arp 299. For the Antennae system we obtained 2 pointings, one centered on the nucleus of NGC 4039 and one on the overlap region between NGC 4038 and NGC 4039. The AGN subsample is restricted to the most nearby systems, where the high spatial resolution of PACS (~ 10 arcsec corresponding to ~ 200 pc at $d = 4$ Mpc) helps separate the AGN-heated gas from most of the gas in the circumnuclear star-forming region.

In most of these galaxies, we measured a set of 7 far-IR CO transitions to provide a coarse but sensitive sampling of the CO SLED over the full FIR range: CO(15-14), CO(16-15), CO(18-17), CO(20-19), CO(22-21), CO(24-23), and CO(30-29). We have carefully inspected our full range (55-200 $\mu$m) scan of Arp 220 (González-Alfonso et al. 2012), which is rich in molecular lines, and verified that these CO lines are not contaminated by other molecular features. For some of the objects, additional PACS high-J CO data are available: with SHINING we obtained full range PACS spectra of NGC 1068, NGC 4418, NGC 4945, and M 82, together with full spectra of Mrk 231 and NGC 6240 from a SHINING-related OT2 programme (PI: J. Fischer). These data cover high-J transitions between $J_{\text{upp}} = 14$ and $J_{\text{upp}} = 50$. In the case of NGC 6240, the CO(16-15), CO(18-17), CO(24-23) data were taken from the shared OT1 programmes of R. Meijerink and S. Hailey-Dunsheath; the CO(14-13) and CO(28-27) lines of NGC 6240 and IC 694 were taken from the Meijerink OT1 programme as well. Combined with
existing ground-based and SPIRE observations, these measurements sample the CO ladder from CO(1-0) to CO(30-29) in a number of well-studied galaxies that are often used as templates, allowing us to address the questions posed in the introduction, e.g. to what extent high-J CO transitions can be used to unambiguously trace the existence and physical properties of AGN-heated gas.

As part of the SHINING observations, we also obtained CO(18-17) and CO(20-19) fluxes or upper limits in 19 ULIRGs of the RBGS (Sanders et al. 2003), in addition to Arp 220, Mrk 231 and NGC 6240. These are local ULIRGs ($z < 0.1$) with total 60 $\mu$m flux density greater than 5.24 Jy (and $L_{IR} > 10^{12}L_{\odot}$). We include these data in our study below in order to assess the use of high-J CO transitions as probes of the excitation mechanisms in luminous dusty sources. The observation details for the PACS data, together with galaxy classifications, are summarized in Table 5.1.

Finally, for a subset of the RBGS ULIRGs for which no CO(6-5) data existed in the literature, we observed this line using APEX with the CHAMP$^+$ receiver (see Table 5.2). The APEX data were reduced with the standard software in CLASS. Calibration was obtained with the APEX calibration software (Muders et al. 2006).

Most of the PACS CO observations were made in PACS range scan mode with a 2600 km s$^{-1}$ velocity coverage, while for the merging systems we increased this to 3000 km s$^{-1}$ to ensure the detection of broad lines. The PACS data reduction was done using the standard PACS reduction and calibration pipeline (ipipe) included in HIPE 6.

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1This part of the publication is based on data acquired with the Atacama Pathfinder Experiment (APEX). APEX is a collaboration between the Max-Planck-Institut fur Radioastronomie, the European Southern Observatory, and the Onsala Space Observatory.
CHAPTER 5. *HIGH-J CO IN NEARBY GALAXIES*

Table 5.1: Observation Details of the PACS Data

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<td>1342225144 to -48</td>
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<td>1342191153 and -54, 1342203120 to -30,</td>
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Table 5.2: The CO J=1-0, 6-5, 18-17, and 20-19 flux measurements for the ULIRG sample

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<th>CO(6-5)</th>
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<th>Log(L$_{AGN}$)</th>
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<td>[W m$^{-2}$]</td>
<td>[W m$^{-2}$]</td>
<td>[W m$^{-2}$]</td>
<td>[W m$^{-2}$]</td>
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<td>F09320+6134</td>
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<td>92±29</td>
<td>42±12</td>
<td>56.9</td>
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<td>11.87</td>
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<td>258±68</td>
<td>289±43</td>
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</tr>
</tbody>
</table>

**Note.** Velocity-integrated line flux densities in central PACS spaxel ($\theta = 9.4''$) in units of 10$^{-19}$ W m$^{-2}$

---

*IRAS name

*Papadopoulos et al. (2012a); Chung et al. (2009); Mirabel et al. (1990); Solomon et al. (1997)

*20551-4259 and 23128-5919 were detected by us with APEX; rest taken from Papadopoulos et al. (2012a)

*PACS measurements

*AGN fractions, taken from Veilleux et al. (2009, 2013), are included for those ULIRGs that appear in the ratio-ratio plot of Figure 5.2. The AGN fractions for Arp 220, NGC 6240, and Mrk 231 are 18.5%, 25.8%, and 70.9% respectively. The AGN luminosities for these three sources are 11.5, 11.32, and 12.45 respectively.

*AGN Luminosity ($= AGN_{frac} * L_{bol}$)
For the final calibration we normalized the spectra to the telescope flux and recalibrated it with a reference telescope spectrum obtained from dedicated Neptune continuum observations. This ‘background normalization’ method is described in the PACS data reduction guide. We also assessed the line flux uncertainties associated with the uncertainties in defining the continuum and estimated an absolute line flux accuracy of 20% with this method.

The PACS spectrometer performs integral field spectroscopy over a 47″ × 47″ FoV, resolved into a 5 × 5 array of 9.4″ spatial pixels (spaxels.) With the exception of M 83, M 82, and NGC 3690, the high-J lines in the PACS range for the remaining sources are all consistent with arising in the central spaxel, with little, if any, flux detected outside of the central spaxel. The fluxes were thus extracted from the central spaxel only (θ = 9.4″), and referenced to a point source by dividing by the recommended point source correction factors as given in the PACS manual. We did spot checks with HIPE 11 and verified that this does not yield significantly different line fluxes or upper limits.

In the case of M 83 and M 82 where the high-J CO emission are extended beyond the central spaxel, the fluxes were derived by integrating over the entire PACS FoV. For NGC 3690, the PACS flux measurements cover both the galaxy, as well as an extended region of star formation where the galaxy disks of NGC 3690 and IC 694 overlap. The high-J line fluxes for this source were thus derived by co-adding the 3 spaxels covering components B and C (as NGC 3690 and the overlap region are respectively referred to in the literature).

To supplement these PACS line observations, we collect low and mid-J line fluxes for these sources from the literature and, when necessary, apply aperture corrections using
available CO maps. For point-like sources such as Arp 220, NGC 6240, and Mrk 231, where the low and mid-J line fluxes are fully contained in the PACS beam, no aperture corrections are necessary. This is also deemed to be the case for NGC 4418 and IC 694, where $^{12}$CO J=1-0, J=2-1, and J=3-2 maps reveal the emission to be fully enclosed within a $\theta \sim 10''$ beam (Sakamoto et al. 2013; Sliwa et al. 2012; Casoli et al. 1999). The morphology of NGC 1068, which is composed of a compact central circumnuclear disk ($\theta \sim 4''$) and an extended ring ($\theta \sim 20-40''$), is slightly more complex. To avoid potential scaling issues, we only consider lines that are probed on the scale of the compact source at the center of NGC 1068, i.e. the interferometric measurements of the $J_{upp} = 1 - 3$ lines integrated over the central 4'' by Krips et al. (2011), and the $J_{upp} = 9 - 13$ lines probed by SPIRE FTS with a beam width of $\theta \sim 17''$ (Spinoglio et al. 2012).

In the case of M 83, aperture corrections are also deemed unnecessary since PACS flux measurements for this source extend over a $\sim 21''$ area, and the low and mid-J lines found in the literature refer to a similar beam size (Bayet et al. 2006; Israel & Baas 2001). Similarly, for M 82, the $J_{upp} = 4 - 13$ $^{12}$CO lines are referenced to the $\sim 43''$ beam size of the SPIRE spectrometer (Kamenetzky et al. 2012) and therefore do not need to be scaled when compared against the high-J lines which fill the PACS FoV ($\theta = 47''$) in this source. The $^{12}$CO J=1-0 map for M 82 indicates that the low-J lines are also not in need of any scaling corrections since the emission is predominately contained within an $\sim 25''$ area, consistent with the FWHP beam of 24.4'' referenced for the $J_{upp} = 1 - 3$ line measurements (Ward et al. 2003).

$^{12}$CO J=1-0, J=2-1, and J=3-2 maps for the Arp 299 merger system show that the source sizes of NGC 3690 and the overlap region are $\theta \sim 2''$ and 4'' respectively, and that the combined emission from these two components does not extend beyond $\theta \sim 19''$ (the
CHAPTER 5. *HIGH-J CO IN NEARBY GALAXIES*

PACS aperture size over which the high-J lines were integrated) (Sliwa et al. 2012). The low-J line fluxes for this region are thus derived by co-adding the flux values presented in the literature for components B and C without any further scaling corrections. The mid-J line fluxes are taken from SPIRE observations which include contributions from both components, B and C (Rosenberg et al. 2014b). Although the SPIRE beam sizes vary (15-42"), it is assumed that the fluxes, too, are mostly contained within a 19" beam and no further scaling is applied.

In the case of NGC 4945 and Circinus, available CO maps of the low-J lines indicate that these sources are spatially resolved and more extended than the PACS single spaxel size (Dahlem et al. 1993; Mauersberger et al. 1996; Curran et al. 2008; Zhang et al. 2014). Since the recorded fluxes fill the respective beams with which they were probed, we assume a uniform distribution of flux and linearly scale the low-J emission with the ratio of the PACS spaxel area and the respective literature beam area. A similar technique is applied to NGC 253, where the extended low and mid-J lines corrected to a 15" beam are assumed to be uniformly distributed over that beam size and are thus scaled linearly with the PACS area (Rosenberg et al. 2014a; Hailey-Dunsheath et al. 2008).

The PACS measurements, along with the (aperture-corrected) low-J line fluxes collected from the literature, are summarized in Tables 5.3 and 5.4.
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

Table 5.3:: CO Line Observations

<table>
<thead>
<tr>
<th>Lines</th>
<th>Flux (10^{-17} \text{ W m}^{-2})</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>NGC 253(^1)</td>
</tr>
<tr>
<td>CO(1-0)</td>
<td>0.4±0.1</td>
</tr>
<tr>
<td>CO(2-1)</td>
<td>4.4±0.7</td>
</tr>
<tr>
<td>CO(3-2)</td>
<td>11.3±1.6</td>
</tr>
<tr>
<td>CO(4-3)</td>
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<td>CO(5-4)</td>
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<td>37.6±13.5</td>
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</tr>
<tr>
<td>CO(28-27)</td>
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</tr>
<tr>
<td>CO(29-28)</td>
<td>...</td>
</tr>
<tr>
<td>CO(30-29)</td>
<td>&lt;14.6</td>
</tr>
</tbody>
</table>

\(^1\)Rosenberg et al. (2014a); Hailey-Dunsheath et al. (2008)

\(^2\)Bayet et al. (2006); Israel & Baas (2001)

\(^3\)Ward et al. (2003); Kamenetzky et al. (2012)
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

Table 5.3 (Continued)

<table>
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<th>Lines</th>
<th>Flux</th>
<th>[10^{-17} W m^{-2}]</th>
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<td></td>
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</tr>
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<td>CO(4-3)</td>
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<tr>
<td>CO(18-17)</td>
<td>2.5±0.5</td>
<td>4.4±0.9</td>
</tr>
<tr>
<td>CO(19-18)</td>
<td>1.5±0.3</td>
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<td>&lt; 1.3</td>
<td>3.0±0.6</td>
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<td>…</td>
</tr>
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<td>CO(24-23)</td>
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\(^4\)Hitschfeld et al. (2008); Weiss (private communication)

\(^5\)Krips et al. (2011); Spinoglio et al. (2012)

\(^6\)Sakamoto et al. (2013); Aalto et al. (2007)

\(^7\)Rosenberg et al. (2014b)

\(^8\)Rangwala et al. (2011); Greve et al. (2009)

\(^9\)Meijerink et al. (2013); Greve et al. (2009)

\(^10\)van der Werf et al. (2010); Papadopoulos et al. (2007)
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

Table 5.3 (Continued)

<table>
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<th>Flux</th>
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<td></td>
<td>NGC 4418^6</td>
<td>IC 694^7</td>
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<tr>
<td>CO(25-24)</td>
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<td>⋯</td>
<td>⋯</td>
</tr>
<tr>
<td>CO(27-26)</td>
<td>⋯</td>
<td>⋯</td>
</tr>
<tr>
<td>CO(28-27)</td>
<td>⋯</td>
<td>&lt; 2.3</td>
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<tr>
<td>CO(29-28)</td>
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<td>⋯</td>
</tr>
<tr>
<td>CO(30-29)</td>
<td>⋯</td>
<td>&lt;2.5</td>
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Note. With the exception of M 83, M 82, and NGC 3690, the line fluxes recorded in this table represent the fluxes contained in a $\theta = 9.4''$ beam for each source. Flux values have been normalized to this beam size when necessary, using aperture corrections discussed in section 5.3. In the case of M 83, M 82, and NGC 3690 the fluxes are those contained in $\theta = 21''$, 47'', and 19'' beams, respectively. References for the $J_{upper} < 14$ line fluxes collected from the literature are given below.

Table 5.4: Additional PACS CO Line Observations

<table>
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<th>Lines</th>
<th>Flux [10^{-17} W m^{-2}]</th>
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<td>Centaurus A</td>
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<tr>
<td>CO(15-14)</td>
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<td>CO(16-15)</td>
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</tr>
<tr>
<td>CO(18-17)</td>
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</tr>
<tr>
<td>CO(20-19)</td>
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<td>CO(22-21)</td>
<td>&lt; 2.6</td>
</tr>
<tr>
<td>CO(24-23)</td>
<td>&lt;2.6</td>
</tr>
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</table>
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

5.4 Excitation Analysis

5.4.1 CO SLEDs and Line Ratios

The observed CO SLEDs of the sources, whose excitation conditions will further be explored in the following sections, display a large variation in overall SLED shapes (Figure 5.1). On a first glance this spread seems to nicely follow the qualitatively expected behavior that the strength of high-J CO lines increases with increasing importance of an AGN in these sources. For instance, the CO SLED of the archetypal starburst galaxy M 82 peaks at around $J_{\text{upp}} = 7$ and then quickly declines towards higher J values, while the archetypal Seyfert 2 galaxy NGC 1068 shows strong CO lines even above $J_{\text{upp}} = 20$. In Mrk 231, the CO SLED rises up to $J_{\text{upp}} = 5$ and then remains relatively flat for the higher-J transitions, consistent with the presence of a central X-ray source illuminating the circumnuclear region. However, other sources do not seem to follow the expected trends. The starburst galaxy NGC 253 and the ULIRG NGC 6240, a mixed source thought to be less dominated by its AGN than e.g. Mrk 231 (based on mid-IR diagnostics) exhibit extremely strong high-J lines, suggesting that other excitation sources, like warm PDRs (as in NGC 253) or strong shocks (as in NGC 6240) have to be considered as well, i.e. that the pure detection of a high-J CO line alone is not an unambiguous signature of an XDR excited by an AGN. In a previous paper (Hailey-Dunsheath et al. 2012), we showed that the well characterized SLED of NGC 1068 could not be uniquely explained with a mixture of PDR, XDR, and shock models. It was only with additional information that an AGN could be identified as the most likely excitation source of the highly excited components. Our new findings here, drawn from a much larger sample, underline the importance of this caveat.
Figure 5.1: Observed CO SLED of sources listed in Table 5.1. Flux values have been normalized with respect to the CO(1-0) flux measurement using aperture corrections when necessary, as explained in section 5.3. Starbursts, Seyfert galaxies, and (U)LIRGs are denoted with squares, triangles, and diamonds respectively. The break in the SEDs separates measurements obtained from the literature from the PACS line measurements.
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

The implication of these findings is particularly relevant in studies of high-redshift galaxies, where the majority of CO detections are limited to high-J transitions. The findings in this paper demonstrate the difficulty in applying high-J CO diagnostics in a simple manner to identify XDRs/AGNs in dusty high-redshift sources. In particular, if only a single or a few CO lines are observed, without a broad coverage of the entire SLED, these line detections can be misinterpreted.

Furthermore, caution must be exercised in calculations of the total molecular gas mass via the so-called CO-to-\(H_2\) conversion factor, \(\alpha_{CO} = \frac{M_{H_2}}{L_{CO(1-0)}}\), (e.g. expressed in units of \(M_\odot/(K \text{ km s}^{-1} \text{ pc}^2)\)). Since at high redshifts, CO detections are limited to \(J > 3\) lines, many studies are forced to first convert an observed mid-J CO line intensity to a \(J = 1\rightarrow 0\) intensity before applying \(\alpha_{CO}\) to arrive at an \(H_2\) gas mass. Usually, line ratios between a mid-J or high-J line and the \(J = 1\rightarrow 0\) line are estimated by comparing the source to a similar galaxy and assuming the typical excitation of the galaxy under consideration (Carilli & Walter 2013). However, the diversity in our observed SLEDs (Figure 5.1) suggests that this approach may be problematic; extrapolating from mid or high-J lines to \(J = 1\rightarrow 0\) using templates based on galaxies with similar inferred physical properties introduces a degree of uncertainty since the high-J to CO(1-0) line ratios can vary by an order of magnitude for otherwise similar sources.

In order to further explore the usefulness of high-J CO lines as a tool for characterizing dusty objects at high redshifts, we construct a ratio-ratio diagram employing just three CO lines: \(J = 1\rightarrow 0, 6\rightarrow 5, \text{ and } 18\rightarrow 17\). The CO(1-0) transition is traditionally used to trace the total molecular gas mass, while the CO(6-5) line traces a warm and dense component that is generally associated with star formation, and is typically one of the brightest transitions in infrared-bright starburst galaxies (see Figure 120).
Figure 5.2: CO(18-17)/CO(1-0) vs. CO(18-17)/CO(6-5) plot. Starbursts, Seyfert galaxies, and (U)LIRGs are denoted with squares, triangles, and diamonds respectively. The ULIRGs are further color-coded according to their AGN fractions (see Table 5.2), where blue, green, and red indicate AGN fractions between 0-25%, 25-50%, and 50-75% respectively. The RBGS ULIRGs are labeled according to the following: 1. IRAS F08572+3915, 2. IRAS 23128-5919, 3. IRAS F12112+0305, 4. IRAS 17208-0014, 5. IRAS F09320+6134, 6. IRAS F10565+2448, 7. IRAS F05189-2524, 8. IRAS 20551-4250, 9. IRAS 23365+3604. Unfilled markers indicate cases where we only have upper limits on the CO(18-17) and/or CO(6-5) line fluxes; these data points thus represent upper bounds in the ratio-ratio plot.
5.1). CO(18-17) is a very high-J line that may offer a large leverage in distinguishing starburst-dominated from AGN-dominated excitation. Figure 5.2 shows the resulting plot of the CO(18-17)/CO(1-0) versus CO(18-17)/CO(6-5) ratios in cases where flux values (or upper limits) for all three rotational lines are available. Since Figure 5.2 is meant to serve as an observational tool, we plot ratios of the observed (unscaled) flux values, as opposed to the line fluxes plotted in Figure 5.1 and tabulated in Table 5.3, which have been scaled to the PACS 9.4” beam size when necessary. (A scaled version of Figure 5.2 demonstrates the same qualitative trends discussed below.)

We find that the CO(18-17) line is weak with respect to both CO(1-0) and CO(6-5) in our starburst galaxies (NGC 253, M 83, M 82), and strong in the prototypical Seyfert NGC 1068 and in the ULIRGs of our sample, which are generally located in a region above the starbursts, in the upper right corner where objects have significant amounts of hot gas. A quantitative treatment of this trend will be presented in section 5.5.

We also searched for potential trends between the ULIRG positions in this diagram and their AGN properties. We collected the AGN luminosities and AGN fractions, i.e. the relative contribution of the AGN (w.r.t. the starburst) to the combined bolometric light in these objects (taken from Veilleux et al. (2009, 2013) and listed in Table 5.2), but did not find a clear trend with either of these two parameters.

5.4.2 LVG Radiative Transfer Model

To quantitatively analyze the CO SLEDs of the sources in our sample, we assemble the lower-J line intensities from the literature (see footnotes in Table 5.3) and employ a large velocity gradient (LVG) model in which the excitation and opacity of the CO
lines are determined by the gas density \( n_{\text{H}_2} \), kinetic temperature \( T_{\text{kin}} \), and the CO-to-H\(_2\) abundance per velocity gradient \( \chi_{\text{CO}}/(dv/dr) \). We use the escape probability formalism derived for a spherical cloud undergoing uniform collapse, with \( \beta = (1-e^{-\tau})/\tau \) (Castor 1970; Goldreich & Kwan 1974). Each source is assumed to consist of a large number of these unresolved clouds, such that the absolute line intensities scale with the beam-averaged CO column density, \( N_{\text{CO}} \). In the following analysis, we assume a canonical value of \( \chi_{\text{CO}} = 10^{-4} \), motivated by abundance measurements in Galactic molecular clouds (Frerking et al. 1982). We assume collisional excitation by H\(_2\) assuming an H\(_2\) ortho/para ratio of 3.

To carry out the computations, we use the Mark & Sternberg LVG radiative transfer code described in Davies et al. (2012), with CO-H\(_2\) collisional coefficients taken from Yang et al. (2010) and energy levels, line frequencies and Einstein A coefficients taken from the Cologne Database for Molecular Spectroscopy (CDMS). For a given set of parameters, \( \{n_{\text{H}_2}, T_{\text{kin}}, dv/dr, N_{\text{CO}}\} \), the code computes the intensities of molecular lines by iteratively solving the equations of statistical equilibrium for the level populations using the escape probability formalism. We calculate a three-dimensional grid of expected CO SLEDs, varying \( n_{\text{H}_2} \) (\( 10^{2.4}\) - \( 10^{8.2} \) cm\(^{-3}\)), \( T_{\text{kin}} \) (30-2500 K), and \( dv/dr \) (0.1-1000 km s\(^{-1}\)pc\(^{-1}\)) over a large volume of parameter space. While these parameters determine the shape of the resulting SLED, the line intensity magnitudes are set by the beam-averaged CO column density, \( N_{\text{CO}} \), which is tweaked to match the observed fluxes and beam sizes. Thus the intensity of each CO line is given by the expression

\[
I_{\text{line}} = \frac{h\nu}{4\pi} x_u A\beta(\tau) N_{\text{CO}} \tag{5.1}
\]

where \( x_u \) is the population fraction in the upper level of the transition, \( h\nu \) is the
transition energy, $A$ is the Einstein radiative coefficient, $\beta(\tau)$ is the escape probability for a line optical depth $\tau$, and $N_{\text{CO}}$ is the beamed averaged column density. The molecular gas mass in the beam (for a spherical geometry) is then given by

$$M_{\text{H}_2} = \pi R^2 \mu m_{\text{H}_2} \frac{N_{\text{CO}}}{\chi_{\text{CO}}} \quad (5.2)$$

where $\mu = 1.36$ takes into account the helium contribution to the molecular weight and $R = D_A \theta/2$ is the effective radius of the beam, with $D_A$ being the angular diameter distance to the source and $\theta$ the beam size of the line observations.

The LVG-modeling technique thus offers an opportunity to derive the CO-to-H$_2$ conversion factor in an extragalactic source in an independent way, using the gas mass estimate from the source’s best-fit LVG model (Mashian et al. 2013). As mentioned above, the molecular hydrogen gas mass is often obtained from the CO(1-0) line luminosity by adopting a mass-to-luminosity conversion factor, $\alpha_{\text{CO}}$. The standard Galactic value, calibrated using several independent methods (Dickman 1978; Bloemen et al. 1986; Solomon et al. 1987; Strong et al. 1988), is $\alpha_{\text{CO}} \sim 4 - 5 \ M_\odot/(K \ \text{km}^{-1}\text{pc}^2)$, while subsequent studies of CO emission in ULIRGs found a significantly smaller ratio, $\alpha_{\text{CO}} \sim 0.8 - 1.0 \ M_\odot/(K \ \text{km}^{-1}\text{pc}^2)$ (Downes & Solomon 1998). These values have been adopted by many (Sanders et al. 1988; Tinney et al. 1990; Wang et al. 1991; Walter et al. 2012) to convert CO J=1-0 line observations to total molecular gas masses, and the question of what value to apply for what type of galaxy has been a controversial issue for decades. Often, consideration is not given to the dependence of $\alpha_{\text{CO}}$ on the average molecular gas conditions (metallicity, temperature, density) in the sources to which they are being applied.

Detailed studies of the conversion factor based on CO SLED modeling of the...
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

objects in our sample are beyond the scope of this paper because of the significant uncertainties associated with our simple models. We do estimate, however, the conversion factors derived using the $L_{CO(1-0)}$ and $M_{H_2}$ values from both the single-component and two-component LVG models for each of the sources in our sample (where the total gas mass, $M_{H_2,\text{total}} = M_{H_2,\text{cool}} + M_{H_2,\text{warm}}$, is used in the two-component case). We note that the sole use of $^{12}$CO lines to derive the CO-to-$H_2$ conversion factor via LVG modeling raises its own concerns. As discussed in Bolatto et al. (2013), this technique is only sensitive to regions where CO is bright and may therefore miss any component of “CO-faint” $H_2$, unless combined with observations of other lines, i.e. [CII], that trace these “CO-faint” molecular regions.

5.4.3 Fitting Procedure

To determine the best-fit set of parameters that characterize the CO SLED of each source, we compare the modeled SLEDs to the observed CO line intensities and generate a likelihood distribution for each of the parameters following a Bayesian formalism outlined in Ward et al. (2003) and Kamenzisky et al. (2012). The Bayesian likelihood of the model parameters, $p$, given the line measurements, $x$, is

$$P(p|x) = \frac{P(p)P(x|p)}{\int dp P(p)P(x|p)}$$  \hspace{1cm} (5.3)

where $P(p)$ is the prior probability of the model parameters and $P(x|p)$ is the probability of obtaining the observed data set given that the source follows the model characterized by $p$. Assuming that the measured line strengths have Gaussian-distributed random
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

errors, \( P(\mathbf{x}|\mathbf{p}) \) is the product of Gaussian distributions in each observation,

\[
P(\mathbf{x}|\mathbf{p}) = \prod_i \frac{1}{\sqrt{2\pi}\sigma_i^2} \exp \left[ -\frac{(x_i - I_i(\mathbf{p}))^2}{2\sigma_i^2} \right]
\]

(5.4)

where \( \sigma_i \) is the standard deviation of the observational measurement for transition \( i \) and \( I_i(\mathbf{p}) \) is the predicted line intensity for that transition and model. The likelihood distribution of any one parameter is thus the integral of \( P(\mathbf{p}|\mathbf{x}) \) over all the other parameters. In our analysis, we use a binary prior probability, choosing priors that are flat in the logarithm of each parameter, and that go to zero for any model that predicts a molecular gas mass which exceeds the source’s dynamical mass (in cases where \( M_{dyn} \) is known through other means; see footnote in Table 5.5).

We first run a calculation with a single-component model, assuming all the CO lines are emitted by a region characterized by a single kinetic temperature, \( \text{H}_2 \) number density, velocity gradient, and column density. It is instructive to examine how far a single gas component can go in reproducing the entire observed CO SLEDs before a given fit becomes inadequate and a second component must be introduced. However, given the fact that many of the sources considered in this paper have had their low- to mid-J emission lines analyzed in previous studies (see Table 5.6) using two-component LVG models, we would like to explore how these “best-fit” multi-component models are modified by the inclusion of the more recent PACS high-J line observations. We therefore divide the line fluxes into two components, one cooler and one warmer (with some mid-J lines receiving significant contributions from both) and follow an iterative procedure, looking for the best solution of one component at a time and subtracting it from the other. This two-step approach thus results in a six parameter model, with three parameters characterizing the shape of the SLED in each respective component. It is
therefore not applied to sources which have fewer than three line intensity measurements in each component, i.e. M83, since in such cases, the problem is underdetermined, i.e. there are more parameters than data points. The detected transitions from NGC 1068 are also not modeled as arising from two different components in this paper since the full SLED has been thoroughly analyzed and fitted with radiative transfer models in previous papers (Hailey-Dunsheath et al. 2012; Spinoglio et al. 2012).

5.5 LVG Results & Discussion

The LVG-modeled SLEDs for the single and two-component fits are shown in the left and right-hand panels of Figure 5.3 respectively. Although the single-component LVG models provide only a crude approximation to the complicated mixture of physical conditions that characterize the emitting source, they nonetheless yield surprisingly good fits to the observed SLEDs in most cases. The constraints provided by the PACS high-J CO line detections drive the “best-fit” kinetic temperatures in these single component LVG models to high values, both relative to their two-component counterparts and relative to CO SLED fits obtained in earlier LVG analyses, when measurements of these high-level excitations were not yet available. Furthermore, demanding that a single set of LVG model parameters reproduce the full CO SLED often results in under-predicted low-J CO transitions. Introducing a separate low-excitation component mitigates both of these issues, accounting for the excess CO(1-0) and CO(2-1) line emissions while yielding a two-component LVG model with more moderate estimates of the kinetic temperature. While a true multi-component model will obviously provide more accurate estimates of these molecular gas properties, the fact that in most cases, a single component LVG
Table 5.5: LVG Model: Best Fit Parameters & Results

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<td>630</td>
<td>500 - 1000</td>
<td>50</td>
<td>20 - 63</td>
<td>316</td>
<td>200 - 400</td>
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<tr>
<td>nH₂ [cm⁻³]</td>
<td>10²¹.⁸</td>
<td>10²⁴. - 10³.⁰</td>
<td>10²⁸.</td>
<td>10²⁴. - 10³.²</td>
<td>10⁴.⁴</td>
<td>10³.² - 10⁴.⁸</td>
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<td></td>
</tr>
<tr>
<td>dv/dr [km s⁻¹ pc⁻¹]</td>
<td>1</td>
<td>0.1 - 2</td>
<td>1</td>
<td>0.1 - 10</td>
<td>32</td>
<td>1 - 1000</td>
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</tr>
<tr>
<td>N_H₂ [cm⁻²]</td>
<td>10²¹.⁹</td>
<td>10²¹.₆ - 10²².⁴</td>
<td>10²².³</td>
<td>10²¹.³ - 10²³.⁵</td>
<td>10²⁰.⁷</td>
<td>10²⁰.³ - 10²¹.⁶</td>
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<td></td>
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</tr>
<tr>
<td>M_H₂ [Mₜ]</td>
<td>10⁹.²</td>
<td>10⁹.⁰ - 10⁹.⁷</td>
<td>10⁹.⁷</td>
<td>10⁸.⁷ - 10¹⁰.⁸</td>
<td>10⁸.⁰</td>
<td>10⁷.⁶ - 10⁸.⁹</td>
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<td></td>
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<tr>
<td>NGC 6240</td>
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<td>160</td>
<td>100 - 200</td>
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<tr>
<td>nH₂ [cm⁻³]</td>
<td>10³.²</td>
<td>10³.⁰ - 10³.⁴</td>
<td>10³.⁴</td>
<td>10³.² - 10³.⁸</td>
<td>10⁷.⁴</td>
<td>10⁷.² - 10⁸.²</td>
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<tr>
<td>dv/dr [km s⁻¹ pc⁻¹]</td>
<td>8</td>
<td>4 - 10</td>
<td>1</td>
<td>0.1 - 2</td>
<td>20</td>
<td>4 - 25</td>
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<td></td>
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<tr>
<td>N_H₂ [cm⁻²]</td>
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<td>10²¹.₂ - 10²¹.⁷</td>
<td>10²².⁴</td>
<td>10²².⁰ - 10²².⁵</td>
<td>10²².⁵</td>
<td>10²².⁰ - 10²⁴.⁴</td>
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</tr>
<tr>
<td>M_H₂ [Mₜ]</td>
<td>10⁹.¹</td>
<td>10⁸.⁸ - 10⁹.³</td>
<td>10¹⁰.⁰</td>
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<td>10¹⁰.¹</td>
<td>10⁹.⁶ - 10¹².⁰</td>
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<td></td>
<td></td>
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<tr>
<td>Mrk 231</td>
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<td></td>
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<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>T [K]</td>
<td>630</td>
<td>500 - 794</td>
<td>50</td>
<td>20 - 63</td>
<td>316</td>
<td>160 - 500</td>
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</tr>
<tr>
<td>nH₂ [cm⁻³]</td>
<td>10²¹.⁴</td>
<td>10²¹.₃ - 10²¹.⁶</td>
<td>10²¹.₀</td>
<td>10²⁰.₈ - 10²¹.⁵</td>
<td>10²⁰.⁴</td>
<td>10¹⁹.⁷ - 10²¹.⁵</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>dv/dr [km s⁻¹ pc⁻¹]</td>
<td>1</td>
<td>0.1 - 2</td>
<td>1</td>
<td>0.1 - 2</td>
<td>200</td>
<td>2 - 1000</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>N_H₂ [cm⁻²]</td>
<td>10²¹.⁴</td>
<td>10²¹.₃ - 10²¹.⁶</td>
<td>10²¹.₀</td>
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<td>10¹⁹.⁷ - 10²¹.⁵</td>
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</tr>
<tr>
<td>M_H₂ [Mₜ]</td>
<td>10⁹.⁴</td>
<td>10⁹.₃ - 10⁹.⁶</td>
<td>10⁹.⁰</td>
<td>10⁸.⁸ - 10⁹.⁵</td>
<td>10⁸.⁴</td>
<td>10⁷.⁷ - 10⁹.⁶</td>
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<td></td>
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</tr>
</tbody>
</table>
Table 5.5 (Continued)

**Note.** (i) With the exception M 83, M 82, and NGC 3690, for which the molecular gas masses contained within $\theta \sim 21''$, 47'', and 19'' beams are given respectively, all other estimates of $M_{H_2}$ correspond to the molecular gas mass in a $\theta = 9.4''$ beam centered on the emission region.

Table 5.6: LVG Results from Previous Studies

<table>
<thead>
<tr>
<th>Source</th>
<th>Component (low/high J)</th>
<th>$T$ [K]</th>
<th>$n_{H_2}$ [cm$^{-3}$]</th>
<th>$dv/dr$</th>
<th>$N_{CO}$ [cm$^{-2}$]</th>
<th>$M_{H_2}$ [M$_\odot$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NGC 253$^1$</td>
<td>low</td>
<td>$\leq 40$</td>
<td>$10^{2.4}$-$10^{3}$</td>
<td>20</td>
<td>$10^{18.2}$-$10^{18.5}$</td>
<td>$10^{7.5}$</td>
</tr>
<tr>
<td></td>
<td>high</td>
<td>80 - 200</td>
<td>$10^{3.8}$-$10^{4.1}$</td>
<td>20</td>
<td>$10^{18.2}$-$10^{18.3}$</td>
<td>$10^{7.1}$-$10^{7.2}$</td>
</tr>
<tr>
<td>NGC 253$^2$</td>
<td>low</td>
<td>60</td>
<td>$10^{3.5}$</td>
<td>–</td>
<td>$10^{17}$ ($N_{CO}$/$\Delta v$)</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>low</td>
<td>40</td>
<td>$10^{4.5}$</td>
<td>–</td>
<td>$10^{17}$ ($N_{CO}$/$\Delta v$)</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>high</td>
<td>110</td>
<td>$10^{5.5}$</td>
<td>–</td>
<td>$10^{17}$ ($N_{CO}$/$\Delta v$)</td>
<td>$10^{7.5}$ (total)</td>
</tr>
<tr>
<td>M 83$^3$</td>
<td>single</td>
<td>40</td>
<td>$10^{5.8}$</td>
<td>–</td>
<td>–</td>
<td>$10^{18.7}$</td>
</tr>
<tr>
<td>M 83$^4$</td>
<td>low</td>
<td>30 - 150</td>
<td>$10^{2.7}$-$10^{3.5}$</td>
<td>–</td>
<td>$10^{17}$-$10^{17.5}$ ($N_{CO}$/$\Delta v$)</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>high</td>
<td>60 - 100</td>
<td>$10^{3.5}$-$10^{5}$</td>
<td>–</td>
<td>$10^{15.8}$-$10^{17}$ ($N_{CO}$/$\Delta v$)</td>
<td>$10^{7.5}$ (total)</td>
</tr>
<tr>
<td>M 82$^5$</td>
<td>high</td>
<td>545</td>
<td>$10^{3.7}$</td>
<td>35</td>
<td>$10^{19}$</td>
<td>$10^{7.1}$</td>
</tr>
<tr>
<td>M 82$^6$</td>
<td>low</td>
<td>14</td>
<td>$10^{3.3}$-$10^{3.8}$</td>
<td>–</td>
<td>$10^{17.8}$-$10^{18.0}$</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>high</td>
<td>170</td>
<td>$10^{2.8}$-$10^{3.0}$</td>
<td>–</td>
<td>$10^{19.5}$</td>
<td>$10^{8.2}$ (total)</td>
</tr>
<tr>
<td>M 82$^7$</td>
<td>low</td>
<td>63</td>
<td>$10^{3.4}$</td>
<td>–</td>
<td>$10^{18.6}$</td>
<td>$10^{7.3}$</td>
</tr>
<tr>
<td></td>
<td>high</td>
<td>447</td>
<td>$10^{4.1}$</td>
<td>–</td>
<td>$10^{18.0}$</td>
<td>$10^{6.1}$</td>
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<tr>
<td>NGC 4945$^8$</td>
<td>single</td>
<td>100</td>
<td>$10^{3.5}$</td>
<td>–</td>
<td>$10^{18.8}$</td>
<td>–</td>
</tr>
<tr>
<td>NGC 4945$^9$</td>
<td>(degenerate solutions)</td>
<td>20</td>
<td>$10^{4.5}$</td>
<td>–</td>
<td>$10^{17.9}$</td>
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<td></td>
<td>100</td>
<td>$10^{3}$</td>
<td>–</td>
<td>$10^{17.8}$</td>
<td>$10^{9}$</td>
</tr>
<tr>
<td>Circinus$^8$</td>
<td>single</td>
<td>50 - 80</td>
<td>$10^{3.3}$</td>
<td>–</td>
<td>$10^{18.3}$</td>
<td>–</td>
</tr>
<tr>
<td>Circinus$^9$</td>
<td>(degenerate solutions)</td>
<td>20</td>
<td>$10^{4}$</td>
<td>–</td>
<td>$10^{17.5}$</td>
<td>$10^{8.8}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>100</td>
<td>$10^{3}$</td>
<td>–</td>
<td>$10^{17.7}$</td>
<td>$10^{8.9}$</td>
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</table>
Table 5.6 (Continued)

<table>
<thead>
<tr>
<th>Source</th>
<th>Component (low/high J)</th>
<th>T [K]</th>
<th>$n_{H_2}$ [cm$^{-3}$]</th>
<th>$dv/dr$ [km s$^{-1}$ pc$^{-1}$]</th>
<th>$N_{CO}$ [cm$^{-2}$]</th>
<th>$M_{H_2}$ [M$_\odot$]</th>
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<tr>
<td>NGC 1068$^{10}$</td>
<td>mid-J</td>
<td>169</td>
<td>$10^{5.6}$</td>
<td>148</td>
<td>–</td>
<td>$10^{6.7}$</td>
</tr>
<tr>
<td></td>
<td>high</td>
<td>571</td>
<td>$10^{6.4}$</td>
<td>269</td>
<td>–</td>
<td>$10^{5.6}$</td>
</tr>
<tr>
<td>IC 694$^{11}$</td>
<td>single</td>
<td>10 - 500</td>
<td>&gt; $10^{2.5}$</td>
<td>–</td>
<td>$10^{18}$ - $10^{18.9}$</td>
<td>$10^{8.8}$</td>
</tr>
<tr>
<td>NGC 3690$^{11}$</td>
<td>single</td>
<td>10 - 1000</td>
<td>&gt; $10^{2.5}$</td>
<td>–</td>
<td>$10^{18}$ - $10^{18.8}$</td>
<td>$10^{8.5}$</td>
</tr>
<tr>
<td>Arp 220$^{12}$</td>
<td>low</td>
<td>50</td>
<td>$10^{2.8}$</td>
<td>1.4</td>
<td>$10^{20.3}$</td>
<td>$10^{9.7}$</td>
</tr>
<tr>
<td></td>
<td>high</td>
<td>1343</td>
<td>$10^{3.2}$</td>
<td>20</td>
<td>$10^{19.4}$</td>
<td>$10^{8.7}$</td>
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<tr>
<td>Mrk 231$^{13}$</td>
<td>low</td>
<td>55 - 95</td>
<td>$10^{3}$</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>mid-J</td>
<td>40 - 70</td>
<td>$10^{4}$ - $10^{4.5}$</td>
<td>–</td>
<td>–</td>
<td>$10^{10.2}$ - $10^{10.6}$</td>
</tr>
</tbody>
</table>

Note. References from which LVG results were extracted and the beam size for mass estimates when provided:

1 Hailey-Dunsheath et al. (2008); $\theta \sim 11''$
2 Rosenberg et al. (2014a); $\theta \sim 32''$
3 Bayet et al. (2006)
4 Israel & Baas (2001); $\theta \sim 20''$
5 Panuzzo et al. (2010); $\theta \sim 46''$
6 Ward et al. (2003); $\theta \sim 40''$
7 Kamenetzky et al. (2012); $\theta \sim 43''$
8 Curran et al. (2001)
9 Hitschfeld et al. (2008)
10 Hailey-Dunsheath et al. (2012); $\theta \sim 10''$
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

model is sufficient to faithfully reproduce the full SED, is a noteworthy result. The CO emission line spectra of star-forming galaxies may often be representable by a single LVG SLED as a function of halo mass and molecular gas mass content.

Below, we present estimates of the best-fit parameters characterizing the molecular gas in each source and compare our results to those obtained in previous studies (Table 5.6) when applicable. A summary of these LVG results can be found in Table 5.5, where “4D Max” refers to the single most probable grid point in the entire multi-dimensional distribution. The sources are listed and discussed in order of increasing distance. We also present estimates of the CO-to-H₂ conversion factors derived from our best-fit LVG models (Table 5.7). For the ULIRGs in our template sample, and with the two-component approach, we derive values in the canonical range 0.4 - 0.5 M_☉(K km⁻¹pc²)⁻¹. The lowest factor is found for M 82 (∼0.2 M_☉(K km⁻¹pc²)⁻¹), while for the other objects it varies between ~0.4 and ~14 M_☉(K km⁻¹pc²)⁻¹. These are all plausible values, keeping in mind that these models refer to the central regions of these starburst, AGN and merger templates. Drawing more firm conclusions from these data sets would require more detailed modeling and a careful analysis of the involved assumptions and error bars. We will address this in future single source studies. Our LVG results are also applied to further analyze the ratio-ratio diagram (Figure 5.2) presented in section 5.4. As previously mentioned, the ULIRGs in our sample tend to be located in the upper right corner of this plot, where objects have significant amounts of hot gas. To obtain a quantitative measure of this trend, we divide 10 of the template objects in Figure 5.2 into two bins by grouping the objects into the lower left and upper right quadrant: 5 objects with CO(18-17)/CO(1-0) < 10 and CO(18-17)/CO(6-5) < 0.2 (lower left quadrant, this group contains NGC 253, M 82, NGC 4945, Circinus, and Arp 220) and 5 objects with...
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

CO(18-17)/CO(1-0) > 10 and CO(18-17)/CO(6-5) > 0.2 (upper right quadrant, this group contains NGC 1068, IC 694, NGC 3690, NGC 6240, and Mrk 231). Using a two-component LVG fit (discussed in section 5.4), we find that the average fractions of highly-excited warm molecular gas (relative to the total gas mass) for the objects in the lower left and upper right quadrants are ~11% and 22% respectively (with standard deviations of 21%). These fractions (found in Table 5.7) are calculated from the mass estimates given in Table 5.5, and from Hailey-Dunsheath et al. (2012) in the case of NGC 1068. (Note: M 83 is not included since we do not have a two-component LVG fit, and consequently, an estimate of the highly-excited gas mass component for this source).

Given the uncertainties in estimating the gas masses and the low number of objects, this difference between the percentage of dense and warm gas estimated for each quadrant is marginal. However, the data we have collected so far demonstrate the abundance of hot molecular gas in ULIRGs, both with respect to the warm phase that produces the bulk of the CO luminosity, and with respect to the total molecular gas mass. Detailed single source studies with careful modeling of PDR, XDR and shock components are needed to better understand the mechanisms that determine the variety of CO SLED shapes and the plausible excitation sources.

5.5.1 NGC 253

NGC 253 is among the nearest and best-studied starburst galaxies. Hailey-Dunsheath et al. (2008) employed a multiline LVG model to analyze NGC 253’s CO SLED, introducing a low-excitation component to model the J=2→1 and J=1→0 emission while using the remaining higher transitions (J_{upp} ≤ 7), including a $^{13}$CO(6-5) detection.
Figure 5.3: SLEDs for $^{12}$CO: Single (left panel) and Two-Component (right panel) LVG Results. Diamonds represent the low-J line intensities extracted from the data in the references listed below Table 5.3. Asterisks represent the observed PACS line intensities while arrows signify upper bounds on the line intensity. Best fit SLEDs, corresponding to the ”Single/Low/High 4D Max” column in Table 5.5, are shown with solid/blue/red lines. The dashed line in the two-component fit is the total fitted SLED, i.e., the sum of the two components.
Figure 5.3 (Continued)
Figure 5.3 (Continued)
Figure 5.3 (Continued)
with ZEUS, to constrain the high-excitation component. Requiring that $T_{\text{kin}} \leq 200$ K and restricting the velocity gradient to $dv/dr \sim 7 - 40$ km s$^{-1}$ pc$^{-1}$, they found a low-excitation component characterized by $T_{\text{kin}} \leq 40$ K and $n_{H_2} = 10^{2.4}$ - $10^{3.0}$ and a high-excitation component with kinetic temperature in the range 80-200 K and $n_{H_2} = 10^{3.8}$ - $10^{4.1}$, with a velocity gradient of 20 km s$^{-1}$ pc$^{-1}$ in both cases.

With the additional CO transition lines observed by SPIRE, Rosenberg et al. (2014a) modeled the CO SLED as arising from three distinct molecular gas phases where the low-J lines ($J_{\text{upp}} < 5$) originate from regions characterized by temperatures $T_{\text{kin}} = 60$ K and $T_{\text{kin}} = 40$ K, and number densities $n_{H_2} = 10^{3.5}$ cm$^{-3}$ and $n_{H_2} = 10^{4.5}$ cm$^{-3}$ respectively, while the mid-to-high-J lines ($5 \leq J_{\text{upp}} \leq 13$) are emitted by a region with a kinetic temperature 110 K and number density of $10^{5.5}$ cm$^{-3}$.

In our analysis, we limit ourselves to two-phase molecular gas and model our “high-excitation” component to fit the recent high-J line PACS observations ($J=15 \rightarrow 14$, $16 \rightarrow 15$, and $18 \rightarrow 17$), in addition to the mid-J lines. We find that the low and high-excitation components are characterized by similar number densities, $n_{H_2} \sim 10^{3.4-3.6}$ cm$^{-3}$, while the temperatures range from 50 K to 1260 K for each respective component. We estimate a total H$_2$ mass of $\sim 5 \times 10^7$ M$_\odot$, only $\sim 2\%$ of which is in the warm phase generating the high-J CO line emission.

5.5.2 M 83

For the nearby, barred starburst galaxy M 83, Israel & Baas (2001) presented two LVG models to fit the $J_{\text{upper}} \leq 4$ CO emission lines: one with $T_{\text{kin}} = 30$-150 K and $n_{H_2} = 10^{2.7}$-10$^{3.5}$ cm$^{-3}$, and one with $T_{\text{kin}} = 60$-100 K and $n_{H_2} = 10^{3.5}$-10$^{5.0}$ cm$^{-3}$. Bayet et al.
(2006), modeling the $J_{\text{upper}} \leq 6$ CO emission lines as originating from a single region, suggested a fit with $T_{\text{kin}} = 40$ K and $n_{H_2} = 10^{5.8}$ cm$^{-3}$.

With only two high-J line measurements for this source, CO(15-14) and CO(16-15), we do not fit a two-component model in this case due to the underdetermined nature of the problem. However, we find that the observed CO SLED for M83 is reasonably well-fitted by a single-component model with a kinetic temperature of $\sim 500$ K and a H$_2$ number density of $10^{2.8}$ cm$^{-3}$. The molecular mass traced by the CO emission within the central 325 pc of the source ($\theta \sim 21''$) in this best-fit model is $1.3 \times 10^7$ M$_\odot$, close to the total gas mass estimate of $3 \times 10^7$ M$_\odot$ derived in Israel & Baas (2001).

### 5.5.3 M82

Due to its proximity, M82 is an extensively studied starburst galaxy. Panuzzo et al. (2010) fit the $^{12}$CO emission spectrum from $J=4\rightarrow3$ to $J=13\rightarrow12$ using a LVG model with $T_{\text{kin}} = 545$ K, $n_{H_2} = 10^{3.7}$ cm$^{-3}$, and $dv/dr = 35$ km s$^{-1}$pc$^{-1}$. Kamenetzky et al. (2012) proposed a two-component model where the cool molecular gas (traced by those lines below $J=4\rightarrow3$) was characterized by a kinetic temperature of 63 K and a H$_2$ number density of $10^{3.4}$ cm$^{-3}$, while the high-J CO lines traced a very warm gas component with $T_{\text{kin}} = 447$ K and $n_{H_2} = 10^{4.1}$ cm$^{-3}$.

With the inclusion of the additional constraints on the high-excitation component provided by the PACS lines CO(15-14), CO(16-15), and CO(18-17), we find that our fitted parameters compare very well with the two-component model set forth in Kamenetzky et al. (2012). Our LVG analysis yields a warm component with $T_{\text{kin}} = 500$ K and $n_{H_2} = 10^{3.4}$ cm$^{-3}$, and a cool component characterized by a kinetic temperature
of 80 K, a H$_2$ number density of $10^{3.2}$ cm$^{-3}$, and a velocity gradient of $\sim 200$ km s$^{-1}$pc$^{-1}$. This high velocity gradient in the low-excitation component is suspected to be the culprit behind the low CO-to-H$_2$ conversion factor in M82, $\alpha_{CO} \sim 0.25 \, M_\odot/(K \, \text{km}^{-1}\text{pc}^2)$. Since the optical depth of the J = 1--0 line is reduced by a large $dv/dr$, less molecular mass is required to produce the observed flux, leading to a reduced estimate of $M_{H_2,tot}$ and consequently, of $\alpha_{CO}$. The total H$_2$ mass within the 47$''$ x 47$''$ PACS beam is estimated to be $\sim 5 \times 10^7 \, M_\odot$, of the same order as the mass estimates derived in Ward et al. (2003), Panuzzo et al. (2010), and Kamenetzky et al. (2012), with 50% of the mass in the warm component.

### 5.5.4 NGC 4945 & Circinus

At distances of $\sim 3.7$ and $\sim 4$ Mpc, NGC 4945 and Circinus are among the nearest and most infrared-bright spiral galaxies in the sky, with observations of their obscured nuclei classifying them as Seyfert galaxies. In both NGC 4945 and Circinus, Hitschfeld et al. (2008) used the ratios of the observed integrated intensities of the $^{12}$CO(1-0) to $^{12}$CO(4-3) lines, as well as the $^{13}$CO(1-0) and $^{13}$CO(2-1) transitions to obtain column densities, H$_2$ number densities, and kinetic temperatures for the two sources. Fitting the CO and $^{13}$CO lines, they found a degeneracy in the best-fit parameters in $n_{H_2}$-$T_{kin}$ plane. Their best fit solution for NGC 4945 was $n_{H_2} = 3 \times 10^4$ cm$^{-3}$ and $T_{kin} = 20$ K, a solution not significantly better than one with $n_{H_2} = 10^3$ cm$^{-3}$ and $T_{kin} = 100$ K. Curran et al. (2001) found a solution with $n_{H_2} = 3 \times 10^3$ cm$^{-3}$ and $T_{kin} = 100$ K from $^{12}$CO observations of the three lowest transitions and $^{13}$CO data of the two lowest transitions.

For Circinus, again, Hitschfeld et al. (2008) found a number of solutions that
### Table 5.7. LVG Model Results: CO-to-H$_2$ conversion factor, $\alpha_{CO}^*$

<table>
<thead>
<tr>
<th>Galaxy</th>
<th>$\alpha_{CO,\text{single-comp}}$</th>
<th>$\alpha_{CO,\text{two-comp}}$</th>
<th>$f_{\text{warm}}^\dagger$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NGC 253</td>
<td>0.57</td>
<td>2.96</td>
<td>2.2</td>
</tr>
<tr>
<td>M 83</td>
<td>0.65</td>
<td>⋮</td>
<td>⋮</td>
</tr>
<tr>
<td>M 82</td>
<td>0.53</td>
<td>0.25</td>
<td>49.6</td>
</tr>
<tr>
<td>NGC 4945</td>
<td>2.43</td>
<td>4.46</td>
<td>1.7</td>
</tr>
<tr>
<td>Circinus</td>
<td>1.68</td>
<td>13.8</td>
<td>0.5</td>
</tr>
<tr>
<td>NGC 1068</td>
<td>0.67</td>
<td>⋮</td>
<td>⋮</td>
</tr>
<tr>
<td>NGC 4418</td>
<td>0.93</td>
<td>11.8</td>
<td>85.8</td>
</tr>
<tr>
<td>IC 694</td>
<td>0.37</td>
<td>0.79</td>
<td>4.1</td>
</tr>
<tr>
<td>NGC 3690</td>
<td>0.26</td>
<td>0.87</td>
<td>18.8</td>
</tr>
<tr>
<td>Arp 220</td>
<td>0.57</td>
<td>1.52</td>
<td>2.0</td>
</tr>
<tr>
<td>NGC 6240</td>
<td>0.52</td>
<td>4.57</td>
<td>57.7</td>
</tr>
<tr>
<td>Mrk 231</td>
<td>0.64</td>
<td>0.39</td>
<td>20.5</td>
</tr>
</tbody>
</table>

* $\alpha_{CO}$ is given in units of [$M_\odot$ (K km s$^{-1}$ pc$^2$)$^{-1}$]

$^\dagger f_{\text{warm}} = M_{H_2,\text{warm}}/M_{H_2,\text{total}}$
provided consistent CO cooling curves for the low-J transitions. The lowest $\chi^2$ was obtained for $n_{H_2} = 10^4$ cm$^{-3}$ and $T_{kin} = 20$ K; a second, degenerate, solution was found with $n_{H_2} = 10^3$ cm$^{-3}$ and $T_{kin} = 100$ K. Their results agreed well with Curran et al. (2001), who found a best-fit solution with $T_{kin} = 50-80$ K and $n_{H_2} = 2\times10^3$ cm$^{-3}$ from observations of the three lowest $^{12}$CO transitions and the two lowest $^{13}$CO transitions in this source.

Our LVG analysis of the $^{12}$CO(1-0) to $^{12}$CO(6-5) lines yields low-excitation components with parameters consistent with those obtained by Hitschfeld et al. (2008). We find best-fit solutions with a kinetic temperature of 50 K for both sources, and an H$_2$ number density of $10^{4.8}$ cm$^{-3}$ and $10^{4.2}$ cm$^{-3}$ in NGC 4945 and Circinus, respectively. Modeling the high-J CO emission lines as originating from a separate region leads to a warmer, denser component characterized by $T_{kin} = 316$ K and $n_{H_2} = 10^5$ cm$^{-3}$ in NGC 4945, and $T_{kin} = 500$ K and $n_{H_2} = 10^{4.2}$ cm$^{-3}$ in Circinus. We estimate a total H$_2$ gas mass of $4 - 5\times10^7$ M$_\odot$ in both sources, of which only $\sim 0.5 - 1\%$ is in the warm phase.

### 5.5.5 NGC 1068

NGC 1068 is one of the brightest and best studied Seyfert 2 galaxies. Its CO SLED, including the PACS high-J lines, has been extensively analyzed by us (Hailey-Dunsheath et al. 2012) and in the works of Spinoglio et al. (2012); we direct the reader to those papers and to Table 5.5 for a summary of the LVG-modeled gas excitation in this source. We only note that our single-component model yields an H$_2$ gas mass of $10^7$ M$_\odot$, twice the total gas mass estimated by Hailey-Dunsheath et al. (2012).
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

5.5.6 NGC 4418

NGC 4418 is a peculiar, single nucleus galaxy, with a LIRG-like luminosity ($\sim 10^{11}L_\odot$) but with other properties similar to warm ULIRGs, like a high $L_{FIR}/M_{H_2}$ ratio, an extreme [C II] deficit (e.g. Graciá-Carpio et al. 2011), and an extremely compact luminosity source (Evans et al. 2003).

We find that a cool gas phase characterized by $T_{kin} = 50$ K and $n_{H_2} = 1000$ cm$^{-3}$ gives rise to the three lowest $^{12}$CO transitions, while the corresponding high-J lines are emitted by a denser, warmer component with $T_{kin} = 100$ K and $n_{H_2} = 10^{5.6}$ cm$^{-3}$. The gas mass is estimated to be $\sim 10^8$ and $10^9$ M$_\odot$ in each of the respective components, indicating that a significant portion of the molecular gas ($\sim 85\%$) is in a dense, warm phase.

5.5.7 IC 694 & NGC 3690

The two galaxies IC 694 and NGC 3690 form the luminous infrared merger system known as Arp 299. The nuclear region of IC 694 shows the typical mid-IR characteristics of ULIRGs (very compact and dust-enshrouded star formation, probably harboring a low-luminosity AGN), while the nuclear region of NGC 3690 hosts a Seyfert 2 AGN and is surrounded by regions of star formation.

Strong $^{12}$CO emission has been detected in the nuclei of both IC 694 and NGC 3690. Sliwa et al. (2012) modeled the ratios of the observed integrated intensities of the $^{13}$CO(2-1) transition and the low-J $^{12}$CO lines in these two sources. Their best-fit LVG solutions for IC 694 and NGC 3690 had kinetic temperatures ranging from 10 to 500 K.
and 10 to 1000 K, respectively, and a H$_2$ number density greater than $10^{2.5}$ cm$^{-3}$ in both cases.

For IC 694, we find that the low and high-J lines can be modeled as arising from two distinct components characterized by the same kinetic temperature, 200 K, but different H$_2$ number densities, $10^{3.4}$ cm$^{-3}$ and $10^{5.8}$ cm$^{-3}$, where the high-J emission originates from the denser component. The molecular gas mass in each of these components is estimated to be $\sim 7\times10^8$ and $3\times10^7$ M$_\odot$, respectively. The total gas mass estimate is consistent with the gas mass estimates of the molecular region modeled after the low-J lines in Sliwa et al. (2012), as well as the mass estimates derived in Rosenberg et al. (2014b) using only PDR heating. However, as evident from the LVG-modeled CO SLED for this source (Figure 5.3), this two-component best-fit model under-predicts the observed mid-J lines ($9 \leq J_{upp} \leq 14$), suggesting that in the case of IC 694, at least three distinct components are necessary in fitting the full CO SLED.

The observed CO SLED for NGC 3690 (including the extended emission region where its’ galaxy disk overlaps with that of IC 694), is well-fit by a two-component LVG model in which the low-J lines arise from a cool gas phase ($T_{kin} = 50$ K) while the high-J line emission originates from a warmer gas phase ($T_{kin} = 250$ K). These two components, which both contribute to the mid-J line emission, are characterized by similar number densities ($4-6\times10^3$ cm$^{-3}$) and have a combined gas mass of nearly $10^9$ M$_\odot$.

5.5.8 Arp 220

At a distance of about 77 Mpc, Arp 220 is one of the nearest and best studied ULIRGs, serving as a template for high-$z$ studies of dusty starbursts. We found that
a single-component model with \( T_{\text{kin}} = 630 \text{ K} \) and \( n_{H_2} = 10^{2.8} \text{ cm}^{-3} \) reproduces the observed CO SLED quite well, yielding an associated \( H_2 \) gas mass of \( \sim 10^9 \text{ M}_\odot \).

Rangwala et al. (2011) found that the low-J transitions trace cold gas with \( T_{\text{kin}} = 50 \text{ K} \) and \( n_{H_2} = 10^{2.8} \text{ cm}^{-3} \), while the mid-J to high-J lines trace a warmer, denser component with \( T_{\text{kin}} = 1350 \text{ K} \) and \( n_{H_2} = 10^{3.2} \text{ cm}^{-3} \), yielding a total gas mass of \( \sim 6 \times 10^9 \text{ M}_\odot \). Our two-component LVG analysis yields identical results for the cool molecular gas region; however, we find that the mid to high-J lines are modeled best as arising from a high-excitation component with \( T_{\text{kin}} = 316 \text{ K} \) and \( n_{H_2} = 10^{4.4} \text{ cm}^{-3} \). The difference in these values when compared against the best-fit parameters obtained in Rangwala et al. (2011) for the high-excitation component may be due to the fact that the high-J CO lines are differentially affected by dust extinction, an effect which Rangwala et al. (2011) argues and accounts for in his modeling, but which was not taken into account in this analysis. Nonetheless, our two-component LVG model yields a total gas mass \( M_{H_2} \sim 6 \times 10^9 \text{ M}_\odot \), (of which only 2% is in the warm phase), consistent with the mass estimates derived in Rangwala et al. (2011).

5.5.9 NGC 6240

NGC 6240 is a nearby luminous infrared galaxy, with a CO SLED similar in shape to that of Mrk 231. Several X-ray studies have firmly established the presence of powerful AGN activity (e.g. Iwasawa & Comastri 1998; Vignati et al. 1999), in fact occurring in both nuclei (Komossa et al. 2003). The system is also known for strong shocked emission in the superwind flow that is driven by the NGC 6240 starburst (van der Werf et al. 1993; Lutz et al. 2003). Although the CO J=8→7 transition has the largest line
intensity, the $J_{\text{upper}} \geq 14$ transitions make a significant contribution, with the intensity of the individual CO lines only slowly decreasing for higher rotational quantum numbers.

Limiting ourselves to a two-component LVG analysis, we find that the low-J lines can be modeled as arising from a region with $T_{\text{kin}} = 126$ K and $n_{\text{H}_2} = 10^{3.4}$ cm$^{-3}$, while the high-J lines are produced by a slightly warmer ($T_{\text{kin}} = 160$ K) and much denser gas phase, with a H$_2$ number density of $10^{7.4}$ cm$^{-3}$. The total gas mass derived for this simplistic model is $2 \times 10^{10}$ M$_\odot$, with close to 60% of the gas in the warmer, denser phase. However, as in the case of IC 694, this two-component LVG model fails to reproduce the observed mid-J lines, suggesting that three distinct components may be necessary to fit the full CO SLED. An alternative approach may be to employ shock models to further analyze the CO excitation in NGC 6240. This was pointed out in Meijerink et al. (2013) when they found, among other things, that even the most optimistic estimate of the AGN X-ray luminosity is not enough to explain the combined H$_2$ and CO observed luminosities.

### 5.5.10 Mrk 231

Mrk 231 is the most luminous of the local ULIRGs and a type 1, low-ionization broad absorption line (LoBAL) AGN. Limited to observations of the CO ladder up to the $J=6\rightarrow5$ transition in Mrk 231, Papadopoulos et al. (2007) found that while the LVG solutions derived solely from the three lowest CO transitions converged to $T_{\text{kin}} = 55 - 95$ K and $n_{\text{H}_2} \sim 10^3$ cm$^{-3}$, the CO(4-3) and CO(6-5) emission lines traced a much denser gas phase with $n_{\text{H}_2} \sim (1-3) \times 10^4$ cm$^{-3}$.

With the additional SPIRE FTS (van der Werf et al. 2010) and PACS high-J lines,
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

we find that the CO lines up to J = 11-10 can be produced by a two-component LVG model, with a cool region at $T_{\text{kin}} = 50$ K and $n_{H_2} = 10^{3.8}$ cm$^{-3}$ emitting the low-J lines ($J_{\text{upper}} < 4$) and a warmer, denser region at $T_{\text{kin}} = 316$ K and $n_{H_2} = 10^{4.2}$ cm$^{-3}$ dominating the mid- to high-J line emissions. These models yield a total associated gas mass of $\sim 10^9$ M$_\odot$, with 20% of the gas in the high-excitation component. However, a challenge is presented by the highest CO rotational lines ($J_{\text{upper}} \geq 12$), which are strongly under-produced by our two-component LVG model. These higher-J lines may signal the presence of a third excitation component which could be a high-excitation PDR, XDR, or shocks, as explained in van der Werf et al. (2010).

5.6 Summary

We have presented the extragalactic detections of FIR CO rotational line emission within the central 10" of a sample of starburst galaxies, Seyfert galaxies, and (U)LIRGs in the local universe. ($z < 0.1$). We have augmented our multi-J $^{12}$CO line dataset ($J_{\text{upp}} \geq 14$), detected with Herschel-PACS, with lower-J CO line measurements collected from the literature to yield a well-sampled set of local CO SLEDs (Tables 5.3 and 5.4). Along with providing a necessary benchmark for the usually more sparsely sampled SLEDs obtained for high redshift galaxies, (e.g. Weiss et al. 2007), these SLEDs demonstrate the uncertainties in relying solely on high-J CO diagnostics to characterize the excitation source of a galaxy. Without a broad coverage of the entire SLED for a given source, a single or few observed CO lines can easily be misinterpreted given the sheer diversity in SLED shapes shown in Figure 5.1. However, while the detection of a high-J CO line alone is not an unambiguous signature of a particular excitation source, the position
CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

of a source on a ratio-ratio diagram may be an indication of the presence, or lack thereof, of a warm, dense molecular gas component. In the CO(18-17)/CO(1-0) versus CO(18-17)/CO(6-5) plot shown in Figure 5.2, the sources that fall in the upper right corner of the diagram, with CO(18-17)/CO(1-0) > 10 and CO(18-17)/CO(6-5) > 0.2, consistently have a higher percentage of highly-excited molecular gas than those that fall in the lower left corner, as verified by the LVG-modeling results for these sources.

Another tracer of high density molecular clouds, which is traditionally used in ground-based mm observations, is provided by low HCN lines. These lines trace similar critical densities as the CO lines in the PACS range (\(n \sim 10^6 - 10^8\) cm\(^{-3}\)). In fact, a similar trend is found if in the above ratio-ratio plot the x-axis is replaced by the HCN(1-0)/CO(1-0) ratios of our objects as presented in Gao & Solomon (2004). However, while both molecules trace dense gas, the energy levels of the upper transitions are different, i.e. the CO traces warmer gas than HCN, and therefore, while HCN lines provide complementary results, they are not 1:1 substitutes for the high-J CO lines.

Furthermore, at high redshifts, the CO lines have moved into the (sub-)mm range and are thus better high density tracers than the low-lying HCN transitions which have moved out of that window.

These results were verified using an LVG radiative transfer modeling technique, which we employed to quantitatively analyze the CO emission from a subset of our detected sources. For each CO SLED, we identify the set of characterizing parameters that best reproduces the observed line intensities. Using both single-component and two-component LVG models to fit the cloud’s kinetic temperature, velocity gradient, gas density, and beam-averaged CO column density, we derive the molecular gas mass and the corresponding CO-to-H\(_2\) conversion factor for each respective source. A summary of
the best-fit LVG parameters is presented in Table 5.5 and the resulting LVG-modeled SLEDs for the single and two-component fits are shown in the left and right panels of Figure 5.3, respectively. Remarkably, the CO emission line spectra of star-forming galaxies may often be representable by a single LVG SLED as a function of halo mass and molecular gas mass content. Furthermore, we find that our two-component LVG model results are mostly consistent with the fits obtained in Kamenetzky et al. (2014) where the $^{12}\text{CO}$ SLEDs from $J=1\rightarrow 0$ to $J=13\rightarrow 12$ are modeled for many of the same sources discussed in this paper.

Estimates of the CO-to-$H_2$ conversion factors derived from our best-fit single and two-component LVG models can be found in Table 5.7. The relatively low $\alpha_{\text{CO}}$ values we find (compared to normal, star-forming galaxies like the Milky Way), are consistent with previous measures of the conversion factor for some of the individual sources as well as the general finding of low $\alpha_{\text{CO}}$’s in the center of bright galaxies (Wild et al. 1992; Bryant & Scoville 1996; Scoville et al. 1997; Bryant & Scoville 1999; Papadopoulos & Seaquist 1999; Israel 2009b,a; Sliwa et al. 2012). Conditions such as low metallicity, high gas temperature, large velocity dispersion, and higher gas density in an extended warm phase outside the GMCs (typical in ULIRGs) all drive $\alpha_{\text{CO}}$ to lower values (Bolatto et al. 2013). While the high velocity gradient is the primary culprit behind the reduced value of $\alpha_{\text{CO}}$ in M82 ($\sim 0.25 \text{M}_\odot(\text{K km}^{-1}\text{pc}^2)^{-1}$), the bulk of our results are due to the higher temperatures and warm-phase gas densities found in our sample targets (which never approach the low-metallicity regime.) However, given our modest sample size and the small degree of variance we find in the warm gas mass fractions, it becomes difficult to identify any specific trend between these physical conditions and the conversion factor.

We also systematically find higher $\alpha_{\text{CO}}$ values for the two-component models which
provide separate fits for the low-and high-J lines, than for the single component models where all CO line emissions trace a single region. This trend is consistent with the existence of a dichotomy, most prominent in (U)LIRGS, pointed out in Papadopoulos et al. (2012b). In their analysis of a CO line survey of (U)LIRGs, Papadopoulos et al. (2012b) find that while one-phase radiative transfer models of the global CO SLEDs yield low $\alpha_{CO}$ values, $\langle \alpha_{CO} \rangle \sim 0.6 \, M_\odot (K \, km^{-1}pc^2)^{-1}$, in cases where higher-J CO lines allow a separate assessment of gas mass at high densities, near-Galactic $\alpha_{CO} \sim (3-6) \, M_\odot (K \, km^{-1}pc^2)^{-1}$ values become possible.

In addition to the CO lines presented here, each of the objects of this study also has (SHINING and other) observations of the FIR fine-structure lines. These will provide further constraints on the physical properties of the photon-dominated regions (PDRs), X-ray dominated regions (XDRs), and shocks in these galaxies, and will augment the interpretation of the CO emission in future detailed studies.

## 5.7 Acknowledgements

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CHAPTER 5. HIGH-J CO IN NEARBY GALAXIES

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Chapter 6

Predicting the Intensity Mapping Signal for multi-J CO lines

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6.1 Abstract

We present a novel approach to estimating the intensity mapping signal of any CO rotational line emitted during the Epoch of Reionization (EoR). Our approach is based on large velocity gradient (LVG) modeling, a radiative transfer modeling technique that generates the full CO spectral line energy distribution (SLED) for a specified gas kinetic temperature, volume density, velocity gradient, molecular abundance, and column...
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

density. These parameters, which drive the physics of CO transitions and ultimately dictate the shape and amplitude of the CO SLED, can be linked to the global properties of the host galaxy, mainly the star formation rate (SFR) and the SFR surface density. By further employing an empirically derived $SFR - M$ relation for high redshift galaxies, we can express the LVG parameters, and thus the specific intensity of any CO rotational transition, as functions of the host halo mass $M$ and redshift $z$. Integrating over the range of halo masses expected to host CO-luminous galaxies, we predict a mean CO(1-0) brightness temperature ranging from $\sim 0.6 \mu K$ at $z = 6$ to $\sim 0.03 \mu K$ at $z = 10$ with brightness temperature fluctuations of $\Delta T_{CO} \sim 0.1$ and $0.005 \mu K$ respectively, at $k = 0.1 \text{ Mpc}^{-1}$. In this model, the CO emission signal remains strong for higher rotational levels at $z = 6$, with $\langle T_{CO} \rangle \sim 0.3$ and $0.05 \mu K$ for the CO $J = 6\rightarrow5$ and CO $J = 10\rightarrow9$ transitions respectively. Including the effects of CO photodissociation in these molecular clouds, especially at low metallicities, results in the overall reduction in the amplitude of the CO signal, with the low- and high-J lines weakening by 2-20% and 10-45%, respectively, over the redshift range $4 < z < 10$.

6.2 Introduction

Within the last decade, spectral line intensity mapping has been proposed as an additional, complementary probe of the large-scale structure (LSS) of star-forming galaxies during the epoch of reionization (EoR) (Suginohara et al. 1999; Righi et al. 2008; Visbal & Loeb 2010). Glimpses into this era have been limited to observations of individual massive galaxies and quasars at high redshifts, provided by the Hubble Space Telescope (HST) and ground-based telescopes. While in the future, we anticipate new
instruments like Atacama Large Millimeter Array (ALMA) and the James Webb Space Telescope (JWST) providing more detailed views of this “cosmic dawn”, they will be restricted by relatively small fields of view and an inability to observe galaxies that are simply too faint to detect individually. Intensity mapping offers a complementary glimpse of the three-dimensional structure of the high-redshift universe by imaging aggregate line emissions from thousands of unresolved objects and studying the large-scale fluctuations in the given line intensity due to the clustering of unresolved sources.

Intensity mapping can be performed using many different spectral lines, the 21 cm neutral hydrogen line being among the most common, given its unique insight into the evolution of the neutral IGM during the EoR (Madau et al. 1997; Loeb & Zaldarriaga 2004; Zaldarriaga et al. 2004; Furlanetto et al. 2006; Morales & Wyithe 2010; Pritchard & Loeb 2011). In this paper, we focus on the millimeter to far-infrared rotational transitions of carbon monoxide (CO), a molecule that forms primarily in star-forming regions and whose intensity maps promise a wealth of information on the spatial distribution of star formation in the universe (Breysse et al. 2014). While CO intensity fluctuations have already been studied, initially as foreground contaminants to cosmic microwave background (CMB) measurements (Righi et al. 2008) and then as probes of LSS (Visbal & Loeb 2010; Carilli 2011; Gong et al. 2011; Lidz et al. 2011; Pullen et al. 2013), these studies have been limited to the lowest order transitions of the molecule, mainly, CO(1-0) and CO(2-1). These lines are often considered because they are typically among the brightest and have redshifted frequencies that can potentially be observed from the ground. However, with the advent of ALMA\(^1\) and its frequency

\(^1\)http://almascience.nrao.edu
coverage (84 - 950 GHz), fluctuations in the line emission of many high-J CO transitions will potentially be available and can be measured and translated into a 3D map of the early universe. Having access to multiple CO rotational lines will further facilitate redshift identification and mitigate line confusion, making it possible to statistically isolate the fluctuations from a particular redshift by cross-correlating the emission from different sets of lines (Visbal & Loeb 2010; Loeb & Furlanetto 2013).

Attempts in the recent literature to obtain a theoretical estimate of the CO emission signal from high redshift galaxies have relied heavily on empirical relations calibrated from local observations and are limited almost exclusively to the $^{12}\text{CO} J=1\rightarrow0$ transition line. To calculate this mean CO brightness, a simple model is often adopted that connects the strength of the CO emission to the abundance of the dark matter halos that host CO luminous galaxies. Visbal & Loeb (2010) construct this model by first approximating a galaxy’s star formation rate (SFR) as a linear function of the mass of the galaxy’s host halo. They then further assume a linear relationship between the line luminosity and SFR and adopt the $L_{\text{CO}}$ to SFR ratio from M 82 to calibrate the proportionality constant. Lidz et al. (2011) embrace a similar approach, adopting the $SFR - M$ relation proposed by Visbal & Loeb (2010), but using a set of empirical scaling relations between a galaxy’s SFR, far-infrared luminosity, and CO(1-0) luminosity that have been measured for galaxies at $z \lesssim 3$. Both studies lead to a simple empirical estimate of the CO luminosity that is linear in halo mass ($L_{\text{CO}} \propto SFR \propto M$) and that relies on the extrapolation of low-redshift calibrations to higher redshifts, redshifts corresponding to the EoR. Gong et al. (2011) arrives at the relation between CO(1-0) luminosity and the halo mass via a different route, making use of the Millennium numerical simulation results of Obreschkow et al. (2009), a study which, although incorporates many physical
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

processes to model the CO emission from high-redshift galaxies, still invokes low-redshift measurements to calibrate the normalization factor of the CO luminosity for a given halo.

These various models, among others, have led to estimates of the CO power spectra amplitude signal that vary over a range spanning two orders of magnitude, illustrating the lack of theoretical understanding of the physics of CO transitions in a high-redshift context (Breysse et al. 2014). In Muñoz & Furlanetto (2013), this problem is addressed and a computation of CO fluxes is presented within an analytic framework that incorporates both global modes of star formation and the physics of molecular rotational lines in \( z \geq 6 \) Lyman-break galaxies. Our paper follows the general direction taken by Muñoz & Furlanetto (2013) and introduces a simpler approach that captures and ties the physics of molecular emission lines to high-redshift \( (z \geq 4) \) observations of star-forming galaxies (Mashian et al. 2016). Our approach is based on large velocity gradient (LVG) modeling, a radiative transfer modeling technique that generates the full CO spectral line energy distribution (SLED) for a specified set of physical parameters. Typically, LVG modeling is employed to quantitatively analyze an observed set of emission lines and determine the set of parameters that best reproduce the observed SED (Mashian et al. 2015b). In this paper, we consider applying the LVG methodology in the reverse direction: given a halo of mass \( M \) with CO-emitting molecular clouds characterized by a kinetic temperature \( T_{\text{kin}} \), velocity gradient \( dv/dr \), gas volume density \( n \), molecular abundance \( \chi \), and column density \( N \), we will derive the full CO SED and compute the mean surface brightness of any CO rotational line emitted by halos with that mass at any given redshift.

Our paper is organized as follows. In section 6.3, we introduce our LVG model
for the specific intensity of CO emission and outline the formalism that relates the set of LVG parameters driving the physics of CO transitions in molecular clouds to the global properties of the host galaxy, mainly, the SFR. Given the empirically determined high-redshift $SFR - M$ relation (Mashian et al. 2016), these parameters, and thus, the specific CO intensity, can ultimately be expressed as functions of the host halo mass $M$ and redshift $z$. In section 6.4 we compute the spatially averaged CO surface brightness from star-forming galaxies, as well as the power spectrum of spatial fluctuations in the CO emission at any given redshift, with a focus on redshifts corresponding to the EoR. We conclude in section 6.5 with a summary of our results and a brief comparison with other related calculations of the CO intensity mapping signal. Throughout we consider a $\Lambda$CDM cosmology parametrized by $n_s = 1$, $\sigma_8 = 0.8$, $\delta_c = 1.69$, $\Omega_m = 0.31$, $\Omega_\Lambda = 0.69$, $\Omega_b = 0.05$, and $h = 0.7$, consistent with the latest measurements from Planck (Planck Collaboration et al. 2016b).

6.3 Modeling the CO Emission

6.3.1 CO Brightness Temperature

To calculate the average CO brightness temperature, we follow the formalism presented by Lidz et al. (2011) and consider the specific intensity of a CO line observed at frequency $\nu_{obs}$ at redshift $z = 0$,

$$I(\nu_{obs}) = \frac{c}{4\pi} \int_0^\infty dz' \frac{\epsilon[\nu_{obs}(1 + z')]}{H(z')(1 + z')^4}$$

as determined by solving the cosmological radiative transfer equation, where $H(z)$ is the Hubble parameter and $\epsilon[\nu_{obs}(1 + z')]$ is the proper volume emissivity of the given line.
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

Since CO is emitted from within halos hosting star-forming galaxies, we take the CO luminosity, $L_{CO}$, to be some function of the halo mass $M$ and redshift, and assume the profile of each CO line is a delta function in frequency,

$$L_{CO} = L(M, z)\delta_D(\nu - \nu_J) \quad (6.2)$$

where $\nu_J$ is the rest frame frequency of the transition of interest. If we then further assume that at any given time, a fraction $f_{duty}$ of halos with mass larger than $M_{\text{min},CO}$ actively emit CO lines, then for a given halo mass function $dn/dM$, the volume emissivity is,

$$\epsilon(\nu, z) = \delta_D(\nu - \nu_J)(1 + z)^3 f_{duty} \int_{M_{\text{min},CO}}^{\infty} dM \frac{dn}{dM}(M, z)L(M, z) \quad (6.3)$$

The specific intensity of a line with rest frame frequency $\nu_J$, emitted by gas at redshift $z_J$ thus simplifies to

$$I_{\nu_{obs}} = \frac{c}{4\pi \nu_J H(z_J)} f_{duty} \int_{M_{\text{min},CO}}^{\infty} dM \frac{dn}{dM}(M, z_J)L(M, z_J) \quad (6.4)$$

or, written as the brightness temperature,

$$\langle T_{CO} \rangle = \frac{c^3}{8\pi k_B \nu_J^2 H(z_J)} f_{duty} \int_{M_{\text{min},CO}}^{\infty} dM \frac{dn}{dM}(M, z_J)L(M, z_J) \quad (6.5)$$

where $k_B$ is the Boltzmann constant.

To determine $L(M, z_J)$, the specific luminosity of a given CO line, we employ large velocity gradient (LVG) modeling, a method of radiative transfer in which the excitation and opacity of CO lines are determined by the kinetic temperature $T_{\text{kin}}$, velocity gradient $dv/dr$, gas density $n$, CO-to-H$_2$ abundance ratio $\chi_{CO}$, and the CO column density of the emitting source. We adopt the escape probability formalism (Castor 1970; Goldreich & Kwan 1974) derived for a spherical cloud undergoing uniform collapse where

$$\beta_J = \frac{1 - e^{\tau_J}}{\tau_J} \quad (6.6)$$
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

is the probability, for a line optical depth $\tau_J$, that a photon emitted in the transition $J \rightarrow J - 1$ escapes the cloud (see Mashian et al. (2013) for a more detailed presentation of the LVG formalism.) Assuming that each emitting source consists of a large number of these unresolved homogeneous collapsing clouds, the corresponding emergent intensity of an emission line integrated along a line of sight can be expressed as

$$I_J = \frac{h\nu_J}{4\pi} A_J x_J \beta_J(\tau_J) N_{CO}$$

(6.7)

where $x_J$ is the population fraction in the $J^{th}$ level, $h\nu_J$ is the transition energy, $A_J$ is the Einstein radiative coefficient, and $N_{CO}$ is the beam-averaged CO column density.

The LVG-modeled specific luminosity of a line emitted by a host halo with disk radius $R_d$, therefore takes the form

$$L_{CO}(M, z_J) = 4\pi^2 R_d^2 I_{J, LVG} = \pi h\nu_J R_d^2 A_J x_J \beta_J(\tau_J) N_{CO}.$$  

(6.8)

We set

$$R_d(M, z) = \frac{\lambda}{\sqrt{2}} \frac{j_d}{m_d} r_{vir}$$

$$= \frac{\lambda}{\sqrt{2}} \frac{j_d}{m_d} \times 1.5 \left[ \frac{\Omega_m}{\Omega_m(z)} \frac{\Delta_c}{18\pi^2} \right]^{-1/3} \left( \frac{M}{10^8 M_\odot} \right)^{1/3} \left( \frac{1 + z}{10} \right)^{-1} \text{kpc}$$

(6.9)

where $\Delta_c = 18\pi^2 + 82d - 39d^2$, $d = \Omega_m(z) - 1$, and $\Omega_m(z) = \Omega_m(1+z)^3/(\Omega_m(1+z)^3 + \Omega_\Lambda)$ (Loeb & Furlanetto 2013). We assume that the specific angular momentum of the material that forms the disk is the same as that of the halo, i.e. $j_d/m_d = 1$, and adopt a spin parameter of $\lambda \approx 0.05$, corresponding to an isolated exponential disk (Mo et al. 1998).

Since the excitation state and optical depth of a given line, $x_J$ and $\tau_J$ respectively, are determined by the set of physical parameters $\{T_{kin}, dv/dr, n, \chi_{CO}\}$ that characterize
the emitting molecular clouds, the task remains to express these parameters as functions of \( M \) and \( z \), global properties of the host halo.

### 6.3.2 The Star Formation Model

As will be physically motivated below, the LVG parameters that dictate the shape of CO SLEDs in galaxies are well correlated with the galaxy’s global star formation rate surface density. The first ingredient of our model is therefore a \( SFR - M \) relation that connects the SFR and host halo mass at the high redshifts we are concerned with in this paper. In Mashian et al. (2016), such an empirical relation is derived by mapping the shape of the observed ultraviolet luminosity functions (UV LFs) at \( z \sim 4-8 \) to that of the halo mass function at the respective redshifts. In this abundance-matching method, each dark-matter halo is assumed to host a single galaxy and the number of galaxies with star formation rates greater than \( SFR \) are equated to the number of halos with mass greater than \( M \),

\[
f_{UV} \int_{M}^{\infty} dM \frac{dn}{dM}(M, z) = \int_{SFR}^{\infty} dSFR \phi(SFR, z)
\]

where \( \phi(SFR, z) \) is the observed, dust-corrected UV LF at redshift \( z \) and \( f_{UV} \) is the starburst duty cycle, i.e. the fraction of halos with galaxies emitting UV luminosity at any given time. Mashian et al. (2016) find that the \( SFR - M \) scaling law remains roughly constant across this redshift range and thus, an average relation can be obtained and applied to even higher redshifts, \( z \gtrsim 8 \), where it faithfully reproduces the observed \( z \sim 9 \) and 10 LFs. This mean scaling law, \( SFR_{av}(M) \), is fairly well parameterized by a
Figure 6.1: Left panel: The mean SFR – M relation in the high redshift universe, i.e. $z \gtrsim 4$, derived empirically via abundance matching and fitted by the double power law given in eq. (6.11) where $\{a_1, a_2, b_1, b_2\} = \{2.4 \times 10^{-17}, 1.1 \times 10^{-5}, 1.6, 0.6\}$ for $f_{UV} = 1$. Right panel: The corresponding SFR surface density, $\Sigma_{SFR}(M, z)$, derived by dividing the SFR by the halo disk area, $\pi R_d(M, z)^2$, at redshifts $z = 6$ (red) and $z = 10$ (blue). For more details and comparison to data, see Mashian et al. (2016).
double power law of the form,

$$SFR_{av}(M) = \begin{cases} a_1 M^{b_1}, & M \leq M_c \\ a_2 M^{b_2}, & M \geq M_c \end{cases} \quad (6.11)$$

with a turnover at a characteristic halo mass $M_c \approx 10^{11.6} \, M_\odot$. Fitting the average relations in the observed SFR range $\simeq 0.1 - 500 \, M_\odot/yr$, we obtain $\{a_1, a_2, b_1, b_2\} = \{2.4 \times 10^{-17}, 1.1 \times 10^{-5}, 1.6, 0.6\}$ for $f_{UV} = 1$. We find it reasonable to assume a UV duty cycle of unity throughout our calculations given that the time between mergers grows shorter than the Hubble time at the high redshifts we are considering and the fact that typical hydrodynamical simulations, where star-formation is driven not just by mergers, find a star-forming galaxy in effectively every halo at these redshifts (Fakhouri et al. 2010).

The corresponding mean SFR surface density, $\Sigma_{SFR}$ (units $M_\odot \, yr^{-1} kpc^{-2}$), is computed by dividing the SFR from eq. (6.11) by the area of the active star-forming halo disk with radius given by eq. (6.9). Figure 6.1 depicts the average $SFR - M$ relation and the resulting SFR surface densities at redshifts $z = 6$ and 10.

### 6.3.3 Theoretical Models for LVG Parameters

The next key step in our LVG-motivated approach to predicting the high redshift CO emission signal is to model the LVG parameters dictating the shape of the CO SLED as functions of the global properties of the host halo. As pointed out in Narayanan & Krumholz (2014), quantities, such as the gas temperature and density, which characterize the CO-emitting molecular interstellar medium (ISM) are well-correlated with the star formation rate surface densities of galaxies. Qualitatively, this makes sense since regions
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

of high SFR density typically arise from denser gas concentrations and have large UV radiation fields, with increased efficiency for thermal coupling between gas and dust. In the following sections, we will outline how each LVG parameter can be expressed in terms of the SFR surface density, $\Sigma_{SFR}$, and thus ultimately as a function of just the halo mass and redshift.

6.3.3.1 Gas Kinetic Temperature

To determine the effective kinetic temperature of the CO-emitting molecular gas, we assume that the gas and dust in the star-forming disk are thermally well-coupled, i.e. $T_{gas} \approx T_{dust}$. The temperature of a dust grain is set by the balance of radiative heating and cooling processes taking place in molecular clouds. The rate of heating due to absorption of optical or UV radiation and the incident cosmic microwave background (CMB) can be written as

$$\left( \frac{dE}{dt} \right)_{abs} = \pi a^2 \int_0^\infty d\nu Q_{abs,UV}(\nu) F(\nu) + \sigma_{SB} T_{CMB}^4$$

(6.12)

where $\sigma_{SB}$ is the Stefan-Boltzmann constant, $a$ is the grain radius, $Q_{abs,UV}(\nu)$ is the emissivity in the UV-optical regime, which we set equal to unity (Chanial et al. 2007), $T_{CMB} = 2.73(1+z)$ is the CMB temperature and $F(\nu)$ is the flux of energy radiated by the central starburst in the disk. Assuming optically thick conditions requires this starlight energy to be totally reemitted in the infrared; the integral on the right-hand side can thus be expressed as $L_{IR}/4\pi R_d^2$ and, adopting the conversion between $L_{IR}$ and $SFR$ presented in Kennicutt (1998b),

$$\left( \frac{L_{IR}}{\text{erg s}^{-1}} \right) = 2.2 \times 10^{43} \left( \frac{SFR}{M_\odot \text{yr}^{-1}} \right),$$

(6.13)
eq. (6.12) takes the final form:

\[
\left( \frac{dE}{dt} \right)_{abs} = \pi a^2 \left[ \frac{2.2 \times 10^{43}}{4\pi} \Sigma_{SFR} \left( \frac{M}{M_\odot \text{yr}^{-1} \text{kpc}^{-2}} \right) + \sigma_{SB}(2.73(1 + z))^4 \right].
\] (6.14)

The rate of cooling of dust grains by infrared emission is given by

\[
\left( \frac{dE}{dt} \right)_{em} = 4\pi a^2 \int_0^\infty d\nu \, Q_{abs,IR}(\nu) B_\nu(\nu, T_d)
\] (6.15)

where \( Q_{abs,IR}(\nu) \sim Q_{abs}(\nu_0)(\nu/\nu_0)\beta \) is the emissivity in the infrared regime, \( \nu_0 \) is the reference frequency, and \( \beta \) is the dust emissivity index. Substituting in for \( Q_{abs,IR}(\nu) \) and \( \pi B_\nu(\nu, T_d) \) (the flux emitted by a black-body), the integral simplifies to

\[
\left( \frac{dE}{dt} \right)_{em} = \pi a^2 \left[ \frac{60\sigma_{SB}}{\pi^4} \left( \frac{k_B}{\hbar} \right)^\beta \frac{Q_{abs}(\nu_0)}{\nu_0^\beta} \Gamma(\beta + 4)\zeta(\beta + 4)T_d^{\beta + 4} \right].
\] (6.16)

At thermal equilibrium, \( (dE/dt)_{abs} = (dE/dt)_{em} \), and the steady-state grain temperature in units of kelvin is

\[
T_d(\Sigma_{SFR}(M, z), z) = \left( \frac{\pi^4 (h/\hbar)^\beta \nu_0^\beta}{60} Q_{abs}(\nu_0) \Gamma(\beta + 4)\zeta(\beta + 4) \right) \left[ \frac{2.3 \times 10^{-3} \Sigma_{SFR}(M, z)}{4\pi\sigma_{SB}} \left( \frac{M_\odot \text{yr}^{-1} \text{kpc}^{-2}}{M_{yr}^{-1} \text{kpc}^{-2}} \right) + (2.73(1 + z))^4 \right]^{1/(\beta + 4)}.
\] (6.17)

In the analysis below, we take the fiducial value of \( \beta = 1.3 \), consistent with the mean emissivity index derived from the SCUBA Local Universe Galaxy Survey (Dunne et al. 2000), and the standard value \( Q_{abs}(125 \mu\text{m}) = 7.5 \times 10^{-4} \) (Hildebrand 1983; Alton et al. 2004; Chanial et al. 2007). A plot of the kinetic temperature as a function of halo mass at different redshifts can be found in the left panel of Figure 6.2.

### 6.3.3.2 Cloud volume density

Another key parameter in determining the shape of the CO SLED is \( n \), the cloud volume density (cm\(^{-3}\)) of the dominant collision partner for CO rotational excitation. Since we
Figure 6.2: Left panel: Gas kinetic temperature assuming the fiducial values $\beta = 1.3$ and $Q_{\text{abs}}(125 \, \mu m) = 7.5 \times 10^{-4}$ in eq. (6.17). Right panel: Cloud volume density of molecular hydrogen as defined by eqs. (6.18)-(6.27) plotted at redshifts $z = 6$ (red) and $z = 10$ (blue).
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

are assuming CO-emitting molecular clouds, \( n \) in this case is the cloud volume density of \( \text{H}_2 \), given by

\[
n_{\text{H}_2} = \frac{3 \Sigma_{cl}}{4 \mu m_{\text{H}_2} r_{cl}} \tag{6.18}
\]

where \( \mu = 1.36 \) takes into account the helium contribution to the molecular weight (assuming cold, neutral gas), \( m_{\text{H}_2} = 3.34 \times 10^{-27} \text{ kg} \), and \( r_{cl} \) is the cloud radius assuming a uniform sphere. At these high redshifts where the ISM is dominated by molecular gas, the surface density of \( \text{H}_2 \) in a given molecular cloud, \( \Sigma_{cl} \), can be related to the beam-averaged gas surface density in the galactic disk, \( \Sigma_{\text{gas}} \).

Empirical studies have found that a correlation exists between the surface density of molecular gas and the surface density of the SFR, a discovery that is consistent with observations that stars form predominantly in the molecular component of the ISM. The Kennicutt-Schmidt (KS) relation (Schmidt 1959; Kennicutt 1989) formulates this correlation in terms of a power-law, \( (\Sigma_{\text{SFR}}) \propto (\Sigma_{\text{gas}})^{N} \), where estimates of the index \( N \) range from super-linear (Kennicutt 1989, 1998b; Bouč et al. 2007; Liu et al. 2011; Momose et al. 2013), to linear (Bigiel et al. 2008; Leroy et al. 2008, 2013), to sublinear (Shetty et al. 2014). Given our paper’s focus on high redshift star-forming sources with CO-emitting molecular clouds, we deemed it most appropriate to adopt the KS relation presented in Genzel et al. (2010),

\[
\Sigma_{\text{SFR}} = (3.3 \pm 0.6) \times 10^{-4} \left( \frac{\Sigma_{\text{gas}}}{1 \text{ M}_\odot \text{ pc}^{-2}} \right)^{1.2 \pm 0.1} \text{ M}_\odot \text{ yr}^{-1} \text{ kpc}^{-2} \tag{6.19}
\]

a relation that was derived from data sets of CO molecular emission in \( z \sim 1-3 \) normal star-forming galaxies and restricted to the regime where molecular gas dominates the ISM at these redshifts, i.e. \( \Sigma_{\text{gas}} \gtrsim 3 \text{ M}_\odot \text{ pc}^{-2} \). Since no evidence of any redshift-dependence of this relation has been found thus far, applying eq. (6.19) at the higher redshifts we
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

consider in this paper, \( z \geq 4 \), is a reasonable extrapolation.

We therefore set \( \Sigma_{cl} \) equal to \( \Sigma_{gas} \), as defined by eq. (6.19), except in cases where \( \Sigma_{gas} \) drops below the threshold surface density for which the cloud is predominantly molecular. This “star-formation” threshold, defined by a molecular gas fraction of \( f_{H_2} = 0.5 \), is derived in Sternberg et al. (2014) for a plane-parallel slab (including \( H_2 \) dust) as a function of metallicity \( Z' \),

\[
\Sigma_{gas,*}(Z') = \frac{2m}{\sigma_g(Z')}(1.6 \ln \left[ \frac{\alpha G(Z')}{3.2} + 1 \right])
\]

where \( m = 2.34 \times 10^{-27} \) kg is the mean particle mass per hydrogen nucleus, \( \sigma_g(Z') = 1.9 \times 10^{-21} Z' \) cm\(^{-2}\) is the dust-grain Lyman-Werner-photon absorption cross section per hydrogen nucleon, and \( \alpha G \) is the dimensionless parameter that defines the LW-band optical depth in the cloud due to HI dust,

\[
\alpha G(Z') = \left( \frac{1 + 3.1Z^{0.365}}{4.1} \right) \frac{6.78}{1 + \sqrt{2.64Z'}}.
\]

We adopt the fundamental metallicity relation (FMR), a tight relation between the gas-phase metallicity \( Z' \), stellar mass \( M_* \), and SFR, to ultimately express \( Z' \) as a function solely of the halo mass and redshift. The FMR was initially observed and formulated in Mannucci et al. (2010) for local galaxies in the mass range \( 9.2 \leq \log M_*/M_\odot \leq 11.4 \). Since then, the FMR has been confirmed to hold for star-forming galaxies at redshifts as high as \( z \sim 3 \) Belli et al. (2013), and to extend smoothly at lower masses (Mannucci et al. 2011), taking the final form,

\[
12 + \log (O/H) = \begin{cases} 
8.90 + 0.37m - 0.14s - 0.19m^2 + 0.12ms - 0.054s^2 & \text{for } \mu_{0.32} \geq 9.5 \\
8.93 + 0.51(\mu_{0.32} - 10) & \text{for } \mu_{0.32} < 9.5
\end{cases}
\]
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

where $\mu_\alpha = \log (M_\star) - \alpha \log (SFR)$, $m = \log (M_\star) - 10$, and $s = \log (SFR)$.

To further parametrize the metallicity as a function of the halo mass and redshift, we rely on observations and models that support the conclusion that the SFR in galaxies at redshifts $z \gtrsim 4$ scales nearly linearly with increasing stellar mass and does not vary by more than a factor of order 2 (Salmon et al. 2015). This behavior is consistent with a crude estimation of the stellar mass of a galaxy with a star formation rate $SFR$:

$$M_\star \sim \int_0^{t_H(z)} dt \ SFR(t) \sim SFR(z) \times t_H(z) \quad (6.23)$$

where $t_H(z)$ is the age of the universe at a given redshift $z$. Since each halo of interest formed at some fraction of the age of the universe, the right-hand side should be multiplied by a factor $\lesssim 1$. We therefore calibrate the above expression using the SFR-$M_\star$ best-fit parameters presented in Salmon et al. (2015) for $z \sim 4 - 6$ and obtain the following relation

$$M_\star(M, z) = (0.28 \pm 0.02) \ SFR_{av}(M) \ t_H(z) \quad (6.24)$$

where $SFR_{av}(M)$ is the average SFR for a halo of mass $M$. We assume this relation continues to apply at redshifts $z > 6$ in the following calculations.

Armed with the parametrization of $SFR$ introduced in section 6.3.2, and thus a metallicity $Z$ expressed solely as a function of halo mass and redshift, we can now return to our model for the cloud surface density, $\Sigma_{cl}$. To ensure the molecular state of each individual cloud, i.e. $f_{H_2} \geq 0.5$, we set $\Sigma_{cl}$ equal to the beam-averaged gas surface density $\Sigma_{gas}(M, z)$ (derived by inverting eq. (6.19)) for all halo masses $M > \bar{M}$ and floor
it to the value $\Sigma_{gas,*}(\tilde{M}, z, f_{H_2} = 0.5)$ for all $M < \tilde{M}$,

$$
\Sigma_{cl}(M, z) = \begin{cases} 
\Sigma_{gas}(M, z) & \text{if } M > \tilde{M} \\
\Sigma_{gas,*}(\tilde{M}, z, f_{H_2} = 0.5) & \text{otherwise}
\end{cases}
$$

(6.25)

where $\tilde{M}$ is the halo mass at which $\Sigma_{gas}(z)$ drops below $\Sigma_{gas,*}(f_{H_2} = 0.5, z)$ at a given redshift $z$.

The other variable that appears in our definition of the $H_2$ volume density is $r_{cl}$, the molecular cloud radius. Assuming that the molecular gas within the clump is in hydrostatic equilibrium, the radius of the cloud can be related to its surface mass density through the relation,

$$
r_{cl} = \frac{c_{s, eff}^2}{\pi G \Sigma_{cl}}
$$

(6.26)

where $G$ is the gravitational constant and $c_{s, eff}$ is the effective sound speed in the gas (taking into account turbulence, $c_{s, eff}^2 = c_s^2 + \sigma_{turbulence}^2$), which we set to 10 km/s. The final expression for the molecular cloud volume density then simplifies to

$$
n_{H_2}(M, z) = \frac{3\pi G}{4\mu m_{H_2} c_{s, eff}^2} \Sigma_{cl}^2(M, z),
$$

(6.27)

a plot of which can be found in the right panel of Figure 6.2. The steep decline in number density at low halo masses, as depicted in Figure 6.2, mirrors the steeply declining $SFR - M$ relation at the low-mass end (see left panel in Figure 6.1); as the star-formation rate diminishes by several orders of magnitude with decreasing halo mass, the SFR surface density drops accordingly and ultimately translates into reduced gas column and number densities at these low masses.
6.3.3.3 Velocity Gradient

For the sake of simplicity, we assume self-gravitating, virialized molecular clouds, in which case, the velocity gradient $dv/dr$ and cloud volume density $n_{H_2}$ are related in the following way (Goldsmith 2001)

$$\frac{dv}{dr} \approx 3.1 \sqrt{\frac{n_{H_2}}{10^4 \text{ cm}^{-3}}} \text{ km s}^{-1} \text{pc}^{-1}$$  \hspace{1cm} (6.28)

where $n_{H_2}$ is defined in eq. (6.27). A plot of $dv/dr$ as a function of halo mass at different redshifts can be found in the left panel of Figure 6.3.

6.3.3.4 CO-to-H$_2$ Abundance Ratio

Studies have shown that at high metallicities, i.e. $Z' \gtrsim 10^{-2}$, the dominant metal-bearing molecule in the ISM is CO. Furthermore, (Bialy & Sternberg 2015) find that even at low metallicities, 30-100% of the available carbon is always locked in CO if the CO is shielded, provided that the hydrogen gas is in molecular form. In this limit, the relative CO-to-H$_2$ abundance varies approximately linearly with metallicity (Bialy & Sternberg 2015), and assuming most of the carbon is in fact locked up in CO, $\chi_{CO}$ is given by,

$$\chi_{CO}(Z) \approx 3 \times 10^{-4}Z'$$  \hspace{1cm} (6.29)

where an expression for the relevant metallicity $Z'$ can be found in eq. (6.22). A plot of $\chi_{CO}$ is shown in the right panel of Figure 6.3.

6.3.3.5 CO Column Density, including photodissociation

The CO column density, which sets the overall scaling and amplitude of the CO SLED, can be expressed most simply as the product of the CO-to-H$_2$ abundance ratio and the
Figure 6.3: Left panel: Velocity gradient $dv/dr$ as a function of halo mass $M$ assuming self-gravitating, virialized clouds as defined by eq. (6.28). Right panel: CO-to-H$_2$ abundance ratio via eq. (6.29), plotted at redshifts $z = 6$ (red) and $z = 10$ (blue).
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

beam-averaged molecular column density,

\[ N_{CO} = \chi_{CO} N_{H_2} \]  

(6.30)

where \( N_{H_2} \) is a power-law function of the SFR surface density, derived by inverting the KS relation in eq. (6.19),

\[ N_{H_2}(\Sigma_{SFR}(M, z)) = 2 \times 10^{-4} \left( \frac{\Sigma_{SFR}}{1 \text{ M}_\odot \text{ yr}^{-1} \text{ kpc}^2} \right)^{1/2} \text{ cm}^{-2} \]  

(6.31)

The above expression for \( N_{CO} \) does not account for conditions under which CO has photodissociated into C and C\(^+\) while the gas continues to remain molecular due to either \( \text{H}_2 \) self-shielding or dust-shielding. Such conditions, which may exist on the surfaces of molecular clouds or the clumps contained within such clouds, ultimately result in a fraction of \( \text{H}_2 \) gas that is “dark” in CO transitions. Observations indicate that the column density of this “dark gas” can be as high as 30\% \((\sim 3 \times 10^{21} \text{ cm}^{-2})\) of the total molecular column density in the local Galaxy \((\sim 10^{22} \text{ cm}^{-2})\) (Wolff et al. 2010). A first-order approximation of the CO column density that accounts for the effects of CO photodissociation is then

\[ N_{CO} = \chi_{CO} \left( N_{H_2} - \frac{3 \times 10^{21}}{Z'} \right) \text{ cm}^{-2} \]  

(6.32)

where, as before, \( Z' \) is the metallicity in solar units. The second term in the above expression is essentially the \( \text{H}_2 \) column required to enable CO dust-shielding under the assumption that the threshold for CO survival is set by a universal dust opacity. This approximation captures the effects of decreasing metallicity on the abundance of CO, reducing the column density as the number of shielding dust grains grows sparse. In the limiting case where \( Z' \) drops so low that there is not enough dust to effectively shield CO, (corresponding to the parenthesized portion of eq. (6.32) growing negative),

174
Figure 6.4: Beam-averaged CO column density derived at redshifts $z=6$ (red) and $z=10$ (blue) under conditions where CO photodissociation is accounted for (solid curves, eq. (6.32)) and neglected (dashed curves, eq. (6.31)). In the case where the effects of CO photodissociation are included, the CO column density drops to zero for halos smaller than $M < 10^{10} \, M_{\odot}$, indicating that the CO in the gas has fully disassociated.
the CO is fully dissociated and $N_{CO}$ is set to zero. We note that eq. (6.32) is only a first-order approximation and that the constant, $3 \times 10^{21}$, can be altered due to variations in UV field intensity or gas clumping factors. The beam-averaged CO column density at different redshifts is plotted in Figure 6.4, both for the case where CO photodissociation is accounted for (solid curves) and neglected (dashed curves).

### 6.3.4 Model CO SLEDs

Equipped with analytic expressions for the LVG parameters that dictate the shape and magnitude of the CO SLED, we can now compute the intensity of each CO line and the resulting SED generated by the molecular clouds in a halo with mass $M$ at redshift $z$. To carry out the computations, we use the Mark & Sternberg LVG radiative transfer code described in Davies et al. (2012), with CO-H$_2$ collisional coefficients taken from Yang et al. (2010) and energy levels, line frequencies, and Einstein $A$ coefficients taken from the Cologne Database for Molecular Spectroscopy (CDMS). For a given set of parameters, $\{T_{kin}, n_{H_2}, dv/dr, \chi_{CO}, N_{H_2}\}$, the code determines the level populations by iteratively solving the equations of statistical equilibrium which balance radiative absorptions, stimulated emission, spontaneous emission, and collisions with H$_2$ using the escape probability formalism discussed in section 6.3.1. Once the level populations are computed, the full CO rotational ladder and line intensities follow from eq. (6.7).

Figure 6.5 shows the CO SLEDs generated by halos at redshift $z = 10$ with masses in the range $M = 10^8$-$10^{13} \, M_\odot$ when the effects of CO photodisassociation are excluded. In the case where photodissociation is considered, the line intensities emitted by low-mass halos with $M < 10^{10} \, M_\odot$ (red and orange curves) entirely disappear, reflecting the full
Figure 6.5: CO SLEDs generated by a halo at redshift $z = 6$ (dashed curves) and $z = 10$ (solid curves) with halo mass ranging from $10^8$ to $10^{13}$ M$_\odot$, neglecting the effects of photodissociation. If CO photodissociation is taken into account, the red and orange curves, corresponding to line emission from halos with $M < 10^{10}$ M$_\odot$, would disappear while the other curves would remain unchanged. The brown curve denotes the expected SLED in the optically-thick case when the population levels are in local thermal equilibrium (LTE); in this limiting case, the intensity at a given level follows the Planck function, $B(\nu, T) d\nu = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT}-1} d\nu$, where $\langle T \rangle \sim 91$ K.
dissociation of CO in these molecular clouds where dust-shielding has grown inefficient. However, the other curves, corresponding to line emission from higher mass halos that have been normalized to the ground state, remain unchanged. This is due to the fact that “turning on” photodissociation merely reduces the beam-averaged CO column density according to eq. (6.32); since $N_{CO}$ controls the overall amplitude of the SLED (and not the shape), adjusting this quantity simply amplifies or reduces the intensity of all the CO lines by the same amount, leaving the ratio between lines unchanged.

As expected, we find that as the physical conditions in the emitting molecular clouds grow more extreme, the CO rotational levels become increasingly populated and the SLED rises accordingly. Consequently, the line intensities not only grow in magnitude, but the peak of the CO SLED also shifts to higher $J$ values, reflecting the excitation of the more energetic states of the molecule.

The curves plotted in Figure 6.5 demonstrate this trend in the case where a UV duty cycle of unity is assumed. In this scenario, the SFR and SFR surface density range from $10^{-4}$-1000 M$_\odot$ yr$^{-1}$ and $10^{-2}$-20 M$_\odot$ yr$^{-1}$ kpc$^{-2}$ respectively, when the halo mass varies from $10^8$ to $10^{13}$ M$_\odot$ (see figure 1). While the corresponding kinetic temperature remains relatively constant for this $\Sigma_{SFR}$ range ($T_{kin} \sim 90$ K), the H$_2$ number density varies significantly, $10^2$ cm$^{-3} \lesssim n_{H_2} \lesssim 3 \times 10^5$ cm$^{-3}$. The variance in the shape of the CO SED computed for $f_{UV} = 1$ reflects this range of physical conditions parameterized by the halo mass at $z = 10$; the SEDs produced by low-mass halos, $M < 10^{10}$ M$_\odot$, peak at $J \approx 4$ before turning over and plummeting (neglecting CO photodissociation). In these low density clouds, with correspondingly small velocity gradients ($dv/dr \sim 0.5$ km s$^{-1}$ pc$^{-1}$) and CO abundances ($\chi_{CO} \sim 5 \times 10^{-6}$), only the low-lying transitions such as CO $J = 1 \rightarrow 0$ are optically thick. In contrast, in more extreme star-forming galaxies, i.e. $M >$
$10^{10} \, M_\odot$, the $H_2$ number densities reach $\sim 10^5 \, \text{cm}^{-3}$, the typical critical density value for high-$J$ CO emission. Consequently, the high-$J$ lines grow optically thick and the line ratios approach thermalization for transitions as high as $J \sim 13$ in these high-mass halos.

### 6.4 Results

#### 6.4.1 Predicted CO Fluxes and Spatially Averaged CO Brightness Temperature

Given our LVG model of the full CO SLED, we can now predict the CO line fluxes generated by a set of molecular clouds residing in a host halo of mass $M$ at redshift $z$, as well as compute the spatially averaged brightness temperature of any CO rotational transition. The former is obtained by converting LVG-derived CO luminosities (eq. (6.8)) into observed, velocity-integrated fluxes, $F_{CO}$, using typical observer units,

$$\frac{L_{CO}}{L_\odot} = 1.040 \times 10^{-3} \left( \frac{D_L}{\text{Mpc}} \right)^2 \frac{\nu_{obs}}{\text{GHz}} \frac{F_{CO}}{\text{Jy km s}^{-1}}$$

where $D_L$ is the luminosity distance. The results are shown in Figure 6.6 for a range of CO rotational lines emitted as a function of host halo mass at $z = 6$ (left panel) and $z = 10$ (right panel). The dashed curves represent the fluxes obtained by including the effects of CO photodissociation in our computations; as expected, the change in flux when accounting for this phenomenon is most pronounced at the low-mass end where $F_{CO}$ drops to zero once the CO is fully photodissociated. At the higher-mass end, we predict that a $\sim 10^{11} \, M_\odot$ halo at redshift $z = 6$ will emit strongest in the $J = 7 \rightarrow 6$ transition with a flux of $\sim 25 \, \text{mJy}$ while a halo with the same mass at $z = 10$ will emit
Figure 6.6: The CO rotational line flux as a function of halo mass at $z = 6$ (left panel) and $z = 10$ (right panel) for $J_{\text{upper}} = 1-8$. Solid and dashed curves denote results obtained by neglecting (eq. (6.31)) and including (eq. (6.32)) the effects of CO photodissociation.
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

strongest in a higher energy state, $J = 10 \rightarrow 9$, but with nearly half the flux, $\sim 14 \text{ mJy}$.

In order to determine the spatially-averaged CO brightness temperature emitted by halos across the mass range, we compute the following integral,

$$
\langle T_{CO}(\nu_J) \rangle = \frac{c^3}{8\pi k_B \nu_J^2 \beta(z_J)} f_{duty} \int_{M_{min,CO}}^{\infty} dM \frac{dn}{dM} (M, z_J) L(M, z_J) \tag{6.34}
$$

where $\nu_J$ is the rest-frame frequency of the specified line. This equation is parameterized by $M_{min,CO}$, the minimum host halo mass for CO luminous halos, and $f_{duty}$, the duty cycle for CO activity. Since CO lines are excited by starburst activity, we generally expect that the duty cycle for CO luminous activity is comparable to the starburst duty cycle. We therefore assume $f_{duty} = f_{UV} = 1$ in our fiducial models. Furthermore, in computing the volume-averaged CO brightness temperature, we vary $M_{min,CO}$ widely between $M_{min,CO} = 10^8$, $10^9$, and $10^{10} \text{ M}_{\odot}$ to illustrate the sensitivity of the results to this parameter. In our model, these halos host CO luminous galaxies with SFRs of $\sim 10^{-4}$, $3 \times 10^{-3}$, and $0.1 \text{ M}_{\odot} \text{ yr}^{-1}$ (left panel of Figure 6.1).

We plot the results in Figure 6.7, where the mean brightness temperature is shown as a function of redshift for different CO rotational lines. As expected, we find that $\langle T_{CO} \rangle$ is a steeply declining function of $z$, a direct consequence of the decreasing number of host halos (per volume) at these high redshifts predicted by the Sheth-Tormen halo mass function (Sheth & Tormen 1999). When CO photodissociation is neglected (solid curves), the redshift evolution of $\langle T_{CO} \rangle$ for the low-$J$ CO lines steepens at the high-$z$ end when larger values are assumed for $M_{min,CO}$.

While halos with masses $M > 10^{10} \text{ M}_{\odot}$ emit the most flux at all redshifts (Figure 6.6), the flux emitted by halos with $M \sim 10^9$-$10^{10} \text{ M}_{\odot}$ makes a non-negligible contribution to the total CO brightness temperature at higher redshifts. An illustration of this is
Figure 6.7: Volume-averaged CO brightness temperature as a function of redshift for a minimum host halo mass of CO luminous galaxies of $M_{\text{min,CO}} = 10^8$ (red), $10^9$ (green), and $10^{10}$ M$_\odot$ (blue curves), neglecting the effects of CO photodissociation. The dashed curves denote the signals obtained when photodissociation is taken into account ($M_{\text{min,CO}} = 10^{10}$). Each panel shows $\langle T_{\text{CO}} \rangle$ for a different line in the CO rotational ladder with $1 \leq J_{\text{upper}} \leq 8$. 
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

Figure 6.7 (Continued)
presented in Figure 6.8 which plots $dT/d\ln M$, the contribution to the mean brightness temperature per logarithmic halo mass for different CO lines as a function of halo mass at $z = 6$ (dashed curves) and $z = 10$ (solid curves). It is clear that at $z = 10$, although the primary component of the CO signal originates from halos with masses in the range $M \sim 10^{10}-10^{11} \, M_\odot$, the CO emission from $\sim 10^9 \, M_\odot$ halos makes up nearly 15% of the total signal for the low-J lines. Thus, raising the minimum host halo mass for CO luminous halos from $10^8 \, M_\odot$ to $10^{10} \, M_\odot$ excludes a population of CO-emitting sources and reduces the amplitude of $\langle T_{CO} \rangle$ for the low-J lines by a factor of $\sim 2$. The effects of raising $M_{\text{min,CO}}$ vanish in the higher energy states since these low-mass halos emit less than 1% of the total signal in these high-J lines; hence, the red, green, and blue solid curves, denoting the mean brightness temperature for models where $M_{\text{min,CO}} = 10^8$, $10^9$, and $10^{10} \, M_\odot$, respectively, are barely distinguishable from one another for the higher energy rotational transitions.

In the case where CO photodissociation is taken into account, we found that the CO becomes fully photodissociated in halos with $M < 10^{10} \, M_\odot$ (Figure 6.4); since these low-mass halos do not emit CO flux in this model, the minimum host halo mass of a CO luminous galaxy is effectively set to $M_{\text{min,CO}} = 10^{10} \, M_\odot$. Accounting for CO destruction in molecular clouds results in an overall reduction in the amplitude of $\langle T_{CO} \rangle$, with the low- and high-J lines weakening by $\sim 2$-20% and 10-45%, respectively, over the range of redshifts shown in Figure 6.7 (dashed curves).

The spatially averaged brightness temperature of the CO J = 1–0 line predicted by our model assuming $M_{\text{min,CO}} = 10^8 \, M_\odot$ ranges from $\sim 0.6 \, \mu K$ at $z = 6$ to $\sim 0.03 \, \mu K$ at $z = 10$ when CO photodissociation is neglected. The strength of the CO signal dwindles for higher-J lines, with $\langle T_{CO}(z = 6) \rangle \sim 0.3 \, \mu K$ and $T_{CO}(z = 10) \sim 0.1 \, \mu K$ for
Figure 6.8: Contribution to the mean brightness temperature per logarithmic mass of different CO lines at redshift \( z = 6 \) (dashed) and \( z = 10 \) (solid), in the case where the effects of CO photodissociation are neglected.
the CO $J = 6 \rightarrow 5$ transition. “Turning on” photodissociation does not significantly effect the mean brightness temperature of the high-J lines, but it does reduce the CO(1-0) signal to $\langle T_{CO} \rangle \sim 0.4$ and $\sim 0.01 \mu K$ at $z = 6$ and 10, respectively.

Without delving into any particular instrumental design, we briefly consider the plausibility of detecting such signals. We use the radiometer equation for the signal-to-noise ratio, $S/N = (T_{CO}/T_{sys})\sqrt{\Delta \nu t_{int}}$ where $T_{sys} \sim 20$ K is the system temperature of the detector, $\Delta \nu$ is the observed bandwidth, and $t_{int}$ is the integration time, which we take to be 1000 hours. We find that at $z = 6$, the predicted brightness temperatures of the 4 lowest-lying CO transitions (neglecting CO photodissociation) can be detected at $5\sigma$ confidence with a bandwidth of $\Delta \nu \sim 10$ GHz, while a bandwidth of $\Delta \nu \sim 100$ GHz is required for detection with $1\sigma$ confidence at $z = 10$. Higher J lines in this model will require even longer integration times to achieve the desired brightness sensitivity.

**6.4.2 CO Power Spectrum**

Given the existence of brighter foreground sources of emission at the relevant frequencies, the mean redshifted CO signal will be difficult, if not impossible, to directly observe. We therefore consider spatial fluctuations in the surface brightness and compute the CO power spectrum predicted by different variations of our model. In contrast to the spectrally smooth foreground sources, the CO signal is expected to have structure in frequency space which can be used to isolate spatial fluctuations in its brightness temperature. Since the power spectrum captures the underlying matter distribution and structure, a map of the CO brightness temperature fluctuations at $z \geq 6$ can be used to
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

probe the spatial distribution of star-forming galaxies during the EoR.

Following the formalism in Gong et al. (2011) and Lidz et al. (2011), the three-dimensional power spectrum of the CO brightness temperature fluctuations is expected to take the form

\[ P_{CO}(k, z) = \langle T_{CO}(z) \rangle \left[ b_{CO}(z)^2 P_{\text{lin}}(k, z) + P_{\text{shot}}(z) \right]. \tag{6.35} \]

Since CO is emitted from within halos, the first term in this expression represents spatial variations due to correlations with the underlying dark matter density field where \( P_{\text{lin}} \) is the linear theory density power spectrum and the bias \( b_{CO} \) is given by

\[ b_{CO}(z) = \frac{\int_{M_{\text{min,CO}}}^{\infty} dM \frac{dn}{dM} L_{\text{CO}}(M, z) b(M, z)}{\int_{M_{\text{min,CO}}}^{\infty} dM \frac{dn}{dM} L_{\text{CO}}(M, z)} \tag{6.36} \]

where \( b(M, z) = 1 + (\nu^2(M, z) - 1)/\delta_c, \nu(M, z) = \delta_c/\sigma(M, z), \) and \( \sigma(M, z) \) is the RMS density fluctuation in a spherical region containing mass \( M \) (Mo & White 2002). The second term of eq. (6.35), the shot noise contribution due to Poisson fluctuations in the number of halos on the sky, can be expressed as

\[ P_{\text{shot}}(z) = \frac{1}{f_{\text{duty}}} \frac{\int_{M_{\text{min,CO}}}^{\infty} dM \frac{dn}{dM} L_{\text{CO}}(M, z)^2}{\left( \int_{M_{\text{min,CO}}}^{\infty} dM \frac{dn}{dM} L_{\text{CO}}(M, z) \right)^2} \tag{6.37} \]

where, in all of our calculations, we adopt the Sheth-Tormen halo mass function for \( dn/dM \).

The power spectra of the CO rotational lines from \( J_{\text{upper}} = 1 \) to \( J_{\text{upper}} = 10 \) are plotted in Figure 6.9 for models which include (dashed) and exclude (solid) the effects of CO photodissociation. The y-axis shows \( \Delta_{\text{CO}}^2(k, z) = k^3 P_{CO}(k, z)/(2\pi^2) \), the contribution to the variance of \( \langle T_{CO} \rangle \) per logarithmic bin, in units of \([\mu\text{K}^2]\). In general, the fluctuations depend strongly on the wavenumber, with the overall shape of the
Figure 6.9: Auto power spectrum of CO brightness temperature fluctuations for lines all the way up to $J_{\text{upper}} = 10$, at $z = 6$ (red) and $z = 10$ (blue). In each panel, the solid curves represent results for the models in which CO photodissociation was neglected and a minimum host halo mass of $M_{\text{CO,min}} = 10^8 \, M_\odot$ was assumed; dashed curves denote results for the case where the effects of CO photodissociation were included, effectively setting the minimum host halo for CO luminous galaxies to $M_{\text{CO,min}} = 10^{10} \, M_\odot$. 
predicted power spectra reflecting the form of eq. (6.35). On large scales, small $k$, the clustering term dominates and the fluctuations in CO brightness temperature mirror the underlying dark matter density field. Conversely, on small scales (large $k$), the shot noise takes over and the fluctuations reach $\Delta_{\text{CO}}^2 \sim 300 - 1300 \mu K^2$ on scales of $k = 10 \text{ Mpc}^{-1}$ at $z = 6$, and $\Delta_{\text{CO}}^2 \sim 4 - 14 \mu K^2$ at $z = 10$ (when photodissociation is neglected). The $J = 1 \to 0$ transition is predicted to produce the strongest signal, with an amplitude that drops by a factor of $\sim 5$-50 across the wavenumber range $k \sim 10^{-2}$-10 Mpc$^{-1}$ when the higher energy state, $J = 10 \to 9$, is considered instead.

The redshift evolution of $\Delta_{\text{CO}}^2$ is ultimately dictated by the behavior of $\langle T_{\text{CO}} \rangle (z)$; although $b_{\text{CO}}^2$ increases as the host halos become more clustered at higher redshifts, this effect is not enough to compensate the declining brightness temperature with $z$. The auto-correlation signal of all the CO lines therefore weakens as the redshift varies from $z = 6$ to 10, dropping by $\sim 2$ orders of magnitude over this redshift range. On the other hand, our results for $\Delta_{\text{CO}}^2$ depend very weakly on our choice of the minimum host halo mass for CO luminous galaxies; therefore, in the fiducial models where photodissociation is neglected, we only plot results for the case where $M_{\text{min,CO}} = 10^8 \text{ M}_\odot$, thereby including the contribution of the low-mass halos to the overall emission signal.

The effects of including CO photodissociation are most prominent for the low-$J$ lines, weakening the signal by, at most, a factor of $\sim 6$ at $z = 10$ on large scales. At $k = 0.1 \text{ Mpc}^{-1}$, we find CO(1-0) brightness temperature fluctuations of amplitude $\Delta_{\text{CO}}^2 \sim 0.1 \mu K^2$ at $z = 6$, whether or not CO photodissociation is taken into account. At $z = 10$, $\Delta_{\text{CO}}^2(k = 0.1 \text{ Mpc}^{-1}) \sim 5 \times 10^{-4}$ and $8 \times 10^{-5} \mu K^2$ for the $J = 1 \to 0$ line in the models where photodissociation is turned “off” (assuming fixed $M_{\text{min,CO}} = 10^8 \text{ M}_\odot$) and “on”, respectively.
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

6.5 Discussion

We have presented a new approach to estimating the mean CO emission signal from the epoch of reionization (EoR) that links the atomic physics of molecular emission lines to high-redshift observations of star-forming galaxies. This method is based on LVG modeling, a radiative transfer modeling technique that generates the full CO SLED for a specified set of characterizing parameters, namely, the kinetic temperature, number density, velocity gradient, CO abundance, and column density of the emitting source. We showed that these LVG parameters, which dictate both the shape and amplitude of the CO SLED, can be expressed in terms of the emitting galaxy’s global star formation rate, $SFR$, and the star formation rate surface density, $\Sigma_{SFR}$. Employing the $SFR-M$ relation empirically derived for high-redshift galaxies, i.e. $z \geq 4$, we can then ultimately express the LVG parameters, and thus, the specific intensity of any CO rotational line, as functions of the host halo mass $M$ and redshift $z$.

Adopting a starburst duty cycle of $f_{UV} = 1$, the average $SFR - M$ relation derived via abundance-matching for $4 < z < 8$ is characterized by a steeply declining slope at the low-mass end, where the star formation rate goes as $SFR \propto M^{1.6}$. With the SFR dropping to values below 0.1 $M_\odot$ yr$^{-1}$ for $M < 10^{10}$ $M_\odot$, the physical conditions in these low-mass halos are not “extreme” enough to substantially excite the high-$J$ CO rotational states. The resulting CO SLEDs correspondingly peak around $J \approx 4$ before turning over, and the overall contribution of CO emission from this halo population grows negligible at lower redshifts. On the other hand, the $H_2$ number density and CO-to-$H_2$ abundance in halos with masses $M \geq 10^{10}$ $M_\odot$ are large enough to keep the high-$J$ population levels thermalized; the CO SLEDs generated by these massive halos
therefore have peaks shifted to $J \geq 10$ and overall higher amplitudes, reflecting the excitation of the more energetic states of the molecule.

We also consider the effects of CO photodissociation on the CO line intensities generated by our fiducial models. Assuming that the threshold for CO survival is set by a universal dust opacity, we adopt a first-order approximation of $N_{CO}$ which effectively reduces the CO column density with decreasing metallicity. In the limiting case where the metallicity drops so low that there is not enough dust to shield CO, the CO is considered fully dissociated and $N_{CO}$ is set to zero. We find that such conditions occur in halos with $M \lesssim 10^{10} \, M_\odot$, causing the line intensities emitted by these low-mass halos to entirely disappear in models where CO photodissociation is accounted for.

Given our LVG model of the full CO SLEDs, we can predict both $F_{CO}$, the CO line flux generated by a set of molecular clouds in a host halo of mass $M$ at redshift $z$, as well as $\langle T_{CO} \rangle$, the spatially averaged brightness temperature of any CO rotational transition. We find that the flux emitted in the $J = 1 \rightarrow 0$ transition by a halo at redshift $z = 6$ with mass $M \sim 10^{11} \, M_\odot$ is $F_{CO(1-0)} \sim 0.8$ mJy km/s. The higher rotational lines are expected to be even brighter, with a $10^{11} \, M_\odot$ halo at $z = 6$ emitting a CO(6-5) flux of $\sim 23$ mJy km/s. These fluxes drop by 25-30% when considering a $10^{11} \, M_\odot$ halo emitting at $z = 10$, with $F_{CO(1-0)} \sim 0.2$ mJy km/s and $F_{CO(6-5)} \sim 7$ mJy km/s.

The CO line fluxes emitted by individual host halos of mass $M$ at redshift $z$ as estimated in this paper, are found to be generally higher than previous estimates obtained in the literature (Obreschkow et al. 2009; Muñoz & Furlanetto 2013). Building an analytic formalism within a paradigm where star formation is a function of gas supply and stellar feedback, the model presented in Muñoz & Furlanetto (2013) provides radial
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

distributions of SFR, $\Sigma_{gas}$, and $T$ which are then used to calculate the masses, sizes, and number of GMCs, and the corresponding total CO line luminosities emitted by these clouds. Consequently, the CO(1-0) flux emitted by a $10^{11} M_\odot$ halo at $z = 6$ as predicted by this model is $\sim 0.01$-$0.03$ mJy km/s, an order of magnitude smaller than the flux estimates derived with our methodology. The flux in the $J = 6 \rightarrow 5$ transition is found to be highly sensitive to the inclusion of turbulent clumps within the GMCs, given that the high densities in such inhomogeneities can effect the thermalization of the higher-$J$ rotational lines; the resulting CO(6-5) flux in the models presented in Muñoz & Furlanetto (2013) thus varies from $10$ mJy km/s to $10^{-3}$ mJy km/s when turbulent clumps are included and excluded, respectively.

While these results are comparable to those derived using the semi-analytic methods of Obreschkow et al. (2009), they are consistently smaller than the values presented in this paper. The prolific number of parameters used to characterize the GMC properties in Muñoz & Furlanetto (2013) make it difficult to ascertain the source of divergence between our results, which both use radiative transfer techniques. However, we suspect these differences can be traced back to the different prescriptions used to set the star formation rate surface density, $\Sigma_{SFR}$, and gas surface density, $\Sigma_{gas}$, the two ingredients which, once related to one another via the Kennicutt-Schmidt relation in our model, determine the shape and amplitude of the resulting CO SLED. Furthermore, Muñoz & Furlanetto (2013) parameterizes the properties of MCs as a function of their position relative to the disk center, and after considering the level populations and optical depth of CO in each cloud directly, computes the resulting flux from the entire galaxy by counting up the number of clouds at each galactic radius. The molecular clouds in our model, on the other hand, are characterized by disk-averaged properties of the host
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

halo disk; to derive the signal from a CO-emitting galaxy, we assume a large number of these identical homogeneous collapsing clouds and scale the line intensities with the disk-averaged CO column density. Based on the sensitivity limits quoted in Muñoz & Furlanetto (2013), our approach predicts that the $J_{\text{upper}} = 1$ line in $z = 6$ halos with mass $M \geq 10^{12} \, M_\odot$ will be observable by JVLA\(^2\) (Jansky Very Large Array) after ten hours of observation; at this redshift, the CO(2-1) and CO(3-2) lines fluxes emitted by halos with $M > 10^{11} \, M_\odot$ are also expected to be observed by JVLA. Similarly, we expect ALMA to detect the CO(6-5) flux emitted by $z = 6$ halos with mass $M \geq 5 \times 10^{10} \, M_\odot$ after ten hours of observation, and higher rotational lines $J_{\text{upper}} \geq 7$ emitted by halos with $M \gtrsim 10^{11} \, M_\odot$.

To obtain an estimate of the spatially averaged brightness temperature of a given line at a particular redshift, we simply integrate $L_{\text{CO}}(M, z)$ over the range of halo masses that are expected to host CO-luminous galaxies. In the case where CO photodissociation is included, the minimum host halo mass of CO-emitting galaxies is set to $M_{\text{CO, min}} \sim 10^{10} \, M_\odot$ by the model itself, since the CO is found to be fully dissociated in halos with $M < 10^{10} \, M_\odot$. When CO photodissociation is ignored, varying $M_{\text{CO, min}}$ from $10^8$ to $10^{10} \, M_\odot$ reduces the low-$J$ line signals at high redshifts, where the CO emission from $\sim 10^9 \, M_\odot$ halos make up a non-negligible percentage of the total emission.

In our fiducial model where CO photodissociation is neglected and $M_{\text{min, CO}} = 10^8 \, M_\odot$, we predict a spatially averaged brightness temperature of $\langle T_{\text{CO}} \rangle \sim 0.5 \, \mu\text{K}$ at $z = 6$ and $0.03 \, \mu\text{K}$ at $z = 10$ for the low-$J$ CO rotational lines, with brightness temperature fluctuations of amplitude $\Delta^2 T_{\text{CO}} \sim 0.1$ and $0.005 \, \mu\text{K}^2$ respectively, at $k = 0.1 \, \text{Mpc}^{-1}$.

\(^2\)http://www.vla.nrao.edu/
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

These CO emission signals are further reduced to \( \langle T_{CO} \rangle \sim 0.4 \) and \( 0.01 \ \mu K \) at \( z = 6 \) and \( 10 \), respectively, for the low-lying states when the effects of CO photodissociation are included in the calculations. (Note that, since CO lines are typically excited by starburst activity, the choice of \( M_{\text{min,CO}} = 10^8 \ M_\odot \) is favored by theoretical and numerical investigations which indicate that \( 10^8 \ M_\odot \) is the minimum mass required for a halo to cool and form stars at these high redshifts (Haiman et al. 1996; Tegmark et al. 1997; Trenti et al. 2010; Loeb & Furlanetto 2013)). Our estimates of \( \langle T_{CO} \rangle \) for the low-\( J \) CO transitions are comparable to the values obtained in previous work by Carilli (2011), Gong et al. (2011), Lidz et al. (2011), and Pullen et al. (2013). Constructing a model based on the required cosmic star formation rate density to reionize the universe, Carilli (2011) obtains an order-of-magnitude estimate of \( \langle T_{CO} \rangle(z = 8) \sim 1 \ \mu K \) for the \( J = 1 \rightarrow 0 \) and \( J = 2 \rightarrow 1 \) transitions. Gong et al. (2011) arrives at a slightly smaller estimate of the CO(1-0) brightness temperature, \( \langle T_{CO} \rangle \sim 0.5 \ \mu K \) for \( z = 6 \) and \( 0.1 \ \mu K \) for \( z = 10 \), by using the Millennium numerical simulation results of Obreschkow et al. (2009) to model the CO emission from high-redshift galaxies. Lidz et al. (2011) assumes a linear \( SFR - M \) relation and a set of low-\( z \) empirical scaling relations between a galaxy’s SFR, \( L_{\text{FIR}} \), and \( L_{CO(1-0)} \) to estimate \( \langle T_{CO} \rangle \) for these low-\( J \) lines; they find a mean brightness temperature of \( \sim 2 \ \mu K \) at \( z \sim 6 \) and \( 0.5 \ \mu K \) at \( z \sim 10 \) with fluctuations \( \Delta^2_{CO} \sim 0.2 \) and \( 0.02 \ \mu K^2 \), respectively, on scales of \( k \sim 0.1 \text{ Mpc}^{-1} \). In a more recent paper, Pullen et al. (2013) follows the approach taken in Lidz et al. (2011) with a few adjustments to the \( SFR - M \) prescription to arrive at brightness temperatures of \( \langle T_{CO} \rangle \sim 0.7 \) and \( 0.2 \ \mu K \) at redshifts \( z = 6 \) and \( 10 \) respectively, assuming \( M_{\text{min,CO}} = 10^9 \ M_\odot \) for the CO(1-0) and CO(2-1) lines.

While these previous works are limited almost exclusively to predicting the signals
CHAPTER 6. INTENSITY MAPPING SIGNAL FOR CO LINES

of the $^{12}$CO J=1→0 and 2→1 transition lines, our LVG-based approach generates the full CO SLED and thus allows us to compute the signal strength of the higher-J energy states as well. For example, we predict a CO(10-9) brightness temperature of $\langle T_{\text{CO}} \rangle \sim 0.05 \, \mu$K at $z = 6$ and 0.003 $\mu$K at $z = 10$ with $\Delta^2_{\text{CO}}(k = 0.1) \sim 0.003$ and $10^{-5}\mu$K$^2$ respectively. We look forward to future experiments, such as the Carbon MonOxide Mapping Array (COMA)$^3$ currently under development, which promise to provide spectral-spatial intensity mapping of CO at the high redshifts characterizing the epoch of reionization.

6.6 Acknowledgements

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[^3]: http://www.stanford.edu/group/church_group/cgi-bin/wordpress/?page_id=515
Chapter 7

Spectral Distortion of the CMB by the Cumulative CO Emission from Galaxies throughout Cosmic History

This thesis chapter originally appeared in the literature as


7.1 Abstract

We show that the cumulative CO emission from galaxies throughout cosmic history distorts the spectrum of the cosmic microwave background (CMB) at a level that is
well above the detection limit of future instruments, such as the Primordial Inflation Explorer (PIXIE). The modeled CO signal has a prominent bump in the frequency interval 100-200 GHz, with a characteristic peak intensity of $\sim 2 \times 10^{-23} \text{ W m}^{-2} \text{ Hz}^{-1} \text{ sr}^{-1}$. Most of the CO foreground originates from modest redshifts, $z \sim 2-5$, and needs to be efficiently removed for more subtle distortions from the earlier universe to be detected.

## 7.2 Introduction

Since the measurements by COBE/Far Infrared Absolute Spectrophotometer (FIRAS), the average cosmic microwave background spectrum (CMB) spectrum is known to be extremely close to a perfect blackbody with a temperature $T_0 = 2.726 \pm 0.001 \text{ K}$ and no detected global spectral distortions to date (Mather et al. 1994; Fixsen et al. 1996; Fixsen 2009). However, the standard model of cosmology predicts tiny deviations from the Planckian spectrum due to cosmological processes which heat, cool, scatter, and create CMB photons throughout the history of the Universe (Sunyaev & Zeldovich 1969; Zeldovich & Sunyaev 1969; Sunyaev & Zeldovich 1970; Illarionov & Siuniaev 1975a,b; Danese & de Zotti 1982; Burigana et al. 1991; Hu & Silk 1993; Burigana & Salvaterra 2003; Chluba et al. 2012; Sunyaev & Khatri 2013). While at redshifts $z \gtrsim 2 \times 10^6$, the thermalization process (mediated by the combined action of double Compton emission, Bremsstrahlung and Compton scattering) is rapid enough to efficiently erase any distortion to unobservable levels, at lower redshifts, the CMB spectrum becomes vulnerable and spectral distortions that form are “locked in” and can thus be theoretically observed today (Chluba & Sunyaev 2012; Chluba 2014; Chluba et al. 2015).

In connection with early energy release, two types of CMB distortions are
traditionally distinguished: chemical potential $\mu$- and Compton $y$- distortions (Sunyaev & Zeldovich 1969, 1970; Illarionov & Sunyaev 1975a,b). In the regime $2 \times 10^6 \lesssim z \lesssim 3 \times 10^5$, the efficiency of double Compton and Bremsstrahlung processes in controlling the number of CMB photons gradually reduces while photons are still efficiently redistributed in energy by the Compton process. In this case, where thermalization stops being complete, electrons and photons are in kinetic equilibrium with respect to Compton scattering, and any energy injection produces a chemical potential characterized by $\mu(\nu)$. At lower redshifts, $z \lesssim 10^4$, up-scattering of photons by electrons also becomes inefficient and photons diffuse only little in energy, creating a $y$-type distortion $y(\nu)$ which is an early-universe analogue of the thermal Sunyaev-Zeldovich effect. Both types of distortions are tightly constrained by COBE/FIRAS measurements, with upper limits of $|\mu| < 9 \times 10^{-5}$ and $|y| < 1.5 \times 10^{-5}$ at 95% confidence (Fixsen et al. 1996).

The amplitude of these signals, predicted within the standard cosmological paradigm, is expected to fall below the bounds set by COBE-FIRAS measurements. The average amplitude of the $y$-parameter, due to the large-scale structure and the reionization epoch, is expected to be $y \approx 10^{-7}$-$10^{-6}$, with the most recent computations predicting $y \approx 2 \times 10^{-6}$ (Hu et al. 1994b; Refregier et al. 2000; Oh et al. 2003; Hill et al. 2015). The $\mu$-distortion signal is expected to be even weaker, with the damping of small-scale acoustic modes giving rise to $\mu \approx 2 \times 10^{-8}$ in the standard slow-roll inflation scenario (Daly 1991; Hu et al. 1994a; Chluba et al. 2012). Although these distortions are small, significant progress in technology in the last two decades promises to detect these spectral distortions. Experimental concepts, like the Primordial Inflation Explorer (PIXIE; Kogut et al. 2011a) and Polarized Radiation Imaging and Spectroscopy Mission (PRISM; André et al. 2014), could possibly improve the absolute spectral sensitivity.
CHAPTER 7. SPECTRAL DISTORTION BY CUMULATIVE CO EMISSION

limits of COBE/FIRAS by 2-3 orders of magnitude and detect the aforementioned signals at the 5σ level, providing measurements at sensitivities $\mu = 5\times10^{-8}$ for a chemical potential distortion and $y = 10^{-8}$ for a Compton distortion (Fixsen & Mather 2002; Kogut et al. 2011a; Chluba 2013; Chluba & Jeong 2014).

However, it is not yet clear what the foreground limitations to measuring these primordial spectral distortions will be. When considering the large angular scales of interest to PIXIE, focus has been geared towards the foreground subtraction of polarized emission from the Milky Way’s interstellar medium (ISM) which is dominated by synchrotron radiation from cosmic ray electrons accelerated in the Galactic magnetic field, and thermal emission from dust grains. Kogut et al. (2011b) claim that the CMB emission can be distinguished from Galactic foregrounds based on their different frequency spectra, as long as the number of independent frequency channels equals or exceeds the number of free parameters to be derived from a multi-frequency fit.

But in addition to these Galactic foregrounds, there is another contaminant which has been primarily neglected in the literature, and that is the diffuse background of CO emission lines from external galaxies. Until recently, Righi et al. (2008) provided the only estimate of this redshift-integrated CO emission signal. Assuming star formation is driven by major mergers, they calculated the resulting star-formation rate (SFR) and then converted it to a CO luminosity, $L_{CO}$, using the measured ratio of $L_{CO}$ to SFR in M82, a low-redshift starburst galaxy. The CO background they found, integrated over all redshifts, is expected to contribute $\sim 1 \mu K$ at $\nu \gtrsim 100$ GHz with an almost flat spectrum. De Zotti et al. (2016) also include estimates of the background contributed by CO lines from star-forming galaxies when they consider the Galactic and extragalactic foreground intensity compared with the CMB spectra. Using the $L_{IR}-L_{CO}$ relations presented in
Greve et al. (2014) for the CO rotational ladder from $J = 1 \rightarrow 0$ to $J = 5 \rightarrow 4$, they find that the CO signal is substantially higher than the PIXIE sensitivity, with the CO(4-3) line alone contributing $\sim 3 \times 10^{-24}$ erg s$^{-1}$ cm$^{-2}$ sr$^{-1}$ at sub-mm wavelengths.

In this paper, we apply the formalism and machinery presented in Mashian et al. (2015a) to predict the total CO emission signal generated by a population of star-forming halos with masses $M \geq 10^{10}$ $M_\odot$ from the present-day, to redshifts as early as $z \sim 15$. Our comprehensive approach is based on large-velocity gradient (LVG) modeling, a radiative transfer modeling technique that produces the full CO spectral line energy distribution (SLED) for a specified set of parameters characterizing the emitting source. By linking these parameters to the global properties of the host halos, we calculate the CO line intensities emitted by a halo of mass $M$ at redshift $z$, and then further integrate these CO luminosities over the range of halo masses hosting CO-luminous galaxies to derive the average surface brightness of each rotational line. We find that over a range of frequencies (30-300 GHz) spanned by a PIXIE-like mission, the signal strength of this diffuse background is 1-3 orders of magnitude larger than the spectral distortion limits PIXIE aims to provide. The CO foreground must be removed in order for the more subtle distortion signals from the earlier universe to be detected.

This Letter is organized as follows. Section 7.3 provides a brief overview of the formalism and key ingredients of our CO-signal modeling technique. Section 7.4 presents the results and Section 7.5 summarizes the main conclusions. We adopt a flat, $\Lambda$CDM cosmology with $\Omega_m = 0.3$, $\Omega_\Lambda = 0.7$, $\Omega_b = 0.045$, $H_0 = 70$ km s$^{-1}$Mpc$^{-1}$ (i.e. $h = 0.7$), $\sigma_8 = 0.82$, and $n_s = 0.95$, consistent with the most recent measurements from Planck (Planck Collaboration et al. 2016b).
7.3 The Formalism

In Mashian et al. (2015a), we developed a novel approach to estimating the line intensity of any CO rotational transition emitted by a host halo with mass $M$ at redshift $z$ in the early universe, $z \geq 4$. Here, we briefly outline the model far enough to calculate the quantities relevant for the present work and refer the reader to our previous paper for further details.

In our formalism, the average specific intensity of a given CO line with rest-frame frequency $v_J$ emitted by gas at redshift $z_J$ is,

$$I_{\nu,\text{obs}} = \frac{c}{4\pi \nu_J H(z_J)} \int_{M_{\text{min},\text{CO}}}^{\infty} dM \frac{dn}{dM}(M, z_J) L(M, z_J)$$  \hspace{1cm} (7.1)

where $H(z)$ is the Hubble parameter, $dn/dM$ is the Sheth-Tormen halo mass function (Sheth & Tormen 1999) and $M_{\text{min},\text{CO}}$ is the minimum host halo mass for CO-luminous galaxies. To determine the specific luminosity of the line, $L(M, z_J)$, we employ LVG modeling, a method of radiative transfer in which the excitation and opacity of CO lines are determined by the kinetic temperature $T_{\text{kin}}$, velocity gradient $dv/dr$, gas density $n$, CO-to-H$_2$ abundance ratio $\chi_{\text{CO}}$, and the CO column density $N_{\text{CO}}$ of the emitting source. A background radiation term with temperature, $T_{\text{CMB}} = T_0(1 + z)$, is included in the LVG calculations; the increasing CMB temperature with $z$ is expected to depress the CO line luminosity at higher redshifts. Adopting the escape probability formalism (Castor 1970; Goldreich & Kwan 1974) for a spherical cloud undergoing uniform collapse and assuming that each emitting source consists of a large number of these unresolved collapsing clouds, the emergent LVG-modeled intensity of an emission line can be expressed as

$$I_J = \frac{h \nu_J}{4\pi} A_J x_J \beta_J (\tau_J) \chi_{\text{CO}} N_{H_2}$$  \hspace{1cm} (7.2)
where \( x_J \) is the population fraction in the \( J^{\text{th}} \) level, \( A_J \) is the Einstein radiative coefficient, \( N_{H_2} \) is the beam-averaged \( H_2 \) column density, and \( \beta_J = (1 - e^{\tau_J})/\tau_J \) is the photon-escape probability. To carry out these computations, we use the Mark & Sternberg LVG radiative transfer code described in Davies et al. (2012).

We showed previously that the LVG parameters, \( \{T_{\text{kin}}, n_{H_2}, dv/dr, \chi_{\text{CO}}, N_{H_2}\} \), which drive the physics of CO transitions and ultimately dictate both the shape and amplitude of the resulting CO SLED, can be linked to the emitting galaxy’s global star formation rate, \( SFR \), and the star formation rate surface density, \( \Sigma_{SFR} \). The analytic expressions for these quantities can be found in section 2.3 of Mashian et al. (2015a), and will not be rederived here. The final ingredient in our model is thus a \( SFR - M \) relation that allows us to express these LVG parameters solely as functions of the global properties of the host halo, i.e. the halo mass \( M \) and redshift \( z \).

For high redshifts, \( z \geq 4 \), we adopt the average \( SFR - M \) relation derived in Mashian et al. (2016) via abundance-matching. Assuming each dark-matter halo hosts a single galaxy, they mapped the shape of the observed ultraviolet luminosity functions (UV LFs) at \( z \sim 4-8 \) to that of the halo mass function at the respective redshifts and found that the \( SFR - M \) scaling law is roughly constant across this redshift range (within 0.2 dex). This average relation, which faithfully reproduces the observed \( z \sim 9 \) - 10 LFs, is therefore employed in our calculations for all redshifts greater than 4. For \( z < 4 \), we rely on the results of Behroozi et al. (2013b,a) which empirically quantified the stellar mass history of dark matter halos, using a comprehensive compilation of observational data along with simulated halo merger trees to constrain a parameterized stellar mass-halo mass relation.
Figure 7.1: The relative CMB spectral distortions due to CO emission from star-forming galaxies at redshifts as high as \( z \sim 15 \) to the present. The contribution of each spectral line, from \( J = 1 \rightarrow 0 \) to \( J = 10 \rightarrow 9 \) is shown, along with the summed signal (black curve). The shaded area corresponds to the 1\( \sigma \) confidence region for the total predicted signal.
7.4 Results

In Figure 7.1, we present our predictions of the contribution of each spectral line to the cumulative CO background from star-forming galaxies at redshifts as high as \( z \sim 15 \) to the present. The low-\( J \) CO lines peak at frequencies corresponding to an emission redshift of \( z \sim 2 \). This emission is dominated by star-forming halos with masses \( 10^{11}-10^{12} \) M\(_{\odot}\), hosting molecular clouds that are characterized by a gas kinetic temperature \( T_{\text{kin}} \sim 40 \) K and H\(_2\) number densities \( n_{\text{H}_2} \sim 100 - 1000 \text{ cm}^{-3} \). The higher-\( J \) \((J > 5)\) CO signal is dominated by emission from \( 10^{11}-10^{12} \) M\(_{\odot}\) host halos residing at \( z \gtrsim 4 \); in the star-forming galaxies at these high redshifts, the physical conditions in the emitting molecular clouds are extreme enough to thermalize the higher-order CO transitions, with gas kinetic temperatures of \( \sim 60 \) K and number densities of order \( 10^{4} \) cm\(^{-3}\). Integrating over the population of CO luminous halos between redshifts \( 0 \leq z \leq 15 \), we find that the total emission (black curve) predicted by our LVG-based model is not completely spectrally smooth, but rather has a prominent bump in the frequency interval \( \sim 100 - 200 \) GHz with a characteristic peak intensity of \( \sim 2 \times 10^{-23} \text{ W m}^{-2} \text{ Hz}^{-1} \text{ sr}^{-1} \), i.e. \( \Delta I_\nu / I_\nu \simeq (5 \pm 2) \times 10^{-6} \). This is the frequency range within which the most prominent redshifted CO line emissions, originating from sources at redshifts \( z \sim 2 - 5 \), fall and accumulate to form the peak in the cumulative signal depicted in Figure 7.1. The total CO intensity is \( \sim 0.01\% \) of the far-infrared background intensity computed in Fixsen et al. (1998) and Lutz (2014), where the former computes a total 125-2000 \( \mu \)m background of \( \sim 14 \) nW m\(^{-2}\)sr\(^{-1}\) and the latter computes a total 8-1000 \( \mu \)m background of \( \sim 27 \) nW m\(^{-2}\)sr\(^{-1}\). The uncertainty in our estimates of the CO signal, represented by the shaded regions in Figures 7.1-7.3, primarily stems from the uncertainty in the average \( SFR - M \) relations.
Figure 7.2: The relative CMB spectral distortions due to CO emission from star-forming galaxies at redshifts as high as $z \sim 15$ to the present. The contribution of each spectral line, from $J = 1 \rightarrow 0$ to $J = 10 \rightarrow 9$ is shown, along with the summed signal (black curve). The shaded area corresponds to the $1\sigma$ confidence region for the total predicted signal.
we adopt to express the LVG parameters as functions of the global properties of the host halos.

In the case where we assume that local sources of CO emission can be identified and subtracted from observations, we find that the predicted foreground signal not only drops in magnitude as expected, but the shape of the CO spectrum is modified as well. These results are clearly demonstrated in Figure 7.2, where each curve is computed by integrating the CO intensity emitted by galaxies from some minimum redshift, $z_{\text{min}}$, out to redshift $z \approx 15$. Starting off with $z_{\text{min}} = 0$, which corresponds to the original results shown in Figure 7.1 where emission from local sources is included in the calculations (black curve), we vary the minimum redshift to values as high as $z_{\text{min}} = 8$. We find that excluding the emission from the population of lower redshift sources results in a sawtooth modulation of the cumulative CO spectrum, with the modulation appearing at the observed frequencies, $\nu_{\text{obs}} = \nu_J/(1 + z_{\text{min}})$, at which the contribution from a given CO transition, $J \rightarrow J - 1$, drops out. For example, in the case where emission sources at redshifts $z < 4$ can be subtracted and thus no longer contribute to the CO foreground (blue curve), the total CO signal strength plummets at $\nu_{\text{obs}} \approx 23$ GHz when the CO(1-0) line contribution disappears, and then again at $\nu_{\text{obs}} \approx 46$ GHz when the CO(2-1) contribution dies out; this pattern continues out to $\nu_{\text{obs}} \approx 922$ GHz, at which point the redshifted CO($J = 40 \rightarrow 39$) line vanishes and no trace of the CO signal emitted by the galaxy population at $z \geq 4$ is left. This sawtooth-shaped form of the resulting CO spectrum highlights both the discrete nature of CO rotational transitions at frequencies, $\nu_J = J\nu_{\text{CO(1-0)}}$, with $\nu_{\text{CO(1-0)}} = 115.3$ GHz and $J = 1, 2, ..., 40$, as well as the significant contribution by modest redshift sources to the overall CO foreground signal.
CHAPTER 7. SPECTRAL DISTORTION BY CUMULATIVE CO EMISSION

Assuming that the more local emission sources are not individually subtracted, the intensity of the predicted CO background is at least 2-100 times weaker than the current COBE/FIRAS upper limits, \( \Delta I_\nu / I_\nu \lesssim 10^{-5} - 10^{-4} \). Therefore, although this foreground is expected to peak in the range of frequencies spanned by COBE/FIRAS, the signal has eluded detection to date. However, as depicted in Figure 7.3, the total emission one expects from the CO background lies 1-3 orders of magnitude above the PIXIE sensitivity to \( \mu \)- and \( y \)-type distortions in the 30-300 GHz frequency range. These spectral distortions take the form

\[
\Delta I_\nu^\mu = \frac{2h\nu^3}{c^2} \times \mu \frac{e^x}{(e^x - 1)^2} \left( \frac{x}{2.19} - 1 \right)
\]

(7.3)

and

\[
\Delta I_\nu^y = \frac{2h\nu^3}{c^2} \times y \frac{xe^x}{(e^x - 1)^2} \left[ x \left( \frac{e^x + 1}{e^x - 1} \right) - 4 \right]
\]

(7.4)

where \( x = h\nu/(k_B T) \) is the dimensionless frequency, \( h \) is Planck’s constant, \( k_B \) is Boltzmann’s constant, and \( T \) is the CMB temperature. The full exploitation of PIXIE’s potential to measure \( \mu \)- and \( y \)-type spectral distortions of \( \mu = 5 \times 10^{-8} \) and \( y = 10^{-8} \) at the 5\( \sigma \) level therefore requires a highly refined foreground subtraction, which is further complicated by the fact that the CO signal is not completely spectrally smooth. At higher frequencies, \( \nu \gtrsim 400 \) GHz, the foreground CO emission grows exponentially weak, \( \Delta I_\nu^{CO} \ll \Delta I_\nu^\mu, \Delta I_\nu^y \), and ceases to pose as a prominent limiting factor in obtaining accurate spectral distortion measurements. The \( y \) distortion from reionization and structure formation (\( z \lesssim 10 - 20; \) green curve), has a relatively large amplitude, \( |y| \sim 2 \times 10^{-6} \), comparable to the predicted cumulative CO signal, and is expected to be visible even without more detailed modeling.
Figure 7.3: The relative CMB spectral distortions due to CO emission from star-forming galaxies at redshifts as high as $z \sim 15$ to the present. The contribution of each spectral line, from $J = 1 \rightarrow 0$ to $J = 10 \rightarrow 9$ is shown, along with the summed signal (black curve). The shaded area corresponds to the $1\sigma$ confidence region for the total predicted signal.
7.5 Discussion

We apply an LVG-based modeling approach to predict the cumulative CO emission signal generated by star-forming galaxies throughout cosmic history. The relative CMB distortion due to this CO foreground is not spectrally smooth, but rather peaks in the frequency range $\nu \sim 100 - 200$ GHz with an amplitude of $\Delta I_{\nu}/I_{\nu} \simeq 5 \times 10^{-6}$. Exploring cases where nearby sources of CO emission can be identified and subtracted from observations, we find that the dominant contributors to the CO signal originate from star-forming halos with masses $M \sim 10^{11}-10^{12}$ M$_{\odot}$ at modest redshifts of $z \sim 2 - 5$. While the intensity of this cumulative CO foreground is at least 2-100 times weaker than the current COBE/FIRAS upper limits, and has thus far evaded detection, it falls well above the detection limit of future instruments, such as PIXIE, which promise to measure CMB spectral distortions with sensitivity improved by 2-3 orders of magnitude compared to COBE/FIRAS.

In standard cosmology, there are a number of different heating/cooling processes in the early Universe which may have given rise to CMB spectral distortions of varying magnitudes and shapes. Silk damping of small-scale perturbations in the primordial baryon-electron-photon fluid is one of them, resulting in CMB distortions with magnitudes of $\Delta I_{\nu}/I_{\nu} \simeq 10^{-8} - 10^{-10}$, depending on the shape and amplitude of the primordial power spectrum at scales $50 \leq k \leq 10^4$ Mpc$^{-1}$ (Daly 1991; Hu et al. 1994a; Chluba et al. 2012). Residual annihilation of dark matter particles throughout the history of the Universe is another, releasing energy that leads to $\mu$ and $y$ distortions of amplitude $\mu \approx 3 \times 10^{-9}$ ($z > 5 \times 10^4$) and $y \approx 5 \times 10^{-10}$ ($z < 5 \times 10^4$), respectively (Chluba & Sunyaev 2012; Chluba & Jeong 2014). The cosmological recombination of
hydrogen and helium is expected to have introduced distortions as well, with amplitudes of \( \Delta I_\nu / I_\nu \approx 10^{-9} \) at redshifts \( z \sim 1100 - 6000 \) (Chluba & Sunyaev 2006; Rubiño-Martín et al. 2006, 2008). Similar magnitude but opposite sign distortions, \( \mu \sim -2.7 \times 10^{-9} \) and \( y \sim -6 \times 10^{-10} \), are expected from energy losses of the CMB to baryons and electrons as they cool adiabatically faster than radiation with the expansion of the Universe (Chluba 2005; Chluba & Sunyaev 2012; Khatri et al. 2012).

Experiments like PIXIE will be able to constrain these spectral distortions in the CMB at the \( 5\sigma \) level, providing measurements at sensitivities \( \mu = 5 \times 10^{-8} \) and \( y = 10^{-8} \). However, as demonstrated above, the cumulative CO foreground is an important contaminant to these cosmological distortions, with a signal strength, \( \Delta I_\nu^{\text{CO}} / I_\nu \sim 5 \times 10^{-6} - 10^{-7} \), that is 1-3 orders of magnitude higher than PIXIE’s sensitivity limits in the frequency range \( \nu \sim 20 - 360 \) GHz. Based on the results depicted in Figure 2, CO luminous sources at redshifts \( z < 8 \) need to be identified and subtracted in order to reduce this cumulative signal to levels that are at least comparable to the \( \mu \) - and \( y \) - type spectral distortions one hopes to constrain. Removing all such sources is challenging, both in terms of exposure time and in terms of field coverage. Even with ten hours of integration time, instruments like the Atacama Large Millimeter Array (ALMA) will miss CO emission from host halos with masses \( M \lesssim 5 \times 10^{10} \ M_\odot \), which contribute tens of percent of the cumulative CO signal at redshifts \( z \gtrsim 4 \). (In this paper, we integrate over the population of CO luminous halos with masses \( M \geq 10^{10} \ M_\odot \) and thus present conservative estimates of the total CO foreground which do not account for contributions from lower mass halos, \( M \lesssim 10^{10} \ M_\odot \).) Removing the aggregate line emission from unresolved sources throughout cosmic history poses its own difficulties. Unlike the spectrally smooth synchrotron and thermal dust foregrounds which can be approximately
CHAPTER 7. SPECTRAL DISTORTION BY CUMULATIVE CO EMISSION

described by power laws, the CO foreground fluctuates in frequency due to the clustering of sources over restricted regions on the sky; accurate foreground subtraction therefore requires knowledge of the emission spectrum to high order of precision, challenging our ability to fully exploit PIXIE’s sensitivity to constrain CMB spectral measurements.

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Part III

Early Planetary Systems
Chapter 8

CEMP Stars: Possible Hosts to Carbon Planets in the Early Universe

This thesis chapter originally appeared in the literature as


8.1 Abstract

We explore the possibility of planet formation in the carbon-rich protoplanetary disks of carbon-enhanced metal-poor (CEMP) stars, possible relics of the early Universe. The chemically anomalous abundance patterns ([C/Fe] \geq 0.7) in this subset of low-mass
CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

Stars suggest pollution by primordial core-collapsing supernovae (SNe) ejecta that are particularly rich in carbon dust grains. By comparing the dust-settling timescale in the protoplanetary disks of CEMP stars to the expected disk lifetime (assuming dissipation via photoevaporation), we determine the maximum distance \( r_{\text{max}} \) from the host CEMP star at which carbon-rich planetesimal formation is possible, as a function of the host star’s \([\text{C}/\text{H}]\) abundance. We then use our linear relation between \( r_{\text{max}} \) and \([\text{C}/\text{H}]\), along with the theoretical mass-radius relation derived for a solid, pure carbon planet, to characterize potential planetary transits across host CEMP stars. Given that the related transits are detectable with current and upcoming space-based transit surveys, we suggest initiating an observational program to search for carbon planets around CEMP stars in hopes of shedding light on the question of how early planetary systems may have formed after the Big Bang.

### 8.2 Introduction

The questions of when, where, and how the first planetary systems formed in cosmic history remain crucial to our understanding of structure formation and the emergence of life in the early Universe (Loeb 2014). In the Cold Dark Matter model of hierarchical structure formation, the first stars are predicted to have formed in dark matter haloes that collapsed at redshifts \( z \lesssim 50 \), about 100 million years after the Big Bang (Tegmark et al. 1997; Barkana & Loeb 2001; Yoshida et al. 2003; Bromm & Larson 2004; Loeb & Furlanetto 2013). These short-lived, metal-free, massive first-generation stars ultimately exploded as supernovae (SNe) and enriched the interstellar medium (ISM) with the heavy elements fused in their cores. The enrichment of gas with metals that had otherwise
been absent in the early Universe enabled the formation of the first low-mass stars, and perhaps, marked the point at which star systems could begin to form planets (Bromm & Loeb 2003; Frebel et al. 2007; Clark et al. 2008). In the core accretion model of planet formation (e.g. Papaloizou & Terquem 2006; Janson et al. 2011), elements heavier than hydrogen and helium are necessary not only to form the dust grains that are the building blocks of planetary cores, but to extend the lifetime of the protostellar disk long enough to allow the dust grains to grow via merging and accretion to form planetesimals (Kornet et al. 2005; Johansen et al. 2009; Yasui et al. 2009; Ercolano & Clarke 2010).

In the past four decades, a broad search has been launched for low-mass Population II stars in the form of extremely metal-poor sources within the halo of the Galaxy. The HK survey (Beers et al. 1985, 1992), the Hamburg/ESO Survey (Wisotzki et al. 1996; Christlieb et al. 2008), the Sloan Digital Sky Survey (SDSS; York et al. 2000), and the SEGUE survey (Yanny et al. 2009) have all significantly enhanced the sample of metal-poor stars with $[\text{Fe/H}] < -2.0$. Although these iron-poor stars are often referred to in the literature as “metal-poor” stars, it is critical to note that $[\text{Fe/H}]$ does not necessarily reflect a stellar atmosphere’s total metal content. The equivalence between ‘metal-poor” and “Fe-poor” appears to fall away for stars with $[\text{Fe/H}] < -3.0$ since many of these stars exhibit large overabundances of elements such as C, N, and O; the total mass fractions, $Z$, of the elements heavier than He are therefore not much lower than the solar value in these iron-poor stars.

Carbon-enhanced metal-poor (CEMP) stars comprise one such chemically anomalous class of stars, with carbon-to-iron ratios $[\text{C}/\text{Fe}] \geq 0.7$ (as defined in Aoki et al. 2007; Carollo et al. 2012; Norris et al. 2013). The fraction of sources that fall into this category increases from $\sim 15$-$20\%$ for stars with $[\text{Fe/H}] < -2.0$, to $30\%$ for $[\text{Fe/H}] < -3.0$, to
CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

\[ \sim 75\% \text{ for } [\text{Fe/H}] < -4.0 \text{ (Beers & Christlieb 2005; Norris et al. 2013; Frebel & Norris 2015). Furthermore, the degree of carbon enhancement in CEMP stars has been shown to notably increase as a function of decreasing metallicity, rising from } [\text{C/Fe}] \sim 1.0 \text{ at } [\text{Fe/H}] = -1.5 \text{ to } [\text{C/Fe}] \sim 1.7 \text{ at } [\text{Fe/H}] = -2.7. \text{ (Carollo et al. 2012). Given the significant frequency and level of carbon-excess in this subset of metal-poor Population II stars, the formation of carbon planets around CEMP stars in the early universe presents itself as an intriguing possibility.}

From a theoretical standpoint, the potential existence of carbon exoplanets, consisting of carbides and graphite instead of Earth-like silicates, has been suggested by Kuchner & Seager (2005). Using the various elemental abundances measured in planet-hosting stars, subsequent works have sought to predict the corresponding variety of terrestrial exoplanet compositions expected to exist (Bond et al. 2010; Carter-Bond et al. 2012a,b). Assuming that the stellar abundances are similar to those of the original circumstellar disk, related simulations yield planets with a whole range of compositions, including some that are almost exclusively C and SiC; these occur in disks with C/O > 0.8, favorable conditions for carbon condensation (Larimer 1975). Observationally, there have also been indications of planets with carbon-rich atmospheres, e.g. WASP-12b (Madhusudhan et al. 2011), and carbon-rich interiors, e.g. 55 Cancri e (Madhusudhan et al. 2012).

In this paper, we explore the possibility of carbon planet formation around the iron-deficient, but carbon-rich subset of low-mass stars, mainly, CEMP stars. In section 8.3, we discuss the origins of the unique elemental abundance patterns among these C-rich objects and their potential implications for the carbon dust content of the gas from which CEMP stars and their protostellar disks form. Comparing the expected disk
lifetime to the dust-settling timescale in these protostellar disks, we then determine the maximum distance from a host CEMP star at which the formation of a carbon-rich planet is possible (section 8.4). In section 8.5, we calculate the theoretical mass-radius relation for such a pure carbon planet and present the corresponding depth and duration of its transit across the face of its host CEMP star in section 8.6. We conclude with a discussion of our findings in section 8.7. Standard definitions of elemental abundances and ratios are adopted in this paper. For element X, the logarithmic absolute abundance is defined as the number of atoms of element X per $10^{12}$ hydrogen atoms, \[ \log \epsilon(X) = \log_{10} \left( \frac{N_X}{N_Y} \right) + 12.0 \]. For elements X and Y, the logarithmic abundance ratio relative to the solar ratio is defined as \[ [X/Y] = \log_{10} \left( \frac{N_X}{N_Y} \right) - \log_{10} \left( \frac{N_X}{N_Y} \right)_\odot \]. The solar abundance set is that of Asplund et al. (2009), with a solar metallicity $Z_\odot = 0.0134$.

### 8.3 Star-forming Environment of CEMP Stars

A great deal of effort has been directed in the literature towards understanding theoretically, the origin of the most metal-poor stars, and in particular, the large fraction that is C-rich. These efforts have been further perturbed by the fact that CEMP stars do not form a homogenous group, but can rather be further subdivided into two main populations (Beers & Christlieb 2005): carbon-rich stars that show an excess of heavy neutron-capture elements (CEMP-s, CEMP-r, and CEMP-r/s), and carbon-rich stars with a normal pattern of the heavy elements (CEMP-no). In the following sections, we focus on stars with $[\text{Fe/H}] \leq -3.0$, which have been shown to fall almost exclusively in the CEMP-no subset (Aoki 2010).

A number of theoretical scenarios have been proposed to explain the observed
elemental abundances of these stars, though there is no universally accepted hypothesis. The most extensively studied mechanism to explain the origin of CEMP-no stars is the mixing and fallback model, where a “faint” Population III SN explodes, but due to a relatively low explosion energy, only ejects its outer layers, rich in lighter elements (up to magnesium); its innermost layers, rich in iron and heavier elements, fall back onto the remnant and are not recycled in the ISM (Umeda & Nomoto 2003, 2005). This potential link between primeval SNe and CEMP-no stars is supported by recent studies which demonstrate that the observed ratio of carbon-enriched to carbon-normal stars with $[\text{Fe/H}] < -3.0$ is accurately reproduced if SNe were the main source of metal-enrichment in the early Universe (de Bennassuti et al. 2014; Cooke & Madau 2014). Furthermore, the observed abundance patterns of CEMP-no stars have been found to be generally well matched by the nucleosynthetic yields of primordial faint SNe (Umeda & Nomoto 2005; Iwamoto et al. 2005; Tominaga et al. 2007; Joggerst et al. 2009; Yong et al. 2013; Keller et al. 2014; Ishigaki et al. 2014; Marassi et al. 2014, 2015; Tominaga et al. 2014; Bonifacio et al. 2015). These findings suggest that most of the CEMP-no stars were probably born out of gas enriched by massive, first-generation stars that ended their lives as Type II SNe with low levels of mixing and a high degree of fallback.

Under such circumstances, the gas clouds which collapse and fragment to form these CEMP-no stars and their protostellar disks may contain significant amounts of carbon dust grains. Observationally, dust formation in SNe ejecta has been inferred from isotopic anomalies in meteorites where graphite, SiC, and $\text{Si}_3\text{N}_4$ dust grains have been identified as SNe condensates (Zinner 1998). Furthermore, in situ dust formation has been unambiguously detected in the expanding ejecta of SNe such as SN 1987A (Lucy et al. 1989; Indebetouw et al. 2014) and SN 1999em (Elmhamdi et al. 2003).
existence of cold dust has also been verified in the supernova remnant of Cassiopeia A by SCUBA’s recent submillimeter observations, and a few solar masses worth of dust is estimated to have condensed in the ejecta (Dunne et al. 2003).

Theoretical calculations of dust formation in primordial core-collapsing SNe have demonstrated the condensation of a variety of grain species, starting with carbon, in the ejecta, where the mass fraction tied up in dust grains grows with increasing progenitor mass (Kozasa et al. 1989; Todini & Ferrara 2001; Nozawa et al. 2003). Marassi et al. (2014, 2015) consider, in particular, dust formation in weak Population III SNe ejecta, the type believed to have polluted the birth clouds of CEMP-no stars. Tailoring the SN explosion models to reproduce the observed elemental abundances of CEMP-no stars, they find that: (i) for all the progenitor models investigated, amorphous carbon (AC) is the only grain species that forms in significant amounts; this is a consequence of extensive fallback, which results in a distinct, carbon-dominated ejecta composition with negligible amounts of other metals, such as Mg, Si, and Al, that can enable the condensation of alternative grain types; (ii) the mass of carbon locked into AC grains increases when the ejecta composition is characterized by an initial mass of C greater than the O mass; this is particularly true in zero metallicity supernova progenitors, which undergo less mixing than their solar metallicity counterparts (Joggerst et al. 2009); in their stratified ejecta, C-grains are found only to form in layers where C/O > 1; in layers where C/O < 1, all the carbon is promptly locked in CO molecules; (iii) depending on the model, the mass fraction of dust (formed in SNe ejecta) that survives the passage of a SN reverse shock ranges between 1 to 85%; this fraction is referred to as the carbon condensation efficiency; (iv) further grain growth in the collapsing birth clouds of CEMP-no stars, due to the accretion of carbon atoms in the gas phase onto the remaining grains, occurs only
if C/O > 1 and is otherwise hindered by the formation of CO molecules.

Besides the accumulation of carbon-rich grains imported from the SNe ejecta, Fischer-Trope-type reactions (FTTs) may also contribute to solid carbon enrichment in the protostellar disks of CEMP-no stars by enabling the conversion of nebular CO and H\(_2\) to other forms of carbon (Llorca & Casanova 1998; Kress & Tielens 2001). Furthermore, in carbon-rich gas, the equilibrium condensation sequence changes significantly from the sequence followed in solar composition gas where metal oxides condense first. In nebular gas with C/O \(\gtrsim\) 1, carbon-rich compounds such as graphite, carbides, nitrides, and sulfides are the highest temperature condensates (\(T \approx 1200-1600\) K) (Larimer 1975). Thus, if planet formation is to proceed in this C-rich gas, the protoplanetary disks of these CEMP-no stars may spawn many carbon planets.

### 8.4 Orbital Radii of Potential Carbon Planets

Given the significant abundance of carbon grains, both imported from SNe ejecta and produced by equilibrium and non-equilibrium mechanisms operating in the C-rich protoplanetary disks, the emerging question is: would these dust grains have enough time to potentially coagulate and form planets around their host CEMP-no stars?

In the core accretion model, terrestrial planet formation is a multi-step process, starting with the aggregation and settling of dust grains in the protoplanetary disk (Lissauer 1993; Beckwith et al. 2000; Papaloizou & Terquem 2006; Nagasawa et al. 2007; Rieke 2008; Armitage 2010; Janson et al. 2011). In this early stage, high densities in the disk allow particles to grow from submicron-size to meter-size through a variety
of collisional processes including Brownian motion, settling, turbulence, and radial migration. The continual growth of such aggregates by coagulation and sticking eventually leads to the formation of kilometer-sized planetesimals, which then begin to interact gravitationally and grow by pairwise collisions, and later by runaway growth (Weidenschilling 1988; J. & Cuzzi 1993; Lissauer 1993). In order for terrestrial planets to ultimately form, these processes must all occur within the lifetime of the disk itself, a limit which is set by the relevant timescale of the physical phenomena that drive disk dissipation.

A recent study by Yasui et al. (2009) of clusters in the Extreme Outer Galaxy (EOG) provides observational evidence that low-metallicity disks have shorter lifetimes (< 1 Myr) compared to solar metallicity disks (∼ 5-6 Myr). This finding is consistent with models in which photoevaporation by energetic (ultraviolet or X-ray) radiation of the central star is the dominant disk dispersal mechanism. While the opacity source for EUV (extreme-ultraviolet) photons is predominantly hydrogen and is thus metallicity-independent, X-ray photons are primarily absorbed by heavier elements, mainly carbon and oxygen, in the inner gas and dust shells. Therefore, in low metallicity environments where these heavy elements are not abundant and the opacity is reduced, high density gas at larger columns can be ionized and will experience a photoevaporative flow if heated to high enough temperatures (Gorti & Hollenbach 2009; Ercolano & Clarke 2010).

Assuming that photoevaporation is the dominant mechanism through which circumstellar disks lose mass and eventually dissipate, we adopt the metallicity-dependent disk lifetime, derived in Ercolano & Clarke (2010) using X-ray+EUV models
where $Z$ is the total metallicity of the disk and $p$ is the power-law index of the disk surface density profile ($\Sigma \propto r^{-p}$). A mean power-law exponent of $p \sim 0.9$ is derived by modeling the spatially resolved emission morphology of young stars at (sub)millimeter wavelengths (Andrews et al. 2009, 2010) and the timescale is normalized such that the mean lifetime for disks of solar metallicity is 2 Myr (Ercolano & Clarke 2010). We adopt the carbon abundance relative to solar $[\text{C}/\text{H}]$ as a proxy for the overall metallicity $Z$ since the opacity, which largely determines the photoevaporation rate, and thus the disk lifetime, is dominated by carbon dust grains in the CEMP-no stars we consider in this paper.

The timescale for planet formation is believed to be effectively set by the time it takes dust grains to settle into the disk midplane. The subsequent process of runaway planetesimal formation, possibly occurring via a series of pairwise collisions, must be quick, since otherwise, the majority of the solid disk material would radially drift towards the host star and evaporate in the hot inner regions of the circumstellar disk (Armitage 2010). We adopt the one-particle model of Dullemond & Dominik (2005) to follow the mass growth of dust grains via collisions as they fall through and sweep up the small grains suspended in the disk. Balancing the gravitational force felt by a small dust particle at height $z$ above the mid-plane of a disk with the aerodynamic drag (in the Epstein regime) gives a dust settling velocity of

\[ v_{sett} = \frac{dz}{dt} = \frac{3\Omega^2_k z m}{4\rho c_s \sigma_d} \]  

where $\sigma_d = \pi a^2$ is the cross-section of the dust grain with radius $a$ and $c_s =$
\[ \sqrt{k_B T(r)/\mu m_H} \] is the isothermal sound speed with \( m_H \) being the mass of a hydrogen atom and \( \mu = 1.36 \) being the mean molecular weight of the gas (including the contribution of helium). \( \Omega_K = \sqrt{GM_*/r^3} \) is the Keplerian velocity of the disk at a distance \( r \) from the central star of mass \( M_* \), which we take to be \( M_* = 0.8 \, M_\odot \) as representative of the low-masses associated with CEMP-no stars (Christlieb et al. 2002; Frebel & Norris 2015). The disk is assumed to be in hydrostatic equilibrium with a density given by

\[ \rho(z, r) = \frac{\Sigma(r)}{h \sqrt{2\pi}} \exp \left( -\frac{z^2}{2h^2} \right) \tag{8.3} \]

where the disk scale height is \( h = c_s/\Omega_k \). For the disk surface density \( \Sigma(r) \) and temperature \( T(r) \) profiles, we adopt the radial power-law distributions fitted to (sub-)millimeter observations of circumstellar disks around young stellar objects (Andrews & Williams 2005; Andrews et al. 2009, 2010),

\[ T(r) = 200 \, \text{K} \left( \frac{r}{1 \, \text{AU}} \right)^{-0.6} \tag{8.4} \]

\[ \Sigma(r) = 10^3 \, \text{g/cm}^2 \left( \frac{r}{1 \, \text{AU}} \right)^{-0.9} \tag{8.5} \]

Although these relations were observationally inferred from disks with solar-like abundances, we choose to rely on them for our purposes given the lack of corresponding measurements for disks around stars with different abundance patterns.

The rate of grain growth, \( \frac{dm}{dt} \), is determined by the rate at which grains, subject to small-scale Brownian motion, collide and stick together as they drift towards the disk mid-plane through a sea of smaller solid particles. If coagulation results from every collision, then the mass growth rate of a particle is effectively the amount of solid material in the volume swept out the particle’s geometric cross-section,

\[ \frac{dm}{dt} = f_{dg} \rho d \left( v_{rel} + \frac{dz}{dt} \right) \tag{8.6} \]
where \(dz/dt\) is the dust settling velocity given by equation (2) and

\[
v_{\text{rel}} = \sqrt{\frac{8k_B T (m_1 + m_2)}{\pi m_1 m_2}} \approx \sqrt{\frac{8k_B T}{\pi m}} \tag{8.7}
\]

is the relative velocity in the Brownian motion regime between grains with masses \(m_1 = m_2 = m\). To calculate the dust-to-gas mass ratio in the disk \(f_{dg}\), we follow the approach in Ji et al. (2014) and relate two expressions for the mass fraction of C: (i) the fraction of carbon in the dust, \(f_{dg} M_{C,dust}/M_{dust}\), where \(M_{dust}\) is the total dust mass and \(M_{C,dust}\) is the carbon dust mass; and (ii) the fraction of carbon in the gas, \(\mu_C n_C/\mu n_H\), where \(\mu_C\) is the molecular weight of carbon (\(\sim 12 m_p\)) and \(n_C\) and \(n_H\) are the carbon and hydrogen number densities, respectively. We then assume that a fraction \(f_{\text{cond}}\) (referred to from now on as the carbon condensation efficiency) of all the carbon present in the gas cloud is locked up in dust, such that

\[
f_{\text{cond}} \frac{\mu C n_C}{\mu n_H} = f_{dg} \frac{M_{C,dust}}{M_{dust}} . \tag{8.8}
\]

Since faint Population III SNe are believed to have polluted the birth clouds of CEMP-no stars, and the only grain species that forms in non-negligible amounts in these ejecta is amorphous carbon (Marassi et al. 2014, 2015), we set \(M_{dust} = M_{C,dust}\). Rewriting equation (8) in terms of abundances relative to the Sun, we obtain

\[
f_{dg} = f_{\text{cond}} \frac{\mu C}{\mu} 10^{[C/H]+\log\epsilon(C)_\odot - 12} \tag{8.9}
\]

where \(\log \epsilon(C)_\odot = 8.43 \pm 0.05\) (Asplund et al. 2009) is the solar carbon abundance.

For a specified metallicity \([C/H]\) and radial distance \(r\) from the central star, we can then estimate the time it takes for dust grains to settle in the disk by integrating eqs. (8.2) and (8.6) from an initial height of \(z(t = 0) = 4h\) with an initial dust grain mass of \(m(t = 0) = 4\pi a_{\text{init}}^3 \rho_d/3\). The specific weight of dust is set to \(\rho_d = 2.28 \text{ g cm}^{-3}\).
reflecting the material density of carbon grains expected to dominate the circumstellar
disks of CEMP-no stars. The initial grain size $a_{\text{init}}$ is varied between 0.01 and 1 $\mu$m to
reflect the range of characteristic radii of carbon grains found when modeling CEMP-no
star abundance patterns (Marassi et al. 2014). Comparing the resulting dust-settling
timescale to the disk lifetime given by eq. (8.1) for the specified metallicity, we can
then determine whether there is enough time for carbon dust grains to settle in the
mid-plane of the disk and there undergo runaway planetesimal formation before the disk
is dissipated by photoevaporation. For the purposes of this simple model, we neglected
possible turbulence in the disk which may counteract the effects of vertical settling,
propelling particles to higher altitudes and thus preventing them from fully settling into
the disk mid-plane (Armitage 2010). We have also not accounted for the effects of radial
drift, which may result in the evaporation of solid material in the hot inner regions of
the circumstellar disk.

As the dust settling timescale is dependent on the disk surface density $\Sigma(r)$ and
temperature $T(r)$, we find that for a given metallicity, $[\text{C/H}]$, there is a maximum
distance $r_{\text{max}}$ from the central star out to which planetesimal formation is possible. At
larger distances from the host star, the dust settling timescale exceeds the disk lifetime
and so carbon planets with semi-major axes $r > r_{\text{max}}$ are not expected to form. A plot
of the maximum semi-major axis expected for planet formation around a CEMP-no star
as a function of the carbon abundance relative to the Sun $[\text{C/H}]$ is shown in Figure 8.1
for carbon condensation efficiencies ranging between $f_{\text{cond}} = 0.1$ and 1. As discovered in
Johnson & Li (2012) where the critical iron abundance for terrestrial planet formation
is considered as a function of the distance from the host star, we find a linear relation
CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

Figure 8.1: The maximum distance $r_{\text{max}}$ from the host star out to which planetesimal formation is possible as a function of the star’s metallicity, expressed as the carbon abundance relative to that of the Sun, $[\text{C/H}]$. The dotted, dashed, and solid black curves correspond to the results obtained assuming carbon condensation efficiencies of 10%, 50%, and 100%, respectively, and an initial grain size of $a_{\text{init}} = 0.1 \ \mu\text{m}$. The gray dash-dotted curve corresponds to the distance at which the disk temperature approaches the sublimation temperature of carbon dust grains, $T_{\text{sub,C}} \sim 2000$ K; the formation of carbon planetesimals will therefore be suppressed at distances that fall below this line, $r \lesssim 0.02$ AU. The colored vertical lines represent various observed CEMP stars with measured carbon abundances, $[\text{C/H}]$. 

226
between \([C/H]\) and \(r_{\text{max}}\),

\[
[C/H] = \log \left( \frac{r_{\text{max}}}{1 \text{ AU}} \right) - \alpha
\]

(8.10)

where \(\alpha = 1.3, 1.7,\) and \(1.9\) for \(f_{\text{cond}} = 0.1, 0.5,\) and \(1\), respectively, assuming an initial grain size of \(a_{\text{init}} = 0.1 \mu\text{m}\). These values for \(\alpha\) change by less than 1% for smaller initial grain sizes, \(a_{\text{init}} = 0.01 \mu\text{m}\), and by no more than 5% for larger initial grain sizes \(a_{\text{init}} = 1 \mu\text{m}\); given this weak dependence on \(a_{\text{init}}\), we only show our results for a single initial grain size of \(a_{\text{init}} = 0.1 \mu\text{m}\). The distance from the host star at which the temperature of the disk approaches the sublimation temperature of carbon dust, \(T_{\text{sub,C}} \sim 2000\) K (Kobayashi et al. 2011), is depicted as well (dash-dotted gray curve). At distances closer to the central star than \(r \simeq 0.02\) AU, temperatures well exceed the sublimation temperature of carbon grains; grain growth and subsequent carbon planetesimal formation are therefore quenched in this inner region.

Figure 8.1 shows lines representing various observed CEMP stars with measured carbon abundances, mainly, HE0107-5240 (Christlieb et al. 2002, 2004), SDSS J0212+0137 (Bonifacio et al. 2015), SDSS J1742+2531 (Bonifacio et al. 2015), G 77-61 (Dahn et al. 1977; Plez & Cohen 2005; Beers et al. 2007), and HE 2356-0410 (Norris et al. 1997b; Roederer et al. 2014). These stars all have iron abundances (relative to solar) \([\text{Fe/H}] < -3.0\), carbon abundances (relative to solar) \([\text{C/Fe}] > 2.0\), and carbon-to-oxygen ratios \(\text{C/O} > 1\). This latter criteria maximizes the abundance of solid carbon available for planet formation in the circumstellar disks by optimizing carbon grain growth both in stratified SNe ejecta and later, in the collapsing molecular birth clouds of these stars. It also advances the possibility of carbon planet formation by ensuring that planet formation proceeds by a carbon-rich condensation sequence in the protoplanetary disk. SDSS J0212+0137 and HE 2356-0410 have both been classified as CEMP-no stars, with
Table 8.1. Basic data\textsuperscript{a} for CEMP stars considered in this paper

<table>
<thead>
<tr>
<th>Star</th>
<th>( \log g^b )</th>
<th>[Fe/H]</th>
<th>[C/Fe]</th>
<th>C/O\textsuperscript{c}</th>
<th>Source\textsuperscript{d}</th>
</tr>
</thead>
<tbody>
<tr>
<td>HE 0107-5240</td>
<td>2.2</td>
<td>-5.44</td>
<td>3.82</td>
<td>14.1</td>
<td>1, 2</td>
</tr>
<tr>
<td>SDSS J0212+0137</td>
<td>4.0</td>
<td>-3.57</td>
<td>2.26</td>
<td>2.6</td>
<td>3</td>
</tr>
<tr>
<td>SDSS J1742+2531</td>
<td>4.0</td>
<td>-4.77</td>
<td>3.60</td>
<td>2.2</td>
<td>3</td>
</tr>
<tr>
<td>G 77-61</td>
<td>5.1</td>
<td>-4.03</td>
<td>3.35</td>
<td>12.0</td>
<td>4, 5</td>
</tr>
<tr>
<td>HE 2356-0410\textsuperscript{e}</td>
<td>2.65</td>
<td>-3.19</td>
<td>2.61</td>
<td>( &gt;14.1 )</td>
<td>6</td>
</tr>
</tbody>
</table>

\textsuperscript{a}Abundances based on one-dimensional LTE model-atmosphere analyses

\textsuperscript{b} Logarithm of the gravitational acceleration at the surface of stars expressed in \( \text{cm s}^{-2} \)

\textsuperscript{c} \( \text{C/O} = \frac{N_C}{N_O} = 10^{[\text{C/O}]+\log \epsilon(C)_{\odot}-\log \epsilon(O)_{\odot}} \)

\textsuperscript{d}References: (1) Christlieb et al. 2004; (2) Collet et al. 2006; (3) Bonifacio et al. 2015; (4) Plez & Cohen 2005; (5) Beers et al. 2007; (6) Roederer et al. 2014.

\textsuperscript{e}CS 22957-027

228
measured barium abundances $[\text{Ba}/\text{Fe}] < 0$ (as defined in Beers & Christlieb 2005); the other three stars are Ba-indeterminate, with only high upper limits on $[\text{Ba}/\text{Fe}]$, but are believed to belong to the CEMP-no subclass given their light-element abundance patterns. The carbon abundance, $[\text{C}/\text{H}]$, dominates the total metal content of the stellar atmosphere in these five CEMP objects, contributing more than 60% of the total metallicity in these stars. A summary of the relevant properties of the CEMP stars considered in this analysis can be found in Table 8.1. We find that carbon planets may be orbiting iron-deficient stars with carbon abundances $[\text{C}/\text{H}] \sim -0.6$, such as HE 2356-0410, as far out as $\sim 20$ AU from their host star in the case where $f_{\text{cond}} = 1$. Planets forming around stars with less carbon enhancement, i.e. HE 0107-5240 with $[\text{C}/\text{H}] \sim -1.6$, are expected to have more compact orbits, with semi-major axes $r < 2$ AU. If the carbon condensation efficiency is only 10%, the expected orbits grow even more compact, with maximum semi-major axes of $\sim 5$ and 0.5 AU, respectively.

8.5 Mass-Radius Relationship for Carbon Planets

Next we present the relationship between the mass and radius of carbon planets that we have shown may theoretically form around CEMP-no stars. These mass-radius relations have already been derived in the literature for a wide range of rocky and icy exoplanet compositions (Zapolsky & Salpeter 1969; Léger et al. 2004; Valencia et al. 2006; Fortney et al. 2007; Seager et al. 2007). Here, we follow the approach of Zapolsky & Salpeter (1969) and solve the three canonical equations of internal structure for solid planets,
CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

1. mass conservation

\[ \frac{dm(r)}{dr} = 4\pi r^2 \rho(r), \]  \hspace{1cm} (8.11)

2. hydrostatic equilibrium

\[ \frac{dP(r)}{dr} = -\frac{Gm(r)\rho(r)}{r^2}, \]  \hspace{1cm} (8.12) and

3. the equation of state (EOS)

\[ P(r) = f(\rho(r), T(r)), \] \hspace{1cm} (8.13)

where \( m(r) \) is the mass contained within radius \( r \), \( P(r) \) is the pressure, \( \rho(r) \) is the density of the spherical planet, and \( f \) is the unique equation of state (EOS) of the material of interest, in this case, carbon.

Carbon grains in circumstellar disks most likely experience many shock events during planetesimal formation which may result in the modification of their structure. The coagulation of dust into clumps, the fragmentation of the disk into clusters of dust clumps, the merging of these clusters into \( \sim 1 \text{ km} \) planetesimals, the collision of planetesimals during the accretion of meteorite parent bodies, and the subsequent collision of the parent bodies after their formation all induce strong shock waves that are expected to chemically and physically alter the materials (Mimura & Sugisaki 2003). Subject to these high temperatures and pressures, the amorphous carbon grains polluting the protoplanetary disks around CEMP stars are expected to undergo graphitization and may even crystallize into diamond (Tielens et al. 1987; Onodera et al. 1988; Papoular et al. 1996; Takai et al. 2003). In our calculations, the equation of state at low pressures, \( P \leq 14 \text{ GPa} \), is set to the third-order finite strain Birch-Murnagham EOS (BME; Birch
CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

1947; Poirier 2000) for graphite,

$$P = \frac{3}{2}K_0 \left( \eta^{7/3} - \eta^{5/3} \right) \left[ 1 + \frac{3}{4} \left( K'_0 - 4 \right) \left( \eta^{2/3} - 1 \right) \right]$$ (8.14)

where $\eta = \rho/\rho_0$ is the compression ratio with respect to the ambient density, $\rho_0$, $K_0$ is the bulk modulus of the material, and $K'_0$ is the pressure derivative. Empirical fits to experimental data yields a BME EOS of graphite ($\rho_0 = 2.25$ g cm$^{-3}$) with parameters

$K_0 = 33.8$ GPa and $K'_0 = 8.9$ (Hanfland et al. 1989). At 14 GPa, we incorporate the phase transition from graphite to diamond (Naka et al. 1976; Hanfland et al. 1989) and adopt the Vinet EOS (Vinet et al. 1987, 1989),

$$P = 3K_0 \eta^{2/3} \left( 1 - \eta^{-1/3} \right) \exp \left[ \frac{3}{2} \left( K'_0 - 1 \right) \left( 1 - \eta^{-1/3} \right) \right]$$ (8.15)

with $K_0 = 444.5$ GPa and $K'_0 = 4.18$ empirically fit for diamond, $\rho_0 = 3.51$ g cm$^{-3}$ (Dewaele et al. 2008). (As pointed out in Seager et al. (2007), the BME EOS is not fit to be extrapolated to high pressures since it is derived by expanding the elastic potential energy as a function of pressure keeping only the lowest order terms.) Finally, at pressures $P \gtrsim 1300$ GPa where electron degeneracy becomes increasingly important, we use the Thomas-Fermi-Dirac (TFD) theoretical EOS (Salpeter & Zapolbsky 1967; equations (40)-(49)), which intersects the diamond EOS at $P \sim 1300$ GPa. Given that the full temperature-dependent carbon EOSs are either undetermined or dubious at best, all three EOSs adopted in this work are room-temperature EOSs for the sake of practical simplification.

Using a fourth-order Runge-Kutta scheme, we solve the system of equations simultaneously, numerically integrating eqs. (8.11) and (8.12) beginning at the planet’s center with the inner boundary conditions $M(r = 0) = 0$ and $P(r = 0) = P_{\text{central}}$, where $P_{\text{central}}$ is the central pressure. The outer boundary condition $P(r = R_p) = 0$ then defines

231
Figure 8.2: Mass-radius relation for solid homogenous, pure carbon planet
CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

the planetary radius $R_p$ and total planetary mass $M_p = m(r = R_p)$. Integrating these equations for a range of $P_{\text{central}}$, with the appropriate EOS, $P = P(\rho)$, to close the system of equations, yields the mass-radius relationship for a given composition. We show this mass-radius relation for a purely solid carbon planet in Figure 8.2. We find that for masses $M_p \lesssim 800 M_{\odot}$, gravitational forces are small compared with electrostatic Coulomb forces in hydrostatic equilibrium and so the planet’s radius increases with increasing mass, $R_p \propto M_p^{1/3}$. However, at larger masses, the electrons are pressure-ionized and the resulting degeneracy pressure becomes significant, causing the planet radius to become constant and even decrease for increasing mass, $R_p \propto M_p^{-1/3}$ (Hubbard 1984). Planets which fall within the mass range $500 \lesssim M_p \lesssim 1300 M_{\odot}$, where the competing effects of Coulomb forces and electron degeneracy pressure cancel each other out, are expected to be approximately the same size, with $R_p \simeq 4.3 R_{\odot}$, the maximum radius of a solid carbon planet. (In the case of gas giants, the planet radius can increase due to accretion of hydrogen and helium.)

Although the mass-radius relation illustrated in Figure 8.2 may alone not be enough to confidently distinguish a carbon planet from a water or silicate planet, the unique spectral features in the atmospheres of these carbon planets may provide the needed fingerprints. At high temperatures ($T \gtrsim 1000$ K), the absorption spectra of massive ($M \sim 10 - 60 M_{\odot}$) carbon planets are expected to be dominated by CO, in contrast with the $\text{H}_2\text{O}$-dominated spectra of hot massive planets with solar-composition atmospheres (Kuchner & Seager 2005). The atmospheres of low-mass ($M \lesssim 10 M_{\odot}$) carbon planets are also expected to be differentiable from their solar-composition counterparts due to their abundance of CO and CH$_4$, and lack of oxygen-rich gases like CO$_2$, O$_2$, and O$_3$ (Kuchner & Seager 2005). Furthermore, carbon planets of all masses at low temperatures
are expected to accommodate hydrocarbon synthesis in their atmospheres; stable long-chain hydrocarbons are therefore another signature feature that can help observers distinguish the atmospheres of cold carbon planets and more confidently determine the bulk composition of a detected planet (Kuchner & Seager 2005).

### 8.6 Transit Properties

The detection of theoretically proposed carbon planets around CEMP stars will provide us with significant clues regarding how early planet formation may have started in the Universe. While direct detection of these extrasolar planets remains difficult given the low luminosity of most planets, techniques such as the transit method are often employed to indirectly spot exoplanets and determine physical parameters of the planetary system. When a planet “transits” in front of its host star, it partially occludes the star and causes its’ observed brightness to drop by a minute amount. If the host star is observed during one of these transits, the resulting dip in its measured light curve can yield information regarding the relevant sizes of the star and the planet, the orbital semi-major axis, and the orbital inclination, among other characterizing properties.

A planetary transit across a star is characterized by three main parameters: the fractional change in the stellar brightness, the orbital period, and the duration of the transit (Borucki et al. 1996). The fractional change in brightness is referred to as the transit depth, $\Delta F$ (with a total observed flux $F$), and is simply defined as the ratio of the planet’s area to the host star’s area (Seager & Mallén-Ornelas 2003),

$$\Delta F = \frac{F_{\text{no transit}} - F_{\text{transit}}}{F_{\text{no transit}}} = \left(\frac{R_p}{R_*}\right)^2. \quad (8.16)$$
Figure 8.3: Transit depth as a function of the planetary mass (for a solid carbon planet transit) for different host stellar radii with an assumed stellar mass of $M_\ast = 0.8 \, M_\odot$. These particular stellar radii were chosen to correspond to the stellar radii of the CEMP stars considered in this paper, mainly HE 0107-5240 (red), G 77-61 (cyan), HE 2356-0410 (blue), SDSS J0212+0137 and SDSS J1742+2531 (magenta), where the last two CEMP objects have the same measured surface gravity $\log g = 4.0$. 

\[
\frac{R_*}{R_\odot} \sim 0.4 \quad (G\,77-61) \\
\frac{R_*}{R_\odot} \sim 1.5 \quad (J0212+0137, J1742+2531) \\
\frac{R_*}{R_\odot} \sim 7.0 \quad (HE\,2356-0410) \\
\frac{R_*}{R_\odot} \sim 12 \quad (HE\,0107-5240)
\]
CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

Given the stellar radius $R_*$, measurements of the relative flux change $\Delta F$ yield estimates of the size of the planet $R_p$, and the corresponding planetary mass $M_p$ if the mass-radius relation for the planet is known. Using the $R_p$-$M_p$ relation derived in section 8.5, we illustrate in Figure 8.3 how the transit depth varies as a function of planetary mass in the case where a pure carbon planet transits across the face of its host CEMP star. Curves are shown for each of the five CEMP stars considered in this study, where we assume a stellar mass of $M_* = 0.8 \, M_\odot$ (representative of the low masses associated with old, iron-poor stellar objects) and derive the stellar radii using the stellar surface gravities $g$ listed in Table 8.1, $R_* = \sqrt{G M_*/g}$.

As can be seen in Figure 8.3, the relative change in flux caused by an Earth-mass carbon planet transiting across its host CEMP star ranges from $\sim 0.0001\%$ for a host stellar radius of $R_* \sim 10 \, R_\odot$ to $\sim 0.01\%$ for a solar-sized stellar object. These shallow transit depths are thus expected to evade detection by ground-based transit surveys, which are generally limited in sensitivity to fractional flux changes on the order of 0.1% (Beichman et al. 2009). To push the limits of detection down to smaller, low-mass terrestrial planets requires space-based transit surveys that continuously monitor a large number of potential host stars over several years and measure their respective transit light curves. There are a number of ongoing, planned, and proposed space missions committed to this cause, including CoRot (COnvection ROtation and planetary Transits), Kepler, PLATO (PLAnetary Transits and Oscillations of stars), TESS (Transiting Exoplanet Survey Satellite), and ASTrO (All Sky Transit Observer), which are expected to achieve precisions as low as 20-30 ppm (parts per million) (Beichman et al. 2009; Winn & Fabrycky 2015). With the ability to measure transit depths as shallow as $\Delta F \sim 0.001\%$, these space transit surveys offer a promising avenue towards detecting the planetary
Figure 8.4: Maximum orbital period of a carbon planet transiting across its host CEMP star as a function of the star’s metallicity, expressed as the carbon abundance relative to that of the Sun, [C/H]. The dotted, dashed, and solid black curves denote the results obtained assuming carbon condensation efficiencies of 10%, 50%, and 100% in the parent CEMP star with mass \( M_\star = 0.8 \, M_\odot \). The colored vertical lines represent the five CEMP stars considered in this paper with measured carbon abundances [C/H].
systems that may have formed around CEMP stars.

The orbital period of a planet $P$, which can be determined if consecutive transits are observed, is given by Kepler’s third law in the case of a circular orbit,

$$P^2 = \frac{4\pi^2a^3}{G(M_\star + M_p)} \approx \frac{4\pi^2a^3}{GM_\star}$$  \hspace{1cm} (8.17)

where $a$ is the orbital semi-major axis and the planetary mass is assumed to be negligible relative to the stellar mass, $M_p \ll M_\star$, in the second equality. Given the relation we derived in eq. (8.10) between the metallicity $[C/H]$ and the maximum semi-major axis allowed for a planet orbiting a CEMP star, the maximum orbital period of the planet can be expressed as a function of the metallicity of the host CEMP star ($M_\star = 0.8 \, M_\odot$),

$$P_{\text{max}} \simeq 365.25 \frac{10^{3([C/H]+\alpha)}}{\sqrt{M_\star/M_\odot}} \text{ days}$$  \hspace{1cm} (8.18)

where $\alpha \simeq 1.3, 1.7,$ and 1.9 for carbon condensation efficiencies of 10%, 50%, and 100%.

As can be seen in Figure 8.4, CEMP stars with higher carbon abundances $[C/H]$, i.e. G 77-61 and HE 2356-0410, and larger efficiencies for carbon dust condensation $f_{\text{cond}}$, can host planets with wider orbits and slower rotations, resulting in transits as infrequently as once every couple hundred years. Conversely, carbon planets orbiting relatively less carbon-rich CEMP stars, like SDSS J0212+0137, are expected to have higher rates of transit reoccurrence, completing rotations around their parent stars every $\sim 1-10$ years. These shorter period planets therefore have a much higher probability of producing an observable transit.

The maximum duration of the transit, $T$, can also be expressed as a function of the metallicity $[C/H]$ of the parent CEMP star. For transits across the center of a star, the total duration is given by,

$$T \simeq 2R_\star \sqrt{\frac{a}{GM_\star}}$$  \hspace{1cm} (8.19)
Figure 8.5: Maximum total transit duration of a carbon planet across its host CEMP star as a function of the star’s metallicity, expressed as the carbon abundance relative to that of the Sun, [C/H]. The dotted, dashed, and solid black curves denote the results obtained assuming carbon condensation efficiencies of 10%, 50%, and 100% in the parent CEMP star. The colored vertical lines represent the five CEMP stars considered in this paper with measured carbon abundances [C/H] and stellar radii derived using \( R_\ast = \sqrt{G M_\ast / g} \) with mass \( M_\ast = 0.8 \, M_\odot \).
CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

with the assumption that $M_p \ll M_*$ and $R_p \ll R_*$. Once again, using the relation from eq. (8.10) to express the maximum orbital distance from the host star in terms of the star’s carbon abundance, we find that the maximum transit duration of a carbon planet across its parent CEMP star ($M_* = 0.8 \, M_\odot$) is

$$T_{\text{max}} \simeq 13 \frac{R_*}{R_\odot} \sqrt{\frac{10|\text{[C/H]}+\alpha}{M_*/M_\odot}} \text{ hrs} \ .$$  \hspace{1cm} (8.20)

In Figure 8.5, these maximum durations are shown as a function of $\text{[C/H]}$ for the various stellar radii associated with the CEMP stars we consider in this paper. Transits across CEMP stars with larger radii and higher carbon abundances are expected to take much longer. While the total transit duration across SDSS J0212+0137 and SDSS J1742+2531 with $R_* \sim 1.5 \, R_\odot$ and metallicities of $\text{[C/H]} \sim -1.3 - -1.2$, is at most $\sim 1$-$2$ days, transits across HE 0107-5240 ($R_* \sim 12 \, R_\odot$, $\text{[C/H]} \sim -1.6$) can take up to 2 weeks ($f_{\text{cond}} = 1$). In general, the geometric probability of a planet passing between the observer and the planet’s parent star increases with stellar radius and decreases with orbital radius, $p_t \simeq R_*/a$ Kane (2007). Therefore, focusing on CEMP stars, such as HE 0107-5240 and HE 2356-0410, with large stellar radii increases the observer’s chance of spotting transits and detecting a planetary system.

8.7 Discussion

We explored in this paper the possibility of carbon planet formation around the iron-deficient, carbon-rich subset of low-mass stars known as CEMP stars. The observed abundance patterns of CEMP-no stars suggest that these stellar objects were probably born out of gas enriched by massive first-generation stars that ended their lives as Type II SNe with low levels of mixing and a high degree of fallback. The formation of
dust grains in the ejecta of these primordial core-collapsing SNe progenitors has been observationally confirmed and theoretically studied. In particular, amorphous carbon is the only grain species found to condense and form in non-negligible amounts in SN explosion models that are tailored to reproduce the abundance patterns measured in CEMP-no stars. Under such circumstances, the gas clouds which collapse and fragment to form CEMP-no stars and their protoplanetary disks may contain significant amounts of carbon dust grains imported from SNe ejecta. The enrichment of solid carbon in the protoplanetary disks of CEMP stars may then be further enhanced by Fischer-Trope-type reactions and carbon-rich condensation sequences, where the latter occurs specifically in nebular gas with C/O ≥ 1.

For a given metallicity [C/H] of the host CEMP star, the maximum distance out to which planetesimal formation is possible can then be determined by comparing the dust-settling timescale in the protostellar disk to the expected disk lifetime. Assuming that disk dissipation is driven by a metallicity-dependent photoevaporation rate, we find a linear relation between [C/H] and the maximum semi-major axis of a carbon planet orbiting its host CEMP star. Very carbon-rich CEMP stars, such as G 77-61 and HE 2356-0410 with [C/H] ≃ 0.7 – 0.6, can host carbon planets with semi-major axes as large ∼ 20 AU for 100% carbon condensation efficiencies; this maximum orbital distance reduces to ∼ 5 AU when the condensation efficiency drops by an order of magnitude.

In the case of the observed CEMP-no stars HE 0107-5240, SDSS J0212+0137, and SDSS J1742+2531, where the carbon abundances are in the range [C/H] ≃ -1.6 – -1.2, we expect more compact orbits, with maximum orbital distances \( r_{\max} \approx 2, 4, \) and 6 AU, respectively, for \( f_{\text{cond}} = 1 \) and \( r_{\max} \approx 0.5 - 1 \) AU for \( f_{\text{cond}} = 0.1 \).

We then use the linear relation found between [C/H] and \( r_{\max} \) (section 8.4), along
CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

with the theoretical mass-radius relation derived for a solid, pure carbon planet (section 8.5), to compute the three observable characteristics of planetary transits: the orbital period, the transit depth, and the transit duration. We find that the relative change in flux, $\Delta F$, caused by an Earth-mass carbon planet transiting across its host CEMP star ranges from $\sim 0.0001\%$ for a stellar radius of $R_\star \sim 10 \, R_\odot$ to $\sim 0.01\%$ for a solar-sized stellar host. While the shallow transit depths of Earth-mass carbon planets around HE 0107-5240 and HE 2356-0410 may evade detection, current and future space-based transit surveys promise to achieve the precision levels ($\Delta F \sim 0.001\%$) necessary to detect planetary systems around CEMP stars such as SDSS J0212+0137, SDSS J1742+2531, and G 77-61.

Short orbital periods and long transit durations are also key ingredients in boosting the probability of transit detection by observers. G 77-61 is not an optimal candidate in these respects since given its large carbon abundance ($[C/Fe] \sim 3.4$), carbon planets may form out to very large distances and take up to a century to complete an orbit around the star for $f_{\text{cond}} = 1$ ($P_{\text{max}} \sim 10$ years for 10\% carbon condensation efficiency). The small stellar radius, $R_\star \sim 0.5 \, R_\odot$, also reduces chances of spotting the transit since the resulting transit duration is only $\sim 30$ hours at most. Carbon planets around larger CEMP stars with an equally carbon-rich protoplanetary disk, such as HE 2356-0410 ($R_\star \sim 7 \, R_\odot$), have a better chance of being spotted, with transit durations lasting up to $\sim 3$ weeks. The CEMP-stars SDSS J0212+0137, and SDSS J1742+2531 are expected to host carbon planets with much shorter orbits, $P_{\text{max}} \sim 16$ years for 100\% condensation efficiency ($P_{\text{max}} \sim 1$ year for $f_{\text{cond}} = 0.1$), and transit durations that last as long as $\sim 60$ hours. If the ability to measure transit depths improves to a precision of 1 ppm, then potential carbon planets around HE 0107-5240 are the most likely to be spotted (among
the group of CEMP-no stars considered in this paper), transiting across the host star at least once every $\sim 5$ months (10% condensation efficiency) with a transit duration of 6 days.

While our calculations place upper bounds on the distance from the host star out to which carbon planets can form, we note that orbital migration may alter a planet’s location in the circumstellar disk. As implied by the existence of ‘hot Jupiters’, it is possible for a protoplanet that forms at radius $r$ to migrate inward either through gravitational interactions with other protoplanets, resonant interactions with planetesimals with more compact orbits, or tidal interactions with gas in the surrounding disk (Papaloizou & Terquem 2006). Since Figure 8.1 only plots $r_{\text{max}}$, the maximum distance out to which a carbon planet with $[\text{C/H}]$ can form, our results remain consistent in the case of an inward migration. However, unless planets migrate inward from their place of birth in the disk, we do not expect to find carbon exoplanets orbiting closer than $r \simeq 0.02$ AU from the host stars since at such close proximities, temperatures are high enough to sublimate carbon dust grains.

Protoplanets can also be gravitationally scattered into wider orbits through interactions with planetesimals in the disk (Hahn & Malhotra 1999; Veras et al. 2009). Such an outward migration of carbon planets may result in observations that are inconsistent with the curves in Figure 8.1. A planet that formed at radius $r \ll r_{\text{max}}$ still has room to migrate outwards without violating the ‘maximum distance’ depicted in Figure 8.1; however, the outward migration of a carbon planet that originally formed at, or near, $r_{\text{max}}$ would result in a breach of the upper bounds placed on the transiting properties of carbon planets (section 8.6). In particular, a carbon planet that migrates to a semi-major axis $r > r_{\text{max}}$ will have an orbital period and a transit duration time
Detection of the carbon planets that we suggest may have formed around CEMP stars will provide us with significant clues regarding how planet formation may have started in the early Universe. The formation of planetary systems not only signifies an increasing degree of complexity in the young Universe, but it also carries implications for the development of life at this early junction (Loeb 2014). The lowest metallicity planetary system detected to date is around BD+20 24 57, a K2-giant with [Fe/H] = -1.0 (Niedzielski et al. 2009), a metallicity already well below the critical value once believed to be necessary for planet formation (Gonzalez et al. 2001; Pinotti et al. 2005). More recent formulations of the minimum metallicity required for planet formation are consistent with this observation, estimating that the first Earth-like planets likely formed around stars with metallicities [Fe/H] \lesssim -1.0 (Johnson & Li 2012). The CEMP stars considered in this paper are extremely iron-deficient, with [Fe/H] \lesssim -3.2, and yet, given the enhanced carbon abundances which dominate the total metal content in these stars ( [C/H] \gtrsim -1.6), the formation of solid carbon exoplanets in the protoplanetary disks of CEMP stars remains a real possibility. An observational program aimed at searching for carbon planets around these low-mass Population II stars could therefore potentially shed light on the question of how early planets, and subsequently, life could have formed after the Big Bang.

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CHAPTER 8. CEMP STARS: POSSIBLE HOSTS TO CARBON PLANETS

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Chapter 9

EPILOGUE

The Darkest of All Ends: Hunting Black Holes with GAIA

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9.1 Abstract

We predict the number of black holes with stellar companions that are potentially detectable with GAIA astrometry over the course of its five-year mission. Our model estimates that nearly $3 \times 10^5$ astrometric binaries hosting black holes and stellar
companions brighter than GAIA’s detection threshold, \( G \sim 20 \), should be discovered with \( 5\sigma \) sensitivity. Among these detectable binaries, systems with longer orbital periods are favored, and black hole and stellar companion masses in the range \( M_{BH} \sim 6 - 10 \, M_\odot \) and \( M_\star \sim 1 - 2 \, M_\odot \), respectively, are expected to dominate.

9.2 Introduction

Stellar evolution models, chemical enrichment by supernovae within the Milky Way, and gravitational microlensing events all indicate that a population of about \( \sim 10^8 - 10^9 \) stellar-mass black holes resides in our Galaxy (Shapiro & Teukolsky 1983; van den Heuvel 1992; Brown & Bethe 1994; Samland 1998; Agol et al. 2002). And yet, despite such high estimates, fewer than fifty stellar black hole candidates have been studied and confirmed, all of which are in X-ray binary systems (G. & van der Klis M. 2006; Casares 2007; Fender et al. 2013; Narayan & McClintock 2013). We are therefore left to wonder, where are all these “missing” black holes and how can we observe them?

While black holes in binary systems with ongoing mass transfer have been preferentially detected via X-rays, we expect that at any given moment, a dominant fraction of stellar black holes reside in binaries with no substantial X-ray emission. The binary system may be an X-ray transient, undergoing dramatic episodes of enhanced mass-transfer followed by quiescent phases where the X-rays switch off and the flux drops by several magnitudes; all known low mass black hole binaries (LMBHBs) fall into this category, demonstrating transient behavior (Tanaka & Lewin 1995; White et al. 1995; J. & R. 2006). Menou et al. (1999) suggested that there may be a population of persistent LMBHBs that are simply dim due to the very low radiative efficiencies of their
advection-dominated accretion flow zones. These systems lack large-amplitude outbursts and thus remain difficult to detect with their persistent, yet faint X-ray emission.

There may be a significant number of stellar black holes residing in detached binary systems with companion stars that have not yet reached, or may never reach, the evolutionary stage of transferring mass by Roche-lobe overflow to their compact primaries (Yungelson et al. 2006). Karpov & Lipunov (2001) suggests the existence of hundreds of times more detached binaries composed of a massive OB star and a stellar-wind accreting black hole that remain impossible to detect through X-ray observations. The spherically symmetric accretion that takes place in these systems can only result in the effective generation of a hard radiation component if equipartition is established between the gravitational and magnetic energies in the flow. Given the magnetic exhaust effect operating in these binaries, such equilibrium is rarely established and most black holes in these systems remain unobservable (Karpov & Lipunov 2001).

Given the difficulties associated with detecting stellar-mass black holes in binary systems with no substantial X-ray emission, we explore the possibility of discovering these elusive, compact objects through astrometric observations. The recent advent of the European Space Agency mission Gaia (Perryman et al. 2001) is expected to transform the field of astrometry by measuring the three-dimensional spatial and velocity distribution of nearly \(1\) billion stars brighter than magnitude \(G \sim 20\) (Lindegren et al. 2016). Over the course of its five-year mission lifetime, Gaia is expected to perform an all-sky survey, observing each source an average of 70 times and yielding final astrometric accuracies of roughly 10 \(\mu\)as (micro-arcsec) between \(G \sim 6 - 12\), 25 \(\mu\)as at \(G \sim 15\), and 300 \(\mu\)as at \(G \sim 20\) (Gaia Collaboration et al. 2016). By surveying an unprecedented \(1\)% of the Galaxy’s total stellar population with unparalleled precision, Gaia will not
only confirm and improve upon observations of the few dozen active X-ray binaries that have already been closely studied, but it will also provide a unique opportunity to detect astrometric binaries that have one invisible component, i.e. a black hole, by observing the motion of the visible companion around the system’s barycenter.

In this Letter, we seek to estimate the number of black holes with stellar companions that are potentially detectable with Gaia astrometry. We outline the components of our model and explore the various constraints on the detectability of these binary systems in section 9.3. Our results are presented and discussed in section 9.4. We adopt a flat, $\Lambda$CDM cosmology with $\Omega_m = 0.3$, $\Omega_{\Lambda} = 0.7$, and $H_0 = 70$ km s$^{-1}$ Mpc$^{-1}$, consistent with the most recent measurements from the Planck satellite (Planck Collaboration et al. 2016b).

### 9.3 The Model

To calculate the number of black holes we expect Gaia to detect astrometrically over its five-year lifetime, our model accounts for several limiting factors: (i) the fraction of stars assumed to end their lives as a black hole in a binary system with a fellow stellar companion; (ii) the fraction of those systems with stellar companions that are still shining and whose astrometric wobbles are thus detectable; (iii) the fraction of those systems with periods in the range that Gaia can observe given its mission lifetime and astrometric precision; and (iv) the volume of space Gaia can probe given its detection threshold of $G \sim 20$. We will now briefly discuss each factor in turn.
9.3.1 Black holes with stellar companions

The massive star progenitors of stellar black holes are commonly found in binaries, with galactic surveys yielding bias-corrected spectroscopic binary fractions of 0.6-0.7 in the Milky Way (Kobulnicky & Fryer 2007; Sana et al. 2012; Dunstall et al. 2015; Sana 2017). Kiminki & Kobulnicky (2012) suggest that the binary fraction among these massive stars may even be as high as 90% for systems with periods up to $10^4$ years. The question then becomes whether these black hole progenitors keep their companions throughout the stellar evolutionary process. Various phenomena can lead to the unbinding of a binary, including dynamical interactions, mass loss, supernova explosions of either companion, and merging of the two sources. Fender et al. (2013) estimate that about one quarter of O-stars merge with their companions during evolution and that nearly 50% of black holes have companions that undergo iron core-collapse supernovae (CCSNe), producing neutron stars with natal kicks that can unbind the system with their large velocities.

The formation of the black hole itself may disturb the binary system depending on the formation mechanism. For the lower mass end of black hole progenitors, a metastable proto-neutron star (PNS) is left behind by a weak CCSN and a black hole appears after fallback accretion of the part of the stellar envelope that was not successfully expelled by the supernova (SN) explosion. In the case of more massive stars with larger iron cores, successful SNe explosions are even more difficult to achieve and black holes are formed through accretion of the entire stellar material, either through direct collapse or as a result of failed SNe (Kochanek et al. 2008; Belczynski et al. 2010; Adams et al. 2016).

This notion that some massive stars undergo collapse without producing an explosion was first invoked by theorists to explain away difficulties in producing SN explosions in
analytical models and hydrodynamic simulations (Woosley & Weaver 1986; Gould & Salim 2002). Since then, failed SNe have gained ground as a possible mechanism for producing cosmological gamma-ray bursts (Woosley 1993) and as a potential solution to the “Red Supergiant Problem”, referring to the statistically significant absence of higher mass ($\gtrsim 16 \, M_\odot$) red supergiants exploding as SNe (Smartt 2009, 2015). Evidence in line with the suggestion that $\gtrsim 16 \, M_\odot$ stars do not explode as optically bright SNe has been mounting in recent years. To date, there have been no observed Type IIP SNe with strong [OII] emission consistent with a zero-age main sequence (ZAMS) progenitor mass $\gtrsim 16 \, M_\odot$ (Jerkstrand et al. 2014). Furthermore, Brown & Woosley (2013) found that Galactic abundances can be reproduced even if no stars with masses above 25 $M_\odot$ contribute metals via SN explosions, a mass threshold that can be even lower if uncertain mass loss parameters and reaction rates are modified. Though simulations suggest that there is no single mass below which all stars explode and above which black holes form by implosion, typically 95% of stars that do explode have masses less than 20 $M_\odot$ (Sukhbold et al. 2016). For those stars that end up as black holes, which are most but not all stars with masses above 20 $M_\odot$, only a few were found to form black holes via fallback (Sukhbold et al. 2016).

Given the theoretical predictions and supporting observations, we assume for the purposes of our calculation that progenitor stars with mass $\gtrsim 20 \, M_\odot$ will collapse to form black holes without undergoing an explosion. The mass loss experienced by these black hole progenitors may effectively disrupt the binary if the system loses more than half of its mass suddenly during stellar collapse; in such cases, the newly formed black hole may receive a natal kick, enhancing binary disruption (Repetto et al. 2012; Lovegrove & Woosley 2013; Kochanek 2015). On the other hand, if the progenitor loses
its mass gradually, i.e. via wind, adiabatic invariants should be preserved and the binary separation will adjust accordingly to accommodate the mass loss, allowing the binary to remain gravitationally bound (Smith 2014). The final fraction of stellar objects assumed to end their lives as a black hole in a binary system is thus,

\[ f_{B.F.} = f \int_{20 M_\odot}^{150 M_\odot} \epsilon(M_*) dM_* , \]  

where \( f \) is fudge factor accounting for the fraction of black hole progenitor stars that either never host a companion, or lose their companion over the course of stellar evolution. Rapid mass loss and SN-like kicks during black hole formation will result in small values of \( f \), while formation via implosion or failed SN of stripped Wolf-Rayet stars imply values closer to unity.

The initial mass function (IMF) of progenitor stars, \( \epsilon(M_*) \), is a multi-part power law taken from Kroupa (2007),

\[ \epsilon(M_*) = k \begin{cases} \left( \frac{M_*}{0.5} \right)^{-1.3} & 0.1 < M_* \leq 0.5 \, M_\odot \\ \left( \frac{M_*}{0.5} \right)^{-2.3} & 0.5 < M_* \leq 150 \, M_\odot \end{cases} \]

where \( k \) is set to normalize the distribution such that \( \int_{0.1 \, M_\odot}^{150 \, M_\odot} dM_* \epsilon(M_*) = 1 \).

9.3.2 Visible binary companions

In order to detect a black hole via the astrometric wobble of its stellar companion, the star must still be shining, i.e. observable in the visual range. To determine the fraction of binary systems with stellar sources that are currently burning fuel, we adopt the simplifying assumption that the Milky Way stars follow the cumulative star-formation
CHAPTER 9. HUNTING BLACK HOLES WITH GAIA

history of the Universe,

$$\rho_\star(z) = (1 - R) \int_0^t \dot{\rho}_\star(t) \, dt = (1 - R) \int_z^\infty \frac{\dot{\rho}_\star(z')}{H(z')(1 + z')} \, dz' \, ,$$  \hspace{1cm} (9.2)

where $R = 0.39$ is the “return fraction”, $H(z') = H_0 [\Omega_m(1 + z')^3 + \Omega_\Lambda]^{1/2}$, and the best-fitting comoving star formation rate density (Madau & Fragos 2016) is

$$\dot{\rho}_\star(z) = 0.01 \frac{(1 + z)^{2.6}}{1 + [(1 + z)/3.2]^{6.2}} \, M_\odot \, yr^{-1} \, Mpc^{-3} \, .$$  \hspace{1cm} (9.3)

If we express the fraction of baryons locked up in stars at a certain redshift as $f_\star(z) = \rho_\star(z)/\rho_b$ where $\rho_b = \Omega_b \rho_{crit}$, then the fraction of stars with ZAMS mass $M_\star$ that are still “alive” today is given by

$$f_{shining}(M_\star) = 1 - \frac{\rho_\star(z(t_{LB} = t_{age}(M_\star)))}{\rho_\star(0)}$$  \hspace{1cm} (9.4)

where the look-back time, $t_{LB}$, is set to the stellar lifetime, $t_{age}(M_\star)$. Stellar lifetimes were calculated using MIST models and the MESA stellar evolution libraries (Paxton et al. 2011; Choi et al. 2016; Dotter 2016) and $f_{shining}(M_\star)$ is set to unity for stars with lifetimes that exceed the age of the Universe.

9.3.3 Accessible range of periods

Binary surveys that probe massive stars often find a uniform distribution in log period, following what is commonly referred to as Öpik’s law (E.J. 2016; Garmany et al. 1980; Kouwenhoven et al. 2007). We therefore adopt a log-flat distribution, $p(\log P) \propto (\log P)^\gamma$ with $\gamma = 0$, to characterize the orbital period distribution of the binary systems under consideration.

For the astrometric signals of these binaries to be detectable by Gaia, the orbital periods should not exceed Gaia’s mission lifetime, $P_{\text{max}} = t_G = 5$ years. There is also a
lower bound on the range of accessible periods that is set by Gaia’s astrometric precision at a given magnitude, $\alpha_G(m)$ (Perryman et al. 2014). The astrometric signature of the binary, which must be at least as large as $\alpha_G$, is given by

$$\alpha = \frac{a_s}{r} = \frac{M_{BH}}{M_{BH} + M_s} \frac{a}{r},$$

(9.5)

where $r$ denotes the distance of the binary system from the Sun, $a_s$ is the observable semi-major axis of the star’s orbit projected onto the sky, and $a$ is the corresponding semi-major axis of the relative orbit of the black hole and companion star, with masses $M_{BH}$ and $M_s$ respectively. Since $a$ is related to the period $P$ through Kepler’s third law, the constraint on the astrometric signature, $\alpha \geq \alpha_G$, translates into a minimum detectable orbital period of

$$P_{\text{min}} = (M_{BH} + M_s) \left( \frac{r \alpha_G(m)}{M_{BH}} \right)^{3/2}.$$

(9.6)

Given that massive binary systems with orbital periods less than 1 day are extremely rare and more likely to be disruptively interactive, we set the minimum orbital period equal to 1 day if $P_{\text{min}}$ in eq. (9.6) drops below this threshold.

### 9.3.4 Volume of space probed by Gaia

The final factor our model accounts for is the fraction of stars Gaia can probe given its detection threshold, $m_{\text{lim}}$. A star of mass $M_s$ with a corresponding luminosity of $L(M_s)$ can be observed out to a distance

$$d_{\text{max}}(M_s) = 0.3 \sqrt{10^{(m_{\text{lim}}+2.72)/2.5} L(M_s)} \text{ pc}$$

(9.7)

where $L(M_s)$ is computed using the previously mentioned MIST models (in units of solar luminosity). We model the stellar density profile with a double exponential thin
and thick disk centered at the solar position in the Galaxy, \((R_\odot, Z_\odot) = (8 \text{ kpc}, 25 \text{ pc})\),
with scale lengths of \(h_{R,\text{thin}} = 2.6 \text{ kpc}\) and \(h_{R,\text{thick}} = 3.6 \text{ kpc}\), scale heights of \(h_{Z,\text{thin}} = 0.3 \text{ kpc}\) and \(h_{Z,\text{thick}} = 0.9 \text{ kpc}\), and a normalization of the thick disk (relative to the thin) of \(f_{\text{thick}} = 0.04\) (Jurić et al. 2008; Yoshii 2013). Normalized further to yield a total stellar mass of \(M_{*,\text{tot}} = 6.08 \times 10^{10} \, M_\odot\) (Licquia & Newman 2015), this stellar number density distribution takes the following form (in spherical coordinates),

\[
n(r, \theta, \phi) = n_0 \left[ \exp \left( -\frac{(r \sin \phi + R_\odot)}{2.6 \text{ kpc}} - \frac{|r \cos \phi + Z_\odot|}{0.3 \text{ kpc}} \right) + 0.04 \exp \left( -\frac{(r \sin \phi + R_\odot)}{3.6 \text{ kpc}} - \frac{|r \cos \phi + Z_\odot|}{0.9 \text{ kpc}} \right) \right]
\]  

(9.8)

where \(n_0 \approx 3 \, \text{ pc}^{-3}\).

Taking into account all these various limiting factors, the resulting total number of black holes we can expect Gaia to observe astrometrically over the course of its five-year mission takes the following form,

\[
N_{\text{tot}} = f_{B.F.} \int_{5 \, M_\odot}^{\infty} dM_{BH} \psi(M_{BH}) \int_{0.1 \, M_\odot}^{150 \, M_\odot} dM_* f_{\text{shining}}(M_*) \epsilon(M_*) \int_0^{2\pi} d\theta \int_0^\pi d\phi \sin \phi \times \
\int_0^{d_{\text{max}}(M_*,M_{\text{lim}})} dr r^2 \int_{\log (\Delta_0)}^{\log (t_G)} d(\log P) \, n(r, \theta, \phi) \frac{p(\log P)}{(\log (\Delta_0))},
\]  

(9.9)

where \(\psi(M_{BH})\) represents the black hole mass distribution adopted from Özel et al. (2010, 2012),

\[
\psi(M_{BH}) = \left\{ A(M_{BH})^\delta + [B(M_{BH})^{-\delta} + C(M_{BH})^{-\delta}]^{-1} \right\}^{1/\delta},
\]  

(9.10)

with \(\delta = -10.0\) and,

\[
A(M_{BH}) = 4.367 - 1.7294 M_{BH} + 0.1713 M_{BH}^2
\]

\[
B(M_{BH}) = 14.24 e^{-0.542 M_{BH}}
\]

\[
C(M_{BH}) = 3.322 e^{-0.386 M_{BH}}.
\]  

(9.11)
CHAPTER 9. HUNTING BLACK HOLES WITH GAIA

9.4 Results & Discussion

Using the model outlined above, we estimate the number of astrometric binaries with stellar black holes that Gaia can potentially detect with $5\sigma$ sensitivity. Figure 9.1 depicts the cumulative number of expected binaries with orbital periods less than some value $P$, assuming various limiting magnitudes in the $G$ band, $m_{\text{lim}}$. Out of the nearly 1 billion stellar sources that will be observed by Gaia, we expect to find $\sim 5500$ binaries with periods $\lesssim 5$ years that host a black hole ($M_{BH} \geq 5 M_\odot$) and a stellar companion brighter than $G \sim 13$. The distribution of orbital periods among these potentially detectable binaries with $G \lesssim 13$ will be roughly uniform across the range $4 \text{ days} \lesssim P \lesssim 5$ years.

Alternatively, if we observe stars as faint as $G \sim 20$, corresponding to the magnitude threshold of Gaia, this number rises to $N_{\text{tot}}(P \leq 5 \text{ yr}) = 3 \times 10^5$, $0.02\%$ of the surveyed sources. Correspondingly, inclusion of these fainter sources results in a period distribution among the detected astrometric binaries that is more heavily weighted towards longer orbital periods (Figure 9.1, right panel). If the mission lifetime is extended to 10 years, Gaia may observe up to $4.6 \times 10^5$ astrometric binaries hosting stellar black holes. We also note that all of these conservative estimates for a $5\sigma$ detection may be modified by the fudge factor, $f$, introduced in 9.3, that accounts for black holes that end up ‘isolated’, either because their progenitor stars never hosted a companion or because they lost their companion over the course of stellar evolution.

Figure 9.2 illustrates how these numbers vary instead with the mass of the black hole (top panel) and stellar companion (bottom). The differential count per logarithmic interval in mass (plotted in the right panel), demonstrates that a significant fraction of the detected astrometric binaries are expected to have black hole masses between 6 and
Figure 9.1: **Left panel**: Cumulative number of detectable astrometric binaries hosting black holes with orbital periods less than $P$, assuming detection thresholds of $m_{\text{lim}} = 13$, 15, and 20 in the $G$ band. **Right panel**: The corresponding differential count per logarithmic interval in $P$. Numbers are shown for a $5\sigma$ detection and may be modified by a multiplicative factor $f$ to account for the fraction of black hole progenitor stars that end their lives isolated.
10 $M_\odot$, reflecting the intrinsic black hole mass distribution which peaks in the range 5-7 $M_\odot$ and rapidly decreases at larger masses (Özel et al. 2010; Farr et al. 2011). The stellar companions in these detectable astrometric binaries are expected to have masses predominately in the solar range, with $dN/d\ln M_*$ peaking around $\sim 1$-2 $M_\odot$.

Astrometric observations provided by Gaia will yield the period of the orbital motion around a binary’s barycenter, as well as $\alpha$, the angular semi-major axis of the luminous companion’s orbit. Kepler’s third law, expressed in terms of these quantities, takes on the form,

$$
\left( \frac{P}{1 \text{ yr}} \right)^{-2} \left( \frac{\alpha D}{1 \text{ AU}} \right)^3 = \frac{M_{\text{dark}}^3}{(M_{\text{dark}} + M_{\text{visible}})^2 M_\odot},
$$

where $M_{\text{dark}}$ and $M_{\text{visible}}$ are the masses of the dark and luminous components, respectively. In cases where $M_{\text{visible}}$ and $D$, the distance to the binary, can be determined independently, astrometric measurements fix the left-hand side of this equation and the mass of the unseen companion, $M_{\text{dark}}$, can easily be derived. Stellar-mass black holes can thus be identified astrometrically in systems where the proper motion of the visible component, i.e. the star, implies the existence of a dark companion with $M_{\text{dark}} \gtrsim 3 M_\odot$.

The invisible companions of astrometrically observed metal-poor, low-mass stars ([Fe/H] < -1, $M_* < 1 M_\odot$) may be stellar remnants from the dawn of the Universe, offering to shed light on the formation of the first stellar black holes in the early stages of galaxy assembly and evolution. Conversely, astrometric binaries with a stellar black hole and a fellow high-mass stellar companion ($M_* > 20 M_\odot$) offer candidate systems for future gravitational-wave observations with the Laser Interferometer Gravitational Wave Observatory (LIGO) or eLISA (Christian & Loeb 2017). By providing astrometric observations of nearly 1 billion galactic stars with unprecedented precision, Gaia promises
Figure 9.2: Left panel: Cumulative number of detectable astrometric binaries hosting black holes with mass less than $M_{\text{BH}}$ (top) and stellar companions with mass less than $M_*$ (bottom). Right panel: The corresponding differential count per logarithmic interval in mass, assuming 5σ detection. The multiplicative factor $f$ accounts for the fraction of isolated black hole progenitors with no stellar companion.
to probe the stellar black hole population, a population that, despite its expected abundance, has mostly evaded detection thus far.

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