H\textsubscript{1}-TO-H\textsubscript{2} TRANSITIONS AND H\textsubscript{1} COLUMN DENSITIES IN GALAXY STAR-FORMING REGIONS

Amiel Sternberg\textsuperscript{1,} Franck Le Petit\textsuperscript{2,} Evelyne Roueff\textsuperscript{2,} and Jacques Le Bourlot\textsuperscript{2,3}

\textsuperscript{1} Raymond and Beverly Sackler School of Physics & Astronomy, Tel Aviv University, Ramat Aviv 69978, Israel
\textsuperscript{2} LERMA, Observatoire de Paris, CNRS, 5 place Jules Janssen, F-92190 Meudon, France
\textsuperscript{3} Université Paris Diderot, 5 rue Thomas-Mann, F-75205 Paris cedex 13, France

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ABSTRACT

We present new analytic theory and radiative transfer computations for the atomic-to-molecular (H\textsubscript{1}-to-H\textsubscript{2}) transitions and the buildup of atomic hydrogen (H\textsubscript{1}) gas columns in optically thick interstellar clouds irradiated by far-UV (FUV) photodissociating radiation fields. We derive analytic expressions for the total H\textsubscript{1} column densities for (one-dimensional (1D)) planar slabs, for beamed or isotropic radiation fields, from the weak- to strong-field limits, for gradual or sharp atomic-to-molecular transitions, and for arbitrary metallicity. Our expressions may be used to evaluate the H\textsubscript{1} column densities as functions of the radiation field intensity and the H\textsubscript{2}\textsuperscript{-dust limited dissociation flux, the hydrogen gas density, and the metallicity-dependent H\textsubscript{2} formation rate coefficient and FUV dust grain absorption cross section. We make the distinction between “H\textsubscript{1}-dust” and “H\textsubscript{2}-dust” opacity, and we present computations for the “universal H\textsubscript{2}-dust limited effective dissociation bandwidth.” We validate our analytic formulae with Meudon PDR code computations for the H\textsubscript{1}-to-H\textsubscript{2} density profiles and total H\textsubscript{1} column densities. We show that our general 1D formulae predict H\textsubscript{1} columns and H\textsubscript{2} mass fractions that are essentially identical to those found in more complicated (and approximate) spherical (shell–core) models. We apply our theory to compute H\textsubscript{2} mass fractions and star-formation thresholds for individual clouds in self-regulated galaxy disks, for a wide range of metallicities. Our formulae for the H\textsubscript{1} columns and H\textsubscript{2} mass fractions may be incorporated into hydrodynamics simulations for galaxy evolution.

Key words: galaxies: ISM – ISM: clouds – ISM: general – ISM: structure – stars: formation

Online-only material: color figures

1. INTRODUCTION

The atomic-to-molecular hydrogen (H\textsubscript{1}-to-H\textsubscript{2}) transition is of central importance for the evolution of the interstellar medium (ISM) and for star formation in galaxies, from local environments in the Milky Way to distant cold gas reservoirs in high-redshift systems. Stars form in molecular gas, plausibly because H\textsubscript{2} formation enhances low-temperature cooling and cloud fragmentation or perhaps simply because the molecular formation rates are elevated in the denser and more shielded components of the gravitationally collapsing regions. The atomic-to-molecular conversion is also the critical initiating step for the atomic-to-molecular transitions and, for arbitrary metallicity. Our expressions may be used to evaluate the H\textsubscript{1} column densities as functions of the radiation field intensity and the H\textsubscript{2}\textsuperscript{-dust limited dissociation flux, the hydrogen gas density, and the metallicity-dependent H\textsubscript{2} formation rate coefficient and FUV dust grain absorption cross section. We make the distinction between “H\textsubscript{1}-dust” and “H\textsubscript{2}-dust” opacity, and we present computations for the “universal H\textsubscript{2}-dust limited effective dissociation bandwidth.” We validate our analytic formulae with Meudon PDR code computations for the H\textsubscript{1}-to-H\textsubscript{2} density profiles and total H\textsubscript{1} column densities. We show that our general 1D formulae predict H\textsubscript{1} columns and H\textsubscript{2} mass fractions that are essentially identical to those found in more complicated (and approximate) spherical (shell–core) models. We apply our theory to compute H\textsubscript{2} mass fractions and star-formation thresholds for individual clouds in self-regulated galaxy disks, for a wide range of metallicities. Our formulae for the H\textsubscript{1} columns and H\textsubscript{2} mass fractions may be incorporated into hydrodynamics simulations for galaxy evolution.

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In this paper, we revisit the theory of the H\textsubscript{1}-to-H\textsubscript{2} transition and the buildup of atomic hydrogen gas layers in fully optically thick interstellar clouds irradiated by far-UV (FUV) radiation fields. Atomic (H\textsubscript{1}) gas produced by rapid stellar FUV “Lyman–Werner” (LW) photodissociation undergoes conversion to H\textsubscript{2}; as the destructive radiation is absorbed. In steady state, a mass of H\textsubscript{1} is maintained in the outer FUV-irradiated photodominated regions (PDRs) of the dense molecular clouds. Much of the (cold) H\textsubscript{1} gas in galaxies may reside in such cloud boundary layers and envelopes, interspersed with the recently formed FUV-emitting OB-type stars.

The study of interstellar H\textsubscript{1}-to-H\textsubscript{2} conversion has had a long and venerable history. Early theoretical discussions (e.g., Spitzer 1948; Gould & Salpeter 1963; Field et al. 1966; Stecher & Williams 1967; de Jong 1972; followed by Aaronson et al. 1974; Glassgold & Langer 1974; Jura 1974; Black & Dalgarno 1977; Federman et al. 1979; van Dishoeck & Black 1986) focused on the competing processes of (grain surface) molecule formation, photodissociation, and shielding in predominantly atomic gas—the classical warm and cold neutral medium (WNM and CNM) and diffuse gas—showing that significant concentrations of H\textsubscript{2} could be expected in the Galactic ISM, especially in dark, dusty clouds with high visual extinctions (Mészáros 1968; Hollenbach et al. 1971; Solomon & Werner 1971; de Jong 1972). This was confirmed observationally with the first direct (FUV LW absorption line) detections of interstellar molecular hydrogen in diffuse clouds and the correlation of the H\textsubscript{2} with E(B–V) color excess and dust extinction (Carruthers 1970; Spitzer et al. 1973; Savage et al. 1977) and with the discovery of fully molecular clouds via proxy millimeter-wave carbon monoxide (CO) emissions (Wilson et al. 1970; Rank et al. 1971).

Absorption line spectroscopy (Ly\alpha for H\textsubscript{1}; LW band for H\textsubscript{2}) has been carried out for H\textsubscript{1}-to-H\textsubscript{2} conversion along many Milky Way sight lines, through low-extinction diffuse-to-translucent gas in the disk, and into the infrared cirrus and high-velocity gas in vertical directions (Savage et al. 1977; Bohlín et al. 1978; Richter et al. 2001; Liszt & Lucas 2002; Rachford et al. 2002, 2009; Gillmon & Shull 2006; Gillmon et al. 2006; Wakker 2006; Liszt 2007; France et al. 2013; Fukui et al. 2014; Röhrer et al. 2014). These studies probe systems in which the H\textsubscript{2} mass fractions range over many orders of magnitude, from $\lesssim10^{-5}$ up to $\sim50\%$ in highly reddened systems. Absorption line observations of damped and sub-damped Ly\alpha absorbers at high redshifts also directly reveal the partial conversion of H\textsubscript{1} to H\textsubscript{2} in optically thin media (Levshakov & Varshalovich 1985; Foltz et al. 1988; Ge & Bechtold 1997; Cui et al. 2005; Ledoux et al. 2014). These studies probe systems in which the H\textsubscript{2} mass fractions range over many orders of magnitude, from $\lesssim10^{-5}$ up to $\sim50\%$ in highly reddened systems. Absorption line observations of damped and sub-damped Ly\alpha absorbers at high redshifts also directly reveal the partial conversion of H\textsubscript{1} to H\textsubscript{2} in optically thin media (Levshakov & Varshalovich 1985; Foltz et al. 1988; Ge & Bechtold 1997; Cui et al. 2005; Ledoux et al. 2014).
by the 1980s, a conceptual switch had occurred with the recognition that much of the hydrogen in galaxies is fully shielded H2 and that in dense gas in star-forming regions the H i is often a surface photodissociation “product,” rather than being the dominant component within which some shielded H2 may be present, as in the diffuse medium. Over the decades, many model computations for the H i-to-H2 transition in optically thick irradiated cloud surfaces, for application to Galactic emission line sources (see also Jura 1974; Hill & Henry 2001; Knapen et al. 2006; Schuster et al. 2007).

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opposed to the (also idealized) planar geometry and beamed fields adopted in much of the earlier PDR literature, including S88.

Our main goal and motivation in this paper is to reintroduce and extend the S88 theory for applications to global galaxy evolution studies. In Section 2 we elaborate on S88 and present a detailed overview and discussion of the basic theoretical ingredients and parameters controlling the H 1-to-H 2 transition in FUV-irradiated clouds. We rederive the fundamental S88 equation for the total H 1 column density produced for beamed radiation into a (1D) optically thick slab. We then extend the theory and consider irradiation by isotropic fields. This will enable our direct comparison with the more complicated (and more approximate) formalism for spheres. In Section 3 we present detailed numerical (Meudon PDR code) radiative transfer computations for the H 1-to-H 2 transitions and integrated H 1 columns for a wide range of interstellar conditions. The ratio of the free-space FUV field intensity (or dissociation rate) to the gas density (or H 2 formation rate) is an essential parameter, as is the metallicity and dust-to-gas mass ratio. We present numerical computations for a verification of our analytic formulae for beamed and isotropic irradiation from the weak- to strong-field limits (gradual to sharp H 1-to-H 2 transitions) and for low- to high-metallicity gas. In Section 4 we compare our planar formulae with the KMT/MK10 theory for spheres. This includes a discussion of the dimensionless parameters and a comparison of the expressions for the total H 1 columns, H 2 mass fractions, and star-formation thresholds, as functions of the metallicity. An important application and comparison is for “self-regulated gas” in which the FUV intensity-to-gas density ratio is set by the condition of two-phased equilibrium for H 1. We demonstrate that our simpler, more general, and fully analytic 1D formulæ predict H 1 columns and H 2 mass fractions that are essentially identical to results for spheres in the more restricted regime in which the spherical models are applicable (intense fields, sharp transitions, low metallicity).

This is a lengthy paper, and we develop the theory and present our step-by-step comparisons in a pedagogical style. In Section 5 we summarize and recap our basic analytic results for the H 1 column densities and molecular mass fractions in FUV-irradiated clouds, including for self-regulated star-forming galaxies. A glossary of symbols is in the Appendix.

2. ANALYTIC OVERVIEW

In this section we present an analytic discussion and overview of the basic processes and quantities that control the H 1-to-H 2 transitions and total H 1 columns in interstellar clouds exposed to photodissociating FUV radiation fields. Our overview anticipates and also provides analytic representations for the detailed numerical results that we present in Section 3. We focus on idealized static 1D semi-infinite uniform density isothermal and optically thick plane-parallel clouds that are irradiated by steady fluxes of FUV LW-band photons. We rederive the S88 formula for the steady state H 1 column densities produced in slabs irradiated by normally incident unidirectional beamed fields as appropriate for interstellar clouds exposed to localized FUV sources. We then show that this formula can be generalized to clouds embedded in isotropic radiation fields. Isotropic irradiation may be more representative of global ambient conditions in galaxies.

We begin with our normalizations for the beamed and isotropic ultraviolet radiation fields and for the associated H 2 photodissociation rates (Section 2.1). We then define the dissociation bandwidth and its derivative—the H 2 self-shielding function (Section 2.2.1). We then describe our treatment of dust grains (Section 2.2.2). The grains provide FUV continuum opacity and are also the H 2 formation sites. The metallicity of the gas then enters as an important parameter because it controls the dust-to-gas mass ratio and therefore also the associated H 2 formation efficiency and the FUV dust optical depth per gas column density. We make the simplifying assumption that the dust-to-gas mass ratio scales linearly with the metallicity. If star formation requires the conversion from H 1 to H 2, the metallicity will be an essential parameter in controlling the star-formation thresholds.

We put the physical ingredients together and write down the density-dependent steady state H 1/H 2 formation–destruction equation for semi-infinite slabs exposed to beamed fields (Section 2.2.3). Crucially, the differential equation is separable, and this enables our definition of the “universal H 2-dust-limited LW dissociation bandwidth” (Section 2.2.4) and the “effective dissociation flux” (Section 2.2.5). The H 2-dust-limited dissociation bandwidth is a fundamental quantity in the theory, and we present analytic expressions and numerical computations for it in this paper.

We then integrate the H 1/H 2 formation–destruction equation to derive our analytic formula for the H 1 column density for clouds irradiated by beamed fields (Section 2.2.6). Our formula gives the H 1 column density as a function of the physical variables, including gas density, FUV intensity, effective dissociation flux, H 2 formation rate coefficient, FUV dust absorption cross section, and metallicity.

As we discuss in Section 2.2.6, the H 1-to-H 2 transition profiles and the total atomic column densities are controlled by a single dimensionless parameter, “αG,” first introduced by S88. In a nutshell, αG determines the LW-band optical depth in the cloud due to the dust associated with the H 1 gas (which we refer to in this paper as “H 1-dust”), whether or not the H 1 is mixed with the H 2. The total H 1-dust optical depth is a critical quantity in the theory; for beamed fields our formula for it (as derived in Section 2.2.6) is

\[ \tau_{1,\text{tot}} = \ln \left[ \frac{\alpha G}{2} + 1 \right] . \]

As we show in Section 2.2.7, αG can be expressed in terms of the physical variables in several ways. Most simply, α (also dimensionless) is the ratio of the free-space photodissociation rate to the H 2 formation rate, and G is a cloud-averaged H 2 self-shielding factor. The product αG is then similar to the ionization parameter “U” for H 1 Strömgren regions, where U is proportional to the ratio of the photionization rate to the H 1 formation rate via electron–proton recombination. However, αG is also a measure of the dust absorption efficiency of the H 2-dissociating photons. For the H 1/H 2 density ratio in an optically thin “free-space” radiation field, αG is the ratio of the H 1-dust to H 2-line absorption rates of LW-band photons that are effectively available for H 2 dissociation. For sufficiently large metallicities, this excludes LW photons “between the lines” that are not effectively available for H 2 absorption. Because of this competition, a metallicity dependence is introduced into G and therefore also into our fundamental parameter αG.

An important physical distinction occurs between the limits of small and large αG (Section 2.2.8). Small αG is the...
“weak-field limit” for which H1-dust opacity is negligible and does not contribute to the absorption of the radiation, although a substantial (observable) atomic column can nevertheless exist in this limit. Large $\alpha G$ is the “strong-field limit” for which the atomic column becomes so large that H1-dust dominates the attenuation of the radiation fields, reducing the fraction of the incident radiation that is absorbed by the H2.

In general, $\alpha G$ is the dimensionless “free parameter” in the problem, with a value that is determined by local conditions (density, radiation intensity, metallicity, etc.). However, as invoked by KMT/MK10, on global scales in star-forming galaxy disks the gas density and radiation intensity may be correlated or self-regulated to conditions enabling a two-phase equilibrium between cold and warm H1 (CNM/WNM multiphase). As we describe in Section 2.2.9, this then drives $\alpha G$ to a narrow range, of order unity, intermediate between the weak- and strong-field limits, and only weakly dependent on the metallicity.

Finally, in Section 2.3 we extend our analysis to slabs exposed to isotropic radiation fields. An angular integration over all photodissociating ray directions is then also required in the computation of the H1 column densities. Our resulting analytic expressions for the atomic columns and associated H1-dust opacities are similar to those for beamed fields, with similar behavior in the weak- and strong-field limits. Our analytic results for slabs irradiated by isotropic fields enable a direct comparison to the KMT/MK10 results for spheres, as we discuss in depth in Section 4. In Section 3 we verify our analytic results with detailed numerical model computations.

2.1. Radiation Fields and H2 Photodissociation Rate

We will consider static, optically thick plane-parallel clouds (slabs) exposed to either isotropic or corresponding beamed LW-band radiation fields. We define the spectral range of the LW band as 912–1108 Å (11.3–13.6 eV) as appropriate for line absorptions occurring out of low-laying rotational levels in the ground vibrational state.

Let $F_{\nu}$ = $4\pi I_{\nu}$, where $I_{\nu}$ is the specific photon intensity (cm$^{-2}$ s$^{-1}$ Hz$^{-1}$ sr$^{-1}$) of an isotropic optically thin “free-space” LW radiation field. If an optically thick gas slab (or semi-infinite slab) is inserted, the flux density of the isotropic field at a cloud surface is equal to $\pi I_{\nu} = F_{\nu}/4$. The corresponding unidirectional beamed field is defined such the LW photons are normally incident on the cloud surface with flux density $2\pi I_{\nu} = F_{\nu}/2$. The surface flux of the isotropic field is half that of the corresponding beamed field, but the energy densities are equal. The energy densities at the cloud surfaces are half that in the (full $4\pi$) free-space radiation field.

In this paper we adopt the standard Draine (1978, 2011) expression

$$I_{\nu}^{\text{ISM}} = \frac{4\pi}{\lambda} \left( \frac{1.068 \times 10^{-3}}{\lambda} - \frac{1.719 \times 10^{6}}{\lambda^{2}} + \frac{6.853 \times 10^{2}}{\lambda^{3}} \right) \text{photons cm}^{-2} \text{Hz}^{-1} \text{sr}^{-1} \ (2)$$

for the specific intensity of the isotropic free-space FUV (5–13.6 eV FUV) radiation field in the Galactic ISM. In Equation (2), $\lambda$ is the photon wavelength in Angstroms. For this spectrum, the specific intensity varies by a factor of eight across the LW band. At 1000 Å, $I_{\nu}^{\text{ISM}} = 2.73 \times 10^{-9}$ photons s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ sr$^{-1}$, and the energy density $4\pi h\nu I_{\nu}/c = 6.8 \times 10^{-14}$ erg cm$^{-3}$ (where $\nu$ is the photon frequency in Hz). The total photon density in the 912–1108 Å LW band is $6.9 \times 10^{-4}$ cm$^{-3}$.

To consider radiation fields with greater or lesser intensities, we multiply by an overall field-strength scaling factor $I_{\text{UV}}$, such that $I_{\text{UV}} = 1$ corresponds to the unit free-space Draine field given by Equation (2). In this paper we do not consider radiation fields with alternate spectral shapes. For completeness we recall that the Draine energy density is 1.7 times larger than the Habing (1968) estimate for the LW energy density at 1000 Å.

For the free-space fields, we define the LW-band photon flux integral

$$F_{\nu} = \int_{v_{1}}^{v_{2}} F_{\nu} dv_{\nu} \ \ (3)$$

where $v_{1}$ to $v_{2}$ is the frequency range of the LW band and $F_{\nu} = 4\pi I_{\nu}^{\text{ISM}}$. For the Draine spectrum, $F_{\nu} = 3.4 \times 10^{-8} I_{\text{UV}}$ photons s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ at 1000 Å, and

$$F_{0} = 2.07 \times 10^{5} I_{\text{UV}} \text{ photons s}^{-1} \text{ cm}^{-2} \text{ s}^{-1}. \ (4)$$

At the cloud surfaces, the 1000 Å flux densities are then $F_{\nu}/4 = 8.6 \times 10^{-9} I_{\text{UV}}$ and $F_{\nu}/2 = 1.7 \times 10^{-8} I_{\text{UV}}$ photons s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ for the isotropic and corresponding beamed fields. The total LW-band surface fluxes are $F_{\nu}/4 = 5.18 \times 10^{-9} I_{\text{UV}}$ and $F_{\nu}/2 = 1.03 \times 10^{-8} I_{\text{UV}}$ photons cm$^{-2}$ s$^{-1}$. For a given $I_{\text{UV}}$, the energy densities of the isotropic and corresponding beamed fields are equal at the cloud surfaces.

The photodissociation of H2 occurs via line absorption of LW photons in allowed transitions from the ground electronic $X^1\Sigma_{g}^{\text{+}}$ state to the excited $B^{1}\Sigma_{u}^{\text{+}}$ or $C^{1}\Pi_{\text{v}}$ states. These are followed by rapid decays to either bound ro-vibrational levels or to the continuum of the ground X state. Decays to the continuum lead to dissociation (P. M. Solomon, private communication in Field et al. 1966; Stecher & Williams 1967; Stephens & Dalgarno 1972; Aggrall et al. 1992). The $B$–X and $C$–X bound–bound transitions are mainly to excited vibrational levels followed by a near-infrared quadrupole radiative cascade (Gould & Harwit 1963; Black & Dalgarno 1976; Shull 1978; Black & van Dishoeck 1987; S88; Sternberg & Dalgarno 1989; Draine & Bertoldi 1996; Neufeld & Spaans 1996). Thus, all of the LW-band photons absorbed by the H2 are removed, but only a fraction of these absorptions (~10%) lead to photodissociation.

The H2 photodissociation rate in the ISM is a fundamental quantity, and we recompute it in Section 3 by assuming the Draine spectrum for a range of assumed gas temperatures, densities, and field intensities. We find that for dissociation out of the 912–1108 Å LW band, the optically thin (full $4\pi$) free-space photodissociation rate is

$$D_{0} = 5.8 \times 10^{-11} I_{\text{UV}} \ \text{ s}^{-1}. \ (5)$$

---

4 We note that in the classical “PDR literature,” the FUV field strength is designated variously as $G_{0}$, $I_{\text{UV}}$, or $\chi$ (e.g., Hollenbach et al. 1971; van Dishoeck & Black 1986; Sternberg & Dalgarno 1989; Draine & Bertoldi 1996). In this paper we adopt $I_{\text{UV}}$ for the field strength to avoid confusion with the “$\alpha G$ factor” defined in Section 2.2.5 or with the KMT/MK10 “$\chi$,” which as we discuss in Section 4 is equivalent to our $\alpha G$ in the low-metallicity limit. The adopted normalizations can be confusing. For example, in the classic Tielens & Hollenbach (1985) paper, $G_{0} = 1$ refers to an FUV field for which the energy density at the surface of an optically thick cloud is equal to the energy density in the free-space (all $4\pi$) Habing (1968) field that is, $G_{0} = 0.5$ for an optically thick slab embedded in a unit (isotropic) Habing field. With our definitions, $I_{\text{UV}} = 1$ (not 0.5) for a cloud inserted into a unit isotropic Draine field with $I_{\nu} = I_{\nu}^{\text{ISM}}$ or for a cloud illuminated by a corresponding beamed field with surface flux density $F_{\nu} = 2\pi I_{\nu}^{\text{ISM}}$. For $I_{\text{UV}} = 1$, the H2 photodissociation rates at the cloud surfaces are equal to half the full $4\pi$ “free-space” rate in a unit Draine field (see also Equation (5)).
At a cloud surface the dissociation rate, \( D(0) \equiv D_0/2 \), is half the free-space rate and

\[
D(0) = 2.9 \times 10^{-11} I_{\text{UV}} \text{s}^{-1}.
\]  

Because the dissociation rate is proportional to the radiation energy density, the dissociation rates for isotropic and corresponding beamed fields are identical at a cloud surface.

The photodissociation rate diminishes with cloud depth due to the combination of H2-line and dust absorptions. The attenuation of the LW radiation field is crucial in determining the depth dependence of the atomic and molecular densities, the shapes of the H1-to-H2 transition profiles, and the resulting atomic hydrogen column densities. The depth-dependent attenuation depends on the assumed field geometry, and we analyze the behavior for both beamed and isotropic fields, starting with beamed fields which are simpler.

2.2. Beamed Fields

We consider the H1-to-H2 transition and total column density of atomic hydrogen on one side of an optically thick plane-parallel slab of gas (or semi-infinite slab) that is exposed to a steady flux of LW-band photons normally incident on the cloud surface as unidirectional beamed radiation.

2.2.1. Dissociation Bandwidth and Self-shielding Function

Let \( N_{2} \) be the H2 column density (cm\(^{-2}\)) at some depth normal to the cloud surface. Then, neglecting dust absorption of the LW photons, and for beamed radiation, the photodissociation rate (s\(^{-1}\)) for a single LW absorption line \( \ell \) may be written as

\[
D_{\ell}(N_{2}) = \frac{1}{2} \int_{0}^{\infty} F_{\ell} \sigma_{v,d} e^{-\sigma_{v,N_{2}}} dv = \frac{1}{2} F_{\ell} \frac{dW_{\ell,d}}{dN_{2}},
\]  

where

\[
W_{\ell,d}(N_{2}) \equiv \int_{0}^{\infty} \left[ 1 - \frac{\sigma_{v,d}}{\sigma_{v}} e^{-\sigma_{v,N_{2}}} \right] dv.
\]

In these expressions, \( F_{\ell} \approx 2 \pi \bar{T}_{\text{VIS}} I_{\text{UV}} \) is the incident beamed flux density (photons cm\(^{-2}\) s\(^{-1}\) Hz\(^{-1}\)) at the cloud surface, \( \sigma_{v,d} \) is the cross section (cm\(^2\)) for absorptions that lead to molecular dissociation,\(^5\) and \( \sigma_{v} \) is the cross section for all photon absorptions (not just those that are followed by dissociation). The dissociation probabilities, \( f_{\text{diss}} \equiv \sigma_{v,d}/\sigma_{v} \), range from \( \approx 0 \) to more than 0.5 for individual LW transitions depending on the rotational quantum number in the excited B or C states. The mean (typical) dissociation probability averaged over all lines is \( \langle f_{\text{diss}} \rangle \approx 0.12 \). For a single absorption line, \( \sigma_{v,d} \equiv \int \sigma_{v,d} dv = f_{\text{diss}} \frac{\pi e^{2}}{m_{e} c} f_{\text{osc}} \approx 2.7 \times 10^{-5} \text{ cm}^{2} \text{ Hz} \) for a typical LW-band oscillator strength of \( f_{\text{osc}} \approx 0.01 \) and dissociation probability of \( f_{\text{diss}} \approx 0.1 \) (and where \( e \) and \( m_{e} \) are the electron charge and mass, and \( c \) is the speed of light).

In Equation (7), we pull \( F_{\ell} \) out of the integral because we assume that the flux density varies very slowly over the narrow line profile (as represented by \( \sigma_{v} \)). In Equation (8), \( W_{\ell,d}(N_{2}) \) is defined as the “equivalent bandwidth” (Hz) of radiation absorbed in H2 dissociations via absorption line \( \ell \), up to molecular column \( N_{2} \). The dissociation rate \( D_{\ell}(N_{2}) \) decreases with the molecular column \( N_{2} \) as the absorption line become optically thick, and the ratio

\[
f_{\ell,\text{shield}}(N_{2}) \equiv \frac{D_{\ell}(N_{2})}{D_{\ell}(0)} = \frac{1}{\sigma_{d}} \frac{dW_{\ell,d}}{dN_{2}}
\]

is the individual H2-line “self-shielding” function. It quantifies the reduction of the line dissociation rate, where \( D_{\ell}(0) \) is the line dissociation rate at the cloud surface. By definition, the self-shielding function is proportional to the derivative of the dissociation bandwidth \( W_{\ell,d}(\text{Fedeman et al. 1979; van Dishoeck & Black 1986; SS8; Draine & Bertoldi 1996}) \).

For the full multiline LW-band system, the dissociation rate (again neglecting dust absorption) may be written compactly as

\[
D(N_{2}) = \frac{1}{2} \bar{F}_{\ell} \frac{dW_{d}}{dN_{2}},
\]

where \( W_{d}(N_{2}) \) is the equivalent dissociation bandwidth \( \text{summed} \) over all of the (possibly overlapping) absorption lines, and \( \bar{F}_{\ell} \) is a mean flux density. A plot of \( W_{d} \) versus \( N_{2} \) is the effective “curve of growth” for the dissociating LW radiation bandwidth in a dust-free cloud. We present computations for \( W_{d}(N_{2}) \) in Section 3 (the blue curve in Figure 3).

The mean flux density in Equation (11) is given by

\[
\bar{F}_{\ell} \equiv 4\pi \sum_{ij} I_{\nu_{ij}} x_{i} \sigma_{ij}^{d}/\sum_{ij} x_{i} \sigma_{ij}^{d}.
\]

Here \( x_{i} \) are the fractional populations of H2 molecules in ro-vibrational levels \( i \) of the ground electronic X state, \( I_{\nu_{ij}} \) is the (full \( 4\pi \)) free-space specific intensity at frequencies \( \nu_{ij} \) of LW-band transitions between levels \( i \) and \( j \) in the excited B or C states, and \( \sigma_{ij}^{d} \) are the absorption line dissociation cross sections (cm\(^2\) Hz). The mean flux density \( \bar{F}_{\ell} \) is weighted by the relative strengths of the dissociation transitions. For the Draine spectrum, \( \bar{F}_{\ell} = 2.46 \times 10^{-8} I_{\text{UV}} \) photons cm\(^{-2}\) s\(^{-1}\) Hz\(^{-1}\).

The denominator in expression (12) is the total (frequency integrated) H2 dissociation cross section (cm\(^2\) Hz) summed over all absorption lines,

\[
\sigma_{d}^{\text{tot}} \equiv \sum_{ij} x_{i} \sigma_{ij}^{d}.
\]

Most of the H2-line absorptions occur out of the lowest few rotational levels, and the total effective dissociation cross section is insensitive to the fractional populations \( x_{i} \). We find that

\[
\sigma_{d}^{\text{tot}} \approx 2.36 \times 10^{-5} \text{ cm}^{2} \text{ Hz}.
\]

The ratio \( \sigma_{d}^{\text{tot}}/\sigma_{d} \approx 80 \) is then the approximate number of strong LW absorption lines involved in the multiline H2 photodissociation process (see also Figure 2 in Section 3).

With these definitions, the free-space photodissociation rate may be expressed as

\[
D_{0} = \bar{F}_{\ell} \sigma_{d}^{\text{tot}}.
\]

At a cloud surface the photodissociation rate is \( D(0) \equiv D_{0}/2 = (1/2) \bar{F}_{\ell} \sigma_{d}^{\text{tot}} \). The ratio

\[
f_{\text{shield}}(N_{2}) \equiv \frac{D(N_{2})}{D(0)} = \frac{1}{\sigma_{d}} \frac{dW_{d}}{dN_{2}}
\]

\(^5\) In our notation, the subscript “d” refers to H2 photodissociation. Thus, \( \sigma_{v,d} \) is the cross section for line absorption followed by dissociation. The subscript “g” refers to dust grains. Thus, \( \sigma_{g} \) is the FUV dust grain absorption cross section (Section 2.2.2).
is then the complete multiline \( \text{H}_2 \) “self-shielding” function. It quantifies the reduction of the total dissociation rate due opacity in all of the absorption lines.

For a single line the self-shielding function varies as \( N_2^{-1/2} \) for large \( N_2 \) because absorptions can always occur far out on the Lorentzian damping wings.\(^6\) Therefore, for a single absorption line, \( W_{e,d} \) as given by Equation (8) diverges as \( N_2^{1/2} \). For strong lines (with \( f_{\text{osc}} \sim 0.01 \)), this “square root” part of the curve of growth begins when \( N_2 \gtrsim 10^{11} \text{ cm}^{-2} \). For the realistic multilinear system, the absorption lines will overlap for sufficiently large (\( \gtrsim 5 \times 10^{20} \text{ cm}^{-2} \)) molecular columns, and \( W_d \) does not diverge as does \( W_{e,d} \). For the multilinear system, the total dissociation bandwidth

\[
W_{d,\text{tot}} = \int_0^{\infty} \frac{dW_d}{dN_2} dN_2 \tag{17}
\]

is limited to a finite maximal value (even in the absence of dust). We find that for the Draine spectrum \( W_{d,\text{tot}} = 9.1 \times 10^{13} \text{ Hz} \) (as computed in Section 3.1.2). In Section 3.1.3 we present our computations for the multilinear self-shielding function (Figure 5). At the cloud surface, \( f_{\text{shield}} = 1 \). As the Doppler cores become optically thick at \( N_2 \gtrsim 10^{15} \text{ cm}^{-2} \), \( f_{\text{shield}} \) becomes small and the molecules are then said to self-shield against the dissociating radiation. The decline is more gradual at intermediate columns, \( 10^{17} \) to \( 10^{22} \text{ cm}^{-2} \), for which most of the absorption is out of the line wings. Finally, as line overlap occurs and the dissociating radiation is fully absorbed, \( f_{\text{shield}} \) becomes vanishingly small.

In the limit of complete line overlap, every photon in the (912–1108 Å) LW band is absorbed in \( \text{H}_2 \)-lines. The product \( (1/2)\bar{F}_v W_{d,\text{tot}} \) is then the LW “dissociation flux” (photons cm\(^{-2}\) s\(^{-1}\)) at the cloud surface. In the absence of dust absorption, this flux is equal to the \( \text{H}_2 \) dissociation rate per unit area. For complete absorption of the LW-band radiation, the mean dissociation probability is

\[
f_{\text{diss}} = \frac{\bar{F}_v W_{d,\text{tot}}}{F_0}, \tag{18}
\]

where \( F_0/2 \) is the total incident LW-band flux. For the radiative transfer computations we present in Section 3, we find that \( f_{\text{diss}} = 0.12 \) and is essentially equal to the simple average over the individual line dissociation probabilities for the matrix of \( X-B \) and \( X-C \) transitions. Our result for \( f_{\text{diss}} \) is consistent with many previous calculations (e.g., Black & van Dishoeck 1987; Draine & Bertoldi 1996; Browning et al. 2003).

2.2.2. Dust and Metallicity

In addition to the \( \text{H}_2 \)-line absorptions, the LW-band photons are also absorbed by dust grains, further reducing the photodissociation rate. We assume that the dust is mixed uniformly with the gas with a dust-to-gas mass ratio that depends linearly on the metallicity of the cloud. For the grain–photon interaction, we assume pure absorption and no scattering (or equivalently only forward scattering). With the inclusion of dust, the local dissociation rate, \( D \), at any cloud depth is then 

\[
D = \frac{1}{2} D_0 f_{\text{shield}}(N_2) e^{-\tau_g}, \tag{19}
\]

where \( D_0 \) is the free-space dissociation rate (Equation (5)). In this expression, \( \tau_g \equiv \sigma_g \bar{N} \) is the dust continuum optical depth, where \( \bar{N} \equiv N_1 + 2N_2 \) is the column density of hydrogen nuclei, in molecules plus atoms. Here \( \sigma_g \) is the dust grain LW-photon absorption cross section (cm\(^2\)) per hydrogen nucleus. With the inclusion of dust attenuation, the dissociation rate given by Equation (19) depends on both \( N_2 \) and the column density of atomic hydrogen \( N_1 \).

For simplicity we also assume that \( \sigma_g \) is independent of photon frequency over the narrow LW band. For a standard interstellar extinction curve, with a total-to-selective extinction ratio of \( R_V = A_V/E(B-V) = 3.1 \), a 1000 Å grain albedo \( \approx 0.3 \), and a scattering asymmetry factor \( \langle \cos \theta \rangle \approx 0.6 \), the effective absorption cross section per hydrogen nucleus \( \sigma_g = 1.9 \times 10^{-21} \text{ cm}^2 \) (Draine 2003); \( R_V = 3.1 \) is for diffuse gas (with densities \( n \sim 10^5 \text{ cm}^{-3} \)). For \( R_V = 3.1 \), \( A_V/N = 5.35 \times 10^{-22} \text{ mag cm}^2 \). In dense regions (\( n \gtrsim 10^6 \text{ cm}^{-3} \), \( R_V \) can be larger (up to \( \sim 5.8 \)) but with an extinction curve that is less steep toward the ultraviolet, with \( \sigma_g \approx 8 \times 10^{-22} \text{ cm}^2 \) (Cardelli et al. 1989; Fitzpatrick 1999; Draine & Bertoldi 1996; Draine 2011). With the assumption that the dust-to-gas mass ratio is linearly proportional to the metallicity \( Z \) of the gas, we therefore set

\[
\sigma_g = 1.9 \times 10^{-21} \bar{\phi}_g Z' \text{ cm}^2, \tag{20}
\]

where \( Z' = 1 \) corresponds to the solar photospheric abundances of the heavy elements (“solar metallicity”) and where \( \bar{\phi}_g \) of order unity depends on the grain composition and size distribution.

Dust grains are also essential for \( \text{H}_2 \) formation (Hollenbach et al. 1971; Jura 1974; Barlow & Silk 1976; Leitch-Devlin & Williams 1985; Pirronello et al. 1997; Takahashi et al. 1999; Cazaux & Tielens 2002; Habart et al. 2004). We assume that per hydrogen nucleon the rate coefficient for \( \text{H}_2 \) formation on grains is given by

\[
R = 3 \times 10^{-17} \left( \frac{T}{100 \text{ K}} \right)^{1/2} Z' \text{ cm}^3 \text{ s}^{-1}, \tag{21}
\]

where \( T \) is the gas temperature in \( \text{K} \). Our standard value is then \( R = 3 \times 10^{-17} \text{ cm}^3 \text{ s}^{-1} \) for \( T = 100 \text{ K} \) and \( Z' = 1 \).

2.2.3. \text{H} i/\text{H}_2 \text{ Formation–Destruction Equation}

For a steady state in which molecular photodissociation is balanced everywhere by grain surface \( \text{H}_2 \) formation, the \( \text{H} i/\text{H}_2 \) formation–destruction equation may be written as

\[
R n_1 = \frac{1}{2} \bar{F}_v \frac{dW_d}{dN_2} e^{-\tau_g} n_2 = \frac{1}{2} D_0 f_{\text{shield}}(N_2) e^{-\tau_g} n_2. \tag{22}
\]

In this equation, \( n_1 \) and \( n_2 \) are the local volume densities (cm\(^{-3}\)) of the \( \text{H} \) atoms and \( \text{H}_2 \) molecules, and

\[
n = n_1 + 2n_2 \tag{23}
\]

is the total volume density of hydrogen nuclei. The right-hand side of Equation (22) is the \( \text{H}_2 \) photodissociation rate per unit volume (s\(^{-1}\) cm\(^{-3}\)) at some cloud depth where the rate is reduced by the combined effects of self-shielding and dust attenuation. The left-hand side is the rate per unit volume of \( \text{H}_2 \) formation on dust grains. We ignore all other formation or destruction processes (such as formation in the gas phase or destruction by X-ray or cosmic-ray ionization).

Given the free parameters \( n, D_0 \) (or equivalently \( I_{\text{UV}} \)), \( R \), and \( \sigma_g \) (or given \( Z' \), which determines \( R \) and \( \sigma_g \)), Equation (22)
together with particle conservation Equation (23) can be solved for the local atomic and molecular densities \( n_1 \) and \( n_2 \) and for the integrated atomic and molecular columns \( N_1 \) and \( N_2 \). If it is assumed that the incident LW radiation is fully absorbed, then (as we show below) Equation (22) gives our fundamental formula for the total atomic column that is maintained in the cloud.

The density ratio \( n_1/n_2 = dN_1/dN_2 \), and Equation (22) may be written as the separable differential equation (S88; see also Jura 1974; Hill & Hollenbach 1978):

\[
Rn \int_0^{N_1} e^{\sigma_g N_1} dN_1' = \frac{1}{2} \tilde{F}_v \int_0^{N_1} dN_2' \int_0^{N_1} N_2' e^{-2\sigma_g N_2'} dN_2'.
\] (24)

In writing the formation–destruction equation this way, a key insight is that the dust opacities associated with the atomic and molecular columns can be considered separately. We will refer to \( "\text{H}_2\text{-dust}" \) or \( "\text{H}_1\text{-dust}" \) as the dust opacities associated with either just the \( \text{H}_2 \) or the \( \text{H}_1 \) gas, respectively, whether or not the \( \text{H}_1 \) gas is mixed with the \( \text{H}_2 \).

Integrating this expression and assuming that \( R \) and \( n \) are constants (i.e., do not vary with depth cloud width)

\[
Rn \int_0^{N_1} e^{\sigma_g N_1} dN_1' = \frac{1}{2} \tilde{F}_v \int_0^{N_1} N_2' e^{-2\sigma_g N_2'} dN_2',
\] (25)

which is a functional relationship, \( N_1(N_2) \), between the atomic and molecular column densities. We note that the independent variable parameterizing the cloud depth is here chosen to be \( N_2 \) rather than the total gas column density \( N \). Choosing \( N_2 \) as the independent variable is essential for our analysis, even though it is \( N \) that is proportional to the visual extinction \( A_V \), or to the length scale \( z \equiv N/n \).

### 2.2.4. H\(_2\)-dust-limited Dissociation Bandwidth

Most importantly, for a given value of \( \sigma_g \), the integral on the right-hand side of Equation (25),

\[
W_g(N_2) \equiv \int_0^{N_1} N_2' e^{-2\sigma_g N_2'} dN_2',
\] (26)

is a function of the molecular column \( N_2 \) only. This is because the exponential cutoff factor in the integrand is due to \( \text{H}_2\)-dust opacity only—it excludes \( \text{H}_1\)-dust—and because \( W_g \) itself depends only on \( N_2 \). Furthermore, \( W_g(N_2) \) is only very weakly dependent on \( n, R, \) or \( D_0 \) and is essentially independent of these parameters (see Section 3). So, for a given \( \sigma_g \), the effective equivalent width \( W_g(N_2) \) is a quantity that can be calculated in advance as a “universal dust-limited curve of growth” for the \( \text{H}_2\)-line absorption of LW radiation, independent of the other parameters, \( n, R, \) or \( D_0 \), that together with \( \sigma_g \) determine the depth-dependent \( \text{H}_1/\text{H}_2 \) density ratios and the \( \text{H}_1/\text{H}_2 \) transition profiles.

Thus, \( W_g(N_2) \) (as opposed to \( W_d[N_2] \)) is the effective bandwidth of dissociating LW radiation in a dusty \( \text{H}_2 \) cloud, where now this bandwidth is limited by \( \text{H}_2\)-dust absorption of LW photons that would otherwise be available for \( \text{H}_2 \) photodissociation in a dust-free cloud. \( \text{H}_2\)-dust opacity is important if it becomes large before the \( \text{H}_2 \) absorption lines can fully overlap.

For sufficiently small \( \sigma_g \), the lines do overlap completely, and then \( W_g(N_2) = W_d(N_2) \) for sufficiently large \( \sigma_g \), the \( \text{H}_2\)-dust provides a cutoff, and then \( W_g(N_2) < W_d(N_2) \) at large \( N_2 \).

It is a remarkable physical coincidence that the \( \text{H}_2 \) column density at which the \( \text{H}_2 \)-lines begin to overlap—a column that depends on the internal molecular oscillator strengths and energy level spacings—is comparable to the \( \text{H}_2 \) column at which the \( \text{H}_2\)-dust opacity \( 2N_2\sigma_g \geq 1 \) for standard interstellar dust absorption cross sections. Thus, both regimes of “small \( \sigma_g \)” and “large \( \sigma_g \)” for the dissociation bandwidth \( W_g(N_2) \) are relevant for the range of interstellar dust properties and metallicities in galaxies. In Section 3.1.2, we present computations of \( W_g(N_2) \) for a wide range of \( \sigma_g \) encompassing these regimes.

As \( N_2 \to \infty \), the equivalent width \( W_g(N_2) \) converges to a finite limit

\[
W_g,\text{tot}(\sigma_g) \equiv \int_0^{\infty} dN_2 e^{-2\sigma_g N_2} dN_2,
\] (27)

either because the exponential \( \text{H}_2\)-dust attenuation factor cuts off the integral (for large \( \sigma_g \)) or because \( dW_d/dN_2 \) itself vanishes as the lines overlap (for small \( \sigma_g \)). Thus, \( W_g,\text{tot}(\sigma_g) \) is the total \( \text{H}_2\)-dust-limited effective dissociation bandwidth. For large \( \sigma_g \), \( W_{g,\text{tot}} < W_d,\text{tot} \), and for small \( \sigma_g \), \( W_{g,\text{tot}} = W_d,\text{tot} \). For large \( \sigma_g \), the absorption lines remain separated but are nevertheless highly damped for most of the integration range up to the \( \text{H}_2\)-dust cutoff.

For a single absorption line, \( dW_d/dN_2 \propto N_2^{-1/2} \) in the damped regime, and it follows from Equation (27) that \( W_{g,\text{tot}}(\sigma_g) \) scales as \( \sigma_g^{-1/2} \). Our numerical computations (Section 3.1.2) show that for large \( \sigma_g \) this scaling behavior is maintained in the full multiline problem to a good approximation. In Section 3, we find that the simple formula

\[
W_{g,\text{tot}}(\sigma_g) \approx \frac{9.9 \times 10^{13}}{1 + (\sigma_g/7.2 \times 10^{-22} \text{ cm}^2)^{1/2}} \text{ Hz}
\] (28)

is an excellent fit to our numerical radiative transfer results. The normalized \( \text{H}_2\)-dust-limited dissociation bandwidth

\[
w \equiv \frac{W_{g,\text{tot}}}{W_{d,\text{tot}}} \approx \frac{1}{1 + (\sigma_g/7.2 \times 10^{-22} \text{ cm}^2)^{1/2}} = \frac{1}{1 + (2.64\phi_Z Z')^{1/2}},
\] (29)

where in the last equality we have assumed \( \sigma_g = 1.9 \times 10^{-21} \phi_Z Z' \) (Equation (20)). In these expressions, \( W_{g,\text{tot}} \to W_{d,\text{tot}} \) and \( w \to 1 \) for small \( \sigma_g \) (low metallicity) and decrease as \( \sigma_g^{-1/2} \) for large \( \sigma_g \) (high metallicity). The normalized bandwidth \( w \) decreases from 0.9 to 0.2 for \( \sigma_g \) ranging from \( 1 \times 10^{-23} \text{ cm}^{-2} \) (small) to \( 6 \times 10^{-21} \text{ cm}^{-2} \) (large) or \( Z' \) ranging from \( 0.01 \) to 3 (assuming \( \sigma_g \propto Z' \)), which is the relevant range for galaxies.

### 2.2.5. Effective Dissociation Flux and Dissociation Probability

Given Equation (18), we may now write

\[
\tilde{F}_v W_{g,\text{tot}} = w \tilde{F}_{\text{diss}} F_0,
\] (30)

and define the effective dissociation probability

\[
\tilde{p}_{\text{diss}} \equiv \frac{\tilde{F}_v W_{g,\text{tot}}}{F_0} \equiv w \tilde{F}_{\text{diss}}.
\] (31)

The product \((1/2)\tilde{F}_v W_{g,\text{tot}}\) is the “effective dissociation flux” for dusty clouds in which \( \text{H}_2\)-dust may absorb some of the incident LW radiation. The effective dissociation flux depends
on the competition between H$_2$-line absorption and H$_2$-dust absorption as given by the dependence of $W_{g,tot}$ on $\sigma_g$. The effective dissociation flux is the H$_2$ photodissociation rate per unit surface area for a dusty and optically thick molecular slab in which H$_1$-dust opacity is negligible.

When H$_2$-dust is negligible, $w = 1$ and $\bar{f}_{diss} = \bar{f}_{diss}$. When H$_2$-dust opacity is significant, $w < 1$ and $\bar{f}_{diss} < \bar{f}_{diss}$. The effective dissociation probability $\bar{f}_{diss}$ is the fraction of the total 912–1108 Å LW-band flux that is absorbed in H$_2$ photodissociation events in a dusty, optically thick, predominantly molecular slab (with vanishing H$_1$-dust opacity). For low $Z'$, $\bar{f}_{diss}$ is 0.12 is a constant. For high $Z'$, $\bar{f}_{diss}$ decreases as $Z'^{-1/2}$.

2.2.6. Formula for the H$_1$ Column Density

Returning now to Equation (25), it follows that

$$ Rn \int_0^{N_1} e^{\tau_g N_1} dN_1 = \frac{1}{\sigma_g} Rn [e^{\tau_g N_1} - 1] = \frac{1}{2} \bar{F}_g W_g(N_2) $$

or

$$ N_1(N_2) = \frac{1}{\sigma_g} \ln \left[ \frac{1}{2} \frac{\bar{F}_g W_g(N_2)}{Rn} + 1 \right]. $$

(32)

Following S88, we now define the dimensionless parameter

$$ \alpha \equiv \frac{D_0}{Rn} = \frac{\sigma_g f_{diss} \bar{F}_g}{Rn}, $$

(34)

where $D_0$ is the free-space dissociation rate, $G$ and we define the dimensionless “G integral”

$$ G(N_2) \equiv \sigma_g \int_0^{N_2} f_{shield}(N_2) e^{-2\tau_g N_2} dN_2 = \frac{\sigma_g}{\sigma_g f_{tot}} W_g(N_2). $$

We can then write

$$ N_1(N_2) = \frac{1}{\sigma_g} \ln \left[ \frac{\alpha G(N_2)}{2} + 1 \right]. $$

(35)

where

$$ \alpha G(N_2) = \frac{\sigma_g f_{diss} \bar{F}_g W_g(N_2)}{Rn}. $$

(36)

Given the “universal” dust-limited curve of growth $W_g(N_2)$, which can be computed “in advance” for any $\sigma_g$, the atomic column is then given by Equation (35) (or Equation (33)) for any surface dissociation rate $D_0$ (or $I_{UV}$), rate coefficient $R$, and density $n$.

We refer to Equation (35) as the “semi-analytic integral H$_1$-to-H$_2$ profile.” It shows that the H$_1$ column at any depth depends only on two quantities—$\sigma_g$ and $\alpha G(N_2)$. In dimensionless form

$$ \tau_1(\tau_2) = \ln \left[ \frac{\alpha G(N_2)}{2} + 1 \right]. $$

(37)

where $\tau_2 = 2\sigma_g N_2$ is the dust optical depth associated with the molecular column, and $\tau_1(\tau_2) \equiv \sigma_g N_1$ is the H$_1$-dust optical depth at $\tau_2$.

As $N_2 \to \infty$, $W_g(N_2) \to W_{g,tot}$. The total atomic column density is therefore finite and is given by

$$ N_1(tot) = \frac{1}{\sigma_g} \ln \left[ \frac{1}{2} \frac{\bar{F}_g W_{g,tot}}{Rn} + 1 \right] = \frac{1}{\sigma_g} \ln \left[ \frac{1}{2} \frac{\bar{f}_{diss} \bar{F}_g W_{g,tot}}{Rn} + 1 \right]. $$

(39)

or

$$ N_1(tot) = \frac{1}{\sigma_g} \ln \left[ \frac{\alpha G}{2} + 1 \right]. $$

(40)

Here the dimensionless parameter

$$ G(\sigma_g) \equiv \frac{\sigma_g}{\sigma_g f_{diss}} W_{g,tot}(\sigma_g) $$

(41)

is the limit of $G(N_2)$ as $N_2 \to \infty$, so that

$$ \alpha G = \frac{D_0 G}{Rn} = \frac{\sigma_g f_{diss} \bar{F}_g W_{g,tot}}{Rn} = \bar{f}_{diss} \frac{\sigma_g w F_0}{Rn}. $$

(42)

We discuss these and additional expressions for $\alpha G$ in Section 2.2.6 below.

Equation (40) for the total H$_1$ column on one side of an optically thick cloud was first derived by S88 (see Equation (9) of that paper), and it is the fundamental relation in our analysis.

The basic assumption is that all of the dissociating LW-band radiation is absorbed, as in a classical “ionization-bounded” H$_1$ region or layer (Str"omgren 1939). However, because of the three-way competition between H$_1$-dust, H$_2$-dust, and H$_2$-lines, the behavior for H$_1$ is more complicated than for H$_1$. For a steady (dust-free) photoionized planar Str"omgren layer, the H$_1$ column equals the ratio of the Lyman continuum flux to the recombination rate, independent of the photoionization cross section. Similarly, in our Equation (39) or Equation (40), the H$_2$-line absorption cross section does not appear explicitly (although it is implicit in our definition of the effective dissociation flux).

The H$_1$ column depends on the ratio of the effective dissociation flux to the H$_2$ formation rate, but this ratio is multiplied by the dust absorption cross section and appears inside a logarithm. We discuss this behavior, and the connection to Str"omgren relations, in our description of the weak- and strong-field limits in Section 2.2.8.

In dimensionless form, the total H$_1$-dust optical depth associated with the total atomic column is

$$ \tau_{1,tot} = \ln \left[ \frac{\alpha G}{2} + 1 \right]. $$

(43)

The total H$_1$-dust optical depth depends on the single dimensionless parameter $\alpha G$ constructed from the cloud variables $D_0$ (or $F_0$ or $I_{UV}$), $n$, $R$, and $\sigma_g$ (or $Z'$, which determines $R$ and $\sigma_g$).

The total gas column $N \equiv N_1(N_2) + 2N_2$. It therefore follows from Equation (35) that the atomic column as a function of the total (atomic plus molecular) column, $N_1(N_2)$, also depends on just $\sigma_g$ and $\alpha G$. Similarly, for $\tau_2 \equiv \sigma_g N_1$, the H$_1$-dust optical depth $\tau_1(\tau_2)$ depends on the single dimensionless parameter $\alpha G$.

Then, since $n_1/n_2 = dN_1/dN_2$ if it follows that the shapes of the H$_1$-to-H$_2$ transition profiles are invariant for identical $\alpha G$. That is, the density fractions $n_1/n$ and $2n_2/n$ expressed as functions

---

* The main goal and result of S88 was an analytic formula for the intensity of UV excited (fluorescent) IR H$_2$ emission lines from PDRs. Because the FUV-pumped H$_2$ vibrational excitation rate is proportional to the dissociation rate, the IR intensity is proportional to the H$_1$ column density, as expressed in Equation (10) of that paper.
of the dust optical depth $\tau_d$ (or visual extinction $A_V$) depend on just the single dimensionless parameter $\alpha G$.

In Section 3.1.4 we present detailed numerical computations for the H I-to-H$_2$ transition profiles. We show that the transitions are “gradual” when $\alpha G < 1$ and are “sharp” when $\alpha G > 1$. An essential feature of our derivation and analytic expression for the total H$_2$ column is that no assumptions need to be made on the shape of the H I-to-H$_2$ transition profile. Our Equation (39) or Equation (40) are universally valid for all profile shapes, gradual or sharp.

2.2.7. $\alpha G$

It is useful to consider the physical meaning of the dimensionless parameters $\alpha$ and $G$ and their product $\alpha G$.

First, $\alpha$ is the ratio of the unattenuated free-space H$_2$ photodissociation rate to the H$_2$ formation rate and can be expressed as

$$\alpha = 1.93 \times 10^4 \left( \frac{D_0}{5.8 \times 10^{-11} \text{ s}^{-1}} \right) \left( \frac{3 \times 10^{-17} \text{ cm}^3 \text{ s}^{-1}}{R} \right) \times \left( \frac{100 \text{ cm}^{-3}}{n} \right).$$

Thus, $\alpha$ is just the free-space atomic-to-molecular density ratio $n_1/n_2$, and $\alpha/2$ is the density ratio at the surface of an optically thick slab. The characteristic interstellar cloud gas density $n \sim 10^2 \text{ cm}^{-3}$, and with $D_0 = 5.8 \times 10^{-11} \text{ I}_{\text{UV}} \text{ s}^{-1}$, the atomic-to-molecular density ratio is $n_1/n_2 \gg 1$ at the cloud edge in the absence of shielding, unless $\text{I}_{\text{UV}}$ is unrealistically small. Conversion to the molecular phase in the ISM generally requires significant attenuation of the ambient and destructive radiation fields.

Now consider the parameter $G$. Defining the H$_2$ dust opacity $\tau_2 = 2\sigma_g N_2$ (see Equation (35)),

$$G \equiv \frac{1}{2} \int_{0}^{\infty} f_{\text{shield}}(\tau_2) e^{-\tau_2} d\tau_2 = \frac{1}{2} \left( f_{\text{shield}} \right) \int_{0}^{1} f_{\text{shield}}(\tau_2) d\tau_2.$$

Thus, $G$ is the average H$_2$ self-shielding factor. The average is over an H$_2$ column for which the H$_2$ dust opacity $\tau_2 \approx 1$. Thus, $(1/2)D_0G$ is the characteristic photodissociation rate for self-shielded H$_2$ in a fully molecular cloud, prior to the onset of any H$_2$-dust attenuation. Because $f_{\text{shield}}$ is already $\ll 1$ for $\tau_2 \ll 1$, the H$_2$ molecules are very self-shielded for an H$_2$-dust opacity $\tau_2 \sim 1$, and $G$ is generally very small.

The product $\alpha G/2 = (1/2)D_0G/Rn$ is then the atomic-to-molecular density ratio $n_1/n_2$ for the average shielded H$_2$ dissociation rate. This is our first interpretation for $\alpha G$ (and as adopted in S88). If $n_1 > 2n_2$ for the shielded dissociation rate, then H I-dust must also contribute to the attenuation of the LW radiation since then $\tau_1 > \tau_2$ within the H$_2$-dust attenuation column. If $n_1 < 2n_2$, then H I-dust attenuation is negligible.

Alternatively, $G \equiv \sigma_g W_{g,\text{tot}}/\sigma_d$ (Equation (41)) is the ratio of the UV continuum dust absorption cross section (cm$^2$) to the total H$_2$-line dissociation cross section (cm$^2$ Hz) averaged over the effective dissociation bandwidth (Hz). Again, $G$ is generally very small because H$_2$-line absorption is so much more efficient than dust absorption. Given $\sigma_g = 1.9 \times 10^{-21} \phi_e \text{ Z} \text{ cm}^2$ (Equation (20)) and our expression (28) for $W_{g,\text{tot}}$, and with $\sigma_d^{\text{tot}} = 2.36 \times 10^{-3} \text{ cm}^2 \text{ Hz}$, we have

$$G \approx \frac{7.97 \times 10^{-5} \phi_e Z}{1 + (2.64 \phi_e \text{ Z})^{1/2}}.$$  

For example, for standard values $Z' = 1$ and $\phi_e = 1$, Equation (46) gives $G = 3.0 \times 10^{-5}$ and the shielded H$_2$ dissociation rate $(1/2)D_0G = 8.7 \times 10^{-16} \text{ I}_{\text{UV}} \text{ s}^{-1}$. For low metallicity, small $\sigma_g$, it follows that $G \propto Z'$ (or $G \propto \sigma_g$). For high metallicity, large $\sigma_g$, $G \propto Z'^{1/2}$ (or $G \propto \alpha G$).

Since $\alpha$ is the free-space atomic-to-molecular density ratio, we have

$$\alpha G = \frac{\sigma_g W_{g,\text{tot}}}{\sigma_d} \frac{n_1}{n_2} \text{ freespace}$$

$$= \frac{\sigma_g \tilde{F}_n W_{g,\text{tot}}}{D_0 n_2} \text{ freespace}$$

$$= \frac{\tilde{f}_{\text{diss}} w F_0 \sigma_g n_1}{D_0 n_2} \text{ freespace},$$

where in the second and third equalities we have used the relations $D_0 \equiv \sigma_d^{\text{tot}} \tilde{F}_n$ and $W_{g,\text{tot}} \equiv \tilde{f}_{\text{diss}} w F_0$. This gives our second interpretation for $\alpha G$. It is the free-space ratio of the H I-dust to H$_2$-line absorption rates of LW photons in the H$_2$-dust-limited dissociation band.

Third, since $D_0 G = \tilde{f}_{\text{diss}} w \tilde{F}_n \sigma_g$ (and $\tilde{p}_{\text{diss}} \equiv w \tilde{f}_{\text{diss}}$), we have

$$\alpha G = \frac{\tilde{f}_{\text{diss}} w \tilde{F}_n}{\tilde{p}_{\text{diss}} Rn} \equiv \frac{\tilde{f}_{\text{diss}} w F_0}{\tilde{p}_{\text{diss}} Rn}.$$  

Thus, $\alpha G$ is the free-space ratio of the dust absorption rate of the effective dissociation flux—per hydrogen atom—to the molecular formation rate per atom.

When $\alpha G \ll 1$, H I-dust plays no role anywhere in the cloud, since it is negligible even for the free-space field where the atomic density is largest. However, when $\alpha G \gg 1$, H I-dust becomes important and absorbs an increasing fraction of the LW photons that are otherwise available for H$_2$ photodissociation.

Thus, with Equations (44) and (46),

$$\alpha G = 1.54 \left( \frac{D_0}{5.8 \times 10^{-11} \text{ s}^{-1}} \right) \left( \frac{3 \times 10^{-17} \text{ cm}^3 \text{ s}^{-1}}{R} \right) \times \left( \frac{100 \text{ cm}^{-3}}{n} \right) \frac{\phi_e Z'}{1 + (2.64 \phi_e \text{ Z}')^{1/2}},$$

or with Equation (48),

$$\alpha G = 1.54 \left( \frac{1.9 \times 10^{-21} \text{ cm}^2}{\sigma_g} \right) \left( \frac{2.07 \times 10^2 \text{ cm}^{-2} \text{ s}^{-1}}{R} \right) \times \left( \frac{3 \times 10^{-17} \text{ cm}^3 \text{ s}^{-1}}{100 \text{ cm}^{-3}} \right) \frac{1}{n} \frac{\phi_e Z'}{1 + (2.64 \phi_e \text{ Z}')^{1/2}}.$$  

With Equation (4) or Equation (5) for $F_0$ or $D_0$, and Equations (20) and (21) for $\sigma_g$ and $R$, we then have

$$\alpha G = 1.54 \frac{I_{\text{UV}}}{(n/100 \text{ cm}^{-3})} \frac{\phi_e}{1 + (2.64 \phi_e \text{ Z}')^{1/2}}.$$
For $\sigma_g$ and $R$ varying the same way with $Z'$ there is a cancellation, but a metallicity dependence still remains via the dissociation bandwidth $u$ (Equation (29)) and its dependence on the competition between $H_2$-dust absorption and $H_2$-line absorption. For low $Z'$ (complete line overlap limit, $w = 1$), $\alpha G$ is independent of the metallicity, but for high $Z'$, $w \sim \sigma_g^{-1/2}$ and $\alpha G \sim Z'^{-1/2}$.

2.2.8. Weak- and Strong-field Limits

Expression (51) also shows that the regimes of large and small $\alpha G$ are both relevant for the widely varying conditions in localized environments of the ISM in galaxies. For example, $I_{UV}$ can range from $\sim 1$ at “average” locations to $\gtrsim 10^5$ near hot stars, whereas $n$ can range from $\sim 10$ cm$^{-3}$ in diffuse gas to $\gtrsim 10^6$ cm$^{-3}$ in dense molecular clouds. On global scales in star-forming galaxy disks, $I_{UV}$ and $n$ may be correlated (see Section 2.2.9). But on small scales, enhanced radiation fields will not necessarily be offset by higher gas densities, and $I_{UV}/n$ may span a wide range from “large” to “small.”

For $\alpha G/2 \ll 1$ the absorption of the LW radiation is dominated by the combination of $H_2$-line absorption and $H_2$-dust absorption, and $H_1$-dust is negligible. For $\alpha G/2 \gg 1$ $H_1$-dust absorption dominates the attenuation of the radiation field. We refer to $\alpha G/2 \ll 1$ as the “weak-field limit” and to $\alpha G/2 \gg 1$ as the “strong-field limit.”

We now consider the behavior of $N_{1,\text{tot}}$ in these two limits. It follows from Equations (40) and (39) that for $\alpha G/2 \ll 1$,

$$N_{1,\text{tot}} = \frac{1}{\sigma_g} \frac{\alpha G}{2} = \frac{1}{2 \sigma_g} \frac{D_0}{R_n} \frac{G}{G} = \frac{1}{2 \sigma_g} \frac{\dot{F}_v}{R_n} \frac{W_{g,\text{tot}}}{R_n} = \frac{1}{2} \frac{\dot{F}_v}{R_n} \frac{wF_0}{R_n}.$$

(52)

So for weak fields, the total $H_1$ column density is equal to the ratio of the effective LW dissociation flux to the $H_2$ formation rate (which is the removal rate of the $H_1$). The atomic column is proportional to the surface dissociation rate $D_0$ (or to the field strength $I_{UV}$) and inversely proportional to the cloud gas density $n$.

In the weak-field limit, the $H_1$-dust opacity associated with the total atomic column $\sigma_gN_{1,\text{tot}} \ll 1$. We again see that $H_1$-dust plays no role in attenuating the LW radiation field in this limit. For weak fields, the total $H_1$ column depends on $\sigma_g$ only via $W_{g,\text{tot}}$, through the possible competition between $H_2$-line absorption and $H_2$-dust absorption. For small $\sigma_g$ where $H_2$-dust is negligible, dust absorption plays no role whatsoever, and $N_{1,\text{tot}}$ is completely independent of $\sigma_g$. In the small-$\sigma_g$ limit, $G \propto \sigma_g$, and the dust absorption cross section cancels out completely. For $R \propto Z'$, we then have $N_{1,\text{tot}} \propto 1/Z'$, and the metallicity dependence enters entirely via the $H_2$ formation rate coefficient. For large $\sigma_g$, $H_2$-dust absorption is non-negligible, and $W_{g,\text{tot}} \propto \sigma_g^{-1/2}$ (and $G \propto \sigma_g^{1/2}$), thus $N_{1,\text{tot}}$ scales as $\sigma_g^{-1/2}$. Then with $\sigma_g \propto Z'$ and $R \propto Z'$, we have $N_{1,\text{tot}} \propto Z'^{-3/2}$.

Expression (52) can be written as the simple “Strömgren relation”

$$RnN_{1,\text{tot}} = \frac{1}{2} \dot{F}_v W_{g,\text{tot}}.$$

(53)

The effective dissociation flux on the right-hand side is the rate per unit area at which dissociating photons (those absorbed in $H_2$-lines but not by $H_2$-dust) penetrate the cloud surface. By definition these photons are fully absorbed by the $H_2$ when $H_1$-dust is negligible, so this is also the photodissociation rate per unit surface area. In steady state this must equal the total $H_2$ formation rate per unit area, which is the left-hand side.

For the strong-field limit $\alpha G/2 \gg 1$, it follows from Equation (40) that

$$N_{1,\text{tot}} = \frac{1}{\sigma_g} \ln \left[ \frac{\alpha G}{2} \right] = \frac{1}{\sigma_g} \ln \left[ \frac{1}{2} \frac{D_0G}{R_n} \right]$$

$$= \frac{1}{\sigma_g} \ln \left[ \frac{1}{2} \frac{\dot{F}_v W_{g,\text{tot}}}{R_n} \right] = \frac{1}{\sigma_g} \ln \left[ \frac{1}{2} \frac{\dot{F}_\text{diss} \sigma_g wF_0}{R_n} \right].$$

(54)

For strong fields, $\tau_{1,\text{tot}} = \sigma_gN_{1,\text{tot}} \gtrsim 1$, and the $H_1$-dust opacity associated with the total atomic column contributes significantly to the attenuation of the incident LW flux. This leads to a saturation and logarithmic dependence of the atomic column on the cloud parameters. For example, increasing the atomic column by increasing the LW-band flux also leads to more effective absorption of the LW photons by the larger $H_1$-dust column. A decreasing fraction of the LW photons is then absorbed by the $H_2$, and the growth of the atomic column is limited. Similarly, increasing the $H_2$ formation rate reduces the atomic column, but the $H_1$-dust opacity is then also reduced, which increases the LW fraction available for photodissociation, thereby moderating the reduction of the $H_1$ column.

If we neglect the logarithmic factor, then up to a factor of order unity, we have

$$N_{1,\text{tot}} \approx 1/\sigma_g$$

(55)

for intense fields. Indeed, if the attenuation is dominated by $H_1$-dust, the atomic column must approach a value such that $\tau_{1,\text{tot}} = \sigma_gN_{1,\text{tot}} \gtrsim 1$. Then, if $\sigma_g \propto Z'$ the $H_1$ column $N_{1,\text{tot}} \propto 1/Z'$ (neglecting the logarithmic factor). In the strong-field limit, the metallicity dependence enters via the grain absorption cross section.

Finally, Equation (54) for the strong-field limit may also be expressed as the Strömgren relation

$$RnN_{1,\text{tot}} = \frac{1}{2} \dot{F}_v W_{g,\text{tot}} u.$$

(56)

Here

$$u \equiv \tau_{1,\text{tot}} e^{-\tau_{1,\text{tot}}}$$

(57)

is a reduction factor that accounts for $H_1$-dust attenuation of the effective dissociation flux. The right-hand side of Equation (56), including the factor $u$, is the $H_2$ photodissociation rate per unit surface area, and this equals the total $H_2$ formation rate per unit area, which is the left-hand side.

9 This limit is often referred to in the literature as the “self-shielding” limit. However, this is potentially confusing if self-shielding is properly understood to be associated with just $H_2$-line absorption. As we have emphasized, $H_2$-dust also absorbs and cannot be ignored for small $\alpha G$, unless the metallicity is very low. So the weak-field limit may be referred to as the “$H_2$-line plus $H_2$-dust” shielding limit.

10 This is analogous to the Strömgren expression, $\sigma_g n_e N_{H^+} = F_{1\nu c}$, for the column density, $N_{H^+}$, of ionized hydrogen in a slab that fully absorbs a flux, $F_{1\nu c}$, of Lyman continuum photons. Here $n_e$ is the electron density, and $\sigma_g$ is the electron–proton recombination coefficient.

11 To see this, note that $e^{-\tau_{1,\text{tot}}} = 1/\sigma_g$ when $\alpha G \gg 1$. 
Galaxy disks may be self-regulated such that the thermal pressures in the H\textsc{i} gas enable a cold/warm (CNM/WMN) two-phased mixture, with cold neutral H\textsc{i} (CNM) accumulating in the UV illuminated PDRs of the star-forming molecular clouds (Ostriker et al. 2010; Faucher-Giguère et al. 2013; Kim et al. 2013). As invoked by KMT\textit{i} for self-regulated systems, independent of \( Z' \). The expected H\textsc{i}/H\textsubscript{2} formation–destruction equation at a molecular column \( N_{2} \) normal to the cloud surface may be written as

\[
D(N_{2}) = \frac{D_{0}}{2} \int_{0}^{1} f_{\text{shield}}(N_{2}/\mu) \, d\mu = 2\pi \bar{I}_{\nu} \int_{0}^{1} \frac{dW_{g}(N_{2}/\mu)}{dN_{2}} \, \mu \, d\mu, 
\]

where \( f_{\text{shield}}(N_{2}) \) is the unidirectional self-shielding function defined by Equation (16), and \( W_{g}(N_{2}) \) is the same effective "multi-line" curve of growth for the (dust-free) dissociating bandwidth that appears in Equation (11) for beamed fields. In Equation (61), the contribution to the angular-integrated dissociation rate is reduced by the self-shielding factor \( f_{\text{shield}}(N_{2}/\mu) \) along each ray. Here \( \bar{I}_{\nu} \equiv \bar{F}_{\nu}/4\pi \) is the free-space specific intensity averaged over the dissociating transitions, as given by Equation (12).

With the inclusion of dust absorption along each ray, the H\textsc{i}/H\textsubscript{2} formation–destruction equation at a molecular column \( N_{2} \) is

\[
Rn \, dN_{1} = 2\pi \bar{I}_{\nu} \int_{0}^{1} \frac{dW_{d}(N_{2}/\mu)}{dN_{2}} \, e^{-2\sigma_{g}N_{2}/\mu} \, e^{-\sigma_{d}N_{1}/\mu} \, d\mu \, dN_{2}. 
\]

Like Equation (24) for beamed fields, this is a differential equation for \( N_{1}(N_{2}) \). However, because of the angular integration, the exponential term \( \exp(-\sigma_{d}N_{1}/\mu) \) for the H\textsubscript{2}-dust attenuation along a ray cannot be moved to the left-hand side as was done in Equation (24). To enable a separation of variables nevertheless, we replace the variable \( \mu \) with some constant average \( \langle \mu \rangle \) in the H\textsc{i}-dust term, and we then move this term to the left-hand side. For H\textsubscript{2}-dust attenuation on the right-hand side, we keep \( \mu \) as a variable in the exponential term.

Making this approximation and integrating over the atomic and molecular columns gives

\[
Rn \int_{0}^{N_{1,\text{tot}}} e^{\langle \sigma_{d}N_{1}/\langle \mu \rangle \rangle} \, dN_{1}' = 2\pi \bar{I}_{\nu} W_{g,\text{tot}} \int_{0}^{\infty} \mu d\mu = \frac{1}{4} \bar{F}_{\nu} W_{g,\text{tot}}, 
\]

where

\[
W_{g,\text{tot}} \equiv \int_{0}^{\infty} \mu \frac{dW_{d}(N_{2}/\mu)}{dN_{2}} \, e^{-2\sigma_{g}N_{2}/\mu} \, d\left(\frac{N_{2}}{\mu}\right). 
\]
that appears here is the same effective total H₂-dust-limited dissociation bandwidth that we defined for beamed radiation in Equation (27) (and represented analytically by Equation (28)). The effective bandwidths are identical for isotropic and beamed fields because the relative fractions of LW photons absorbed by H₂-lines versus H₂-dust along a ray do not depend on the ray’s orientation. The product \( \tilde{F}_\nu W_{g,\text{tot}}/4 \) is then the effective dissociating flux for the isotropic field. It follows from Equation (63) that the total H1 column is given by

\[
N_{1,\text{tot}} = \langle \mu \rangle \sigma_g \ln \left( \frac{1}{\langle \mu \rangle} \frac{\sigma_g \tilde{F}_\nu W_{g,\text{tot}}}{Rn} + 1 \right)
\]

or

\[
N_{1,\text{tot}} = \frac{\langle \mu \rangle}{\sigma_g} \ln \left( \frac{1}{\langle \mu \rangle} \frac{\alpha G}{4} + 1 \right).
\]

Equations (65), (66), and (67) for isotropic fields are very similar to Equations (39), (40), and (43) for beamed fields. The values of \( \alpha \) are equal for corresponding beamed and isotropic fields (i.e., fields with the same \( I_{\text{UV}} \)). Furthermore, \( G \) is independent of the field geometry. A geometrical factor of 1/4 appears for slabs irradiated by isotropic fields (as opposed to 1/2 for beamed fields).

The average angle \( \langle \mu \rangle \) appears in Equations (65), (66), and (67) because the radiation fraction absorbed by H₂-dust does depend on the field geometry and is larger for isotropic fields for which the relative H₁-dust attenuation is increased along inclined rays. In Section 3.1.5 we calculate \( \langle \mu \rangle \) by fitting these analytic expressions to the results of our numerical computations for the atomic columns for isotropic fields. We find that universally and to an excellent approximation \( \langle \mu \rangle \approx 0.8 \), independent of \( \alpha G \) or \( Z' \), i.e., independent of the cloud parameters \( n, R, D_0, \) or \( \sigma_g \).

We again consider the weak- and strong-field limits. For weak fields \( \alpha G/4 \ll 1 \),

\[
N_{1,\text{tot}} = \frac{1}{\sigma_g} \frac{\alpha G}{4} = \frac{1}{\sigma_g} \frac{D_0}{4} G = \frac{1}{4} \frac{\tilde{F}_\nu W_{g,\text{tot}}}{Rn} = \frac{1}{4} \tilde{f}_\text{diss} \frac{w F_0}{Rn},
\]

and the H₁-dust opacity \( \sigma_g N_{1,\text{tot}}/\langle \mu \rangle \) is negligible and plays no role in attenuating the LW flux. The total atomic column depends on \( \sigma_g \) only via the dissociation bandwidth \( W_{g,\text{tot}} \), i.e., via the competition between H₂-line absorption and H₂-dust absorption. As for beamed radiation, Equation (68) is a simple Strömgren relation, and \( N_{1,\text{tot}} \) is equal to the ratio of the effective dissociation flux (or dissociation rate per unit surface area) to the H₂ formation rate. In the weak-field limit, and for a given \( \alpha G \) and \( \sigma_g \), i.e., for a given \( D_0 \) (or \( F_0 \) or \( I_{\text{UV}} \)), \( n, R, \) and \( \sigma_g \) (or \( Z' \)), the atomic column for isotropic radiation is equal to half that produced by a corresponding beamed field. This is simply due to the factor-of-two difference in the LW photon fluxes for corresponding isotropic versus beamed fields for a given field strength \( I_{\text{UV}} \).

In the strong-field limit, \( \alpha G/4 \gg 1 \),

\[
N_{1,\text{tot}} = \frac{\langle \mu \rangle}{\sigma_g} \ln \left( \frac{\alpha G}{4} \right) = \frac{\langle \mu \rangle}{\sigma_g} \ln \left( \frac{1}{4} \frac{D_0 G}{Rn} \right) = \frac{\langle \mu \rangle}{\sigma_g} \ln \left( \frac{1}{4} \frac{\tilde{F}_\nu W_{g,\text{tot}}}{Rn} \right).
\]

For strong fields, \( \sigma_g N_{1,\text{tot}} \gg 1 \) and the H₁-dust opacity is significant and dominates the attenuation of the radiation. As for beamed fields, the total atomic column saturates, and \( N_{1,\text{tot}} \) is insensitive to the cloud parameters except for \( \sigma_g \). Up to the logarithmic factor of order unity, we then have

\[
N_{1,\text{tot}} \approx \frac{\langle \mu \rangle}{\sigma_g}.
\]

Because \( \langle \mu \rangle \approx 0.8 \), the saturation columns are only slightly smaller for isotropic versus beamed fields for large \( \alpha G \), and they are not very different.

### 3. NUMERICAL MODEL COMPUTATIONS

With our analytic results (Section 2) in mind, we now present detailed numerical calculations for the H₁-to-H₂ transition profiles and the associated buildup of the atomic hydrogen columns for planar clouds illuminated by either beamed or isotropic FUV LW-band radiation fields. For this purpose we use the Meudon PDR code\(^{12}\) (Le Petit et al. 2006) for the computation of the UV radiative transfer and depth-dependent photodissociation rates and for the steady state atomic and molecular hydrogen gas densities. The code implements the “extended spherical harmonics” method (Flannery et al. 1980; Goicoechea & Le Bourlot 2007) for an exact numerical solution of the coupled H₂-line and dust scattering and absorption radiative transfer. An adaptive frequency grid is employed with sufficient resolution (\( \Delta \nu/\nu \approx 10^{-5} \)) to capture the contributions of the narrow H₂-line Doppler cores and broad wings to the total ultraviolet opacities. The competition between dust absorption and scattering and H₂-line absorptions, and the important effects of H₂-line overlap, are included in the calculation of the local radiation field intensities and H₂ photodissociation rates.

A principal feature of the Meudon PDR code is that the radiative transfer can be calculated for either beamed or isotropic fields. We assume the Draine spectrum (Equation (2)), and we calculate models for beamed and isotropic configurations. As defined in Section 2.2, for corresponding beamed and isotropic fields the radiation energy densities at the cloud surfaces are identical (Section 2.1). We compare our numerical results with the analytic formulae discussed above.

One of our main goals is the accurate computation of the effective H₂-dust-limited dissociation bandwidth \( W_{g,\text{tot}}(\sigma_g) \) (Equation (27)) summed over all of the LW-band absorption lines, for a wide range of FUV dust absorption cross sections \( \sigma_g \) (as set by the metallicity \( Z' \)). We also calculate H₁-to-H₂ transition profiles and the resulting atomic hydrogen columns from the weak- to strong-field limits (small to large \( \alpha G \)), for both beamed and isotropic fields and for a wide range of metallicities.

For computational efficiency in our large parameter space and for direct comparisons with our analytic formulæ, we have made several simplifying assumptions and modifications to the standard Meudon PDR code. First, instead of considering a full

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\(^{12}\) Publically available at http://pdr.obspm.fr.
range of grain sizes and wavelength-dependent absorption and scattering properties, we assume a single representative $\sigma_g$ for each metallicity (as given by Equation (20)), independent of photon frequency within the narrow LW band. We assume pure forward scattering by the grains and neglect the (small) effects of back-scattering discussed by Goicoechea & Le Bourlot (2007). Thus, our $\sigma_g$ enters as a simple effective absorption cross section. We have verified by spot checks within our parameter space that our assumption of a constant $\sigma_g$ alters the results for the computed H I columns by no more than 10% for any metallicity compared with computations incorporating a standard grain-size distribution.

Second, we decouple the H I/H$_2$ formation–destruction equation from the complex gas and grain networks that govern the heavy element chemistry. We assume that the H$_2$ is formed on grain surfaces only with a rate coefficient $R$ as given by Equation (21) and is destroyed only by (depth-dependent) LW photodissociation. We exclude gas-phase formation, e.g., via the equation $H^+ + e \rightarrow H + v$, $H^+ + H \rightarrow H^2 + e$,\textsuperscript{13} or destruction by cosmic-ray or X-ray secondary ionization (and we set the ionization rate $\xi$ equal to zero). Thus, at depths where the LW radiation field is fully absorbed, the atomic density vanishes, and the entire H I column is maintained by photodissociation.

Third, we consider isothermal clouds rather than solving a heating–cooling equation for the gas temperature $T$. Our standard is $T = 100$ K, for which the H$_2$ formation rate coefficient $R = 3 \times 10^{-17}$ cm$^3$ s$^{-1}$ for $Z = 1$. And fourth, we assume that the total hydrogen nucleon density, $n = n_1 + 2n_{12}$, is a constant independent of cloud depth, so that the local H$_2$ formation rate $Rn$ ($s^{-1}$) is also constant for any given model.

Fifth, we ignore absorption by neutral atomic carbon (C I) in the H$_2$ photodissociation layers. The carbon (continuum) photoionization band 1100–912 Å coincides almost exactly with the LW band for H$_2$ photodissociation, and C I, H$_3$, and dust compete for the same photons. The carbon photoionization cross section is $1.6 \times 10^{-15}$ cm$^2$ (van Dishoeck et al. 2006), so that the C I opacity $\tau_{C1} = 1.6 \times 10^{-17} AZ' N_{C1} \approx 1.6 \times 10^{-21} Z' N_{X1}$, where $N$ is the hydrogen gas column, $A$ $\approx$ $10^{-4}$ is the gas-phase carbon abundance for solar ($Z = 1$) metallicity, and $x_{C1}$ is the fraction of carbon present in atomic form. For $x_{C1} \approx 1$, $\tau_{C1}$ is competitive with the dust opacity $\tau_D = \sigma_D N \approx 1.9 \times 10^{-21} N$. However, the carbon is primarily C$_2^+$ and $x_{C2}$ is generally very small in the dust-limited or H$_2$–line-limited absorption layers in which the H I columns are built up. As the absence of dust or H$_2$ absorption, and assuming that C I absorbs the entire LW flux in maintaining an outer and optically thick C$_2^+$ layer, then $F_{C} \approx \alpha_{C} n_{C}^2 \ell = \alpha (A Z')^2 n_{N}$, where $F_{C} = 2 \times 10^7 I_{\text{UV}}$ is the ionizing photon flux (Equation (3)), $\alpha \approx 2 \times 10^{-11}$ cm$^3$ s$^{-1}$ is the electron–carbon recombination rate coefficient (Wolfire et al. 2008), $n_{C} = AZ'n$ is the volume density of C$_2^+$ ions, $\ell$ is the length scale of the optically thick C$_2^+$ Strömgren layer, and $N$ is the hydrogen gas column associated with the C$_2^+$ layer. We are assuming that the carbon ions are neutralized by recombination with free electrons and that $n_{e} \approx n_{C}$. However, if the dust opacity associated with this gas column is large, i.e., if $\sigma_D N \gtrsim 1$, then the C$_2^+$ layer is limited by dust and C I absorption may be ignored. The condition $\sigma_D N \gtrsim 1$ may be expressed as $\sigma_D F_{0}/(AZ')^2 n_{N} \gtrsim 1$, or $I_{\text{UV}}/n \gtrsim 5 \times 10^{-6} Z'$, or $\alpha G \gtrsim 10^{-3} Z'$. Thus, unless $\alpha G$ is unusually small, C I absorption is negligible. Using our PDR code, and turning on the effects of additional C$^+$ neutralization processes such as dust-assisted recombination and chemical removal processes, we find that even for $Z = 1$ the C I absorption is less than a 10% effect for $\alpha G = 0.01$ and is negligible for larger $\alpha G$.

Sixth, we ignore H I Lyman-series line absorption of the LW-band photons. These atomic lines (beginning with Ly$\beta$ at 1026 Å) do appear within the molecular LW absorption band (e.g., Draine & Bertoldi 1996), and the Meudon PDR code includes them. However, very large atomic columns are required for the atomic line equivalent widths to contribute significantly to the absorption. We find that an H I column of $\sim 10^{24}$ cm$^{-2}$ is required for the summed equivalent widths of the Ly-series lines to equal half the LW bandwidth (most of this absorption is due to just Ly$\beta$). Such large H I columns are produced only for very small values of $\sigma_D$ and $Z'$, even in the strong-field large $\alpha G$ limit. For example, for $\alpha G \sim 100$ it follows from Equation (40) that $N_{\text{tot}} \gtrsim 10^{24}$ cm$^{-2}$ requires $\sigma_D \lesssim 3.9 \times 10^{-24}$ cm$^2$, or $Z' \lesssim 2 \times 10^{-3}$. Thus, for the relevant range of metallicities, the atomic line absorptions can be ignored, and we exclude them in the radiative transfer.

With the above assumptions, the basic inputs to the code are the intensity, $I_{\text{UV}}$, and spectral shape of the radiation field (we assume the Draine representation, Equation (2)), in either a beamed or isotropic configuration, the total gas density $n$, the associated H$_2$ formation rate $Rn$ (temperature and metallicity dependent), and the dust grain absorption cross section $\sigma_g$ (metallicity dependent). The dimensionless parameter $\alpha_G$ is formed from these cloud variables as described in Sections 2.2.5 and 2.2.6.

For any set of parameters the critical numerical computation is for the depth-dependent line-plus-continuum absorptions and the attenuation of the H$_2$ photodissociation rate. For the H$_2$, our code includes all 302 ro-vibrational $vj$ levels in the $X^1\Sigma^+$ ground electronic state and the entire matrix of Lyman and Werner transitions to discrete $v'/j'$ levels in the excited $B^1\Sigma^+$ and $C^1\Pi_u$ states. We exclude transitions with energies greater than the hydrogen ionization energy of 13.59 eV. (As is standard, we assume that any ionizing photons are always absorbed in adjacent H II regions outside of the PDRs.) Our code includes transitions out of excited $v$ levels of the X state. However, for almost all conditions of interest and throughout most of the H I–H$_2$ transition zones, the dominating line absorptions are from the lowest few rotational levels $(j = 0$ to $5)$ of the $v = 0$ level.\textsuperscript{14} Thus, the relevant UV transitions lie between 1108 and 912 Å, and this is the wavelength range of our “standard LW band.”

The fractional populations, $x_{vj}$, of the $vj$ levels in the X state are computed assuming population and depopulation by the upward and downward $X$–$B$ and $X$–$C$ transitions, quadrupole radiative (cascade) transitions between the X-state $vj$ levels, and excitations and deexcitations in collisions with He, H$^+$, H, and other H$_2$ molecules. We use the Abgrall et al. (1993a) and Abgrall et al. (1993b) LW-band oscillator strengths and transition wave-numbers and the Abgrall et al. (2000) probabilities

\textsuperscript{13} With our assumption that the grain surface H$_2$ formation rate coefficient $R$ is linearly proportional to the metallicity, the gas-phase formation routes become important for $Z' \gtrsim 5 \times 10^{-3}$, depending on the temperature and fractional ionization, $x_e$, of the gas. For an estimate of the effective rate coefficient, $R_e$, for H$_2$ formation via the negative-ion $H^-$ intermediary, see, e.g., Equation (A7) of MK10, $R_e = 8 \times 10^{-19} x_{e-1} T_8^{0.88}$ cm$^3$ s$^{-1}$.

\textsuperscript{14} Photodissociation out of excited vibrational levels becomes significant when $I_{\text{UV}} \gtrsim 10^5$ and the UV excitation rates become comparable to the quadrupole vibrational decay rates (Shull 1978). However, even for such intense fields, the excitation rates become small as the lines rapidly become optically thick, and for most of the H I layer absorption out of excited vibrational states is negligible (S88).
for spontaneous radiative dissociations from the individual ro-vibrational levels in the excited B and C states. For the radiative quadrupole transitions, we use the Einstein-A values computed by Wolniewicz et al. (1998). For the collisional processes we use quadrupole transitions, we use the Einstein-A values computed by Le Bourlot et al. (1999) and Wrathmall et al. (2007) in their study of H2 excitation in astrophysical media.

As an example of our radiative transfer computations, we show in Figure 2 the energy density (erg cm\(^{-3}\) Å\(^{-1}\)) at a cloud column depth of \(N = 3.74 \times 10^{20}\) cm\(^{-2}\), or \(\tau_V = 0.7 (A_V = 0.2)\), for \(\sigma_g = 1.9 \times 10^{-21}\) cm\(^2\) (Z' = 1) for a model computation with \(I_{UV} = 35.5\) (isotropic) and \(n = 1000\) cm\(^{-3}\), or \(\alpha G/2 = 1\). At this depth the cores of the individual absorption line are very optically thick, but the continuum between the lines has not yet been significantly attenuated by overlapping line wings. Around 80 strong lines are visible in Figure 2, consistent with our analytic estimate \(\sigma_g/\sigma_d \approx 80\) for the number of lines involved in the photodissociation process, as discussed in Section 2.2.1.

### 3.1. Results

We now present our numerical code results for (1) the unattenuated free-space H2 photodissociation rate; (2) the curves of growth for the H2-dust-limited dissociation bandwidth \(W_g(N_2)\); (3) the total dissociation bandwidth \(W_{g,\text{tot}}(\sigma_g)\); (4) the self-shielding function \(f_{\text{shield}}(N_2)\); and (5) the mean self-shielding factor \(\langle G(Z')\rangle\). We then present H1-to-H2 transition profiles and total integrated H1 columns for beamed and isotropic fields and for a range of \(\alpha G\) and metallicities Z'.

#### 3.1.1. Free-space H2 Photodissociation Rate

The optically thin (full 4\(\pi\)) free-space (optically thin) H2 photodissociation rate, \(D_0\), is a fundamental parameter for ISM and galaxy evolution studies, and we have recalculated it here for the Draine FUV spectrum (Equation (2)). In Table 1, and for \(I_{UV} = 1\), we list the free-space UV excitation rates, \(P_{vj}\) (s\(^{-1}\)) out of the 14 lowest-lying H2 \((v, j)\) ro-vibrational levels. Each rate is summed over all upward LW transitions. We also list the mean dissociation probabilities \(f_{\text{diss}}(v, j)\), averaged over all of the transitions, and the resulting dissociation rates, \(D_{vj}\) (s\(^{-1}\)) out of each \((v, j)\) level. Our numbers are consistent with Draine & Bertoldi (1996) (see their Table 2), who used our basic input molecular data sets.

### Table 1

| \((v, j)\) | \(E_i\) (cm\(^{-1}\)) | \(P_{oj}\) (s\(^{-1}\)) | \(f_{\text{diss}}(v, j)\) | \(D_{vj}\) (s\(^{-1}\)) |
|------------|-----------------|-----------------|-----------------|-----------------|
| (0, 0)     | 0.000           | 4.71(−10)       | 0.117           | 5.51(−11)       |
| (0, 1)     | 118.505         | 4.75(−10)       | 0.119           | 5.65(−11)       |
| (0, 2)     | 354.363         | 4.83(−10)       | 0.123           | 5.94(−11)       |
| (0, 3)     | 705.567         | 4.95(−10)       | 0.130           | 6.44(−11)       |
| (0, 4)     | 1168.825        | 5.11(−10)       | 0.145           | 7.41(−11)       |
| (0, 5)     | 1740.277        | 5.30(−10)       | 0.141           | 7.47(−11)       |
| (0, 6)     | 2414.852        | 5.57(−10)       | 0.160           | 8.91(−11)       |
| (0, 7)     | 3187.691        | 5.86(−10)       | 0.160           | 9.38(−11)       |
| (0, 8)     | 4051.884        | 6.19(−10)       | 0.175           | 1.08(−10)       |
| (0, 9)     | 4831.595        | 7.43(−10)       | 0.107           | 4.24(−11)       |
| (1, 0)     | 4161.259        | 7.14(−10)       | 0.051           | 3.64(−11)       |
| (1, 1)     | 4273.913        | 7.21(−10)       | 0.055           | 3.97(−11)       |
| (1, 2)     | 4497.992        | 7.31(−10)       | 0.057           | 4.17(−11)       |
| (1, 3)     | 5002.162        | 6.58(−10)       | 0.197           | 1.30(−10)       |

The total dissociation rate is weighted by the population fractions \(\chi \) but is insensitive to the gas temperature or density when the excitation is mainly out of the lowest few j levels. For \(T\) between 10 to 10\(^3\) K, and for \(n\) ranging from 10 to 10\(^6\) cm\(^{-3}\), we find that to within at most a 2% variation, \(D_0 = 5.8 \times 10^{-11}\) s\(^{-1}\) for \(I_{UV} = 1\). The dissociation rate is essentially proportional to the field intensity. For very intense fields, the rate is increased by enhanced excitation of the rotational states and photodissociation out of these states by photons longward of 1108 Å, outside our nominal LW band. For \(T = 100\) K, and \(n = 100\) cm\(^{-3}\), we find that for \(I_{UV}\) from 1 to 10\(^3\), \(D_0 = 5.8 \times 10^{-11}\phi_{\text{ex}} I_{UV}\) s\(^{-1}\), where the “rotational excitation factor” \(\phi_{\text{ex}}\) increases from 1 to 1.5 for this range of field intensities. We have also computed the mean flux density in the free-space radiation field, as defined by Equation (12). For the Draine spectrum, we find that \(F_\nu = 2.46 \times 10^{-8}\phi_{\text{ex}} I_{UV}\) photons cm\(^{-2}\) s\(^{-1}\) Hz\(^{-1}\) for the same range of \(T, n,\) and \(I_{UV}\). For the analysis we present in Section 2, we assume \(\phi_{\text{ex}} = 1\).

As discussed in Section 2.2.4, the “H2-dust-limited dissociation bandwidth” \(W_g(N_2)\) (Equation (26)) is a fundamental quantity for the H1-to-H2 transitions and the buildup of the H1 column densities.

In Figure 3 we plot our curve-of-growth computations for \(W_g(N_2)\) integrated over all of the LW-band absorption lines, for \(\sigma_g\) ranging from 1.9 \times 10^{-22} to 1.9 \times 10^{-23} cm\(^2\), corresponding to metallicities Z’ from 0.01 to 10. We set the Doppler-\(b\) parameters for all of the lines equal to a typical ISM cloud value of 2 km s\(^{-1}\). Our results are insensitive to the precise choice for \(b\) because the dominant absorption lines are very highly damped. We extract the \(W_g(N_2)\) curves from our numerical radiative transfer computations for the radiation flux absorbed in the lines, self-consistently accounting for the flux reduction due to the presence of H2-dust. For any \(\sigma_g\), the curve of growth \(W_g(N_2)\) depends primarily on the internal molecular oscillator strengths, line profile cross sections, and dissociation probabilities for the excited states. We have verified by explicit computations that \(W_g(N_2)\) is indeed very insensitive to external
cloud parameters such as the field intensity $I_{\text{UV}}$ and/or gas density $n$, or temperature $T$. The curves of growth are also insensitive to the rotational-level distributions and ortho-to-para $\text{H}_2$ ratio. The specific curves displayed in Figure 3 were insensitive to the rotational-level distributions and ortho-to-para ratio. The curves of growth are also insensitive to the rotational-level distributions and ortho-to-para ratio set equal to 3 (with $\text{H}^-\text{H}_2$ proton exchange reactions turned off).

For $N_2 \lesssim 10^{14}$ cm$^{-2}$, all of the lines are optically thin, and $W_g$ increases linearly with $N_2$. Between $10^{15}$ and $10^{17}$ cm$^{-2}$, the growth is logarithmic as the Doppler cores become optically thick. At larger columns, $W_g$ increases more rapidly again as absorptions start occurring out of the line wings. For $N_2$ between $10^{18}$ and $10^{20}$ cm$^{-2}$, we find that $W_g$ grows as $N_2^{3/8}$, a bit more slowly than for a single damped line (for which it would be $N_2^{1/2}$).

The $W_g$ saturates at sufficiently large $\text{H}_2$ columns. When $\text{H}_2$-dust is negligible, the entire LW band is absorbed in fully overlapping lines, and $W_g$ reaches a maximal value of $9 \times 10^{13}$ Hz, for $N_2 \gtrsim 10^{22}$ cm$^{-2}$. In Figure 3 the absorption is essentially dust-free for $\sigma_g = 1.9 \times 10^{-21}$ cm$^2$, since the lines overlap before the $\text{H}_2$-dust opacity becomes significant, and for the (blue) curve $W_g(N_2) = W_d(N_2)$ (see Sections 2.2.1 and 2.2.4). For larger $\sigma_g$, and for $N_2 \gtrsim 1/(2\sigma_g)$, the asymptotic $W_g$ is limited by $\text{H}_2$-dust opacity.

Figure 4 shows our results for the “total dust-limited bandwidth” $W_{g,\text{tot}}(\sigma_g)$ (Equation (27)) for $\sigma_g$ from $10^{-24}$ to $10^{-20}$ cm$^2$. The points are our numerical results, and the solid curve is our analytic representation

$$W_{g,\text{tot}}(\sigma_g) \approx \frac{9.9 \times 10^{13}}{1 + (\sigma_g/7.2 \times 10^{-22} \text{ cm}^2)^{1/2}} \text{ Hz},$$

as already introduced in Section 2. This expression is accurate to within 4% compared with the numerical results. The transition from the line overlap to $\text{H}_2$-dust-limited regimes (small to large $\sigma_g$) occurs at $\sigma_g \sim 7.2 \times 10^{-22}$ cm$^2$. Line overlap is just starting to become important for solar ($Z \sim 1$) metallicities. For a fully molecular slab, most of the LW-band radiation is absorbed by $\text{H}_2$-dust for $Z' \gtrsim 0.5$. For $Z' \lesssim 0.5$, most of the radiation is absorbed in $\text{H}_2$-lines. Our results show that the regimes of small and large $\sigma_g$ are both relevant for the realistic range of metallicities in galaxies.

To a good approximation $W_{g,\text{tot}} \propto \sigma_g^{-1/2}$ for large $\sigma_g$, as indicated by our numerical results and Equation (28). This is the expected scaling for a single (effective) damped absorption line in competition with $\text{H}_2$-dust (see Section 2.2.4). We adopt $W_{g,\text{tot}} \propto \sigma_g^{-1/2}$ for large $\sigma_g$ for our analytic scaling relations in Section 2, although $W_g(N_2)$ grows somewhat more slowly with $N_2$ than for a single line.

3.1.3. Self-shielding Function and $G(Z)$

By definition, the $\text{H}_2$ “self-shielding function” $f_{\text{shield}}(N_2) \equiv (1/\sigma_g^{\text{tot}})dW_d/dN_2$, where $W_d(N_2)$ is the dissociation bandwidth for vanishing $\sigma_g$ (see Equation (16)).
In Figure 5 we plot (solid curve) our numerically computed derivative \( f_{\text{shield}}(N_2) \). We also plot (dashed) the Draine & Bertoldi (1996) fit (their Equation (37)) for the shielding function, given by

\[
f_{\text{shield}}(N_2) = \frac{0.965}{(1 + x/b_3)^2} + \frac{0.035}{(1 + x)^{0.5}} \times \exp[-8.5 \times 10^{-4}(1 + x)^{0.5}],
\]

where \( x = N_2/5 \times 10^{14}\text{cm}^{-2} \) and \( b_3 = b/10^5 \text{ cm s}^{-1} \) (we assume \( b_3 = 2 \)). It is evident that our computed shielding function is in excellent agreement with this formula.

At low \( N_2 \), the lines are optically thin and \( f_{\text{shield}} = 1 \). As the line cores become optically thick for \( N_2 \gtrsim 10^{14}\text{cm}^{-2} \), the molecules “self-shield” and \( f_{\text{shield}} \) decreases. By \( 10^{18}\text{cm}^{-2} \), \( f_{\text{shield}} = 5 \times 10^{-4} \). Between \( 10^{18} \) and \( 10^{20} \text{cm}^{-2} \), the shielding function declines as \( N_2^{-5/8} \), as expected given the (integral) behavior of \( W_d(N_2) \) in this range. Finally, at larger columns \( f_{\text{shield}} \) drops sharply as the lines fully overlap. As found by Draine & Bertoldi (1996), the reduction due to line overlap sets in at a column of \( 3 \times 10^{20}\text{cm}^{-2} \). We again see that attenuation due to line overlap becomes important for \( Z' \lesssim 1 \).

For such metallicities, \( \text{H}_2 \)-dust opacity becomes significant only at columns \( 1/(2\sigma_x) \gtrsim 3 \times 10^{20}\text{cm}^{-2} \), at which point the lines have already overlapped and the LW photons fully absorbed.

In Figure 6 we plot the “average self-shielding factor,” \( \equiv (\sigma_g/\sigma_d^{\text{tot}})W_d,\text{tot}(\sigma_g) \) (Equation (41) or Equation (45)), as a function of the metallicity, assuming \( \sigma_g = 1.9 \times 10^{-21}Z'^{-2}\text{cm}^{-2} \) (\( \phi_g = 1 \)). The points are our numerical results, and the curve is our analytic fitting formula Equation (46). As expected, for low metallicity (full overlap) \( G \propto Z' \), but for high metallicity \( G \propto Z'^{1/2} \) because of the \( \text{H}_2 \)-dust cutoff. For \( Z' = 10, 1, 0.1, \) and 0.01, we find that \( G \) equals \( 1.3 \times 10^{-4}, 2.8 \times 10^{-5}, 5.4 \times 10^{-6}, \) and \( 7.1 \times 10^{-7} \). For these metallicities, the average self-shielded dissociation rates are \( D_0G/2 = 3.8 \times 10^{-15}, 8.1 \times 10^{-16}, 1.6 \times 10^{-16}, \) and \( 2.1 \times 10^{-17}\text{ s}^{-1} \). As discussed in Section 2.2.6 the average is over an \( \text{H}_2 \)-dust optical depth \( \tau_{\text{g}} \sim 1 \). For low metallicities, \( D_0G/2 \) becomes very small because the LW radiation is fully absorbed in lines at very low \( \text{H}_2 \)-dust optical depths.

3.1.4. H\(_1\)-to-H\(_2\) Transition Profiles

We now present illustrative computations for the \( \text{H}_1 \)-to-\( \text{H}_2 \) transition profiles for a range of \( G \alpha G \) spanning the weak- to strong-field limits, and for metallicities \( Z'/n \) from high to low, for beamed and isotropic fields.

As discussed in Section 2.2.5, the profile shapes, i.e., the density ratios \( n_1/n \) and \( 2n_2/n \) as functions of the dust optical depth \( \tau_{\nu} \equiv \sigma_g N \) (where \( N' \equiv N_1 + 2N_2 \)), depend on just the single dimensionless parameter \( \alpha G \equiv D_0G/\dot{\kappa} \). This includes the locations of the \( \text{H}_1 \)-to-\( \text{H}_2 \) transition points expressed in terms of \( \tau_{\nu} \). We define the transition point as the cloud depth where \( n_1/n = 2n_2/n = 0.5 \). For both beamed and isotropic fields we compute the transition profiles for \( \alpha G/2 = 0.01, 0.1, 1, 10, \) and \( 10^2 \), for \( Z' = 1 \) and \( \sigma_g = 1.9 \times 10^{-21}\text{cm}^{-2} \) (\( \phi_g = 1 \)). These sequences illustrate the change in profile shapes, from “gradual” to “sharp,” from the weak-field (\( \text{H}_1 \)-dust negligible) to strong-field limits (\( \text{H}_1 \)-dust dominant). In these computations \( G = 2.8 \times 10^{-5} \) as appropriate for \( Z' = 1 \), and we set \( D_0 = 2 \times 10^{-9}\text{s}^{-1} (I_{\text{UV}} \approx 35) \) and \( R = 3 \times 10^{-17}\text{cm}^3\text{s}^{-1} \) (\( T = 100\text{K} \)). To alter \( \alpha \) and \( \alpha G \), we vary \( n \) from 10 to \( 10^5\text{cm}^{-3} \).

For each \( \alpha G/2 \) we plot the atomic and molecular fractions, \( n_1/n \) and \( 2n_2/n \), as functions of the total (atomic plus molecular) column density, \( N \). For fully atomic gas \( n_1/n = 1 \), and for fully molecular gas \( 2n_2/n = 1 \). For each model we also plot the
Figure 7. H\textsubscript{i}/H\textsubscript{2} transitions for beamed (left panels) and isotropic (right panels) radiation fields, for \(\alpha G/2\) ranging from 0.01 (top panels) to 100 (bottom panels). The solid curves show the atomic and molecular gas fractions, \(n_1/n\) and \(2n_2/n\), as functions of the total gas column density \(N\) into the cloud. The (blue) dashed curves are the normalized atomic columns, \(\tilde{N}_1 \equiv N_1/N_{1,\text{tot}}\), as functions of cloud depth. (A color version of this figure is available in the online journal.)

Normalized atomic column, \(\tilde{N}_1 \equiv N_1/N_{1,\text{tot}}\), also as a function of \(N\). Thus, \(\tilde{N}_1 \to 1\) at sufficiently large cloud depths where the LW radiation is fully absorbed. The curves for \(\tilde{N}_1\) show how and where the atomic column is built up relative to the atomic-to-molecular transition points.

Figure 7, left panels, display the H\textsubscript{i}-to-H\textsubscript{2} transition profiles for the five beamed-field models with varying \(\alpha G\).

Several important features can be seen in these plots. First, the atomic-to-molecular transition points move deeper into the cloud with increasing \(\alpha G\). For \(\alpha G/2 = 0.01, 0.1, 1, 10,\) and \(10^2\), the total gas columns \(N_{1\to2}\) at the transition points equal \(5.6 \times 10^{17}, 1.4 \times 10^{19}, 3.0 \times 10^{20}, 1.2 \times 10^{21},\) and \(2.4 \times 10^{21}\) cm\textsuperscript{-2}. For the assumed \(\sigma_g = 1.9 \times 10^{-21}\) cm\textsuperscript{-2}, these columns correspond to total dust optical depths \(\tau_d = 1.05 \times 10^{-3}, 2.6 \times 10^{-5}, 0.58, 2.3,\) and 4.5. The H\textsubscript{i}-dust optical depths at the transition points are \(9.0 \times 10^{-4}, 2.0 \times 10^{-2}, 0.45, 2.1,\) and 4.2. In the weak-field limit, the transition depths increase rapidly with \(\alpha G\). In the strong-field limit, the UV penetration is moderated by H\textsubscript{i}-dust absorption, and the transition depths increase slowly.

Second, the profile shapes vary with \(\alpha G\). In the weak-field limit, the atomic-to-molecular conversion is controlled by H\textsubscript{2}-line self-shielding, but significant H\textsubscript{i} exists beyond the transition point up to the H\textsubscript{2}-dust cutoff. In the weak-field limit, most of the H\textsubscript{i} column is built up past the transition point where the gas is predominantly molecular. In the strong-field limit, the transition point is controlled by (exponential) H\textsubscript{i}-dust absorption, and most of the H\textsubscript{i} is built up in an outer full atomic layer. Thus, in the weak-field limit the transitions are gradual, and in the strong-field limit the transitions are sharp. For example, at the H\textsubscript{i}-to-H\textsubscript{2} transition points, the normalized atomic column
and the transition columns grow inversely with \( Z' \). For these four models, \( N_{1\to 2} = 3.0 \times 10^{19}, 3.7 \times 10^{20}, 4.0 \times 10^{21}, \) and \( 4.2 \times 10^{22} \text{ cm}^{-2} \), corresponding to dust opacities \( \tau_{\nu} = 0.57, 0.70, 0.76, \) and 0.78. The H\( \text{I} \)-dust opacities at the transition points are 0.46, 0.56, 0.63, and 0.70. This behavior is in excellent agreement with the analytic theory presented in Section 2. For two-phased equilibrium, \( \alpha G/2 \sim 1 \) for all metallicities and is intermediate between the weak- and strong-field limits for which H\( \text{I} \)-dust opacity is just becoming significant.

Figure 8, lower panel, shows the \( n_1/n \) curves for \( Z' = 10, 1, 0.1, \) and 1 for the isotropic-field models, with \( \alpha G/2 = (\alpha G)\text{CNM}(Z')/2 \) as for the beamed-field models. Again, because \( \alpha G \) is about the same for all four models, the profile shapes are very similar. The transition point columns are \( N_{1\to 2} = 1.6 \times 10^{19}, 1.9 \times 10^{20}, 2.1 \times 10^{20}, \) and \( 2.2 \times 10^{22} \text{ cm}^{-2} \), or \( \tau_{\nu} = 0.31, 0.36, 0.40, \) and 0.42. The H\( \text{I} \)-dust optical depths at the transition points are 0.25, 0.29, 0.33, and 0.37. The transition columns and optical depths for all of the isotropic-field models are smaller than for the beamed-field models because of the factor-of-two reductions in the incident fluxes for corresponding isotropic fields with the same \( \alpha G \).

### 3.1.5. Total H\( \text{I} \) Columns

A key goal is the computation of the total atomic column densities, \( N_{1\text{tot}} \), for beamed and isotropic fields for a comparison with our analytic formulae.

In Figure 9, upper panel, we display \( N_{1\text{tot}} \) for beamed fields, as a function of \( \alpha G/2 \) spanning the range from 0.01 to 100, for \( Z' = 10, 1, 0.1, \) and 0.01.

For our numerical models, we again set \( D_0 = 2 \times 10^{-9} \text{ s}^{-1} \) and \( R = 3 \times 10^{17} Z' \text{ cm}^3 \text{ s}^{-1} \) and vary the gas density \( n \) (to select \( \alpha \equiv D_0/Rn \)), and we set \( \sigma_g = 1.9 \times 10^{-21} \text{ cm}^2 \). For the given input parameters \( D_0, R, n \), and \( \sigma_g \), we compute the total integrated atomic column density and also calculate \( W_{g,\text{tot}} \) and the associated average self-shielding factor \( G = (\sigma_g/\sigma_g^{\text{is}})W_{g,\text{tot}} \). For each model we compute \( N_{1\text{tot}} \) for the corresponding \( \alpha G \) and \( \sigma_g \). The points in Figure 9 are our model results for selected \( \alpha G \) and \( Z' \). Again, for the four metallicities, \( G = 1.3 \times 10^{-4}, 2.8 \times 10^{-5}, 5.4 \times 10^{-6}, \) and \( 7.1 \times 10^{-7} \). The curves in Figure 9 are as given by our fundamental analytic formula for beamed fields

\[
N_{1\text{tot}} = \frac{1}{\sigma_g} \ln \left[ \frac{\alpha G}{2} + 1 \right],
\]

where \( 1/\sigma_g = 5.3 \times 10^{20}/Z' \text{ cm}^{-2} \) as for the numerical models.

Our analytic and numerical results are in excellent agreement from the weak- to strong-field regimes. For weak fields (high gas densities), \( N_{1\text{tot}} = (1/\sigma_g)\alpha G/2 = (1/2)F \left( W_{g,\text{tot}}/Rn \right) \) (Equation (52)). In this regime the total atomic column is proportional to the field intensity (dissociation flux) and varies inversely with the gas density. For strong fields (low densities), the dependence is logarithmic and \( N_{1\text{tot}} = (1/\sigma_g)\ln(\alpha G) \) (Equation (54)). In this regime the atomic column is weakly dependent on \( I_{1\nu}/n \), and it is limited to values close to \( 1/\sigma_g \) because of the dominating H\( \text{I} \)-dust absorption. For example, for \( Z' = 1 \) and \( \alpha G/2 = 0.01 \) and 0.01, 1, 10, and 100, our model computations give \( N_{1\text{tot}} = 5.6 \times 10^{13}, 5.3 \times 10^{14}, 3.8 \times 10^{20}, 1.2 \times 10^{21}, \) and \( 2.4 \times 10^{21} \text{ cm}^{-2} \), as also given by our analytic formula.

Expressed as a function of \( \alpha G \), \( N_{1\text{tot}} \propto 1/Z' \). However, we recall that for large \( \sigma_g \) (\( Z' \gtrsim 1 \)), \( \alpha G \) is itself metallicity dependent and \( \alpha G \propto Z'^{1/2} \) (see Equation (51)). Thus, for high metallicities in the weak-field limit, \( N_{1\text{tot}} \propto Z'^{-3/2} \).
In this regime the column decreases by one power of $Z'$ because of enhanced $H_2$ formation efficiency and decreases by an additional factor of $Z'^{1/2}$ because of the reduction of the effective dissociation flux by the $H_2$-dust. For low metallicities in the weak-field limit, the dissociation flux is maximal, and $N_{1,\text{tot}} \propto Z'^{-1}$. In the strong-field limit, the atomic column is only weakly (logarithmically) dependent on $\alpha G$, and the metallicity dependence is mainly via the $H_1$-dust opacity, and $N_{1,\text{tot}} \propto Z'^{-1}$ for all metallicities. These metallicity scalings, discussed in Section 2.2.8, are validated by our numerical model results for all metallicities.

In Figure 9 we also plot a (red) curve for $(\alpha G)_{\text{CNM}}(Z')$ as given by Equation (59) for self-regulated multiphased H$_1$. As is again illustrated in Figure 9, $(\alpha G)_{\text{CNM}}(Z')/2 \sim 1$. Given the assumptions underlying Equation (59), the H$_1$ columns for self-regulated multiphased gas are intermediate between the linear (weak-field) and logarithmic (strong-field) regimes for all metallicities.

Our computational results show that our analytic expression for $N_{1,\text{tot}}$ is valid for all transition profile shapes, whether gradual (weak fields) or sharp (strong fields), regardless of where the atomic column is built up (whether in the molecular zone or in the outer fully atomic layer). Indeed, in our analytic derivation we did not make any assumptions on the profile shape. Our expression is universal and valid for all regimes (weak and strong fields, high and low metallicities) and for all transition profile shapes (gradual or sharp). We emphasize this point again in our alternate derivation via the KMT/MK10 “transfer-dissociation equation” (Section 4.1.1).

In Figure 9, lower panel, we plot the total atomic columns for our isotropic-field models. For these models we select $D_0$ and $R$, and vary $n$ to set $\alpha_0$, and we compute the total H$_1$ column. As discussed in Section 3.2, the total dust-limited dissociation bandwidth, $W_{\text{tot}}$, and the average self-shielding factor, $G$, are identical for beamed and isotropic fields. In Figure 12 we plot $N_{1,\text{tot}}$ as a function of $\alpha G$, where for each $Z'$ we use the $(G(Z'))$ computed using beamed fields. Again, $\alpha G$ ranges from 0.01 to 100, and we present results for $Z'$ from 10 to 0.01. The $(\alpha G)_{\text{CNM}}(Z')$ curve is also displayed. In Figure 9, the points are our numerical results, and the curves are as given by our fundamental analytic formula for isotropic fields (Section 2.3),

$$N_{1,\text{tot}} = \frac{\langle \mu \rangle}{\sigma_g} \ln \left[ \frac{1}{\langle \mu \rangle} \alpha G \frac{4}{4} + 1 \right],$$

where again $1/\sigma_g = 5.3 \times 10^{20}/Z'/\text{cm}^{-2}$. To obtain the match between the numerical results and analytic formula shown in Figure 9, we have fit for the average angle factor $\langle \mu \rangle$. We find that

$$\langle \mu \rangle = 0.8$$

provides an excellent fit for all $\alpha G$ and for all $\sigma_g \propto Z'$.

For isotropic fields in the weak-field limit, $N_{1,\text{tot}} = (1/\sigma_g)\alpha G/4 = (1/4)\bar{F}_W g_{\text{tot}}R/n$ (Equation (68)). As discussed in Section 2.3, this is half the column for the corresponding beamed field because of the factor-of-two difference in the incident dissociation fluxes. For weak fields, $N_{1,\text{tot}}$ is independent of $\langle \mu \rangle$. In the strong-field limit, $N_{1,\text{tot}} = (\langle \mu \rangle/\sigma_g)\ln(\alpha G/4(\mu))$ (Equation (69)), and the column is reduced by the factor $\langle \mu \rangle = 0.8$ compared with beamed-field models (neglecting the small difference in the logarithms). For example, for $Z' = 1$ and $\alpha G/2 = 0.01$ 0.1, 1, 10, and 100, our model results for the total atomic column are $3.1 \times 10^{18}$, $2.9 \times 10^{19}$, $2.1 \times 10^{20}$, $7.7 \times 10^{20}$, and $1.6 \times 10^{21}$ cm$^{-2}$, smaller in the expected way compared with beamed-field models. The linear and logarithmic behaviors for small and large $\alpha G \propto f_{\text{UV}}/n$ and the scaling with $Z'$ are identical for isotropic and beamed fields.

Our expression for the total column for isotropic fields is also valid for all profile shapes, from gradual to sharp.

4. COMPARISON WITH KMT/MK10

In a series of papers, Krumholz et al. (2008, 2009) and McKee & Krumholz (2010; hereafter KMT/MK10) considered the interstellar atomic-to-molecular transition in the context of galaxy-wide conditions for star formation. For this purpose, KMT/MK10 developed analytic models for the $H_1$-to-$H_2$ transitions in spherical clouds irradiated by isotropic radiation fields. They also considered planar models. KMT/MK10 were particularly interested in exploring the role of metallicity in setting star-formation thresholds, and in MK10 they applied their spherical models to compute metallicity-dependent $H_2$ mass fractions in star-forming clouds as functions of the gas mass surface densities in galaxy disks. The integral $H_2$ mass fraction, $f_{H_2}$, may be a critical parameter in galaxy-wide Kennicutt–Schmidt (KS) relations, especially if conversion to $H_2$ is required for star formation.
formation.\textsuperscript{15} For spheres, $f_{\theta}\equiv M_{\text{H\,II}}/M_{\text{gas}}$, where $M_{\text{H\,II}}$ and $M_{\text{gas}}$ are the molecular and total gas masses within the volumes. For slabs $f_{\theta}\equiv \Sigma_{\text{H\,II}}/\Sigma_{\text{gas}}$, where $\Sigma_{\text{H\,II}}$ and $\Sigma_{\text{gas}}$ are the molecular and total gas mass surface densities in the normal directions.

The assumption of spherical versus plane-parallel geometry complicates the analysis and computation of the H\,I-to-H\,2 transition because for spheres oblique rays cross through the clouds even when optically thick H\,2 cores are present. Optically thick slabs are simpler because all rays are absorbed. To proceed, KMT/MK10 made the simplifying assumption that the H\,I-to-H\,2 transitions are always sharp, such that any atomic layer has a well-defined length scale. For the spheres, fully atomic and dusty H\,I shells are then assumed to surround fully molecular H\,2 cores. Rays that cross through the H\,I shells are either unattenuated or are absorbed by dust, or by H\,2-lines under the assumption that the molecular fractions in the shells are small. Rays that impinge on the H\,2 cores are fully attenuated. MK10 employ a “variable Eddington factor” formalism to close the angular moments of the radiative transfer equation for the radiation fields in the H\,I shells. For a given total cloud mass and radiation field intensity, a complicated iterative procedure then yields the spherical and nested H\,I/H\,2 structures, and associated H\,2 mass fractions.

KMT/MK10 implicitly assumed that the H\,2–shells are always in the fully overlapping regime, independent of $Z'$ and $\sigma_z$, and they did not consider the possible reduction of the effective dissociation bandwidth by H\,2-dust. KMT/MK10 did not make the distinction between H\,I-dust and H\,2-dust that we have been emphasizing.

According to KMT/MK10, the spherical H\,I/H\,2 “shell–core” structures depend on two dimensionless parameters, “$\chi$” and “$\tau_r$.” In their definition, “$\chi/f_1$ is the ratio of the number of LW photons absorbed by dust to the number absorbed by H\,2,” where $f_1$ is the fraction of gas in atomic form. As we clarify below, $\chi$ is actually identical to our $\alpha G$ in the low-$Z'$, small-$\sigma_z$, $(w = 1)$ limit where H\,2-dust absorption is negligible. The second parameter, $\tau_r \equiv n\sigma r$, is the “dust optical depth associated with the cloud radius $r$, where $n$ is the hydrogen nucleon density at the cloud surface. For a slab (of finite width) the corresponding second parameter is the total dust optical depth $\tau_z \equiv \sigma_z n \Sigma$ through the slab, where $z$ is the linear extent. The parameters $\tau_r$ and $\tau_z$ will enter into our discussion of the H\,2 mass fractions for spheres and slabs (Section 4.2).

We wish to compare our analytic theory for the H\,I column densities for planar clouds with the KMT/MK10 formulae for spheres. This will enable us to also compare results for the H\,2 mass fractions. We will show that any differences between corresponding (i.e., properly normalized) slabs and spheres are very small and that it is therefore advantageous to use our much simpler and fully analytic plane-parallel formalism.

We start (in Section 4.1) by clarifying the relationship between the KMT/MK10 $\chi$ and our $\alpha G$. To do this we reanalyze the “transfer-dissociation equation” presented by Krumholz et al. (2008). This also enables a comparison of our formulae for the H\,I columns with KMT/MK10’s similar, though not identical, expressions for the atomic columns for planar geometry. In Section 4.2.1 we develop a simple expression for $f_{\theta}$ for optically thick slabs for two-sided irradiation using our analytic expressions for the total H\,I-dust optical depths for one-sided irradiation of semi-infinite clouds, for isotropic or beamed fields. In Section 4.2.2 we re-express the MK10 formulae for uniform density (isochoric) spheres and (isobaric) “atomic–molecular complexes” for (1) the critical H\,I-dust optical depths required for the formation of H\,2 cores and (2) the H\,2 mass fractions as functions of the total cloud optical depths (or gas masses). This will enable a clear comparison with our expressions for slabs.

We find that for corresponding spheres and slabs embedded in isotropic fields, the predicted H\,I columns are very similar. The differences are no greater than 20% for $\alpha G$ ranging from 0.01 to 100. For two-phased H\,I equilibria for which $\alpha G/2 \sim 1$, the differences between spheres and slabs are negligible, and the H\,I columns for spheres and slabs are essentially identical. In fact, we show that switching from a beamed to an isotropic field for a slab is much more significant than switching from a slab to a sphere for a fixed isotropic field. We then show that for proper normalization of the three configurations—uniform sphere, complex, or slab—the predicted H\,2 mass fractions as functions of total cloud masses or columns are also very similar.

4.1. $\chi$ and $\alpha G$

To clarify the relationship between the KMT/MK10 $\chi$ and our $\alpha G$, it is useful to consider the “transfer-dissociation equation” developed by Krumholz et al. (2008), here for beamed radiation into a slab. This discussion will also provide an alternate derivation of our fundamental formula (Equation (40)) for the total H\,I column density.

4.1.1. Transfer-dissociation Equation

Let $F_\nu(z)$ be the flux density (photons $\text{cm}^{-2} \text{s}^{-1} \text{Hz}^{-1}$) at frequency $\nu$ of beamed LW radiation at linear depth $z$ into a slab. The radiation flux ($\text{cm}^{-2} \text{s}^{-1}$) between frequencies $\nu_1$ and $\nu_2$ is then

$$F(z) \equiv \int_{\nu_1}^{\nu_2} F_\nu(z) \, d\nu. \tag{76}$$

At the cloud surface $F(0) = F_0/2$, where $F_0$ is the flux integral (our Equation (3)) for the free-space radiation field.

The transfer equation for $F(z)$ is

$$\frac{dF}{dz} = -n\sigma z F - n_2 \int_{\nu_1}^{\nu_2} \sigma_\nu F_\nu \, d\nu. \tag{77}$$

Here $n \equiv n_1 + 2n_2$ is the total (atomic plus molecular) hydrogen gas volume density, and $\sigma_z$ is the (“complicated”) cross section for the multiline H\,2 absorption process.\textsuperscript{16} The first term on the right-hand side of Equation (77) is the dust absorption rate of the local radiative flux. The second term is the H\,2-line absorption rate.

The steady state H\,2 formation–destruction equation is

$$R_{\text{nn}} = \tilde{f}_{\text{diss}} n_2 \int_{\nu_1}^{\nu_2} \sigma_\nu F_\nu(z) \, d\nu, \tag{78}$$

where in this expression, $\tilde{f}_{\text{diss}}$ (as defined in Section 2) is the mean fraction of all H\,I-line absorptions that lead to photodissociation. Following Krumholz et al. (2008) and our discussion in Section 2, we assume that $\tilde{f}_{\text{diss}}$ is independent of cloud depth.
The “complicated” integral in Equation (77) may be eliminated to give the transfer-dissociation equation (Krumholz et al. 2008)

$$\frac{dF}{dz} = -n\sigma g F - \frac{R_{\text{nn}}}{\chi_{\text{diss}}}. \quad (79)$$

In dimensionless form

$$\frac{d\mathcal{F}}{d\tau} = -\mathcal{F} - \frac{2}{\chi} f_1, \quad (80)$$

where $\mathcal{F} \equiv F/F(0)$ is the normalized depth-dependent flux, $\tau \equiv \sigma g z$ is the dust optical depth, and $f_1(\tau) \equiv n_1/n$ is the depth-dependent fraction of gas in atomic form.

In Equation (80)

$$\chi \equiv \frac{\chi_{\text{diss}} \sigma g F_0}{R n}. \quad (81)$$

This is the KMT/MK10 $\chi$, here introduced for one-sided irradiation of a slab by a beam field with incident LW flux $F(0) \equiv F_0/2$.\(^\text{17}\) Compared with our Equation (48) it is already clear that $\chi = \alpha G$ for $w = 1$.

Because the product $\sigma g n F_0$ is the dust absorption rate per unit volume of the surface LW radiation flux, and because $R n^2 f_1/\chi_{\text{diss}}$ is the H$_2$-line absorption rate per unit volume, KMT/MK10 interpret $\chi/f_1$ as the ratio of the number of LW photons absorbed by dust to the number absorbed by H$_2$-lines at the optically thin cloud surface (with one factor of $n$ canceling when doing the division). In this interpretation, the dust absorption being referred to in the numerator is independent of whether the gas is atomic or molecular.

However, as we now show, if the dust absorption term in the transfer-dissociation equation is redefined to refer to H$_1$-dust absorption only, we will recover our fundamental formula for the H$_1$ column density, including a method for “renormalizing” the dissociation flux to account for H$_2$-dust absorption. We demonstrate this by analyzing the transfer-dissociation equation in the following three steps.

4.1.2. Step 1: Transition Assumed Sharp

First, we assume—as done by KMT/MK10—that the atomic-to-molecular transition is always sharp. We impose this assumption even though we know that it is good only if our $\alpha G \gg 1$, i.e., only if $F_0/n$ and $\chi$ are sufficiently large. Nevertheless, in seeking a solution for Equation (80), we assume that for any $\chi$ the atomic fraction $f_1 = 1$ everywhere $\mathcal{F}$ is non-zero, up to the (unknown) transition point where $\mathcal{F}$ vanishes. At that point the gas switches suddenly from H$_1$ to H$_2$.

Setting $f_1 = 1$, the solution to Equation (80) is

$$\mathcal{F}(\tau) = \frac{\chi + 2}{\chi} e^{-\tau} - \frac{2}{\chi}. \quad (82)$$

It is evident that the flux vanishes for $\tau = \tau_{1,\text{tot}}$, where

$$\tau_{1,\text{tot}} = \ln \left[ \frac{\chi}{2} + 1 \right]. \quad (83)$$

\(^{17}\) When Krumholz et al. (2008) defined their $\chi$ via the transfer-dissociation equation, they wrote the surface flux $F(0)$ in the numerator, rather than the full $4\pi$ free-space $F_0$. However, when discussing spherical models, KMT/MK10 redefine their $\chi$ and replace $F(0)$ with $F_0$ in the numerator. In this paper we use the free-space $F_0$ throughout, including here in our discussion of the transfer-dissociation equation. With this adjustment a factor of two appears in the second term on the right-hand side of Equation (80), which is not there in Krumholz et al. (2008).

and this is then the solution for the transition point (Krumholz et al. 2008). The total atomic column density up to the transition point is

$$N_{1,\text{tot}} = \frac{1}{\sigma g} \ln \left[ \frac{\chi}{2} + 1 \right]. \quad (84)$$

because by assumption there is no H$_2$ in the photodissociated layer and $\tau_{1,\text{tot}}$ is the optical depth due to H$_1$-dust only.

We immediately recognize Equations (83) and (84). They are identical to our expressions (40) and (43) for the total H$_1$-dust optical depth and H$_1$ column density, except that here the argument is $\chi$, as given by Equation (81), rather than our $\alpha G$ as defined by the similar but not quite identical Equation (48). Indeed, it is apparent that $\alpha G = w \chi$, where $w$ is the normalized effective dissociation bandwidth as defined by Equation (31). (This identity is clarified in Step 3.)

For $\chi \gg 1$, the attenuation of the LW flux is dominated by dust absorption, and $\mathcal{F}(\tau) \approx e^{-\tau}$. An exponentially attenuating flux is precisely what produces a sharp transition profile. Therefore, for $\chi \gg 1$ the assumption that the transition is sharp is consistent. Furthermore, the exponential attenuation is due specifically to H$_1$-dust absorption. Sharp profiles occur when H$_1$-dust dominates the attenuation.

For $\chi \ll 1$, dust absorption is negligible compared with H$_2$-lines, $\tau \ll 1\,$ throughout the atomic layer, and $\mathcal{F}(\tau) = 1 - 2\tau/\chi$ to first-order in $\tau$. For small $\chi$, Equation (83) gives $\tau_{1,\text{tot}} = \chi/2$, so that

$$N_{1,\text{tot}} = \frac{1}{\sigma g} \frac{\chi}{2} \quad (85)$$

in this limit. However, when H$_2$-lines dominate the attenuation the transition is not sharp, and the assumption that $f_1 = 1$ is inconsistent.

Nevertheless, as we now show in Step 2, the above expressions for $\mathcal{F}(\tau)$, $\tau_{1,\text{tot}}$, and $N_{1,\text{tot}}$ for large and small $\chi$ are valid for any varying $f_1$, whether or not the H$_1$/H$_2$ transition is sharp, provided that H$_2$-dust is always negligible compared with H$_1$-dust or H$_2$-lines, so that $\tau$ in Equation (80) can be redefined as the optical depth associated with H$_1$-dust absorption only.\(^{18}\)

4.1.3. Step 2: H$_2$-dust Negligible, and $\tau$ Redefined

With the neglect of H$_2$-dust absorption, Equation (79) is

$$\frac{dF}{dz} = -n_1 \sigma g F - \frac{R_{\text{nn}}}{\chi_{\text{diss}}}, \quad (86)$$

where now $n$ has been replaced by $n_1$ in the first term on the right-hand side, or

$$\frac{d\mathcal{F}}{d\tau} = -\mathcal{F} - \frac{2}{\chi}, \quad (87)$$

where $\chi$ is again given by Equation (81) but where now

$$\tau = \sigma g \int_0^\tau n_1 \, dz \quad (88)$$

is defined in advance as the optical depth associated with H$_1$-dust only.

\(^{18}\) Indeed, we know that our Equations (40) and (43) are valid for all $\alpha G$, whether or not the H$_1$ to H$_2$ transition is sharp. This suggests that although we assumed $f_1 = 1$ to derive Equations (83) and (84), they are valid even when $\chi$ is small and the transition is not sharp.
In Equations (86) and (87), a factor \( f_1 \equiv n_1/n \) does not appear. The solutions are still given by Equations (84) and (85) for large and small \( \chi \) but now with no assumptions on the shapes of the transition profiles.

For large \( \chi \) the transition is sharp because the radiation flux is attenuated exponentially by the H\(_2\)-dust, as shown in Step 1. However, for low \( \chi \), for which \( \tau_{\text{tot}} \) is small, the transition need not be sharp. In this limit we again have,

\[
N_{1,\text{tot}} = \frac{1}{\sigma_g} \frac{\chi}{2} = \frac{f_{\text{diss}} F_0/2}{Rn}. \tag{89}
\]

But this is just a Strömgren relation (as also noted by MK10). Therefore, it must hold independent of the shape of the H\(_1\)/H\(_2\) profile, provided only that the incident dissociation flux, \( f_{\text{diss}} F_0/2 \), is fully absorbed by H\(_2\)-lines, which it indeed will be for small \( \tau_{\text{tot}} \). Again, \( RnN_{1,\text{tot}} \) is the integrated H\(_2\) formation rate per unit area, and in steady state this equals the fully absorbed dissociation flux \( f_{\text{diss}} F_0/2 \) impinging on the surface, independent of profile shape. In fact, we know that for low \( \chi \) (i.e., for small \( F_0/n \) and \( \alpha G \)) the transition profile is gradual, with most of the H\(_1\) column built up in the molecular zone, as we have shown and discussed in Section 3.

Although Krumholz et al. (2008) derived their expression (83) for the dust optical depth assuming a sharp transition, it is actually valid for all \( \chi \), large and small, for sharp and gradual atomic hydrogen profiles, provided that H\(_2\)-dust absorption is negligible compared with H\(_1\)-dust and H\(_2\)-lines.

4.1.4. Step 3: H\(_2\)-dust and Renormalization of the Dissociation Flux

We now include H\(_2\)-dust. In Equations (79) and (80), the original dust absorption term, \( n_0 \sigma_g F \), is not necessarily negligible—even when \( \chi \ll 1 \)—if the atomic fraction \( f_1 \) is sufficiently small. This is the regime where H\(_2\)-dust absorption may be significant, even if H\(_1\)-dust is negligible.

Because of H\(_2\)-dust absorption of radiation “between the lines,” not all of the photons in the LW band are absorbed by the H\(_2\), even for a fully molecular slab. The effective dissociation flux is then smaller than \( f_{\text{diss}} F_0/2 \). The Strömgren relation then implies that for \( \chi \ll 1 \) the total H\(_1\) optical depth \( \tau_{1,\text{tot}} \) must be smaller than \( \chi/2 \), rather than equal to \( \chi/2 \) as given by Equation (89).

If \( \tau \) is redefined to refer to H\(_1\)-dust only as in Step 2, the effect of H\(_2\)-dust absorption can be included in the transfer-dissociation equation by a simple “renormalization” of the effective dissociation flux. We replace \( F_0/2 \) with a suitably reduced \( wF_0/2 \) equal to the flux of LW photons absorbed in H\(_2\)-lines in a dusty molecular slab, excluding in advance photons that are inevitably absorbed by H\(_2\)-dust. The renormalization factor can be computed in advance for any given \( \sigma_g \), and we immediately recognize \( w \) as the (normalized) effective dissociation bandwidth that we defined and computed in Sections 2 and 3.

The transfer-dissociation equation for the renormalized LW flux is

\[
\frac{d(w F)}{dz} = -n_1 \sigma_g w F - \frac{RnN_1}{f_{\text{diss}}}, \tag{90}
\]

where again the dust term on the right-hand side refers to H\(_1\)-dust absorption only. Photons absorbed by H\(_2\)-dust anywhere in the slab are excluded from consideration “in advance.”

In dimensionless form

\[
\frac{d\mathcal{F}}{d\tau} = -\mathcal{F} - \frac{2}{\chi}, \tag{91}
\]

where \( \mathcal{F} \equiv F/F(0), \) \( d\tau \equiv n_1 \sigma_g z, \) and

\[
\chi' = w \chi = \frac{\bar{f}_{\text{diss}} \sigma_g w F_0}{Rn}. \tag{92}
\]

We see that \( \chi' \) is just our \( \alpha G \) (Equation (48)). Thus,

\[
\alpha G = w \chi \tag{93}
\]

as already indicated in Step 1.

Most importantly, in Equations (90) and (91) a factor “\( f_1 \)” does not appear at all. The solution is

\[
\mathcal{F}(\tau) = \frac{\chi' + 2}{\chi'} e^{-\tau} - \frac{2}{\chi'}, \tag{94}
\]

where \( \tau \) is the H\(_1\)-dust optical depth, and there are no assumptions on the shape of the H\(_1\)-to-H\(_2\) transition profile. The flux vanishes for \( \tau = \tau_1 \), where

\[
\tau_{1,\text{tot}} = \ln \left( \frac{\chi' + 1}{2} \right) = \ln \left[ \alpha G \left( \frac{2}{\chi'} + 1 \right) \right], \tag{95}
\]

and the expression for the total atomic column is then

\[
N_{1,\text{tot}} = \frac{1}{\sigma_g} \ln \left[ \frac{\alpha G}{2} + 1 \right]. \tag{96}
\]

We have thus recovered our original expressions (39) and (40) for the total atomic column and H\(_1\)-dust opacity for beamed radiation into a slab. It is again clear that these expressions are general. They are valid for large or small \( \alpha G \) (strong or weak fields) for the regimes of significant H\(_1\)-dust and/or H\(_2\)-dust absorption and are independent of the profile shapes (gradual or sharp). We also have in Equation (94) a closed-form expression for the depth-dependent LW-band flux as a function of the H\(_1\)-dust optical depth.

We again see that \( \alpha G \) is the fundamental dimensionless parameter. Physically, \( \alpha G \) is the ratio of the H\(_1\)-dust to H\(_2\)-line absorption rates of the effective dissociation flux, excluding any LW photons that are absorbed by H\(_2\)-dust. The relationship between \( \chi \) and our \( \alpha G \) is now clear. Specifically, \( w \chi \equiv \alpha G \), where crucially our factor \( w \) accounts for H\(_2\)-dust absorption and the resulting reduction of the effective dissociation flux. In the low-Z\(_2\), small-\( \sigma_g \) limit, H\(_2\)-dust is negligible, \( w = 1 \), and \( \chi = \alpha G \). For high Z\(_2\) and large \( \sigma_g \), \( w < 1 \) (decreasing as \( \sigma_g^{-1/2} \) or as \( Z_2^{-1/2} \)), and then \( \alpha G < \chi \). KMT/MK10 did not make the distinction between H\(_1\)-dust and H\(_2\)-dust and ignored the effects of H\(_2\)-dust entirely in their definition of \( \chi \). As we have discussed in Sections 2 and 3, H\(_2\)-dust can reduce the effective dissociation bandwidth by a factor \( \sim 4 \) for the (realistic) range of metallicities in galaxies.

In Figure 10 we again schematically summarize the four regimes that are incorporated by our formula for the total H\(_1\) column density. In each quadrant, large or small \( \alpha G \) for large or small \( Z_2 \), we indicate the shape of the H\(_1\)-to-H\(_2\) transition (sharp or gradual), the dominant source of opacity (H\(_1\)-dust, H\(_2\)-lines, or H\(_2\)-lines plus H\(_2\)-dust), and the expression for the H\(_1\)-dust opacity in terms of the parameters \( \sigma_g, F_0, Rn \), and \( w \).

4.2. Critical H\(_1\)-dust Opacities and H\(_2\) Mass Fractions: Slabs versus Spheres

4.2.1. Slabs

Given our expressions (Equation (40) or Equation (65)) for the total H\(_1\)-dust optical depths in semi-infinite slabs, we can write
direction), the H2 mass fraction is simply

\[ \alpha G/2 \quad w<1 \]








Figure 10. Dominant sources of far-UV absorption (H-dust, H2-lines, and H2-dust). H1-to-H2 transition profile shapes (gradual or sharp), and total H1-dust opacities (large or small), in the \( \alpha G = D_0G/(Rn) = f_{\text{diss}}\sigma gF_0/Rn \equiv w\chi \) vs. \( Z' \) plane.

Figure 11. H2 mass fractions as given by Equations (97), (100), and (102), for plane-parallel slabs ("p"), uniform-density spheres ("s"), and complexes ("c"), as functions of the normalized H1-dust optical depth \( y \).

down a simple formula for the integrated H2 mass fraction, \( f_{H2} \), for planar geometry for a comparison with the KMT/MK10 results for spheres. Our main focus is a comparison of slabs and spheres irradiated by isotropic fields, but we also consider beamed radiation for slabs.

For an isotropic field with a given \( I_{\text{UV}} \), a uniformly illuminated sphere corresponds to two-sided irradiation of a slab of finite width, with properly normalized total optical depths for the sphere and slab. For a slab with total dust thickness \( \tau_c \equiv \sigma_cn z = \sigma_cN \) (where \( N \) is the total gas column density in the normal direction), the H2 mass fraction is simply

\[ f_{H2}^p = 1 - \frac{1}{y}, \quad (97) \]

where \( y \equiv \tau_c/\tau_1 \), and \( \tau_1 \) is the H1-dust depth summed over both sides of the slab (the superscript "p" indicates plane-parallel slab). By definition, \( y \geq 1 \). We plot \( f_{H2}^p \) versus \( y \) in Figure 11.

For optically thick slabs in which the radiation incident on both sides is fully absorbed, and for illumination by isotropic fields, \( \tau_1 = \tau_{1}^{p} \), where

\[ \tau_{1}^{p} = 2(\mu) \ln \left[ \frac{\alpha G/4 + 1}{\langle \mu \rangle} \right] = 1.6 \ln \left[ \frac{\alpha G}{2} \right]. \quad (98) \]

This is twice the optical depth given by our Equation (66) for one-sided illumination of a semi-infinite slab. (We have set \( \langle \mu \rangle = 0.8 \), as found in Section 3.) For beamed radiation \( \tau_1 = \tau_{1}^{p,b} \), where

\[ \tau_{1}^{p,b} = 2 \ln \left[ \frac{\alpha G/2 + 1}{1} \right], \quad (99) \]

given our Equation (39) for one-sided illumination (the superscript "b" is for beamed radiation). We plot \( \tau_{1}^{p} \) and \( \tau_{1}^{p,b} \) versus \( \alpha G \) in Figure 12.

For two-sided illumination of optically thick slabs, Equation (97) for \( f_{H2} \), together with Equation (98) or Equation (99) for the total H1-dust optical depths may be used to compute the integral H2 mass fractions whether the H1-to-H2 transitions are gradual or sharp. For \( \alpha G \gg 1 \), an optically thick slab consists of a simple H1-H2-H1 sandwich structure, with two fully atomic layers outside an inner H2 zone, with sharp transitions between the atomic and molecular layers. For sharp transitions a "critical" optically thick slab occurs for \( y = 1 \) for which an H2 layer just appears at the midplane, and \( \tau_{1}^{p} \) or \( \tau_{1}^{p,b} \) are then the critical H1-dust optical depths. The planar sandwich for sharp transitions corresponds to the spherical core–shell structures considered by KMT/MK10, as illustrated in Figure 13.

4.2.2. Spheres

MK10 carried out their iterative radiative transfer procedure to compute spherical H1 shell and H2 core structures for two types of systems. First, they considered "uniform density" spheres for which the density of hydrogen nuclei, \( n = n_1 + 2n_2 \), is constant through the spheres as in our slabs. Second, they considered "atomic–molecular complexes" in which the H2 gas density, \( n_2 \), is 10 times the atomic density, \( n_1 \), for approximate pressure equilibrium between the shells and the cores. MK10 then presented fitting formulae (their Equations (82) and (93)) for \( f_{H2} \) in uniform density spheres and complexes, as functions of their cloud parameters \( \chi \) and \( \tau_1 \).
We can re-express the MK10 formulae for $f_{H_2}$ as simple functions of $y$, similar to our Equation (97) for slabs. For spheres $y \equiv \langle \tau \rangle / (\tau_1)$, where $\langle \tau \rangle \equiv \sigma_\tau \langle N \rangle$ is the area-averaged total dust column density of the sphere and where $\langle N \rangle \equiv M_{\text{gas}}/m_\pi r^2$ is the average gas column density, $r$ is the cloud radius, and $m_\pi$ is the mean particle mass per hydrogen nucleon. For a uniform density sphere, the total optical depth $\langle \tau_1 \rangle = \langle \tau_1 \rangle \equiv (4/3)\sigma_\tau m_\pi r$, so for a complex, $\langle \tau_1 \rangle = (4/3)\sigma_\tau m_\pi r = \langle \tau_1 \rangle$, where $n_1$ is the gas density in the atomic shell. The parameter $y$ is defined such that the total optical depth $\langle \tau \rangle$ is normalized relative to the critical (area-averaged) dust depth $\langle \tau_1 \rangle$ required for the appearance of an H$_2$ core at $r = 0$. The critical depths $\langle \tau_1 \rangle$ are auxiliary quantities also computed by MK10 for the uniform density spheres and complexes, assuming irradiation by isotropic radiation fields. The $\langle \tau_1 \rangle$ for spheres correspond to our $r_1^2$ for two-sided illumination of slabs by isotropic fields. In our terminology, these are the (total) H$_2$-dust optical depths in spheres and slabs. For sharp transitions these are critical optical depths.

The MK10 fitting formula (their Equation (82)) for the H$_2$ mass fraction in uniform density spheres may be rewritten as

$$f_{H_2}^s \simeq 1 - \frac{1.5}{y + 0.5y^{-1.8}}$$

(100)

(where the superscript “s” is for spheres). Their critical H$_2$-dust optical depth is

$$\langle \tau_1 \rangle = 1.1 \times \ln[1 + 0.6\alpha G + 0.01(\alpha G)^2].$$

(101)

Again, in Equation (100) $y \equiv \langle \tau \rangle / (\tau_1)$. In Figures 11 and 12 we plot $f_{H_2}^s$ versus $y$ and $\langle \tau_1 \rangle$ versus $\alpha G$ for comparisons with our expressions for slabs.

For complexes, the MK10 fit formula for the H$_2$ mass fraction (their Equation (93)) may be rewritten as

$$f_{H_2}^c \simeq 1 - \frac{1.5}{y + 0.5}.$$  

(102)

(The superscript “c” is for complexes.) Fully atomic complexes and uniform density spheres are identical, so the critical H$_2$-dust depth $\langle \tau_1 \rangle$ for complexes is also given by Equation (101). Because of the compression of the molecular gas, the functional form for $f_{H_2}$ is altered compared with uniform density spheres, and the $y^{-1.8}$ factor in the denominator of Equation (100) is replaced by unity in Equation (102). We also plot $f_{H_2}^c$ for the complexes in Figure 11.

Figure 12 shows the similarity in the critical H$_2$-dust optical depths for slabs and spheres. For isotropic fields, and for $\alpha G$ ranging from 0.01 to 10$^2$, the differences are no greater than 20%. Furthermore, Figure 12 shows that switching from isotropic to corresponding beamed radiation for a slab is in fact much more significant than switching from a slab to a sphere for an isotropic field. For isotropic fields, the H$_2$-dust optical depths for slabs and complexes are equal for $\alpha G \approx 1.5$, so for two-phased H$_1$ equilibrium ($\alpha G_{\text{CNM}}/2 \sim 1$) the differences between the H$_2$-dust optical depths for spheres and slabs are negligible. Thus, for $\alpha G \sim 1$ any differences between spheres and slabs arise only because of any remaining differences in the functional forms for $f_{H_2}$. 

Figure 11 shows the similarity and small differences in $f_{H_2}$ for slabs, uniform-density spheres, and complexes, as given by Equations (97), (100), and (102). For slabs, our formula (97) for $f_{H_2}$ is unaltered if the molecular gas is assumed to be denser than the atomic gas, and there is no distinction between uniform-density and isobaric conditions. The differences are all small. For example, for a spherical complex compared with a slab, the percentage difference in $f_{H_2}(y)$ is at most 40% at $y = 3$.

4.2.3. H$_2$ Mass Fractions and Star-formation Thresholds in Self-regulated Gas

If H$_2$ is a requirement for star formation, we may define the cloud gas column at which $f_{H_2} = 0.5$ as the “star-formation threshold.” This is a plausible definition for sharp H$_1$-to-H$_2$ transitions for which a “sterile” atomic layer is well defined. As given by Equations (97), (100), and (102), $f_{H_2} = 0.5$ for $y = 2, 2.93,$ and 2.5, for slabs, uniform density spheres, and complexes. We define $\Sigma_{\text{gas,}}$ as the threshold gas mass surface density for which $f_{H_2} = 0.5$.

For estimates of metallicity-dependent H$_2$ mass fractions and star-formation thresholds in Kennicutt–Schmidt relations for galaxy disks, we adopt the KMT/MK10 “self-regulation” ansatz that the H$_1$ in star-forming clouds is typically driven to the CNM densities/pressures required for two-phase equilibria as set by the stellar FUV radiation fields. Thus, for any Z' we assume that $\alpha G = \alpha G_{\text{CNM}}(Z')$ (Equation (59)). Because $(\alpha G_{\text{CNM}} \sim 1$ to 2 for all Z'), the H$_1$-to-H$_2$ transitions are sharp to a good approximation (as argued by KMT/MK10). For our
slabs we therefore assume H$_2$-H$_2$-H$_1$ sandwich structures, for which critical optically thick slabs occur at $y = 1$ (as discussed in Section 4.2.1).

We present four sets of computations to compare results for spheres versus slabs.

First, in Figure 14, panel (a), we use Equations (102) and (101) to reproduce the MK10 results for $f_{H_2} (\Sigma_{gas})$ for spherical atomic–molecular complexes (Figure 5 in MK10). Here $\Sigma_{gas} \equiv (m/\sigma_g)(\tau)$ is the area-averaged gas mass surface density, where $m$ is the mean particle mass per hydrogen nucleus and $\tau$ is the area-averaged dust opacity. Thus, in Equation (102) $y = \Sigma_{gas}/\Sigma_1$, where $\Sigma_1 \equiv (m/\sigma_g)(\tau_1)$, and where $\langle \tau_1 \rangle$ is given by Equation (101) for each ($\alpha G)_{CNM}$. We set $m = 2.34 \times 10^{-24}$ g as appropriate for a cosmic hydrogen–helium mixture. KMT/MK10 assume that the dust cross section scales with metallicity as $\sigma_g = 1.0 \times 10^{-21} Z' \text{ cm}^2$, so we set our $\phi_g = 1/1.9$ (see Equation (20)). MK10 also implicitly assume that H$_2$-dust absorption is negligible for all $Z'$, so we exclude our H$_2$-dust term, $(2.64 \phi_g Z')^{1/2}$, in the denominator of Equation (59). The resulting curves for $f_{H_2}$ as functions of $\Sigma_{gas} \ (M_\odot \text{ pc}^{-2})$ are displayed in Figure 14 for $Z'$ ranging from 0.01 to 10. They are a precise reproduction of the MK10 results (their Figure 5). For example, with the above assumptions, $Z' = 1$ gives $(\alpha G)_{CNM} = 3.6$ so that $\langle \tau_1 \rangle = 1.3$, and a molecular core appears ($y = 1$) for $\Sigma_{gas} = 14.6 M_\odot \text{ pc}^{-2}$. The $f_{H_2} = 0.5$ star-formation threshold ($y = 2.5$) is then $\Sigma_{gas, crit} = 36.5 M_\odot \text{ pc}^{-2}$. For smaller (larger) $Z'$, the curves shift to the right (left) exactly as in Figure 5 of MK10.

Second, in Figure 14, panel (b), we show results for spherical complexes, again with $\phi_g = 1/1.9$ but now with the H$_2$-dust term included in the estimate for $(\alpha G)_{CNM}(Z')$. As expected, for very low $Z'$ the $f_{H_2}$ curves and the corresponding star-formation thresholds are unaltered, since this is the complete line overlap regime for which H$_2$-dust is negligible. However, for $Z' \gtrsim 0.3$ the curves start to shift to the left and the thresholds are reduced to smaller gas mass surface densities. These shifts are due to the reductions of the effective dissociation fluxes by the non-negligible H$_2$-dust opacities. For example, when H$_2$-dust is included for $Z' = 1$ we have $(\alpha G)_{CNM} = 1.6$ (for $\phi_g = 1/1.9$) so that $\langle \tau_1 \rangle = 0.77$, and the H$_2$ core appears at $\Sigma_{gas, crit} = 8.6 M_\odot \text{ pc}^{-2}$ and $\Sigma_{gas, crit} = 21.5 M_\odot \text{ pc}^{-2}$. The inclusion of H$_2$-dust in the estimate for $(\alpha G)_{CNM}$ modifies the MK10 results for solar and super-solar metallicities.

Third, in Figure 14, panel (c), we again adopt the MK10 assumptions, $\phi_g = 1/1.9$ and negligible H$_2$-dust for any $Z'$ but for slabs instead of spheres, and we use Equation (97) to compute...
The fundamental dimensionless parameter in the problem is

\[ \alpha G = \frac{D_0 G}{R_n} = \frac{\sigma_f \bar{f}_I W_{g,\text{tot}}}{R_n} = f_{\text{disc}} \sigma_g w F_0 \frac{R_n}{R_n} = 1.54 \frac{I_{UV}}{(n/100 \text{ cm}^{-3})} \left(1 + (2.64 \phi_g Z)^{1/2}\right). \]

(See also expressions (49) and (50).) Here \( I_{UV} \) is the free-space FUV intensity (relative to the Draine field), \( D_0 \) is the free-space (optionally thin) \( \text{H}_2 \) photodissociation rate \( (s^{-1}) \), \( n \) is the total hydrogen gas volume density \( (\text{cm}^{-3}) \), \( R \) is the \( \text{H}_2 \) formation rate coefficient \( (\text{cm}^3 \text{ s}^{-1}) \), \( G \) (dimensionless) is the mean self-shielding

\[ \Sigma_{\text{gas, s}}(Z') = \frac{12}{\phi_{s'} Z'} M_\odot \text{ pc}^{-2}. \]
| Symbol | Definition | Units |
|--------|------------|-------|
| $\tilde{Z}_0$ | Far-UV specific photon intensity. | photons cm$^{-2}$ s$^{-1}$ Hz$^{-1}$ sr$^{-1}$ |
| $\tilde{Z}_i^\text{ISM}$ | Free-space far-UV specific intensity (Equation (21)). | photons cm$^{-2}$ s$^{-1}$ Hz$^{-1}$ sr$^{-1}$ |
| $I_{\text{UV}}$ | Intensity scaling factor relative to the unit free-space Draine field. | ... |
| $F_i$ | Flux density, $F_i \equiv 4\pi \tilde{Z}_i$. | photons cm$^{-2}$ s$^{-1}$ Hz$^{-1}$ |
| $\tilde{F}_l$ | Mean flux density in LW band (Equation (12)). | photons cm$^{-2}$ s$^{-1}$ Hz$^{-1}$ |
| $F_{(z)}$ | Free-space LW band photon flux integral (Equations (3) and (4)). | photons cm$^{-2}$ s$^{-1}$ |
| $F_{(z)}(\sigma)$ | Beamed photon flux density at linear depth $z$ in a slab. | photons cm$^{-2}$ s$^{-1}$ Hz$^{-1}$ |
| $\sigma_{\nu,d}$ | H$_2$ photodissociation cross section at frequency $\nu$ (Equations (7) and (77)). | cm$^2$ |
| $\sigma_d$ | Individual H$_2$-line photodissociation cross section (Equation (9)). | cm$^2$ Hz |
| $\sigma_{\nu,d}^\text{tot}$ | H$_2$ photodissociation cross section summed over all lines (Equation (13)). | cm$^2$ Hz |
| $D$ | Depth-dependent H$_2$ photodissociation rate. | s$^{-1}$ |
| $D_0$ | Free-space H$_2$ photodissociation rate (Equation (5) and (15)). | s$^{-1}$ |
| $D(0)$ | H$_2$ photodissociation rate at the surface of a optically thick slab (Equation (6)). | s$^{-1}$ |
| $P_{ij}$ | LW photon H$_2$ pumping rate out of ro-vibrational level $ij$ (Table 1). | ... |
| $f_{\text{diss}}(ij)$ | Mean dissociation probability out of level $ij$ (Table 1). | ... |
| $f_{\text{diss}}$ | Mean dissociation fraction per absorbed LW photon (Equation (18)). | ... |
| $\sigma_g$ | Far-UV grain absorption cross section per hydrogen nucleon (Equation (20)). | cm$^2$ |
| $\phi_g$ | Order unity grain composition factor. | ... |
| $Z'$ | Metallicity relative to solar abundances. | ... |
| $R$ | Grain surface H$_2$ formation rate coefficient (Equation (21)). | cm$^3$ s$^{-1}$ |
| $T$ | Gas temperature. | K |
| $n_1$ | Atomic hydrogen (H I) volume density. | cm$^{-3}$ |
| $n_2$ | Molecular hydrogen (H$_2$) volume density. | cm$^{-3}$ |
| $n$ | Total hydrogen gas volume density, $n \equiv n_1 + 2n_2$. | cm$^{-3}$ |
| $N_1$ | H I column density. | cm$^{-2}$ |
| $N_2$ | H$_2$ column density. | cm$^{-2}$ |
| $N$ | Hydrogen gas column density, $N \equiv N_1 + 2N_2$. | cm$^{-2}$ |
| $\tau_g \equiv \sigma_g N$ | Dust opacity in normal direction. | ... |
| $N_{1,\text{tot}}$ | Total H I column density on one side of an optically thick slab. | cm$^{-2}$ |
| $\tau_{1,\text{tot}} \equiv \sigma_g$ | H I-dust opacity in normal direction. | ... |
| $W_d(N_2)$ | H$_2$-line overlap limited dissociation bandwidth. | Hz |
| $W_{d,I}^2(N_2)$ | H$_2$-dust-limited dissociation bandwidth. | Hz |
| $W_{d,\text{tot}}$ | Total H$_2$-dust-limited dissociation bandwidth. | Hz |
| $w$ | Normalized H$_2$-dust-limited dissociation bandwidth (Equation (29)). | ... |
| $f_{\text{shield}}(N_2)$ | H$_2$ self-shielding function (Equations (16) and (72)). | ... |
| $(\mu)$ | Mean ray-angle factor for H I-dust opacity (Equations (63) and (75)). | ... |
| $\alpha \equiv D_0/(Rn)$ | Free-space atomic-to-molecular density ratio (Equations (34) and (44)). | ... |
| $G(\sigma_g)$ | Mean self-shielding factor (Equations (41), (45)–(48)). | ... |
| $\alpha G$ | Fundamental dimensionless parameter for the HI-to-H$_2$ transition (Equations (49)–(51)). | ... |
| $\rho_{\text{CNM}}$ | CNM gas density for multiphased H I equilibrium (Equation (58)). | cm$^{-3}$ |
| $(\alpha G)_{\text{CNM}}$ | $\alpha G$ for two-phase H I equilibrium (Equation (59)). | ... |
| $\Sigma_{\text{H}_2}$ | H$_2$ mass surface density in plane-parallel slab. | $M_\odot$ pc$^{-2}$ |
| $\Sigma_{\text{gas}}$ | Total gas mass surface density in plane-parallel slab. | $M_\odot$ pc$^{-2}$ |
| $M_{\text{H}_2}$ | H$_2$ gas mass within sphere. | $M_\odot$ |
| $M_{\text{gas}}$ | Total gas mass within sphere. | $M_\odot$ |
| $\tau_z \equiv n_2 \sigma_g z$ | Total dust optical depth through slab of finite linear width $z$. | ... |
| $\tau_r \equiv n_2 \sigma_g r$ | Dust optical depth along radius $r$ of a sphere. | ... |
| $y$ | Total dust optical depth normalized to the H I-dust optical depth (Equation (97)). | ... |
Table 2
(Continued)

| Symbol | Definition | Units |
|--------|------------|-------|
| $f_{\text{H}_2}$ | H$_2$ mass fraction for slab (Equation (97)). | ··· |
| $f_{\text{H}_2}$ | H$_2$ mass fraction for uniform density sphere (Equation (100)). | ··· |
| $f_{\text{H}_2}$ | H$_2$ mass fraction for spherical atomic-molecular complex (Equation (102)). | ··· |
| $\Sigma_{\text{gas},*}$ | Star-formation threshold gas surface density at which $f_{\text{H}_2} = 0.5$. | $M_\odot$ pc$^{-2}$ |

Our formulae for the H$_1$ columns and H$_2$ mass fractions may be incorporated easily into hydrodynamics simulations for galaxy evolution.

For $\alpha G/2 \lesssim 1$ the H$_1$-to-H$_2$ transitions are gradual, and the atomic columns are built up in the predominantly molecular portions of the cloud. For $\alpha G/2 \gtrsim 1$ the transitions are sharp, and the H$_1$ is built up in outer fully atomic layers. For sharp transitions, the H$_1$-H$_2$-H$_1$ sandwich structure for slabs corresponds to H$_1$ shell and H$_2$ core structures for spheres. If star-formation requires the conversion to H$_2$, then a threshold surface density, $\Sigma_{\text{gas},*}$, may be defined at which the molecular fraction $f_{\text{H}_2} = 0.5$. For $\alpha G/2 \gtrsim 1$ and sharp transitions we then have $\Sigma_{\text{gas},*} \equiv 2\Sigma_{\text{H}_1}$.

For self-regulated galaxy disks (ala KMT/MK10) in which the H$_1$ is driven to two-phased thermal equilibrium (and heated by FUV photoelectric emission from dust grains), the dimensionless parameter $\alpha G$ is restricted to a narrow range close to $(\alpha G)_{\text{CNM}}$, where

$$
\frac{(\alpha G)_{\text{CNM}}}{2} \approx 1,
$$

independent of the metallicity $Z'$. For such self-regulated systems, our theory then predicts a metallicity-dependent H$_1$-to-H$_2$ star-formation threshold for individual clouds

$$
\Sigma_{\text{gas},*}(Z') \approx \frac{12}{\phi_g Z'} M_\odot \text{ pc}^{-2}.
$$

This appears consistent with Galactic and extragalactic observations, at least for solar metallicity systems.

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APPENDIX

GLOSSARY OF SYMBOLS

Table 2 is a glossary of symbols we have used in this paper. In this listing we also refer to the equations in which the various symbols appear and/or are defined.
