A Theory for the Excitation of CO in Star Forming Galaxies

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ABSTRACT
Observations of molecular gas in high-z star-forming galaxies typically rely on emission from CO lines arising from states with rotational quantum numbers \( J > 1 \). Converting these observations to an estimate of the CO \( J = 1 - 0 \) intensity, and thus inferring \( \text{H}_2 \) gas masses, requires knowledge of the CO excitation ladder, or spectral line energy distribution (SLED). The few available multi-\( J \) CO observations of galaxies show a very broad range of SLEDs, even at fixed galaxy mass and star formation rate, making the conversion to \( J = 1 - 0 \) emission and hence molecular gas mass highly uncertain. Here, we combine numerical simulations of disk galaxies and galaxy mergers with molecular line radiative transfer calculations to develop a model for the physical parameters that drive variations in CO SLEDs in galaxies. An essential feature of our model is a fully self-consistent computation of the molecular gas temperature and excitation structure. We find that, while the shape of the SLED is ultimately determined by difficult-to-observe quantities such as the gas density, temperature, and optical depth distributions, all of these quantities are well-correlated with the galaxy’s mean star formation rate surface density (\( \Sigma_{\text{SFR}} \)), which is observable. We use this result to develop a model for the CO SLED in terms of \( \Sigma_{\text{SFR}} \), and show that this model quantitatively reproduces the SLEDs of galaxies over a dynamic range of \( \sim 200 \) in SFR surface density, at redshifts from \( z = 0 - 6 \). This model should make it possible to significantly reduce the uncertainty in deducing molecular gas masses from observations of high-\( J \) CO emission.

Key words: ISM: clouds – ISM: molecules – galaxies: ISM – galaxies: interactions – galaxies: star formation – galaxies: starburst

1 INTRODUCTION
Stars form in giant clouds in galaxies, comprised principally of molecular hydrogen, \( \text{H}_2 \). Due to its low mass, \( \text{H}_2 \) requires temperatures of \( \sim 500 \) K to excite the first quadrupole line, while GMCs in quiescent galaxies have typical temperatures of \( \sim 10 \) K (e.g. Fukui & Kawamura 2010; Dobbs et al. 2013). The relatively low abundance of emitting \( \text{H}_2 \) in molecular clouds has driven the use of the ground state rotational transition of carbon monoxide, \( ^{12}\text{CO} \) (hereafter, CO), as the most commonly observed tracer molecule of \( \text{H}_2 \). With a typical abundance of \( \sim 1.5 \times 10^{-4} \times \text{H}_2 \) at solar metallicity, CO is the second most abundant molecule in clouds (Lee, Bettsens & Heber 1998). Via a (highly debated) conversion factor from CO luminosities to \( \text{H}_2 \) gas masses, observations of the \( J = 1 - 0 \) transition of CO provide measurements of molecular gas masses, surface densities, and gas fractions in galaxies at both low and high-redshifts.

CO can be excited to higher rotational states via a combination of collisions with \( \text{H}_2 \) and He, as well as through radiative absorptions. When the CO is thermalized, then level populations can be described by Boltzmann statistics, and the intensity at a given level follows the Planck function at that frequency.

While the conversion factor from CO luminosities to \( \text{H}_2 \) gas masses is based solely on the \( J = 1 - 0 \) transition, directly detecting the ground state of CO at high-z is challenging. Only a handful of facilities operate at long enough wavelengths to detect the redshifted 2.6 mm CO \( J = 1 - 0 \) line, and consequently the bulk of CO detections at high-redshift are limited to high-\( J \) transitions (see the compendia in recent reviews by Solomon & Vanden Bout 2005; Carilli & Walter 2013). Thus, to arrive at an \( \text{H}_2 \) gas mass, one must first down-convert from the observed high-\( J \) CO line intensity to a \( J = 1 - 0 \) intensity before applying a CO-to-\( \text{H}_2 \) conversion factor. This requires some assumption of the CO excitation ladder, or as it is often monikered in the literature, the Spectral Line Energy Distribution (SLED).

Typically, line ratios between a high-\( J \) line and the \( J = 1 - 0 \) line are assumed based on either an assumption of thermalized level populations, or by comparing to a similar galaxy (selected either via similar methods, or having similar inferred physical properties such as SFR) (e.g. Geach & Papadopoulos 2012; Carilli & Walter 2013). However, this method is uncertain at the order of magnitude level, even for lines of modest excitation such as \( J = 3 - 2 \).

As an anecdotal example, consider the case of high-z sub-
millimeter galaxies (SMGs). These 850 µm-selected galaxies typically live from \( z = 2 - 4 \), have star formation rates well in excess of \( 500 \, M_\odot \, \text{yr}^{-1} \), and are among the most luminous galaxies in the Universe (see the review by Blain et al. 2002). Originally, it was assumed that the gas was likely thermalized in these systems, given their extreme star formation rates (and likely extreme ISM densities and temperatures) (e.g. Greve et al. 2003; Coppin et al. 2008; Tacconi et al. 2008). However, subsequent CO \( J = 1 - 0 \) observations of a small sample of SMGs with higher \( J \) detections by Hainline et al. (2006) and Harris et al. (2010) showed that a number of SMGs exhibit subthermal level populations, even at the modest excitation level of \( J = 3 \). Since then, it has become increasingly clear that SMGs are a diverse population (e.g. Bothwell et al. 2013; Hayward et al. 2011, 2012, 2013; Hodge et al. 2013; Karim et al. 2013), with a large range in potential CO excitation ladders. To quantify this, in Figure 1 we have compiled all of the CO SLEDs published to date for all high-\( z \) SMGs with a CO \( J = 1 - 0 \) detection. The diversity in the observed SLEDs is striking, even for one of the most extreme star forming galaxy populations known. It is clear that no “template” SLED exists for a given population.

Nor can one do much better simply by comparing an observed galaxy to another galaxy with a known SLED and a similar luminosity or SFR. For example, turning again to Figure 1 we highlight the SLED of a single quasar host galaxy denoted by the red line (the Cloverleaf quasar), and compare it to SMG SMM 163650 (purple). Both galaxies have estimated star formation rates of roughly ~ 1000 \( M_\odot \, \text{yr}^{-1} \) (Ivison et al. 2011; Solomon et al. 2003; Weiß et al. 2003), but they have dramatically different SLEDs. For the \( J = 6 - 5 \) line, there is roughly a factor of five difference in the SLEDs, and the discrepancy likely grows at even higher levels. It is clear from this example that extrapolating from high \( J \) lines to \( J = 1 - 0 \) using templates based on galaxies with similar global SFRs is a problematic approach.

The consequences of uncertainty in the excitation of CO are widespread in the astrophysics of star formation and galaxy formation. For example, observed estimates of the Kennicutt-Schmidt star formation relation at high redshift, an often-used observational test bed for theories of star formation in environments of extreme pressure (e.g. Ostriker & Shetty 2011; Krumholz, Dekel, 

\[ I_{\text{CO}}/ L_{\text{IR}} \] 

= 10^{-7}. In \( \S 4 \) we provide a discussion, and we conclude in \( \S 5 \) to validate their underlying galaxy formation model. We lack a first-principles physical model for the origin of the shape of SLEDs in galaxies, and the relationship of this shape to observables. The goal of this paper is to provide one. The principle idea is that CO excitation is dependent on the gas temperatures, densities and optical depths in the molecular ISM. Utilizing a detailed physical model for the thermal and physical structure of the star-forming ISM in both isolated disk galaxies, and starbursting galaxy mergers, we investigate what sets these quantities in varying physical environments. We use this information to provide a parameterization of CO SLEDs in terms of the star formation rate surface density (\( \Sigma_{\text{SFR}} \)), and show that this model compares very favorably with observed SLEDs for galaxies across a range of physical conditions and redshifts.

This paper is organized as follows. In \( \S 2 \) we describe our numerical modeling techniques, including details regarding our hydrodynamic models, radiative transfer techniques, and ISM specification. In \( \S 3 \) we present our main results, including the principle drivers of SLED shapes, as well as a parameterized model for observed SLEDs in terms of the galaxy \( \Sigma_{\text{SFR}} \). In \( \S 4 \) we provide discussion, and we conclude in \( \S 5 \).

2 NUMERICAL MODELING

2.1 Overview of Models

The basic strategy that we employ is as follows, and is nearly identical to that employed by Narayanan et al. (2011b, 2012). We first simulate the evolution of idealized disk galaxies and galaxy mergers over a range of masses, merger orbits, and halo virial properties utilizing the smoothed particle hydrodynamics (SPH) code, GADGET-3 (Springel & Hernquist 2003; Springel, 2010 RAS, MNRAS 000, 1–77).
we elaborate further in the remainder of this section. Interested in the technical aspects of the simulation methodology, we determine full CO rotational ladder for each cloud in a given system. Properties of the molecular ISM in post-processing. In particular, we project the physical conditions of the SPH particles onto an adaptive mesh, and calculate the physical and chemical properties of the molecular ISM in post-processing. In particular, we determine the temperatures, mean cloud densities, velocity dispersions, $H_2$-
H I balance, and fraction of carbon locked in CO. Determining the thermodynamic structure of the ISM involves balancing heating by cosmic rays and the grain photoelectric effect, energy exchange with dust, and CO and C II line cooling. To calculate the line cooling rates, we employ the public code to Derive the Energetics and SPectra of Optically Thick Interstellar Clouds (DESPOTIC; Krumholz 2013), built on the escape probability formalism. The radiative transfer calculations determine the level populations via a balance of radiative absorptions, stimulated emission, spontaneous emission, and collisions with $H_2$ and He. With these level populations in hand, we determine full CO rotational ladder for each cloud within our model galaxies. The observed SLED from the galaxy is just the combination of the CO line intensities at each level from each cloud in a given system.

At this point, the general reader should have enough background to continue to the Results (§3) if they so wish. For those interested in the technical aspects of the simulation methodology, we elaborate further in the remainder of this section.

Table 1. Galaxy evolution simulation parameters. Column 1 refers to the model name. Galaxies with the word ‘iso’ in them are isolated disks, and the rest of the models are 1:1 major mergers. Column 2 is the baryonic mass in $M_\odot$. Columns 3-6 refer to the orbit of a merger (with “N/A” again referring to isolated discs). Column 7 is the initial baryonic gas fraction of the galaxy, and Column 8 refers to the redshift of the simulation.

| Model          | $M_{\text{bar}}$ | $\theta_1$ | $\phi_1$ | $\theta_2$ | $\phi_2$ | $f_g$ | $z$ |
|----------------|------------------|------------|--------|------------|--------|-----|---|
| z3iso06        | 3.8 $\times$ 10^{11} | N/A | N/A | N/A | N/A | 0.8 | 3 |
| z3iso05        | 1.0 $\times$ 10^{10} | N/A | N/A | N/A | N/A | 0.8 | 3 |
| z3iso04        | 3.5 $\times$ 10^{10} | N/A | N/A | N/A | N/A | 0.8 | 3 |
| z3b5e          | 2.0 $\times$ 10^{11} | 30 | 60 | -30 | 45 | 0.8 | 3 |
| z3b5i          | 2.0 $\times$ 10^{11} | 0 | 0 | 71 | 30 | 0.8 | 3 |
| z3b5j          | 2.0 $\times$ 10^{11} | -109 | 90 | 71 | 90 | 0.8 | 3 |
| z3b5l          | 2.0 $\times$ 10^{11} | -109 | 30 | 180 | 0 | 0.8 | 3 |
| z0iso05        | 4.5 $\times$ 10^{10} | N/A | N/A | N/A | N/A | 0.4 | 0 |
| z0iso04        | 1.6 $\times$ 10^{10} | N/A | N/A | N/A | N/A | 0.4 | 0 |
| z0iso03        | 5.6 $\times$ 10^{10} | N/A | N/A | N/A | N/A | 0.4 | 0 |
| z0d4e          | 3.1 $\times$ 10^{11} | 30 | 60 | -30 | 45 | 0.4 | 0 |
| z0d4h          | 3.1 $\times$ 10^{11} | 0 | 0 | 0 | 0 | 0.4 | 0 |
| z0d4i          | 3.1 $\times$ 10^{11} | 0 | 0 | 71 | 30 | 0.4 | 0 |
| z0d4j          | 3.1 $\times$ 10^{11} | -109 | 90 | 71 | 90 | 0.4 | 0 |
| z0d4k          | 3.1 $\times$ 10^{11} | -109 | 30 | 71 | -30 | 0.4 | 0 |
| z0d4l          | 3.1 $\times$ 10^{11} | -109 | 30 | 180 | 0 | 0.4 | 0 |
| z0d4m          | 3.1 $\times$ 10^{11} | -109 | -30 | 71 | 30 | 0.4 | 0 |
| z0d4n          | 3.1 $\times$ 10^{11} | -109 | 30 | 71 | -30 | 0.4 | 0 |

2.2 Hydrodynamic Simulations of Galaxies in Evolution

The main purpose of the SPH simulations of galaxies in evolution is to generate a large number of realizations of galaxy models with a diverse range of physical properties. To this end, we simulate the hydrodynamic evolution of both idealized disks, as well as mergers between these disks. Here, we summarize the features of the simulations most pertinent to this paper, and we refer the reader to Springel & Hernquist (2002, 2003) and Springel, Di Matteo & Hernquist (2005) for a more detailed description of the underlying algorithms for the hydrodynamic code employed, GADGET-3.

The galaxies are exponential disks, and are initialized following the Mo, Mao & White (1998) formalism. They reside in live dark halos, initialized with a Hernquist (1990) profile. We simulate galaxies that have halo concentrations and virial radii scaled for $z = 0$ and $z = 3$, following the relations of Bullock et al. (2001) and Robertson et al. (2006). The latter redshift choice is motivated by the desire to include a few extreme starburst galaxies in our simulation sample. The gravitational softening length for baryons is 100 $h^{-1}$pc, and 200 $h^{-1}$pc for dark matter.

The gas is initialized as primordial, with all metals forming as the simulation evolves. The ISM is modeled as multi-phase, with clouds embedded in a pressure-confining hotter phase (e.g. McKee & Ostriker 1977). In practice, this is implemented in the simulations via hybrid SPH particles. Cold clouds grow via radiative cooling of the hotter phase, while supernovae can heat the cold gas. Stars form in these clouds following a volumetric Schmidt (1959) relation, with index 1.5 (Kennicutt 1998a; Cox et al. 2009; Narayanan et al. 2011a; Krumholz, Dekel & McKee 2012). We note that in Narayanan et al. (2011b), we explored the effects of varying the Kennicutt-Schmidt star formation law index, and

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found that the ISM thermodynamic properties were largely unchanged so long as the index is $\geq 1$. In either case, observations (e.g. Bigiel et al. 2008), as well as theoretical work (e.g. Krumholz, McKee & Tumlinson 2009b; Ostriker & Shetty 2011) suggest that the index may be superlinear in high-surface density starburst environments.

The pressurization of the ISM via supernovae is implemented via an effective equation of state (Springel, Di Matteo & Hernquist 2005). In the models scaled for present epoch, we assume a modest pressurization ($q_{\text{EOS}} = 0.25$), while for the high-$z$ galaxies, we assume a more extreme pressurization ($q_{\text{EOS}} = 1$). Tests by Narayanan et al. (2011b) show that the extracted thermodynamic properties of the simulations are relatively insensitive to the choice of EOS. Still, we are intentional with these choices. The high-$z$ galaxies would suffer from runaway gravitational fragmentation, preventing starbursts, without sufficient pressurization. Because the simulations are not cosmological, and do not include a hot halo (e.g. Moster et al. 2011, 2012) or resolved feedback (Krumholz & Dekel 2011; Krumholz & Thompson 2012, 2013; Hopkins et al. 2013), the early phases of evolution would quickly extinguish the available gas supply without sufficient pressurization. Despite this pressurization, large scale kpc-sized clumps do still form from dynamical instabilities in high-$z$ systems, similar to observations (Elmegreen, Klessen & Wilson 2008; Elmegreen et al. 2009a, b) and simulations (e.g. Dekel et al. 2009; Ceverino, Dekel & Bournaud 2010).

For the galaxy mergers, we simulate a range of arbitrarily chosen orbits. In Table 1, we outline the basic physical properties of the galaxies simulated here.

### 2.3 The Physical and Chemical Properties of the Molecular ISM

We determine the physical and chemical properties of the molecular interstellar medium in postprocessing. We project the physical properties of the SPH particles onto an adaptive mesh, utilizing an octree memory structure. Practically, this is done through the refinement criteria that the density divided by the solar metallicity. We motivate the usage of the Krumholz, McKee & Tumlinson (2009b) model for H$_2$ formation and destruction for two reasons. First, observations by Fumagalli, Krumholz & Hunfi (2010) and Wong et al. (2013) of dwarf galaxies suggest that the adopted method in Equation 1 may fare better at low metallicities than observed empirical pressure-based relations (e.g. Blitz & Rosolowsky 2006). Second, Krumholz & Gnedin (2011) find that Equation 1 compares well to full numerical time-dependent chemical reaction networks and radiative transfer models for H$_2$ formation and destruction (Pelupessy, Paradisoulos & van der Werf 2006; Gnedin, Tassis & Kravtsov 2008; Gnedin & Kravtsov 2010; Christensen et al. 2012a, b; Munshi et al. 2013) above metallicities of $\sim 0.1 Z_{\odot}$. The mass-weighted metallicity in our star-forming galaxies are always above this threshold.

In order to account for the turbulent compression of gas, we scale the volumetric densities of the clouds by a factor $e^{s^2/2}$, where $s^p$ is approximated by:

$$s^p \approx \ln(1 + 3 M_{1D}/4)$$

based on insight from numerical simulations (Ostriker, Stone & Gammie 2001; Padoan & Nordlund 2002; Lemaster & Stone 2008). Here, $M_{1D}$ is the one-dimensional Mach number of the turbulence. In order to calculate the Mach number, we assume the temperature of the GMC is 10 K. This represents a minor inconsistency in our modeling, as for the remainder of the gas specification, we utilize a fully radiative model to determine the gas thermal properties (5.2). The 1D velocity dispersion of in the cloud is determined by:

$$\sigma = \max(\sigma_{\text{cell}}, \sigma_{\text{vir}})$$

where $\sigma_{\text{cell}}$ is the mean square sum of the subgrid turbulent velocity dispersion within the GMC and the resolved nonthermal velocity dispersion. The external pressure from the hot ISM determines the subgrid turbulent velocity dispersion using $\sigma^2 = P/\rho_{\text{cell}}$ with a ceiling of 10 km s$^{-1}$ imposed. This ceiling value comes from average values seen in turbulent feedback simulations (Dib, Bell & Burkert 2008; Joung, Mac Low & Bryan 2009; Ostriker & Shetty 2011). The resolved non-thermal component is determined via the mean of the standard deviation of the velocities of the nearest neighbour cells in the $\hat{x}$, $\hat{y}$ and $\hat{z}$ directions. In cases where the GMC is unresolved, a floor velocity dispersion, $\sigma_{\text{vir}}$ is set assuming the GMC is in virial balance with virial parameter $\alpha_{\text{vir}} = 1$.

### 2.4 Thermodynamics and Radiative Transfer

A key part to calculating the observed SLED is the determination of the gas temperature in the model GMCs. The model is rooted in algorithms presented by Goldsmith (2001) and Krumholz, Leroy & McKee (2011), and tested extensively in models presented by Narayanan et al. (2011b, 2012). Muñoz & Furlanetto (2013a,b) also use a similar approach. All our calculations here make use of the DESPOTIC package (Krumholz 2013), and our choices of physical parameters match the defaults in DESPOTIC unless stated otherwise.

The temperature of the H$_2$ gas is set by a balance of heating and cooling processes in the gas, heating and cooling in the dust,

$$f_{\text{H}_2} \approx 1 - \frac{3}{4} \frac{s}{1 + 0.25s}$$

for $s < 2$ and $f_{\text{H}_2} = 0$ for $s \geq 2$, where $s = \ln(1 + 0.6 \chi + 0.01 \chi^2)/(0.6\tau_e), \chi = 0.7(1 + 3.1 Z_{\odot}^{0.365})$, and $\tau_e = 0.066 \Sigma_{\text{cloud}}/(10^4 \text{pc}^2) \times Z'$. Here $Z'$ is the metallicity divided by the solar metallicity. We motivate the usage of the Krumholz, McKee & Tumlinson (2009b) model for H$_2$ formation and destruction for two reasons. First, observations by Fumagalli, Krumholz & Hunfi (2010) and Wong et al. (2013) of dwarf galaxies suggest that the adopted method in Equation 1 may fare better at low metallicities than observed empirical pressure-based relations (e.g. Blitz & Rosolowsky 2006). Second, Krumholz & Gnedin (2011) find that Equation 1 compares well to full numerical time-dependent chemical reaction networks and radiative transfer models for H$_2$ formation and destruction (Pelupessy, Paradisoulos & van der Werf 2006; Gnedin, Tassis & Kravtsov 2008; Gnedin & Kravtsov 2010; Christensen et al. 2012a, b; Munshi et al. 2013) above metallicities of $\sim 0.1 Z_{\odot}$. The mass-weighted metallicity in our star-forming galaxies are always above this threshold.

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$$s^p \approx \ln(1 + 3 M_{1D}/4)$$

based on insight from numerical simulations (Ostriker, Stone & Gammie 2001; Padoan & Nordlund 2002; Lemaster & Stone 2008). Here, $M_{1D}$ is the one-dimensional Mach number of the turbulence. In order to calculate the Mach number, we assume the temperature of the GMC is 10 K. This represents a minor inconsistency in our modeling, as for the remainder of the gas specification, we utilize a fully radiative model to determine the gas thermal properties (5.2). The 1D velocity dispersion of in the cloud is determined by:

$$\sigma = \max(\sigma_{\text{cell}}, \sigma_{\text{vir}})$$

where $\sigma_{\text{cell}}$ is the mean square sum of the subgrid turbulent velocity dispersion within the GMC and the resolved nonthermal velocity dispersion. The external pressure from the hot ISM determines the subgrid turbulent velocity dispersion using $\sigma^2 = P/\rho_{\text{cell}}$, with a ceiling of 10 km s$^{-1}$ imposed. This ceiling value comes from average values seen in turbulent feedback simulations (Dib, Bell & Burkert 2008; Joung, Mac Low & Bryan 2009; Ostriker & Shetty 2011). The resolved non-thermal component is determined via the mean of the standard deviation of the velocities of the nearest neighbour cells in the $\hat{x}$, $\hat{y}$ and $\hat{z}$ directions. In cases where the GMC is unresolved, a floor velocity dispersion, $\sigma_{\text{vir}}$ is set assuming the GMC is in virial balance with virial parameter $\alpha_{\text{vir}} = 1$.
and energy exchange between the gas and dust. The principal gas heating processes are via cosmic rays and the grain photoelectric effect, and energy exchange with dust. The principle coolant is CO when the bulk of the carbon is in molecular form, else C II when in atomic form. The dominant heating mechanism for dust is absorption of radiation, while the cooling occurs via thermal emission. Formally, the equations of thermal balance for gas and dust are:

\begin{align}
\Gamma_{\text{gas}} + \Gamma_{\text{CR}} - \Lambda_{\text{line}} + \Psi_{\text{gd}} &= 0 \\
\Gamma_{\text{dust}} - \Lambda_{\text{dust}} - \Psi_{\text{gd}} &= 0
\end{align}

where \( \Gamma \) terms represent heating rates, \( \Lambda \) terms are cooling rates, \( \Psi_{\text{gd}} \) is the dust-gas energy exchange rate, which may be in either direction depending on their relative temperatures. We solve these equations by simultaneously iterating on the gas and dust temperatures.

The grain photoelectric effect heats the gas via FUV photons ejecting electrons from dust grains. Because FUV photons likely suffer heavy extinction in clouds, we attenuate the grain photoelectric heating rate by half the mean extinction in the clouds in order to account for reduced heating rates in cloud interiors:

\[ \Gamma_{\text{pe}} = 4 \times 10^{-26} c \varepsilon' e^{-N_{\text{H}} \sigma_d/2} \text{ erg s}^{-1} \]

where \( G_0' \) is the FUV intensity relative to the Solar neighborhood, and \( \sigma_d \) is the dust cross section per H atom to UV photons (given by the value \( \sigma_d = 1 \times 10^{-21} \text{ cm}^2 \)). We assume that \( G_0' \) scales linearly with the galaxy SFR, normalized by a Milky Way SFR of 2 M\(_{\odot}\) yr\(^{-1}\) (Robitaille & Whitney 2010).

The cosmic ray heating rate is driven by heated electrons freed by cosmic-ray induced ionizations, and is given by:

\[ \Gamma_{\text{CR}} = \zeta' \Phi_{\text{CR}} \text{ s}^{-1} \]

where \( \zeta' \) is the cosmic ray primary ionization rate (assumed to be 2 \times 10\(^{-17} \text{ Z'} \text{ s}^{-1} \)), and \( \Phi_{\text{CR}} \) is the thermal energy increase per cosmic ray ionization. The values for \( \Phi_{\text{CR}} \) are given in Appendix B1 of Krumholz (2013). As with \( G_0' \) before, we assume the cosmic ray ionization rate scales linearly with the SFR of the galaxy.

The carbon abundance is set to \( X_c = 1.5 \times 10^{-4} \) (Lee, Bettens & Herbst 1996), where the fraction of carbon locked into CO molecules is approximated by the semi-analytic model of Wolfire, Hollenbach & McKee (2010):

\[ f_{\text{CO}} = f_{\text{H}2} \times e^{-4(0.53 - 0.045ln(n) + 0.097ln(Z'))/A_v} \]

This model agrees well with the fully numerical calculations of Glover & Mac Low (2011). When \( f_{\text{CO}} \) is above 50%, the cooling is assumed to happen via CO line cooling; otherwise, we assume that C II dominates the carbon-based line cooling. The cooling rates are determined by full radiative transfer calculations, which also determine the CO line luminosity for each GMC in our model galaxies, as described below.

The dust cooling rate is:

\[ \Lambda_{\text{dust}} = \sigma_d (T_d) \mu_{\text{H}2} T_d^3 \]

where the bulk of the dust heating happens via IR radiation in the centers of star-forming clouds. The mean dust cross section per H nucleus, \( \sigma_d \), varies with the dust temperature, \( T_d \) as a powerlaw:

\[ \sigma_d = \sigma_{d,10} \times (T_d/10)^2 \]

1 In Narayanan et al. (2011b), we explored models that included the effects of turbulent heating on molecular clouds via both adiabatic compression as well as viscous dissipation. These tests found only modest differences between our fiducial model and models that included turbulent heating.
Figure 3. Distribution of GMCs in density-temperature phase space for two example simulated galaxies, one with low $\Sigma_{SFR}$ (left panel) and one with high $\Sigma_{SFR}$ (right panel). The main result from this figure is that gas in starburst environments is significantly warmer and denser than in quiescent environments. The left panel shows a galaxy with $\Sigma_{SFR} \approx 2 \times 10^{-2} M_\odot$ yr$^{-1}$ kpc$^{-2}$ (i.e. comparable to nearby quiescent disk galaxies), while the right shows a starburst with $\Sigma_{SFR} \approx 650 M_\odot$ yr$^{-1}$ kpc$^{-2}$ (i.e. comparable to the nuclear regions of local ULIRGs and high-z submillimeter galaxies). The innermost contour shows the region in the $n - T$ plane where the H$_2$ mass density exceeds $5.5 \times 10^7 (1 \times 10^9) M_\odot$ dex$^{-2}$ in the left (right) panel, and subsequent contours are spaced evenly in increments of $5.5 \times 10^7 (1 \times 10^9) M_\odot$ dex$^{-2}$. The horizontal dashed lines show $E_{\text{upper}}/k$ for transitions CO $J = 1 \rightarrow 0$ through $9 \rightarrow 8$ (alternating), and the vertical solid lines show the critical density, $n_{\text{crit}}$, for the same transitions at an assumed temperature of $T = 100 K$, and are taken from the Carilli & Walter (2013) review. We note that critical densities depend on temperature (via collisional rates), though only weakly.

$$\Psi_{\nu} = \alpha_{\nu} n_H T_g^{1/2} (T_d - T_b)$$  \hspace{1cm} (11)$$

where the thermal gas-dust coupling coefficient is $\alpha_{\nu} = 3.2 \times 10^{-34} Z' \text{ cm}^3 \text{ K}^{-3/2}$ for H$_2$, and $\alpha_{\nu} = 1 \times 10^{-35} Z' \text{ cm}^3 \text{ K}^{-3/2}$ for H (Krumholz 2013).

The CO line cooling rates, and CO line luminosities are calculated from every GMC in our model galaxies using the escape probability algorithms built into DESPORTIC. The CO intensities from a GMC are set by the level populations. The source function at a frequency $\nu$, $S_\nu$ for an upper transition to lower $u - l$ is governed by

$$S_\nu = \frac{n_u A_{ul} \nu}{(n_l B_{ul} - n_u B_{ul})}$$  \hspace{1cm} (12)$$

where $A_{ul}$, $B_{ul}$, and $B_{ul}$ are the Einstein coefficients for spontaneous emission, absorption, and stimulated emission, respectively, and $n$ are the absolute level populations.

The molecular levels are determined by balancing the excitation and deexcitation processes of the CO rotational lines. The relevant processes are collisions with H$_2$ and He, stimulated emission, absorption, and spontaneous emission. Formally, these are calculated via the rate equations

$$\sum_l (C_{lu} + \beta_{lu} A_{lu}) f_l = \left[ \sum_u (C_{ul} + \beta_{ul} A_{ul}) \right] f_u$$  \hspace{1cm} (13)$$

$$\sum_l f_l = 1$$  \hspace{1cm} (14)$$

where $C$ are the collisional rates, $f$ the fractional level populations, and $\beta_{ul}$ is the escape probability for transition $u \rightarrow l$. The rate equations can be rearranged as an eigenvalue problem, and solved accordingly. The Einstein coefficients and collisional rates are taken from the publicly available Leiden Atomic and Molecular Database (Schoier et al. 2008). In particular, the CO data are originally from Yang et al. (2010).

For a homogeneous, static, spherical cloud, Draine (2011) shows that the escape probability, averaged over the line profile and cloud volume can be approximated by

$$\beta_{ul} \approx \frac{1}{1 + \frac{1}{2} \tau_{ul}}$$  \hspace{1cm} (15)$$

where the optical depth is given by

$$\tau_{ul} = \frac{g_u}{g_l} \frac{3 A_{ul} \lambda_{ul}^3}{16 (2\pi)^3 \hbar^2 c Q N_H f_l} \left( 1 - \frac{f_u g_u}{f_l g_l} \right).$$  \hspace{1cm} (16)$$

Here $Q$ is the abundance of CO with respect to H$_2$, $g_l$ and $g_u$ are the statistical weights of the levels, $N_H$ is the column density of H$_2$ through the cloud, $\lambda_{ul}$ is the wavelength of the transition, and $\sigma$ is the velocity dispersion in the cloud.

DESPORTIC simultaneously solves Equations (13) and (16) with Equations (11) and (12) using an iteration process. We refer readers to Krumholz (2013) for details. We perform this procedure for every GMC in every model snapshot of every galaxy evolution simulation in Table I. The result is a self-consistent set of gas and dust temperatures, and CO line luminosities, for every simulation snapshot. These form the basis for our analysis in the following section.

3 RESULTS

The CO SLED from galaxies represents the excitation of CO, typically normalized to the ground state. As the CO rotational levels are increasingly populated, the intensity (c.f. Equation 12) increases, and the SLED rises. When the levels approach local thermodynamic equilibrium (LTE), the excitation at those levels saturates. This is visible in the observational data shown in Figure 1 where we showed the SLEDs for all SMGs with CO $J = 1 \rightarrow 0$ detections. The Eyelash galaxy has modest excitation, with the SLED turning over at relatively low $J$-levels. By comparison, HFLS3, an extreme starburst at $z \approx 6$ (Riechers et al. 2013), has levels saturated at $J \approx 7$, with only a weak turnover at higher lying lines.

Our simulated galaxies reproduce, at least qualitatively, this range of behaviors. We illustrate this in Figure 2 which shows our theoretically-computed SLEDs for a sample of snapshots from model galaxy merger z3d4e. Each snapshot plotted has a different CO mass-weighted mean gas density and temperature. With increasingly extreme physical conditions, the populations in higher $J$ levels rise, and the SLED rises accordingly. Eventually the intensity from a given level saturates as it approaches thermalization.

In this Section we more thoroughly explore the behavior of the
SLEDs in our simulations. First, in §3.1 we strive to understand the physical basis of variations in the SLEDs. Then, in §3.2 we use this physical understanding to motivate a parameterization for the SLED in terms of an observable quantity, the star formation surface density. We show that this parameterization provides a good fit to observed SLEDs in §3.3.

3.1 The Drivers of SLED Shapes in Galaxies

The principal physical drivers of CO excitation are from collisions with H$_2$, and absorption of resonant photons. Generally, non-local excitation by line radiation is relatively limited on galaxy-wide scales (Narayanan et al. 2008b), and so the populations of the CO levels are set by a competition between collisional excitation and collisional and radiative de-excitation. Thus the level populations in a given cloud are driven primarily by the density and temperature in that cloud, which affect collisional excitation and de-excitation rates, and by the cloud column density, which determines the fraction of emitted photons that escape, and thus the effective rate of radiative de-excitation. In this Section we examine these factors in three steps, first considering the gas temperature and density distributions, then the optical depth distributions, and finally the implications of the temperature on the shape of the SLED for thermalized populations.

In what follows, we will refer heavily to Figures 3 and 4. Figure 3 shows the distribution of GMCs in density and temperature for two example model galaxies: a quiescent galaxy ($\Sigma_{SFR} \sim 2 \times 10^{-2} M_{\odot} yr^{-1} kpc^{-2}$) and a starburst ($\Sigma_{SFR} \sim 650 M_{\odot} yr^{-1} kpc^{-2}$). For comparison, the figure also shows the temperatures corresponding to the upper energy level of various CO transitions ($T_{upper} = E_{upper}/k$; horizontal dashed lines), as well as the critical densities of the upper levels evaluated at a gas temperature of $T \approx 100$ K (vertical solid lines). Here we define the critical density for a particular $J$ level as

$$n_{crit}(J) = \frac{A_{J,J-1}}{C_{J,J-1}},$$

where $A_{J,J-1}$ is the Einstein coefficient for spontaneous de-excitation from level $J$ to level $J-1$, and $C_{J,J-1}$ is the rate coefficient for collisional de-excitation between the levels. In Figure 3 we plot the CO mass-weighted H$_2$ gas densities, kinetic temperatures, and velocity dispersions of all of our model galaxies as a function of galaxy star formation rate surface density ($\Sigma_{SFR}$) (though note that the trends are very similar for the H$_2$ mass-weighted quantities). The reason for plotting $\Sigma_{SFR}$ on the abscissa will become apparent shortly.

3.1.1 Gas Density and Temperature

By and large, molecular clouds in normal, star-forming disk galaxies at $z \sim 0$ (like the Milky Way) have relatively modest mean gas densities, with typical values $n \approx 10 - 500$ cm$^{-3}$. This is evident from both Figures 3 and 4. Three major processes can drive deviations from these modest values, and greatly enhance the mean gas density of molecular clouds. First, very gas rich systems will be unstable, and large clumps of gas will collapse to sustain relatively high star formation rates. These galaxies are represented by early-phase snapshots of both our model disks, and model mergers, and serve to represent the modest increase in galaxy gas fraction seen in high-$z$ star-forming galaxies (Narayanan, Bothwell & Dave 2012, Haas et al. 2013, Tyson et al. 2013). Second, galaxy mergers drive strong tidal torques that result in dense concentrations of nuclear gas, again associated with enhanced star formation rates (Mihos & Hernquist 1994a,b; Younger et al. 2009, Hayward et al. 2013c, Hopkins et al. 2013d). The mass weighted mean galaxy-wide H$_2$ gas density in the most extreme of these systems can exceed $10^3$ cm$^{-3}$, with large numbers of clouds exceeding $10^4$ cm$^{-3}$ (c.f. Figure A2 of Narayanan et al. 2011b). This is highlighted by the right panel of Figure 3, which shows the distribution of molecular gas in the $n$–$T$ plane for such a nuclear starburst. Finally, large velocity dispersions in GMCs can enhance the mean density via a turbulent compression of gas (c.f. Equation 3). In all three cases, the increased gas densities are correlated with enhanced galaxy-wide SFR surface densities, in part owing to the enforcement of a Kennicutt-Schmidt star formation law in the SPH simulations.

Increased gas kinetic temperatures can also drive up the rate of collisions between CO and H$_2$, thereby increasing molecular excitation. As discussed by Krumholz, Leroy & McKee (2011) and Narayanan et al. (2011b), the gas temperature in relatively quiescent star-forming GMCs is roughly $\sim 10$ K. In our model, this principally owes to heating by cosmic rays. At the relatively low densities ($10 - 100$ cm$^{-3}$) of normal GMCs, heating by energy exchange with dust is a relatively modest effect, and cosmic rays tend to dominate the gas heating. For a cosmic ray ionization rate comparable to the Milky Way’s, a typical GMC temperature of $\sim 10$ K results (Narayanan & Hopkins 2013).

As galaxy star formation rates increase, however, so do the gas temperatures. This happens via two dominant channels. In our models, the cosmic ray ionization rate scales linearly with the galaxy-wide star formation rate, motivated by tentative trends observed by Acciari et al. (2009), Abdo et al. (2010), and Hailey-Dunsheath et al. (2008a). As noted by Papadopoulos (2010), Papadopoulos et al. (2011), and Narayanan & Dave (2012b), increased cosmic ray heating rates can substantially drive up gas kinetic temperatures, depending on the density of the gas and cosmic ray flux. Second, at gas densities above $\sim 10^4$ cm$^{-3}$, the energy exchange between gas and dust becomes efficient enough that collisions between H$_2$ and dust can drive up the gas temperature as well. Because high star formation rates accompany high gas densities, and high dust temperatures typically accompany high star formation rates (e.g. Narayanan et al. 2010), the gas temperature rises with the galaxy SFR. At very large densities ($n \gg 10^4$ cm$^{-3}$) we find that the dust temperatures are typically warm enough that the heating by cosmic rays is a minor addition to the energy imparted to the gas by collisions with dust. As is evident from Figure 3 because both heating channels scale with the observable proxy of SFR surface density, the mean galaxy-wide gas temperature does as well. For galaxies undergoing

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$^2$ It is worth noting that this definition does not include terms associated with stimulated emission, nor does it include collisional de-excitation to levels other than the $J - 1$ level. Both of these are sometimes included in the denominator when defining the critical density.

$^3$ It is important to note that not all of the aforementioned drivers of enhanced gas density are causally correlated with increased SFR surface densities. For example, the calculation of internal GMC velocity dispersions (and resultant turbulent compression of gas) are done in post-processing, while the galaxy-wide SFRs are calculated on the fly in the hydrodynamic simulations. As a result, the two are not causal.

$^4$ This is what drives the apparent low temperature cut-off in the left panel of Figure 3 and top-right of Figure 4.
intense star formation, the mean gas temperature across the galaxy can approach $\sim 100$ K.

### 3.1.2 Line Optical Depths

From §3.1.1 it is clear that at increased star formation rate surface densities, the gas temperatures and densities rise, which will drive up molecular excitation. The next question is, how quickly will these levels approach LTE, and saturate the observed SLED? The critical density provides a rough guide to this, but in optically thick regions, line trapping can increase excitations at a level above what would be expected if the photons could escape easily (Evans 1999, Reiter et al. 2011). In the escape probability approximation, we can define an effective critical density

$$n_{\text{crit,eff}}(J) = \beta_{J,J-1} \frac{A_{J,J-1}}{C_{J,J-1}}$$

where $\beta_{J,J-1}$ is the probability that a photon emitted at a frequency corresponding to the energy difference between levels $J$ and $J-1$ will escape the cloud without being absorbed. Recall from Equation [15] that $\beta_{J,J-1}$ can be approximated by $1/[1 + (3/8)\tau_{J,J-1}]$ (Draine 2011), so for $\tau_{J,J-1} \gg 1$, the effective density needed to thermalize a given level decreases by roughly a factor of $\tau_{J,J-1}$.

In Figure 5 we show the median CO luminosity-weighted optical depth for a sample of CO transitions as a function of galaxy star formation rate surface density. The lines in Figure 5 can be thought of as the typical optical depth for different CO lines within the GMCs in our model galaxies. In short, low-$J$ CO transitions are always optically thick, while high-$J$ lines only become optically thick in more extreme star-forming galaxies. Referring to Equation [16] the qualitative trends are straightforward to interpret, and arise from a combination of both the varying level populations, as well as changing physical conditions as a function of galaxy $\Sigma_{\text{SFR}}$. Low lying transitions such as CO $J = 1 - 0$ are typically thermalized in most clouds in galaxies (even at low $\Sigma_{\text{SFR}}$), owing to the relatively low critical densities and high optical depths. Hence, in even more dense conditions in high $\Sigma_{\text{SFR}}$ systems, the relative level populations stay approximately constant. However, the optical depth is inversely proportional to the gas velocity dispersion which tends to rise with star formation rate surface density (c.f. Figure 4). Hence, at increased $\Sigma_{\text{SFR}}$, the optical depths of low-$J$ transitions decreases slightly, though they remain optically thick. The opposite trend is true for high-$J$ transitions. These transitions are typically subthermally populated in low density clouds. As densities and temperatures rise with $\Sigma_{\text{SFR}}$, so do the level populations. This rise offsets the increase in gas velocity dispersion, and the optical depths in these lines increase in more extreme star forming systems.

The net effect of the mean trends in CO optical depths in molecular clouds in star forming galaxies, as summarized in Figure 5 is that galaxies of increased gas density and temperature (as parameterized here by increased $\Sigma_{\text{SFR}}$) have increased optical depths in high-$J$ CO lines. This drives down the effective density, and lets the levels achieve LTE more easily. This will be impor-

Figure 4. CO mass-weighted H$_2$ gas densities, kinetic temperatures, and velocity dispersions of GMCs in each of our model galaxy snapshots as a function of galaxy $\Sigma_{\text{SFR}}$. Each point represents a single snapshot from a single simulation. Notice that, at high $\Sigma_{\text{SFR}}$, the physical conditions become increasingly extreme in our model galaxies.
3.1.3 Line Ratios for Thermalized Populations

Thus far, we have been principally concerned with the physical drivers of CO excitation, as well as the influence of optical depth in lowering the effective density for thermalization of a given CO line. These have given some insight as to roughly when SLED lines will saturate. We now turn our attention to what values line ratios will reach as the gas velocity dispersion increases, and photons in these lines are more easily able to escape, decreasing the optical depths. For high-\(J\) transitions, the level populations begin at modest levels, and the optical depths are low. Broadly, at increased \(\Sigma_{\text{SFR}}\), the level populations rise owing to increased gas densities and temperatures, which drives the optical depths up.

![Figure 5. CO line luminosity-weighted line optical depths as a function of galaxy \(\Sigma_{\text{SFR}}\). Each line represents the median luminosity-weighted line optical depth for all snapshots within bins of \(\Sigma_{\text{SFR}}\). The low-\(J\) CO lines start off roughly thermalized. At increased \(\Sigma_{\text{SFR}}\), the gas velocity dispersions increase, and photons in these lines are more easily able to escape, decreasing the optical depths. For high-\(J\) transitions, the level populations begin at modest levels, and the optical depths are low.](image1)

![Figure 6. CO line luminosity-weighted median gas kinetic temperatures as a function of galaxy \(\Sigma_{\text{SFR}}\). The horizontal dashed lines show the temperature \(T_{\text{upper}} = E_{\text{upper}}/k\) that corresponds to the upper level energy of a given CO transition (with the same color coding as the solid lines). At even modest \(\Sigma_{\text{SFR}}\), gas temperatures as such that lines through CO \(J = 4 - 3\) are well into the Rayleigh-Jeans limit. In contrast, even at the most extreme \(\Sigma_{\text{SFR}}\) values in our library, the median gas temperature is never high enough to exceed \(T_{\text{upper}}\) for \(J_{\text{upper}} \geq 7\).](image2)

3.2 A Parameterized Model for CO SLEDs

Owing to both a desire for high-resolution and sensitivity, as well as the general prevalence of (sub)mm-wave detectors that operate between 800 \(\mu\)m and \(\sim 3\) mm, observations of high-\(z\) galaxies are often of rest-frame high-\(J\) CO lines. Because physical measurements of \(H_2\) gas masses require conversion from the CO \(J = 1 - 0\) line, we are motivated to utilize our model results to derive a parameterized model of the CO excitation in star forming galaxies.

From Figure 2 it is clear that the SLED from galaxies rises with increasing \(H_2\) gas density and kinetic temperature. How rapidly these SLEDs rise depend on the exact shape of the density and temperature probability distribution function (PDF), as well as the line optical depths. As we showed in §3.1.3 the SLED tends to saturate at roughly \(J^2\) for \(J_{\text{upper}} \lesssim 6\) at high \(\Sigma_{\text{SFR}}\), owing to large gas kinetic temperatures (c.f. Figure 6). For higher lying lines, when the levels are in LTE, the SLED will saturate at the ratio of the Planck functions between \(J_{\text{upper}}\) and the ground state.

In principle, the SLED would best be parameterized by a combination of the gas densities, temperatures and optical depths. Of course, these quantities are typically derived from observed SLEDs, not directly observed. However, as shown in Figures 3-5 these quantities are reasonably well-correlated with the star formation rate surface density of galaxies. Qualitatively this makes sense - more compact star forming regions arise from denser gas concentrations. Similarly, regions of dense gas and high star formation rate densities have large UV radiation fields (and thus warmer dust temperatures), increased efficiency for thermal coupling between gas and dust, and increased cosmic ray heating rates.

Motivated by these trends, we fit the simulated line ratios for all model snapshots in our galaxies as a power law function of the star formation rate surface density utilizing a Levenberg-Marquardt algorithm. The power-law fit encapsulates the behaviour expected for line intensity ratios (with respect to the ground state) as a function of \(\Sigma_{\text{SFR}}\): at low \(\Sigma_{\text{SFR}}\), the line ratios rise as the levels ap-
Table 2. Fits to Equation[19] for Resolved Observations of Galaxies.

| Line Ratio   | A     | B     | C     |
|--------------|-------|-------|-------|
| (I_0 / I_1-0) |       |       |       |
| CO J = 2 – 1 | 0.09  | 0.49  | 0.47  |
| CO J = 3 – 2 | 0.17  | 0.45  | 0.66  |
| CO J = 4 – 3 | 0.32  | 0.43  | 0.60  |
| CO J = 5 – 4 | 0.75  | 0.39  | 0.006 |
| CO J = 6 – 5 | 1.46  | 0.37  | -1.02 |
| CO J = 7 – 6 | 2.04  | 0.38  | -2.00 |
| CO J = 8 – 7 | 2.63  | 0.40  | -3.12 |
| CO J = 9 – 8 | 3.10  | 0.42  | -4.22 |

Table 3. Fits to Equation[19] for Unresolved Observations of Galaxies.

| Line Ratio   | A     | B     | C     |
|--------------|-------|-------|-------|
| (I_0 / I_1-0) |       |       |       |
| CO J = 2 – 1 | 0.07  | 0.51  | 0.47  |
| CO J = 3 – 2 | 0.14  | 0.47  | 0.64  |
| CO J = 4 – 3 | 0.27  | 0.45  | 0.57  |
| CO J = 5 – 4 | 0.68  | 0.41  | -0.05 |
| CO J = 6 – 5 | 1.36  | 0.38  | -1.11 |
| CO J = 7 – 6 | 1.96  | 0.39  | -2.14 |
| CO J = 8 – 7 | 2.57  | 0.41  | -3.35 |
| CO J = 9 – 8 | 2.36  | 0.50  | -3.70 |

Table 2 provides reliable parameters for a SLED construction from the SFR surface density \( \Sigma_{SFR} \), and shows how the functional form of the best-fit SLED varies with \( \Sigma_{SFR} \). The parameterized form given by Equation [19] is valid for SFR surface densities \( \Sigma_{SFR} \geq 1.5 \times 10^{-2} \) M\(_{\odot}\) yr\(^{-1}\) kpc\(^{-2}\), as this is the range above which our fits are well-behaved.

In principle, the numbers presented in Table 3 allow for the calculation of the full SLED of a galaxy given a measured \( \Sigma_{SFR} \). This said, an essential point to the SLED calculations presented thus far is that CO intensities for a given line are resolved at the level of our finest cell in our adaptive mesh (~ 70 pc). Thus, Table 2 provides reliable parameters for a SLED construction from the SFR surface density given that the emitting region in each line is resolved. In other words, if a given high-J line is observed from a galaxy (say, CO J = 4 – 3), to convert down to the J = 1 – 0 transition utilizing Equation [19] and the fit parameters in Table 2 for unresolved observations share the same assumed emitting area, and therefore depress the SLEDs at high-J because the emitting gas occupies a smaller area, and therefore suffers beam dilution when averaged over the same area as the low-J lines.

![Figure 7](https://sites.google.com/a/ucsc.edu/krumholz/codes) Parameterized model for SLEDs. The model SLED shape is a function of \( \Sigma_{SFR} \), and is given in Equation[19] with fit parameters listed in Tables 2 and 3. The solid lines show the perfectly resolved case, while the dashed lines (of the same color) show the case for unresolved models. Unresolved observations share the same assumed emitting area, and therefore depress the SLEDs at high-J because the emitting gas occupies a smaller area, and therefore suffers beam dilution when averaged over the same area as the low-J lines.

3.3 Comparison to Observations

In an effort to validate the parameterized model presented here, in Figure 8 we present a comparison between our model for CO excitation in galaxies and observations of 15 galaxies from present epoch to \( z > 6 \). Most of the observational data comes from galaxies at moderate to high-redshift owing to the fact that it is typically easier to access the high-J submillimeter CO lines when they are redshifted to more favorable atmospheric transmission windows than it is at \( z \sim 0 \). With the exception of NGC 253, we use our fits for unresolved observations in this comparison. For NGC 253 we use the resolved model, because that galaxy is only \( \sim 3.3 \) Mpc proach LTE, then plateau as the levels are thermalized at high \( \Sigma_{SFR} \). Our model line ratios are well fit by a function:

\[
\log_{10} \left( \frac{I_0}{I_1-0} \right) = A \times \log_{10}(\Sigma_{SFR}) - \chi B + C
\]

where the \( \Sigma_{SFR} \) is in M\(_{\odot}\) yr\(^{-1}\) kpc\(^{-2}\), and the offset \( \chi = -1.85 \); this value is chosen to ensure that our fit produces purely real values for \( I_0 / I_1-0 \), and is determined primarily by the range of \( \Sigma_{SFR} \) values sampled by our simulation library. We list the best fit values for model parameters A, B, and C in Table 2 and show how the functional form of the best-fit SLED varies with \( \Sigma_{SFR} \) in Figure 7. The parameterized form given by Equation [19] is valid for SFR surface densities \( \Sigma_{SFR} \geq 1.5 \times 10^{-2} \) M\(_{\odot}\) yr\(^{-1}\) kpc\(^{-2}\), as this is the range above which our fits are well-behaved.

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4 DISCUSSION

4.1 The Parameterization of SLEDs

We have presented a model the physical origins of SLEDs in star forming galaxies, and derived a rough parameterization of the SLED in terms of an observable quantity, the star formation rate surface density. As discussed in §3.2, as well as in Figure 9, the global SFR alone provides a poor parameterization of the CO SLED, and more generally, the physical conditions in the molecular clouds in the galaxy.

A number of other works have arrived at similar conclusions, though via notably different methods. As an example, Rujopakarn et al. (2011) showed that galaxies with similar infrared luminosity densities across different redshifts shared more common observed properties (such as aromatic features) than simply galaxies at a shared infrared luminosity. This is akin to the idea that ULIRGs at $z \sim 0$ do not lie on the SFR-$L_*$ main sequence, while galaxies of a comparable luminosity at high-$z$ do (Daddi et al. 2005; Rodighiero et al. 2011). In contrast, normalizing by the spatial scale of the emitting (or star-forming) region allows for a more straightforward comparison of galaxies even at vastly different redshifts. A similar point was made by Hopkins et al. (2010), who showed that with increasing redshift, the fraction of galaxies at a given luminosity comprised of galaxy mergers and starbursts decreases dramatically.

This point is related to that made by Díaz-Santos et al. (2013), when examining the [C II]-FIR deficit in galaxies. At $z \sim 0$, galaxies with large infrared luminosity tend to have depressed [C II] 158 µm emission as compared to what would be expected for the typical [C II]-FIR scaling at lower luminosities (Malhotra et al. 1997; Luhman et al. 1998; de Looze et al. 2011; Farrah et al. 2013).

While the origin of the deficit is unknown, early indications suggest that a similar deficit may exist in high-$z$ galaxies, though offset in infrared space (e.g. Stacey et al. 2010; Graciá-Carpio et al. 2011; Wang et al. 2013). However, Díaz-Santos et al. (2013) showed that when comparing to a galaxy’s location with respect to the specific star formation rate main sequence, galaxies at both low and high-$z$ follow a similar trend.

As a result of this, there are no “typical” values of CO SLEDs for a given galaxy population. Populations such as ULIRGs or SMGs are generally selected via a luminosity or color cut. This can result in a heterogeneous set of physical conditions in galaxies, and therefore heterogeneous CO emission properties. This was shown explicitly by Paradisopoulos et al. (2012), who demonstrated that local luminous infrared galaxies (LIRGs; $L_{\text{IR}} \geq 10^{11} L_{\odot}$) exhibit a diverse range of CO excitation conditions. Similarly, Downes & Solomon (1998), Tacconi et al. (2008), Magdis et al. (2011), Hodgson et al. (2012), Magnelli et al. (2013), Ivison et al. (2013), and Fu et al. (2013) showed that the CO-H$_2$ conversion factor, $X_{\text{CO}}$, for ULIRGs and high-$z$ SMGs each show a factor \(~ \geq 10^{11} \) in observationally derived values. A template for the CO emission properties is not feasible for a given galaxy population given the wide variation in ISM physical conditions that can be found in luminosity-selected populations.

4.2 Relationship to Other Models

Over the last few years, a number of theoretical groups have devoted significant attention to predicting CO emission from star-forming galaxies. Here, we review some previous efforts to predict CO SLEDs, and place our current work into this context. In
short, a number of analytic and semi-analytic models have explored the simulated SLEDs from model galaxies, but no comprehensive model for the origin of SLEDs has been reported thus far. Most works focus on validation of a given galaxy formation model.

To date, no work investigating SLEDs has utilized bona fide hydrodynamic simulations of galaxy evolution that directly simulate the physical properties of the interstellar medium to calculate the CO excitation from galaxies. They have instead relied on either analytic or semi-analytic models to describe the physical properties of galaxies and giant molecular clouds within these galaxies, and coupled these analytic models with numerical radiative transfer calculations to derive the synthetic CO emission properties.

On the purely analytic side, Armour & Ballantyne (2012) and Muñoz & Furlanetto (2013b) developed models for quiescent disk galaxy evolution (constructing such a model for merger-driven starbursts would be quite difficult) in order to predict CO emission...
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from nuclear starburst disks around AGN, and from $z \gtrsim 6$ galaxies, respectively. 

Armour & Ballantyne (2012) construct single phase nuclear disks that rotate around a central AGN. The SFR is forced to be such that Toomre’s $Q$ parameter is unity, and the vertical support of the disk owes to radiative feedback following the theory of Thompson, Quataert & Murray (2005). The CO SLEDs are calculated by applying RATRAN radiative transfer calculations to the model grid (Hogerheijde & van der Tak 2000). These authors find that nuclear starbursts are extremely dense, and therefore thermalized line ratios will be common. A subset of the models show strong correspondence with the M82, Mrk 231 and Arp 220, with potentially some under-prediction of the highest $J$ transitions ($J > 8$). Interestingly, a subset of the models by Armour & Ballantyne (2012), fall into CO line absorption at large $J_{upper}$ ($J_{upper} > 11$), owing to the steep temperature and density gradients within the starburst.

Muñoz & Furlanetto (2013b) develop analytic models of high-$z$ galaxy disks that also are forced to maintain vertical hydrostatic equilibrium by radiation pressure, similar to the aforementioned study by Armour & Ballantyne (2012). Muñoz & Furlanetto (2013b) place their galaxies in a cosmological context by allowing for gas accretion from the intergalactic medium (IGM) following parameterizations from cosmological dark matter simulations, as well as allow for momentum driven winds following the Oppenheimer & Davé (2008) prescriptions. Within the disks, GMCs are assumed to have a threshold floor surface density of $85 \, M_{\odot} \, pc^{-2}$, and $H_2$ fractions that depend on the stellar and cloud surface density. The CO fraction follows the Wolfire, Hollenbach & McKee (2010) model, as in our work, and the GMCs have lognormal density distribution following from supersonic turbulence. After accounting for the modulation of critical densities by line optical depths, Muñoz & Furlanetto (2013b) calculate the CO excitation of their model $z \sim 6$ galaxies utilizing a precursor code to DESPOTIC, with identical underlying algorithms. These authors focused specifically on the observable CO $J = 6 - 5$ line. They find that the high $J$ lines from these galaxies will be observable with ALMA, as long as the ISM clumps similarly to local galaxies. If turbulence does not provide the principal support for the clouds, however, and they are more homogenous, and the excitation of high $J$ levels will be greatly reduced. This said, Muñoz & Furlanetto (2013a) suggest that their model may overpredict the expected CO $J = 6 - 5$ emission from extreme star-formers at high-$z$ such as the $z \sim 6$ SMG HFLS3, in part due to the high gas velocity dispersions (and thus an increased gas mean density due to turbulent compression of gas; c.f. equation [2]). Indeed their model has similar velocity dispersions for HFLS3-like systems as our own ($\sim 100 \, km \, s^{-1}$). While it is difficult to exactly compare our model with that of Muñoz & Furlanetto (2013a) owing to the starkly different modeling methods (analytic versus coupled hydrodynamic and radiative transfer), one possible origin in the difference in predicted SLEDs for HFLS3-like systems is in the radial density distribution within the gas. In our model, a sufficiently large low-density emitting-region exists even in high $\Sigma_{\text{SFR}}$ galaxies that the unresolved model SLED is depressed at high $J$ levels.

Turning to semi-analytic models, Lagos et al. (2012) coupled the GAlFORM SAM with the 1D photodissociation region (PDR) code ucl_PDR (Bayet et al. 2011) to analyze the model CO emission from analytic galaxies painted on to dark matter halos taken from N-body simulations. These authors assume $H_2$ fractions that derive from the empirical relations provided by Blitz & Rosolowsky (2006) for normal star-forming galaxies, and an $H_2$ fraction of unity in starbursts. The PDR modeling assumes the gas is confined to a 1-zone slab geometry illuminated on one side by a UV field, which scales with $\Sigma_{\text{SFR}}$ in the Lagos et al. (2011, 2012) version of GALFORM. For the majority of their models, Lagos et al. (2012) assume isodensity gas of $\rho_{H2} = 10^4 \, M_{\odot} \, cm^{-3}$, and calculate the SLEDs accordingly. They find that on average the SLEDs of galaxies that are LIRGs (ULIRGs) at $z = 0$ peak at $J = 4(5)$, though there is significant dispersion in the high-$J$ excitation. While difficult to directly compare with our own work, the range of SLEDs derived by Lagos et al. (2012) is certainly consistent with the range found here.

Following on this, Popping et al. (2013) and Popping, Somerville & Trager (2013) coupled a semi-analytic model for galaxy formation (Somerville & Eales 2008), with the radiative transfer code $\beta$3D (Poelman & Spaans 2005, 2006; Pérez-Beaupuits, Wada & Spaans 2011) to model the CO (among other species) emission from their model galaxies. The $H_2$ fraction is based on fitting functions from cosmological zoom simulations by Gnedin & Kravtsov (2011), dependent on the stellar and gas surface densities. Star formation follows a modified Kennicutt-Schmidt star formation relation (Kennicutt 1998b, Kennicutt & Evans 2012), and clouds occupy a volume filling factor of $f_{\text{cloud}} = 0.01$. These authors find excellent agreement in the dense gas fractions returned by their models (as traced by observed dense gas line ratios – Narayanan et al. 2005; Bussmann et al. 2008; Juneau et al. 2009; Hopkins et al. 2013a) and observations. Relevant to the present study, Popping et al. (2013) find that galaxies with higher FIR luminosities have CO SLEDs that peak at higher excitation levels, similar to the work by Lagos et al. (2012). Galaxies at a fixed FIR luminosity in this model, though, peak at higher CO levels at high redshifts than at low redshifts. In the Popping et al. (2013) model, this owes to the fact that galaxies at high-$z$ at a fixed FIR have warmer and denser cold gas than their low-$z$ counterparts do. While we are unable to make a similar comparison, in our model this could be ascribed to galaxies at high-$z$ at a fixed luminosity having higher $\Sigma_{\text{SFR}}$ than their low-$z$ analogs. This is likely the case in the Popping et al. (2013) model, as the disk sizes of galaxies at a fixed stellar mass are smaller at high-$z$ than present epoch (Somerville et al. 2008a).

Popping et al. (2013) show a steeply rising relation between CO level populations and $\Sigma_{\text{gas}}$ (which is presumably similar to the relation with $\Sigma_{\text{SFR}}$ given their star formation law), and a much more moderate relationship between molecular level populations and global galaxy SFR. In this sense our work is seemingly in very good agreement with the Popping et al. (2013) model.

4.3 Applications of this Model

With the powerlaw fit presented in Equation [19] and Tables 2 and 3 we have provided a mechanism for calculating the full CO rotational ladder through the $J = 9 - 8$ transition given a constraint on the star formation rate surface density. With this, in principle one can utilize a CO observation of a high-$z$ galaxy at an arbitrary...
transition, and then down-convert to the CO $J = 1 - 0$ transition flux density.

To convert from the CO $J = 1 - 0$ flux density to the more physically meaningful H$_2$ gas mass, one needs to employ a CO-H$_2$ conversion factor. While there have been numerous observational (Donovan Meyer et al. 2012; Magdis et al. 2011; Genzel et al. 2012; Hodge et al. 2012; Schruba et al. 2012; Bolatto, Wolfire & Leroy 2013; Blanc et al. 2013; Fu et al. 2013; Sandstrom et al. 2013) and theoretical (Glover & Mac Low 2011; Genzel et al. 2012; Hodge et al. 2012; Schruba et al. 2012; Lagos et al. 2012) attempts to constrain the CO-H$_2$ conversion factor, significant uncertainty exists in the calibration.

In Narayanan et al. (2012), utilizing the same simulations presented here to derive a smooth functional form for the CO-H$_2$ conversion factor in galaxies:

$$X_{CO} = \frac{\min \left[ 4, 6.75 \times \left( \frac{S_{CO}}{Z} \right)^{0.32} \right] \times 10^{20}}{Z^{0.65}}$$ (20)

$$\alpha_{CO} = \frac{\min \left[ 6.3, 10.7 \times \langle S_{CO} \rangle^{0.32} \right] \times 10^{-3}}{Z^{0.65}}$$ (21)

where $X_{CO}$ is in cm$^{-2}$/K-km s$^{-1}$, $\alpha_{CO}$ in M$_{\odot}$ pc$^{-2}$ (K-km s$^{-1}$)$^{-1}$, $\langle S_{CO} \rangle$ is the resolved velocity-integrated CO intensity in K-km s$^{-1}$, and $Z'$ is the metallicity of the galaxy in units of solar metallicity.

The coupling of the model for CO SLEDs in this work, with the formalism for deriving H$_2$ gas masses in Equations 20 and 21 in principle could allow for the direct determination of an H$_2$ gas mass of a high-z galaxy with measurements (or assumptions) of a CO surface brightness (at any $J$ level up to $J = 9 - 8$), a $\Sigma_{SFR}$, and a gas phase metallicity. This may have implications for the gas mass of high-z galaxies.

For example, galaxy baryonic gas fractions at high-z are measured to be substantially larger than in the local Universe (e.g. Daddi et al. 2010; Tacconi et al. 2010; Geach et al. 2011; Sandstrom et al. 2013). Correctly measuring these and relating them to galaxy formation models in which the gas fraction is set by a combination of accretion from the IGM, star formation and gas outflows (e.g. Dave, Finlator & Oppenheimer 2012; Gabor & Bournaud 2013) will depend on the conversion from CO $J = 1 - 0$ to H$_2$ gas masses (cf. Narayanan, Bothwell & Dave 2012), but also a correct downconversion from the measured excited CO emission line to the ground state. Systematic trends in the excitation with galaxy physical property will, of course, muddy comparisons between observation and theory further.

Similarly, measurements of the Kennicutt-Schmidt star formation relation at high-z are sensitive dependent on gas excitation in galaxies. In principle, if there is a strong relationship between gas excitation and galaxy physical conditions, one might expect that inferred star formation laws form high-excitation lines will be flatter than the true underlying relation (Krumholz & Thompson 2007; Narayanan et al. 2008) and Narayanan, Cox & Hernquist (2008) showed that the local SFR- L$_{CO}$ relation can be strongly affected by increasing level populations of the HCN molecule. This work was furthered by Narayanan et al. (2011) who used a more rudimentary model of the calculations presented here to find that inferred lower star formation laws at high-z potentially suffered from differential excitation, and that the true underlying slope was steeper. As large surveys of galaxies at high-z fill in the $\Sigma_{SFR} - \Sigma_{gas}$ relation, accurate conversions from highly excited lines to the $J = 1 - 0$ line will become increasingly necessary.

Finally, forthcoming (sub)millimeter and radio-wave deep fields will determine the cosmic evolution of molecular gas masses and fractions in galaxies (e.g. Decarli et al. 2013; Walter et al. 2013). At a fixed receiver tuning, the observations will probe increasingly high excitation lines with redshift. Because the line ratios depend on (as observational parameterizations) the star formation rate surface density, and the CO-H$_2$ conversion factor depends on CO surface brightness and gas phase metallicity, potential biases in these deep fields may impact the predicted measurements of the molecular gas history of the Universe. We will discuss these issues in a forthcoming article.

### 4.4 Caveats

There are two notable regimes where our model may potentially fail. The first is when considering the gas in the vicinity of an active galactic nucleus (AGN). van der Werf et al. (2010) and Meijerink et al. (2013) used observations with the Herschel Space Observatory to constrain the excitation of very high $J$ lines in nearby active galaxies Mrk 231 and NGC 6240, respectively. Both galaxies showed extremely high excitation in the high $J$ CO lines. van der Werf et al. (2010) found that UV radiation from star formation could account for the excitation through the $J = 8$ state, but that the luminosities of the higher-$J$ lines could be explained only by invoking X-ray heating from an accreting supermassive black hole. Similarly, Meijerink et al. (2013) attributed the high excitation of gas in NGC 6240 to CO shock heating. While we do include accreting black holes in our hydrodynamic and dust radiative transfer calculations, we cannot easily resolve their impact on the thermal structure of the gas. Accordingly, we are unable to model the potential impact of AGN on the $J > 10$ CO emission lines. This said, we note that our model fit from Table 3 performs extremely well for both galaxies Mrk 231 and NGC 6240 from $J = 1 - 0$ through $J = 9 - 8$, even without the inclusion of AGN. It is reasonable to expect, then, that the heating provided by star formation, coupled to the high densities found in these rapidly-star-forming galaxies, are sufficient to explain the emission up to the $J = 9 - 8$ line without the aid of additional AGN-driven heating.

Second, our model does not account for the potential extinction very high $J$ CO lines may encounter after leaving their parent cloud. A key example of this is the extreme ULIRG, Arp 220. Arp 220 has potentially the highest $\Sigma_{SFR}$ ever measured, at nearly $1000$ M$_{\odot}$ yr$^{-1}$ kpc$^{-2}$ (Kennicutt 1998b). Despite this, the observed CO SLED in this system is not comparably extreme -- rather, the high $J$ lines appear depressed compared to what one might expect given other high $\Sigma_{SFR}$ sources. Papadopoulos, Isaak & van der Werf (2010) raised the possibility that this may owe to obscuration at FIR/submillimeter wavelengths. When applying a correction for this, the SLED approached thermalized populations. This is straightforward to understand. The observed gas surface densities of ~ $2.75 \times 10^{-4}$ M$_{\odot}$ pc$^{-2}$ in Arp 220 (Sco Gloss, Yun & Brynd 1997) translate to a dust optical depth of $\tau \sim 5$ at the wavelength of the CO $J = 5 - 4$ line, and $\sim 15$ at the $J = 9 - 8$ line, assuming solar metallicities and
Weingartner & Draine (2001) $R_\text{e} = 3.15$ dust opacities (as updated by Draine & Li 2007). In Figure 11 we show a projection map of the CO $J = 9 - 8$ optical depth in a model merger with $\Sigma_{\text{SFR}}$ comparable to Arp 220.

On the other hand, Rangwala et al. (2011) utilized Herschel measurements to derive an observed SLED for Arp 220, and found more modest dust obscuration than the aforementioned calculations. These authors find optical depths of unity at wavelengths near the CO $J = 9 - 8$ line. We show the Rangwala et al. (2011) SLED in Figure 10 alongside our model prediction for a $\Sigma_{\text{SFR}} \approx 1000 \, M_\odot \, \text{yr}^{-1} \, \text{kpc}^{-2}$ galaxy. Clearly the model over-predicts the SLED compared to the Rangwala et al. (2011) measurements. The factor of 10 difference in estimated optical depths from the Rangwala et al. (2011) observations, and our estimation likely drive the difference between the observed SLED and our model SLED. If the Rangwala et al. (2011) dust corrections are correct, this may prove to be a challenge for our model. On the other hand, given the excellent correspondence of our model with a large sample of observed galaxies (Figure 8), and the extreme star formation rate surface density of Arp 220, it may be that the dust obscuration is in fact quite extreme in this galaxy, and the true SLED is closer to thermalized.

5 SUMMARY AND CONCLUSIONS

Observations of galaxies at low and high-$z$ show a diverse range of CO excitation ladders, or Spectral Line Energy Distributions (SLEDs). In order to understand the origin of variations in galaxy SLEDs, we have combined a large suite of hydrodynamic simulations of idealized disk galaxies and galaxy mergers with molecular line radiative transfer calculations, and a fully self-consistent model for the thermal structure of the molecular ISM. Broadly, we find that the CO ladder can be relatively well-parameterized by the galaxy-wide star formation rate surface density ($\Sigma_{\text{SFR}}$).

(i) We find that the CO excitation increases with increasing gas densities and temperatures, owing to increased collisions of CO with H$_2$ molecules. The average gas density and temperature in the molecular ISM of in turn increases with $\Sigma_{\text{SFR}}$. As a result, the SLED rises at higher $J$’s in galaxies with higher SFR surface densities.

(ii) High SFR surface density galaxies tend to have increased line optical depths. This effect, which comes from the increased population of high-$J$ levels, in turn drives down the effective density for thermalization of the high-$J$ lines.

(iii) The gas temperatures in extreme $\Sigma_{\text{SFR}}$ systems rises owing to an increase in cosmic ray ionization rates, as well as increased efficiency in gas-dust energy transfer. For $J_{\text{upper}} \lesssim 6$, the lines tend to be in the Rayleigh-Jeans limit ($E_{\text{upper}} \ll kT$), and once the density is high enough to thermalize the levels, this produces lines whose intensity ratios scale as $J^2$. Lines arising from $J \gtrsim 7$, however, do not reach the Rayleigh-Jeans limit even for the most extreme star formation rates currently detected, and thus the SLED is always flatter than $J^2$ for $J \gtrsim 7$.

(iv) CO line ratios can be well-parameterized by a powerlaw function of $\Sigma_{\text{SFR}}$. We provide the parameter fits for both well-resolved observations, as well as for the more typical unresolved observations where the same emitting area is assumed for all lines (Equation 15 and Tables 2 and 3). Our functional form for the CO line ratios quantitatively matches multi-line observations of both local and high-$z$ galaxies over a large dynamic range of physical properties. In principle, this model can allow for the full reconstruction of a CO SLED with an arbitrary CO line detection (below $J_{\text{upper}} \leq 9$), and a star formation rate surface density estimate.

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