ANALYTIC H I-to-H2 PHOTODISSOCIATION TRANSITION PROFILES

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ABSTRACT

We present a simple analytic procedure for generating atomic (H I) to molecular (H2) density profiles for optically thick hydrogen gas clouds illuminated by far-ultraviolet radiation fields. Our procedure is based on the analytic theory for the structure of one-dimensional H I/H2 photon-dominated regions, presented by Sternberg et al. Depth-dependent atomic and molecular density fractions may be computed for arbitrary gas density, far-ultraviolet field intensity, and the metallicity-dependent H2 formation rate coefficient, and dust absorption cross section in the Lyman–Werner photodissociation band. We use our procedure to generate a set of H I-to-H2 transition profiles for a wide range of conditions, from the weak- to strong-field limits, and from super-solar down to low metallicities. We show that if presented as functions of dust optical depth, the H I and H2 density profiles depend primarily on the Sternberg “αG parameter” (dimensionless) that determines the dust optical depth associated with the total photodissociated H I column. We derive a universal analytic formula for the H I-to-H2 transition points as a function of just αG. Our formula will be useful for interpreting emission-line observations of H I/H2 interfaces, for estimating star formation thresholds, and for sub-grid components in hydrodynamics simulations.

Key words: galaxies: star formation – ISM: clouds – methods: analytical – photon-dominated region (PDR) – radiative transfer

1. INTRODUCTION

Stars form in dense molecular hydrogen (H2) cores that are shielded from external ultraviolet (UV) radiation. The H2 plays a crucial role in the chemistry that occurs, and its formation leads to the subsequent production of other molecules such as CO, OH, and H2O (e.g., Herbst & Klemperer 1973; Sternberg & Dalgarno 1995; Tielens 2013; van Dishoeck et al. 2013; Bialy et al. 2015). These species are efficient coolants, and are able to cool the gas to very low temperatures ~10–20 K, reducing the Jeans masses and enabling fragmentation. Star formation may be triggered by the atomic-to-molecular (H I-to-H2) phase transition. Alternatively, production of H2 may be enhanced in the denser and optically thicker gas. Theoretically, the atomic gas converts to molecular form once the H I column density reaches a critical value. Such a threshold is expected since the H I is often a dissociation product of penetrating far-ultraviolet (FUV) radiation in a photon-dominated region (PDR). With increasing column density, the combination of H2 self-shielding and dust absorption attenuate the radiation field, and a conversion from H I to H2 occurs.

Theoretically, the H I-to-H2 conversion in PDRs has been widely investigated through analytic and numerical studies (e.g., Federman et al. 1979; van Dishoeck & Black 1986; Sternberg 1988; Draine & Bertoldi 1996; Kaufman et al. 1999; Browning et al. 2003; McKee & Krumholz 2010; Gnedin & Draine 2014; Liszt 2015), as well as in hydrodynamics simulations (e.g., Robertson & Kravtsov 2008; Gnedin et al. 2009; Glover et al. 2010; Bisbas et al. 2012; Davé et al. 2013; Thompson et al. 2014; Lagos et al. 2015).

Sternberg et al. (2014, hereafter S14) presented analytic and detailed radiative transfer computations for the H I-to-H2 transitions in one-dimensional gas slabs irradiated by isotropic or beamed FUV radiation, and with emphasis on the build-up of the photodissociated H I columns in optically thick gas. They considered depth-dependent multi-line H2 photodissociation, and derived analytic formulae for the resulting total H I columns. An important quantity is the dust opacity, τ1,tot, associated with the total H I column. S14 refer to this as “H I-dust” opacity and derived the analytic expression

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

for a slab exposed to beamed radiation. Here \( \sigma_g \) (cm2) is the metallicity-dependent dust absorption cross-section per hydrogen nucleon in the 11.2–13.6 eV Lyman–Werner (LW) photodissociation band, and \( N_{1,tot} \) is the total H I column produced by photodissociation in optically thick clouds, in which all of the radiation is absorbed. The basic dimensionless parameter, \( \alpha G \), that appears in this expression depends on several quantities (see Equation (20) in Section 2) and is proportional to the ratio of the FUV intensity to gas density. For realistic ISM conditions, \( \alpha G \) may range from large (\( \gg 1 \)) to small (\( \ll 1 \)), and the H I dust opacity may or may not be significant.

In this paper, we extend the S14 formalism to develop a simple analytic procedure for the construction of complete depth-dependent atomic and molecular density profiles for FUV-illuminated gas. The “density profiles” are the local volume gas densities of H I and H2 as functions of cloud depth, as parameterized by the total gas column density, or alternatively by the dust optical depth and/or visual extinction. The analytic procedure we present in this paper provides a simple and quick method to generate such density profiles for a
wide range of gas densities and radiation field intensities, and also the \( \text{H}_2 \) formation efficiencies and dust absorption cross-sections, as specified by the dust-to-gas mass ratio and the overall metallicity. Following the formalism presented in S14, we show that the density profiles depend on the same two parameters, \( \sigma \) and \( \alpha_G \), that determine the total \( \text{H} \) I columns. We use our procedure to generate \( \text{H} \) I-to-\( \text{H}_2 \) density profiles for a wide range of conditions, including for very low metallicities and dust-to-gas ratios.

Of particular interest are the gas columns and/or dust optical depths at which the conversion from atomic-to-molecular form occurs. We will show that when expressed in terms of the dust optical depth, the transition points, \( \tau_{\text{tran}} \), depend almost entirely on just \( \alpha_G \), just as for the expression for \( \tau_{\text{log}} \). Remarkably, this is irrespective of whether the conversion point is governed by \( \text{H}_2 \) line self-shielding or \( \text{H} \) I dust opacity. We derive a universal fitting formula for the transition optical depth, given by

\[
\tau_{\text{tran}} \equiv \sigma \frac{N_{\text{tran}}}{N_{\text{gas}}} = \beta \ln \left( \frac{\alpha G}{2} \right)^{1/\beta} + 1.
\]

In this expression \( N_{\text{tran}} \) is the gas column, atomic plus molecular, at which the transition occurs. For dust-to-gas ratios within 0.1–10 times the standard ISM value, we find that \( \beta = 0.7 \) gives the transition point to high accuracy, for any \( \alpha_G \).

Our formula will be useful for interpreting observations since the \( \text{H} \) I/\( \text{H}_2 \) transition layers are expected sources of rovibrational emissions from warm molecules (e.g., Timmermann et al. 1996; Rosenthal et al. 2000; Rodríguez-Fernández et al. 2001; Allers et al. 2005; Shaw et al. 2009; Sheffer et al. 2011). Our formula will also be useful as a “sub-grid” ingredient in simulations that incorporate atomic-to-molecular conversion (GNedin et al. 2009; Mac Low & Glover 2012; Davé et al. 2013; Valdivia & Hennebelle 2014; Thompson et al. 2014; Bahe et al. 2016). This is because with our formula, the transition point may be expressed in terms of external parameters only (i.e., those that enter \( \alpha_G \)) without requiring a solution for the detailed density profiles or the consideration of molecular self-shielding functions.

The structure of our paper is as follows. In Section 2 we briefly review the S14 formalism, and elaborate on it to show that \( \alpha_G \) and \( \sigma \) fully determine the \( \text{H} \) I and \( \text{H}_2 \) density profiles. In Section 3 we develop our analytic procedure for the construction of the atomic and molecular density profiles and we present formulae for the necessary auxiliary functions. In Section 4 we present our set of density profiles computed for a wide range of \( \alpha_G \) and \( \sigma \), and we discuss their properties. We then derive our fitting formula for the atomic-to-molecular transition points, and also present attenuation factors. In Section 5 we obtain a threshold for the gas mass surface density required for star formation. We summarize and conclude in Section 6.

2. THEORY

In this section we describe the basic analytic theory for the depth-dependent variation of the atomic and molecular gas densities through steady-state PDRs. We follow the S14 theoretical framework for semi-infinite gas slabs. S14 considered irradiation by isotropic or beamed fields. Here we assume beamed irradiation.

This theoretical analysis is for \( \text{H}_2 \) photodissociation by FUV LW photons. \( \text{H}_2 \) destruction by cosmic-ray and/or X-ray ionization requires a separate treatment (e.g., Maloney et al. 1996; Meijerink & Spaans 2005; Bialy & Sternberg 2015).

2.1. Basic Equations

For steady-state conditions, and for beamed radiation into one side of an optically thick slab,

\[
R n m = \frac{1}{2} D_0 f_{\text{att}} n_2.
\]

The left-hand side is the \( \text{H}_2 \) formation rate per unit volume (\( \text{cm}^{-3} \text{ s}^{-1} \)), where \( R \) is the \( \text{H}_2 \) formation rate coefficient (cm\(^{-3} \) s\(^{-1} \)). The right-hand side is the local (attenuated) photodissociation rate per unit volume, where \( D_0 \) is the free-space (unattenuated) photodissociation rate (s\(^{-1} \)), and \( f_{\text{att}} \) is the depth-dependent attenuation factor accounting for \( \text{H}_2 \)-self-shielding and dust absorption. In Equation (1), \( n_1 \) and \( n_2 \) are the local atomic and molecular volume densities (\( \text{cm}^{-3} \)) and \( n \equiv n_1 + 2n_2 \) is the total gas density. For steady state this equality holds at every cloud depth.

The free-space \( \text{H}_2 \) photodissociation rate is \( D_0 = \sigma_{d} F_{\nu} \), where \( F_{\nu} \) is the mean LW band flux density (photons cm\(^{-2} \) s\(^{-1} \) Hz\(^{-1} \)). As computed by S14, \( \sigma_d = 2.36 \times 10^{-3} \text{ cm}^{2} \text{ s}^{-1} \) Hz\(^{-1} \) is the total \( \text{H}_2 \)-line photodissociation cross-section, summed over all the lines. For a Draine (1978) far-UV radiation spectrum \( F_{\nu} = 2.46 \times 10^{-4} I_{\nu, \text{UV}} \text{ photon cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1} \), and \( D_0 = 5.8 \times 10^{-11} I_{\nu, \text{UV}} \text{ s}^{-1} \), where \( I_{\nu, \text{UV}} \) is the radiation strength relative to the Draine field, for which \( I_{\nu, \text{UV}} = 1 \). The factor 1/2 in Equation (1) accounts for the removal of half of the free-space energy density by the optically thick slab.

Equation (1) is the fundamental relation for PDR theory, and it must be solved, either numerically or analytically, for the depth-dependent atomic and molecular volume densities, and the conversion from \( \text{H} \) I to \( \text{H}_2 \).

With increasing cloud depth the photodissociation rate is reduced by a combination of \( \text{H}_2 \)-line self-shielding and dust opacity, and the molecular fraction increases. In Equation (1), \( f_{\text{att}} \leq 1 \) is the attenuation factor,

\[
f_{\text{att}} (N_2, N) = f_{\text{shield}} (N_2) e^{-\tau},
\]

and is the product of the dust attenuation term, \( e^{-\tau} \), and the \( \text{H}_2 \)-self-shielding function \( f_{\text{shield}} (N_2) \). Here

\[
\tau \equiv \sigma_{g} N
\]

is the dust opacity in the LW band, where \( N = N_1 + 2N_2 \) is the hydrogen column density, in atoms plus molecules, from the cloud surface to the given cloud depth, and \( \sigma_g \) is the LW band dust absorption cross-section per hydrogen nucleon.\(^1\) In Equation (2) we assume absorption (and pure forward scattering) by the grains, and neglect the (small) effects of back-scattering discussed by (Goicoechea & Le Bourlot 2007, see also S14).

The visual extinction is related to \( \tau \) through

\[
A_{V} = 5.3 \times 10^{-22} N \text{ cm}^{2} \text{ mag}
= 0.28 \tau \text{ mag}.
\]

\(^1\) In this paper we are following the S14 notation for which the subscript “d” refers to photodissociation, and “g” refers to dust grains. Thus, \( \sigma_d \) is the photodissociation cross-section, and \( \sigma_g \) is the dust-grain absorption cross-section.
Both $\sigma_g$ and $A_V/N$ are proportional to the dust-grain surface area, and therefore depend strongly on the dust-to-gas ratio. The dust-to-gas ratio may be further related to the overall gas metallicity.

For standard interstellar dust and assuming a linear relation between the dust-to-gas ratio and gas metallicity

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

(5)

where $Z'$ is the metallicity relative to solar and $\phi_g$ is a factor of the order of unity (Draine 2003, S14). For low metallicities the dust-to-gas ratio may scale superlinearly with the metallicity (Rémy-Ruyer et al. 2014) and $\sigma_g$ will then scale accordingly.

In our discussion below we consider $\sigma_g$ as a variable, and we define a normalized cross-section

$$\bar{\sigma}_g \equiv \frac{\sigma_g}{1.9 \times 10^{-21} \text{ cm}^2},$$

(6)

relative to the standard Galactic value.

As discussed in S14, $f_{\text{shield}}$ depends on the molecular column, $N_2$, only, and its basic definition is

$$f_{\text{shield}}(N_2) = \frac{1}{\sigma_d} \frac{dW_d(N_2)}{dN_2}.$$  

(7)

In this expression $W_d(N_2)$ is the bandwidth (Hz) of LW radiation absorbed in molecular photodissociations up to $N_2$, in a dust-free cloud, and is referred to as the “dust-free $N_2$-line photodissociation bandwidth.” Both $W_d(N_2)$ and its derivative $f_{\text{shield}}(N_2)$ are very weakly dependent on the internal molecular excitation state (see S14) and hence may be computed in advance independent of external cloud parameters such as the gas density and field intensity. We discuss analytic forms for $f_{\text{shield}}(N_2)$ and $W_d(N_2)$ in Section 3.

In Equation (1)

$$\alpha = \frac{D_0}{R n} = \frac{\sigma_d F_d}{R n}$$

$$= 5.8 \times 10^4 I_{\text{UV}} \left(\frac{10^{-17} \text{ cm}^2 \text{s}^{-1}}{R}\right) \frac{\left(100 \text{ cm}^{-3}/n\right)}{n},$$

(8)

is the (dimensionless) ratio of the free-space $N_2$ photodissociation rate to the $H_2$ formation rate. The parameter $\alpha$ is proportional to the ratio $I_{\text{UV}}/n$, but it also depends on the $H_2$ rate coefficient $R$. The $H_2$ formation rate coefficient depends on several quantities, including the gas-to-dust ratio and the gas and dust temperatures (e.g., Hollenbach & McKee 1979; Cazaux & Spaans 2004; Le Bourlot et al. 2012). A characteristic value for $R$ is

$$R = 3 \times 10^{-17} \bar{\sigma}_g \text{ cm}^3 \text{s}^{-1},$$

(9)

with the further assumption that $R \propto \sigma_g$ since both quantities depend on the dust-grain surface area. This gives

$$\alpha = 1.9 \times 10^4 I_{\text{UV}} \left(\frac{100 \text{ cm}^{-3}/n}{n}\right) \frac{1}{\bar{\sigma}_g}. $$

(10)

Therefore, as long as $H_2$ formation is dominated by dust catalysis, $\alpha$ is inversely proportional to the dust absorption cross-section. For very low metallicities, $H_2$ formation is dominated by gas phase reactions (e.g., Cazaux & Spaans 2004; Bialy & Sternberg 2015), independent of $\sigma_g$.

In terms of $\alpha$, Equation (1) may be rewritten as

$$\frac{n_1}{n_2} = \frac{1}{2} \alpha f_{\text{att}}. $$

(11)

At the cloud boundary $f_{\text{att}} \rightarrow 1$ and the $H_1$ to $H_2$ density ratio $n_1/n_2 \rightarrow 0.5\alpha$. Since $n = n_1 + 2n_2$ the $H_1$ and $H_2$ fractions at the cloud boundary are $2n_2/n = 1/(1 + 0.25\alpha)$ and $n_1/n = 0.25\alpha/(1 + 0.25\alpha)$. For most astrophysical conditions $\alpha \gg 1$ and the gas is predominantly atomic at the unshielded boundaries, with $n_1/n \approx 1$ and $2n_2/n \approx 4/\alpha$.

The essential problem is to solve Equation (11) for $n_1$ and $n_2$ as functions of cloud depth, as parameterized by the gas column $N = N_1 + 2N_2$ (or visual extinction via Equation (4)). The solution is non-trivial because the attenuation factor depends on $N_2$ and $N$ in combination, not just on $N$ alone. Thus, to obtain a solution for $n_1(N)$ and $n_2(N)$, one has to first solve for $N_2$ as a function of $N$.

2.2. No Dust Absorption

A simplifying case is the limit where dust absorption is negligible, i.e., $\alpha \ll 1$, for which $f_{\text{att}} \rightarrow f_{\text{shield}}$ and self-shielding dominates. Assuming $R n$ constant, and with Equation (7) for $f_{\text{shield}}$, and with $n_1/n_2 = dN_1/dN_2$ for slab geometry, integration gives

$$N_2(N_1) = \frac{1}{2} \alpha \frac{W_d(N_1)}{\sigma_d} = \frac{1}{2} \frac{F_d W_d(N_1)}{R n}, $$

(12)

for the accumulated $H_1$ column as a function of $N_2$. For any $\alpha$, and given the precomputed $W_d(N_1)$, and with $N = N_1 + 2N_2$, Equation (12) gives $N_1(N)$ and $N_2(N)$.

Equation (11) with $n = n_1 + 2n_2$ then gives $n_1(N)$ and $n_2(N)$. Thus, when dust absorption is negligible, the $H_1$ and $H_2$ density profiles are fully determined by the dimensionless parameter $\alpha$. This solution is valid only up to gas columns $N \lesssim 5 \times 10^{20}/\bar{\sigma}_g \text{ cm}^{-2}$ (for which $\alpha \lesssim 1$). For larger columns, dust absorption becomes significant.

2.3. Inclusion of Dust Absorption

With the inclusion of dust absorption, $f_{\text{att}}$ becomes a function of both $N_2$ and $N$, and $\sigma_g$ enters as a parameter. However, since $e^{-\alpha} \equiv e^{-\sigma_g N} = e^{-\sigma_g N_1} \times e^{-2\sigma_g N_2}$, Equation (11) is separable and may be written as

$$e^{-\sigma_g N_1} dN_1 = \frac{\alpha}{2} f_{\text{shield}}(N_2) e^{-2\sigma_g N_2} dN_2$$

$$= \frac{\alpha}{2} \frac{dW_d}{dN_2} dN_2,$$

(13)

where again $n_1/n_2 = dN_1/dN_2$, as appropriate for slab geometry. With this separation, and again assuming that $R n$ is constant through the cloud, $N_1$ can still be expressed as a function of $N_2$, as follows.

The derivative on the right-hand side of Equation (14) is of the form

$$W_d(N_2; \sigma_g) = \int_0^{N_2} \frac{dW_d(N_2)}{dN_2} e^{-2\sigma_g N_2} dN_2'$$

$$= \sigma_d \int_0^{N_2} f_{\text{shield}}(N_2') e^{-2\sigma_g N_2'} dN_2'. $$

(14)
Importantly, the exponential term in the integrand definition of \( W_\ell(N_2; \sigma_g) \) accounts for the dust opacity associated with the H\(_2\) column only ("H\(_2\)-dust"). Thus, as discussed in S14, \( W_\ell(N_2; \sigma_g) \) is the "H\(_2\)-dust limited dissociation bandwidth." \( W_\ell(N_2; \sigma_g) \) may be viewed as a curve-of-growth for the accumulating absorption of dissociating photons in a cloud that is fully molecular but also dusty. The function \( W_\ell(N_2; \sigma_g) \) may be computed in advance for any assumed \( \sigma_g \), and is independent of the gas density or the radiation field strength. S14 presented detailed numerical radiative transfer computations for \( W_\ell(N_2; \sigma_g) \).

For small H\(_2\) columns, H\(_2\)-dust absorption is negligible compared to H\(_2\)-line absorption so that \( W_\ell(N_2) \rightarrow W_\ell(N_2; \sigma_g) \), and the solutions approach the dust-free solutions given by Equation (12). For larger H\(_2\) columns \( W_\ell(N_2; \sigma_g) < W_\ell(N_2) \) when some of the LW photons are absorbed by H\(_2\)-dust rather than in H\(_2\) photodissociations. For sufficiently large H\(_2\) columns the dissociation bandwidth reaches a total (asymptotic) value. Following S14 we refer to this asymptotic bandwidth as \( W_\ell(tot) \). The asymptotic bandwidth is maximal for complete H\(_2\) line overlap, and is reduced by H\(_2\)-dust opacity for sufficiently large \( \sigma_g \). The product \((1/2) W_\ell W_\ell(tot) \) is then the effective dissociation photon flux through the H\(_2\)-dust opacity, excluding photons absorbed by H\(_2\)-dust, in fully molecular gas.

It is convenient to also define the normalized (dimensionless) curve-of-growth

\[
\tilde{w}(N_2; \sigma_g) \equiv \frac{W_\ell(N_2; \sigma_g)}{W_\ell(tot)(\sigma_g)}.
\]

which has the property that for any \( \sigma_g \), \( \tilde{w} \rightarrow 1 \) as \( N_2 \rightarrow \infty \). In Section 3 we plot the functions \( W_\ell, \tilde{w}, \) and \( W_\ell(tot) \) (Figures 2 and 3) and also derive analytic forms for these quantities based on the numerical radiative transfer results presented by S14.

Equation (15) may be integrated with \( N_2 \) the independent variable. This gives

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

In this expression

\[
G \equiv \frac{\sigma_g}{\sigma_d} W_\ell(tot) = 3.0 \times 10^{-5} \bar{\sigma}_g \left( \frac{9.9}{1 + 8.9 \bar{\sigma}_g} \right)^{0.37},
\]

where we have used the analytic form we develop for \( W_\ell(tot)(\sigma_g) \) in Section 3.3 below (Equation (29)). As discussed by S14, the parameter \( G \) is generally \( \ll 1 \), and may be viewed as the average H\(_2\)-self-shielding attenuation factor, averaged over an H\(_2\)-dust optical depth \( \sim 1 \). The product \( D_0 G \) is then the characteristic shielded dissociation rate.

With the inclusion of dust absorption, Equation (16) replaces Equation (12) for \( N_1(N_2) \). Together with \( N = N_1 + 2N_2 \) this gives \( N_1 \) and \( N_2 \) as functions of the gas column \( N \). This then gives the attenuation factor, \( f_{\text{att}} \), as a function of \( N \) alone, determining the density profiles \( n_1 \) and \( n_2 \) versus the total gas column.

### 2.4. Total H\(_1\) Column and the \( \alpha G \) Parameter

For \( N_2 \rightarrow \infty \), \( \tilde{w} \rightarrow 1 \), and we recover the basic S14 expression for the total H\(_1\) column density

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

This is for one side of an optically thick slab irradiated by a beamed field. The H\(_1\)-dust opacity associated with the total H\(_1\) column is then simply

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

In Equations (18) and (19) the dimensionless parameter is

\[
\alpha G \equiv \frac{D_0}{R} \frac{\sigma_g}{\sigma_d} W_\ell(tot) = \frac{\sigma_g}{\sigma_d} \frac{W_\ell(tot)}{W_\ell}. \quad (20)
\]

and it accounts for both H\(_2\)-self shielding and dust absorption. This was a key result in S14 (see also Sternberg 1988). The basic dimensionless parameter for \( \tau_{1,\text{tot}} \) is always \( \alpha G \), not \( \alpha \) alone. As shown by Equation (20), \( \alpha G \) may be expressed as the ratio of the shielded dissociation rate to the H\(_2\) formation rate. Alternatively, it is the ratio of the H\(_1\)-dust absorption rate of the effective dissociation flux to the H\(_2\) formation rate.

Using Equations (8) and (17) for \( \alpha \) and \( G \) we may write \( \alpha G \) in the normalized form

\[
\alpha G = 1.76 I_{\text{UV}} \bar{\sigma}_g \left( 10^{-17} \text{cm}^3 \text{s}^{-1} \right) \left( \frac{100 \text{ cm}^{-3}}{n} \right) \times \left( \frac{9.9}{1 + 8.9 \bar{\sigma}_g} \right)^{0.37}\).
\]

For H\(_2\) formation on dust grains (Equation (9)),

\[
\alpha G = 0.59 I_{\text{UV}} \left( \frac{100 \text{ cm}^{-3}}{n} \right) \left( \frac{9.9}{1 + 8.9 \bar{\sigma}_g} \right)^{0.37}. \quad (22)
\]

Like \( \alpha \), the product \( \alpha G \) is also proportional to the ratio \( I_{\text{UV}}/n \), but the pre-factor is of the order of unity. Both large and small \( \alpha G \) are relevant for the realistic range of interstellar conditions. The remaining factor \( 1/(1 + 8.9 \bar{\sigma}_g)^{0.37} \) accounts for the reduction in the total dissociation bandwidth by H\(_2\)-dust absorption, which becomes important for \( \bar{\sigma}_g \gtrsim 0.1 \). Because \( \alpha G \) itself depends on \( \bar{\sigma}_g \), the ratio \( I_{\text{UV}}/n \) must be adjusted if \( \alpha G \) is held constant for varying \( \bar{\sigma}_g \). For example, for \( \alpha G = 1 \), \( I_{\text{UV}}/n = 9 \times 10^{-3}, \quad 2 \times 10^{-2}, \quad 4 \times 10^{-2} \text{ cm}^{-3} \), for \( \bar{\sigma}_g = 0.1, \quad 1, \quad \text{and} \quad 10, \) respectively.

In Figure 1 we plot \( \tau_{1,\text{tot}} \) as a function of \( \alpha G \) (solid curve). For \( \alpha G \ll 1 \), \( \tau_{1,\text{tot}} \) increases linearly with \( \alpha G \). This is the "weak-field" limit. For \( \alpha G \gtrsim 1 \), \( \tau_{1,\text{tot}} \gtrsim 1 \), H\(_1\)-dust dominates the absorption of the LW band radiation, and the H\(_1\) column is "self-limited." This is the "strong-field" limit.

For \( \alpha G \ll 1 \), \( \tau_{1,\text{tot}} \ll 1 \) and H\(_1\)-dust absorption is negligible. In this limit \( N_1(N_2) \rightarrow 0.5 a G \tilde{w} / \sigma_d = 0.5 a W_\ell / \sigma_d \) (notice that \( \sigma_d \) drops out). If H\(_2\)-dust is also negligible \( W_\ell \rightarrow W_d \) and we recover Equation (12) for the dust-free conditions.

In Figure 1 we also plot (dashed curve) the analytic expression we derive in Section 4.3 for the dust optical depth \( \tau_{\text{dust}} \), at which the H\(_1\)-to-H\(_2\) transition occurs (see Equation (39)). We first present our procedure for generating the
atomic and molecular density profiles. These will determine the transition points as functions of \( \alpha G \) and \( \bar{\sigma}_q \).

2.5. Timescales

The above analysis, beginning with the formation-destruction Equation (1) is for steady-state conditions. The timescale to reach steady state is given by

\[
\tau_{\text{eq}} = \frac{1}{D + 2Rn}.
\]

where \( D \) is the local (attenuated) photodissociation rate and \( Rn \) is the formation rate. When \( D/(2Rn) \gg 1 \), \( \tau_{\text{eq}} \) is the dissociation time \( \approx 1/D \), and the gas becomes atomic on a short timescale. For example, in free-space \( D = D_0 \) and \( \tau_{\text{eq}} \approx 5.5 \times 10^3/t_{\text{UV}} \) year. When \( D/(2Rn) \ll 1 \), \( \tau_{\text{eq}} \) is the molecular formation time \( \approx 1/(2Rn) \approx 5 \times 10^8/n \) year. Because the molecular formation time is long, non-equilibrium effects (e.g., Liszt 2007) may become important beyond the H\( 1 \)-to-H\( 2 \) transition points.

3. ANALYTIC PROCEDURE FOR GENERATING PROFILES

Differentiating Equation (16) gives a formal expression for the atomic-to-molecular density ratio as a function of just the molecular column,

\[
\frac{n_1}{n_2}(N_2) = \frac{1}{\sigma_q} \times \frac{\alpha G \tilde{w}'(N_2; \sigma_q)}{\alpha G \tilde{w}(N_2; \sigma_q) + 2},
\]

where \( \tilde{w}' = d\tilde{w}/dN_2 \). Together with Equation (16) this can be converted to \( n_1/n_2 \) as a function of the total gas column \( N \), since \( N = N_1(N_2) + 2N_2 \). Because the functions on the right-hand side of Equations (16) and (24) depend on just \( \sigma_q \) and \( \alpha G \), so do \( n_1/n_2 \), \( n_1/n \) and \( n_2/n \), all as functions of \( N \).

Equation (24) can be reexpressed in the computationally convenient form

\[
\frac{n_1}{n_2}(N_2) = \frac{\alpha f_{\text{shield}}(N_2)}{\alpha G \tilde{w}(N_2; \sigma_q) + 2} \frac{e^{-2\sigma_q N_2}}{f_{\text{shield}}(N_2) e^{-2\sigma_q N_2}} = \left( \frac{\sigma_q}{\sigma_g} \right) \frac{\alpha G f_{\text{shield}}(N_2)}{\alpha G W_e(N_2; \sigma_q) + 2W_{\text{g,tot}}(\sigma_q)}. \quad (25)
\]

The depth-dependent atomic and molecular densities may then be constructed in a simple procedure:

1. Select values for \( \sigma_q \) and \( \alpha G \) (Equations (6) and (22)).
2. Evaluate \( n_1/n_2 \) as a function of \( N_2 \) using Equation (25), with the analytic forms for \( f_{\text{shield}} \), \( W_e \), and \( W_{\text{g,tot}} \) (Equations (26), (27), and (29) below).
3. Compute \( N_2(N) \) using Equation (16) for \( N_1(N_2) \) together with the relation \( N = N_1 + 2N_2 \).
4. Convert \( n_1/n_2 \) versus \( N_2 \) to \( n_1/n_2 \) as a function of \( N \).
5. Obtain \( n_1/n \) and \( 2n_2/n \) as functions of \( N \), assuming constant gas density \( n = n_1 + 2n_2 \).

In the remainder of this section we provide the analytic expressions for \( f_{\text{shield}} \), \( W_e \), and \( W_{\text{g,tot}} \) required to evaluate Equation (25).
3.1. Self-shielding Function $f_{\text{shield}}(N_2)$

The self-shielding function $f_{\text{shield}}(N_2)$ as defined by Equation (7) was computed via multi-line radiative transfer in S14. The results (see Figure 2 of S14) are in excellent agreement with the Draine & Bertoldi (1996) fitting function

$$f_{\text{shield}} = \frac{0.965}{(1 + x/b_2)^2} + \frac{0.035}{(1 + x)^{0.5}} \times \exp[-8.5 \times 10^{-4}(1 + x)^{0.5}].$$

(26)

Here, \(x \equiv N_2/(5 \times 10^{14} \text{ cm}^{-2})\) and \(b_2 \equiv b/(5 \times 10^5 \text{ cm s}^{-1})\) is the normalized Doppler parameter. In our computations we assume \(b_2 = 2\) as a compromise between purely thermal and turbulent broadened linewidths. As we discuss further below (Section 4.2) the positions of the transition points depend weakly on \(b\).

In Figure 2 (upper panel) we plot $f_{\text{shield}}$ as a function of $N_2$ for $b_2 = 1, 2, 4$. The onset of self-shielding occurs at small H$_2$ columns, \(\sim 10^{14} \text{ cm}^{-2}\), the exact value depending on \(b\). At $N_2 \geq 10^{17} \text{ cm}^{-2}$ the absorption occurs out of the radiative damping wings and the self-shielding is independent of the Doppler parameter. Finally, at very large columns, $N_2 \geq 10^{22} \text{ cm}^{-2}$, the absorption lines overlap and $f_{\text{shield}}$ drops sharply.

As we discuss in Section 4.3 below in our analysis of the transition points, a simple power-law approximation $f_{\text{shield}} \propto N_2^{-\beta/2}$, is useful. For the range $10^{14} < N < 10^{21.2} \text{ cm}^{-2}$, a power-law index $\beta = 0.7$ provides a good approximation. This is shown as the red dotted line in Figure 2 (upper panel).

3.2. H$_2$-dust Limited Dissociation Bandwidth $W_g(N_2; \sigma_g)$

S14 presented radiative transfer computations for the H$_2$-dust limited dissociation bandwidth, $W_g(N_2; \sigma_g)$, for four discrete values of $\sigma_g$, ranging from $\sigma_g = 0.01$ to 10. Recall that $\sigma_g$ is the normalized dust cross section, normalized to $1.9 \times 10^{-21} \text{ cm}^2$.

Those computations were carried out using the Meudon PDR code.2 The numerical S14 results for $W_g(N_2; \sigma_g)$ are the circles in Figure 2 (middle panel). For our purposes we require analytic expressions that vary smoothly with $N_2$ for any $\sigma_g$ within this range. That we find that an excellent fit to the S14 calculations is

$$W_g(N_2; \sigma_g) = a_1 \ln \left[ \frac{a_2 + y}{1 + y/a_3} \right] \left( \frac{1 + y/a_3}{1 + y/a_4} \right)^{0.4}.$$  

(27)

where

\[
y = \frac{N_2}{10^{14} \text{ cm}^{-2}}.
\]

\[
a_1 = 3.6 \times 10^{11} \text{ Hz}
\]

\[
a_2 = 0.62
\]

\[
a_3 = 2.6 \times 10^3
\]

\[
a_4 = 1.4 \times 10^3 \times (1 + 8.9\sigma_g)^{-0.93}
\]

The analytic fits are displayed as the solid curves in Figure 2 (middle panel). Our analytic formula for $W_g(N_2; \sigma_g)$ is accurate to within 6% of the numerical results for $N_2 > 10^{14} \text{ cm}^{-2}$ and for any $\sigma_g \leq 10$.

3.3. Total Dissociation Bandwidth $W_{g,\text{tot}}(\sigma_g)$

As $N_2$ becomes large $W_g(N_2; \sigma_g)$ approaches the total H$_2$-dust dissociation bandwidth $W_{g,\text{tot}}(\sigma_g)$. The circles in Figure 3 are the radiative transfer numerical results as computed by S14 for $W_{g,\text{tot}}(\sigma_g)$.

$$W_{g,\text{tot}}(\sigma_g) = \frac{9.9 \times 10^{13} \text{ Hz}}{1 + (2.6\sigma_g)^{y/2}}.$$  

(28)

Here we adopt an alternative and more accurate expression

$$W_{g,\text{tot}}(\sigma_g) = \frac{8.8 \times 10^{13} \text{ Hz}}{(1 + 8.9\sigma_g)^{0.37}},$$

(29)

plotted as the solid curve in Figure 3. This expression is obtained by taking the limit $N_2 \rightarrow \infty$ in our formula for $W_g(N_2; \sigma_g)$ (Equation (27)). For large $\sigma_g$, $W_{g,\text{tot}}$ decreases as an increasing fraction of the LW band radiation is absorbed by H$_2$-dust, before complete line overlap occurs. For $\sigma_g < 0.1$, H$_2$-line absorption dominates, and $W_{g,\text{tot}} \rightarrow W_{d,\text{tot}} \equiv 8.8 \times 10^{13} \text{ Hz}$, independent of $\sigma_g$.

Given our analytic forms for $W_g$ and $W_{g,\text{tot}}$ we can compute the normalized curve-of-growth $\widehat{\nu}(N_2) \equiv W_g(N_2)/W_{g,\text{tot}}$. In the lower panel of Figure 2 we plot $\widehat{\nu}$ for $\sigma_g = 0.01, 0.1, 1, 10$. By definition $\widehat{\nu}$ is normalized such that it approaches unity for

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2 Publicly available at http://pdr.obspm.fr.
large \( N_2 \). Therefore, for any \( N_2 \) prior to saturation, \( \tilde{w} \) is larger for larger values of \( \sigma_g \).

4. DENSITY PROFILES AND TRANSITION POINTS

Starting with Equation (25), we use our analytic procedure to generate \( \text{H} \) and \( \text{H}_2 \) density profiles for a wide range of \( \alpha G \) and \( \sigma_g \). We are particularly interested in the metallicity behavior so we consider large variations in the dust cross-section. We present results for \( 4 \times 4 \) combinations of \( \alpha G = 0.01, 0.1, 1, 10 \), and \( \sigma_g = 0.01, 0.1, 1, 10 \), where \( \alpha G \) and \( \sigma_g \) are treated as independent variables. We then use the profiles to derive an analytic scaling relation for the \( \text{H} \) to \( \text{H}_2 \) transition points.

4.1. \( \text{H} \) and \( \text{H}_2 \) Densities versus Gas Column

In Figure 4 we plot (blue solid curves) the atomic and molecular density fractions, \( n_1/n \) and \( 2n_2/n \), as functions of the total gas column density \( N \), for all \( 4 \times 4 \) combinations of \( \alpha G \) and \( \sigma_g \). As shown by the curves in each panel, for sufficiently small \( N \) the gas is entirely atomic, and for large \( N \) the gas is molecular. We define the transition points as the depths at which \( n_1 = 2n_2 \). These are indicated by the red dots in Figure 4.

For \( N \to 0 \) the ratio \( n_1/n_2 \to \alpha/2 \equiv D_0/(2Rn) \), or equivalently \( 2n_2/n \to 4/\alpha \) since \( n_1/n \approx 1 \) at the cloud boundaries. We stress that in each row in Figure 4 it is \( \alpha G \) that is held constant, not \( \alpha \). For \( \alpha G \) constant, \( \alpha \) must be altered with the dust cross-section as \( (1 + 8.9\sigma_g)^{0.37}/\sigma_g \). In Figure 4, this is reflected in the increasing molecular fraction at the cloud boundary, as \( \sigma_g \) is increased. For example, for \( \alpha G = 0.1 \), and for \( \sigma_g \) from 0.01 to 10, \( \alpha \) decreases from \( 1.5 \times 10^5 \) to \( 7.4 \times 10^3 \). The corresponding molecular fractions at the boundaries increase from \( 2n_2/n = 2.7 \times 10^{-2} \) to \( 5.3 \times 10^{-3} \).

In each panel we also plot (dashed curves) the normalized accumulated \( \text{H} \) columns

\[
\tilde{N}_1 = \frac{N_1(N)}{N_{1, \text{tot}}}. \tag{30}
\]

Here \( N_1(N) \) is obtained from step 3 of the procedure (Section 3), and \( N_{1, \text{tot}} \) is the total \( \text{H} \) column (Equation (18)). The curves for \( \tilde{N}_1 \) show how the \( \text{H} \) columns are built up with increasing cloud depth, finally reaching the maximal values when all of the photodissociating radiation has been absorbed. As discussed...
by S14, in the strong-field limit ($\alpha G \gtrsim 1$) most of the H\textsc{i} column density is built up in an outer fully photodissociated layer, prior to the conversion points (e.g., see the lowest row in Figure 4). These are the strong-field “sharp” transitions. In contrast, in the weak-field limit ($\alpha G \lesssim 1$), the transitions are “gradual” and most of the H\textsc{i} column density is built up past the transition points where the gas is predominantly molecular (e.g., see top row in Figure 4).

In Figure 4, for any $\sigma_2$, the transition points occur at greater cloud depths as $\alpha G$ is increased, i.e., as the free-space dissociation rate is increased relative to the H$_2$-formation rate. When $\alpha G$ is small, the transition points are controlled by H$_2$-self-shielding. For large $\alpha G$, the transition points are limited by H\textsc{i}-dust in addition to self-shielding. For example, for fixed $\sigma_2 = 1$, the transition point occurs at gas columns $N_{\text{tran}} = 1.5 \times 10^{17}, 3.5 \times 10^{18}, 1.2 \times 10^{20}$, and $8.3 \times 10^{20}$ cm$^{-2}$, for $\alpha G = 0.01, 0.1, 1$, and 10 (top to bottom in Figure 4).

For fixed $\alpha G$, the transition points occur at greater gas columns as $\sigma_2$ is reduced. In the strong-field limit ($\alpha G \gtrsim 1$), this is simply because the gas column required to achieve a large ($\gtrsim 1$) H\textsc{i}-dust optical depth grows as the dust absorption cross-section is reduced. Thus, for example, for $\alpha G = 10$, the transition column increases from $10^{20}$ to $10^{23}$ cm$^{-2}$, as $\sigma_2$ is reduced from 10 to 0.01 (see bottom row of Figure 4).

For small $\alpha G$ the behavior is more complicated. Dust absorption plays no role, but a dependence on $\sigma_2$ remains. For example, for $\alpha G = 0.01$, the transitions occur at gas columns equal to $2.5 \times 10^{16}, 1.5 \times 10^{17}, 1.3 \times 10^{18}$, and $4.3 \times 10^{19}$, as $\sigma_2$ is reduced from 10 to 0.01 (see top row of Figure 4). This is because we have assumed that the grain surface H$_2$ formation rate coefficient, $R$, is proportional to $\sigma_2$ (see Equations (9) and (22)), with both quantities scaling in the same way with the dust-to-gas ratio. Thus, for small $\alpha G$ the transition points occur at larger gas columns as $\sigma_2$ is reduced due to the associated reduction in the H$_2$ formation efficiency. The behavior is nonlinear however, because of the dependence on the H$_2$ self-shielding function.

Our analytically generated profiles in Figure 4, and the profiles computed using the full multi-line radiative transfer in S14 (see their Figure 7) are in excellent agreement.

### 4.2. H\textsc{i} and H$_2$ Densities versus Dust Opacity

The overall behavior becomes simpler if the density profiles are plotted as functions of the dust optical depth $\tau \equiv \sigma_2 N$, instead of the gas column $N$. A very useful scaling relation for the transition point is also revealed by making this transformation. In Figure 5 we show $n_1/n, 2n_2/n, \text{and } N_2$ as functions of $\tau$ as log-log plots. In Figure 6 we display the profiles as log-linear plots. The transition points are again indicated by the red dots.

The dust optical depth at the transition is

$$\tau_{\text{tran}} \equiv \sigma_2 (N_{\text{tran}} + 2N_{2,\text{tran}}),$$

where $N_{\text{tran}}$ and $N_{2,\text{tran}}$ are the integrated atomic and molecular columns up to the transition point (where $n_1 = 2n_2$). As expected, for $\alpha G \gtrsim 1$ H\textsc{i}-dust absorption becomes significant and $\tau_{\text{tran}} \gtrsim 1$. For $\alpha G \ll 1$, self-shielding dominates and $\tau_{\text{tran}} \ll 1$. Remarkably, as can be seen by inspecting Figures 5 or 6, for any $\alpha G$, $\tau_{\text{tran}}$ is quite insensitive to $\sigma_2$, especially in the astrophysically important range 0.1–10. Indeed to an excellent approximation, the profiles structures depend only on $\alpha G$. This is indicated by the almost identical profiles in each row of Figure 6 in the linear-log displays that suppress the differences in the free-space H\textsc{i}/H$_2$ ratios near the boundaries.

This behavior is not surprising for large $\alpha G$, for which the transitions all occur at $\tau_{\text{tran}} \sim 1$. However, for small $\alpha G$ this result is less immediate, and depends on the complex interplay between H$_2$ self-shielding and the connection between the H$_2$ formation rate coefficient and the dust cross section, and on the definition of the effective dissociation bandwidth.

The precise locations of the transition points do also depend on the assumed absorption-line Doppler parameter when $\alpha G \ll 1$ and $\sigma_2 \gtrsim 1$ since then self-shielding at the transition point occurs near the Doppler cores. In Figure 5, the horizontal bars indicate the variation in the location of the transition points for $b_2 = 1$ to 4 (from left to right), a factor of two variation in our assumed Doppler parameter $b_2 = 2$. As $\sigma_2$ becomes small (still at $\alpha G \ll 1$), the self-shielding at the transition points occurs within the damping wings, and the H\textsc{i}-to-H$_2$ transition is then independent of $b$.

### 4.3. Analytic Expression for the Transition Point

That the transition optical depth $\tau_{\text{tran}}$ depends mainly on the single parameter $\alpha G$ is a primary result of this paper, and we now present an analysis for this behavior.

In Figure 7 we plot $\tau_{\text{tran}}$ versus $\alpha G$ ranging from $10^{-3}$ to $10^3$, for the four values of $\sigma_2$. We computed these curves using our procedure for generating the depth-dependent profiles for any $\alpha G$, and then extracted the transition points. For comparison, we also plot (dashed curve) the total H\textsc{i}-dust optical depth $\tau_{1,\text{tot}}$ as given by Equation (19) (see also Figure 1). For large $\alpha G$, the curves for $\tau_{\text{tran}}$ all converge to $\tau_{1,\text{tot}}$ as expected in this limit for which the H\textsc{i}-to-H$_2$ transitions are sharp. Thus for large $\alpha G$

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

and independent of $\sigma_2$.

For small $\alpha G$, $\tau_{\text{tran}} \ll \tau_{1,\text{tot}}$, since the transitions are controlled by H$_2$-self-shielding and most of the H\textsc{i} columns are built up past the transition points. Figure 7 shows that $\tau_{\text{tran}}$ remains insensitive to $\sigma_2$ even as $\alpha G$ becomes small. For $\sigma_2$ between 0.1 and 10, the transition optical depths do not deviate by more than a factor 2 for any $\alpha G$ down to $10^{-3}$. For smaller $\sigma_2$ the transition optical depths increase somewhat as indicated by the curve for $\sigma_2 = 0.01$.

This behavior may be understood analytically as follows. When $\alpha G$ is small, $\tau \ll 1$, and dust absorption may be neglected at the transition point. The H\textsc{i} and H$_2$ column densities at the transition are then given by Equations (11) and (12), evaluated for $n_1 = 2n_2$, giving the pair of equations

$$\frac{n_1}{n_2} = 2 = \frac{1}{2} \alpha f(N_{2,\text{tran}}),$$

and

$$N_{1,\text{tran}} = \frac{\alpha}{2} \frac{W_d(N_{2,\text{tran}})}{\sigma_d}.$$  

To obtain simple solutions for the two unknowns $N_{1,\text{tran}}$ and $N_{2,\text{tran}}$, we approximate the H$_2$ shielding function as a power-law $f \propto N_2^{-\beta}$, so that $W_d \propto N_2^{-1-\beta}$ (see Equation (7)). It follows
that

\[ N_{1,\text{tran}} \propto N_{2,\text{tran}} \propto \alpha^{1/\beta}. \]  

The optical depth at the transition point then obeys

\[ \tau_{\text{tran}} \propto \bar{\sigma}_g \alpha^{1/\beta}. \]  

If expressed in terms of \( \alpha \) alone \( \tau_{\text{tran}} \) is proportional to \( \bar{\sigma}_c \).

To express Equation (36) in terms of \( \alpha G \), we multiply and divide \( \alpha \) by \( G \times (1 + 8.9 \bar{\sigma}_g)^{0.37} \). This gives

\[ \tau_{\text{tran}} \propto \bar{\sigma}_g^{(3-1)/\beta} (1 + 8.9 \bar{\sigma}_g^{0.37}/\beta) (\alpha G)^{1/\beta}. \]  

Thus, when considering \( \tau_{\text{tran}} \) in terms of \( \alpha G \) rather than \( \alpha \), two important limits arise:

\[ \tau_{\text{tran}} \propto (\alpha G)^{1/\beta} \times \begin{cases} \bar{\sigma}_g^{(\beta - 0.63)/\beta} & \text{for } \bar{\sigma}_g \gg 0.1 \\ \bar{\sigma}_g^{(3-1)/\beta} & \text{for } \bar{\sigma}_g \ll 0.1. \end{cases} \]  

As discussed in Section 3.1, for \( N_2 \) in the range \( 10^{14} - 10^{21} \) cm\(^{-2} \), \( \bar{I}_{\text{shield}} \propto N_2^{-\beta} \) with \( \beta \approx 0.7 \) is a good approximation. The dependence of \( \tau_{\text{tran}} \) on \( \bar{\sigma}_c \) is then very weak, especially for \( \bar{\sigma}_c \geq 0.1 \), for which \( \tau_{\text{tran}} \propto \bar{\sigma}_g^{0.10} \). Furthermore, in this approximation \( \tau_{\text{tran}} \) varies as a power-law \( (\alpha G)^{1/\beta} \) as seen in Figure 7.

An excellent fitting formula for \( \tau_{\text{tran}} \) as a function of \( \alpha G \) only is therefore

\[ \tau_{\text{tran}} = \beta \ln \left( \frac{\alpha G}{2} \right)^{1/\beta} + 1. \]  

For \( \alpha G \gg 1 \), this gives \( \tau_{\text{tran}} \rightarrow \ln(\alpha G/2) \) as it should (Equation (32)). For \( \alpha G \ll 1 \) the power-law behavior \( \tau_{\text{tran}} \propto (\alpha G)^{1/\beta} \) is recovered (Equation (37)), with prefactor \( \beta \) of the order of unity. The gray strip in Figure 7 shows \( \tau_{\text{tran}} \) as given by Equation (39) with \( \beta = 0.7 \), with a width indicating \( \pm 0.2 \) dex variations from the formula. This choice of \( \beta \) provides the best accuracy for \( \bar{\sigma}_g \gg 0.1 \). The maximal absolute deviations over the whole \( \alpha G \) range are 0.16, 0.21, and 0.20 dex, and the medians (in log space) are 0.03, 0.02, and 0.04 dex, for \( \bar{\sigma}_g = 0.1, 1, \) and 10, respectively. For \( \bar{\sigma}_g = 0.01 \), the median and maximum absolute deviations are 0.15 and 0.49 dex. For factor-of-two variations in the Doppler parameter \( \beta \) varies by less than 5%.

We stress that our universal scaling relation for \( \tau_{\text{tran}} \) depends on the inclusion of the H\(_2\)-dust absorption term in the definition of \( \alpha G \), i.e., \((1 + 8.9 \bar{\sigma}_g)^{-0.37} \). Without this metallicity-

Figure 5. H I and H\(_2\) density profiles \( n_1/n \) and \( 2n_2/n \) (blue solid curves) and the normalized accumulated H I column \( \tilde{N}_1 \) (dashed black curves), as functions of the dust opacity \( \tau \equiv \sigma_d N_\nu \), for the \( 4 \times 4 \) combinations of the basic parameters \( \alpha G = 0.01, 0.1, 1, 10, \) and \( \bar{\sigma}_g = 0.01, 0.1, 1, 10 \). The horizontal bars (mainly seen in the upper right panels) indicate the variation of the transition points for varying Doppler parameter \( b_c = 1 - 4 \). The profile shapes (sharp vs. gradual) and the positions of the H I- to-H\(_2\) transition points are determined mainly by the \( \alpha G \) parameter.
dependent term built into the definition of $\alpha G$, the transition point would depend on $\alpha G$ and $\sigma_g$ independently.

As examples for how our formula may be used, we compute the gas column density for the transition point for an incident radiation field with $I_{UV} = 1$, and cloud gas density $n = 10^3$ cm$^{-3}$, assuming a standard gas-to-dust ratio, i.e., $\sigma_g = 1.9 \times 10^{-21}$ cm$^2$, and $R = 3 \times 10^{-17}$ cm$^3$ s$^{-1}$. For these conditions $\sigma_g = 1$ and $\alpha G = 5.7 \times 10^{-2}$. Plugging $\beta = 0.7$ into Equation (39) gives $\tau_{\text{tran}} = 4.3 \times 10^{-3}$, or $N_{\text{tran}} = 2.3 \times 10^{18}$ cm$^{-2}$. This is only 15% of the total H$_1$ column for this value of $\alpha G$, which is $1.5 \times 10^{19}$ cm$^{-2}$. Reducing the metallicity by a factor of 10, and with the assumption that this implies a linear decrease in the dust cross section, this gives $\sigma_g = 0.1$ and $\alpha G = 0.14$, for which $\tau_{\text{tran}} = 1.5 \times 10^{-2}$ and $N_{\text{tran}} = 8.2 \times 10^{19}$ cm$^{-2}$.

For $\alpha G = 1$, the critical value between the weak- and strong-field limits $\tau_{\text{tran}} = 0.22$, and is approximately half the value of $\tau_{\text{tot}}$.

### 4.4. Attenuation Factor

Given solutions for the depth-dependent atomic and molecular density ratios $n_i/n_2$, we can compute the corresponding depth-dependent attenuation factors for the H$_2$ photodissociation rate. These are given by

$$ f_{\text{att}}(N; \alpha G, \sigma_g) = \frac{2}{\alpha} \frac{n_i}{n_2}(N), $$

where as discussed above, any pair $(\alpha G, \sigma_g)$ gives $n_i/n_2$ versus $N$, and determines $\alpha$. In Figure 8 we plot $f_{\text{att}}$ as a function of the total gas column $N$ (left panels) and of the dust opacity $\tau \equiv \sigma_g N$ (right columns). Each panel is for a fixed $\alpha G$, and shows four curves for the different $\sigma_g$ values. The transition points are marked by the red dots. The crosses indicate the points where the dust opacity $\tau = 1$. 

Figure 6. H$_1$ and H$_2$ density profiles as functions of dust optical depth in a log-linear display.

Figure 7. Optical depths at the H$_1$-to-H$_2$ transition points $\tau_{\text{tot}}$ (the red dots in Figure 5), as functions of the $\alpha G$ parameter, for $\sigma_g = 0.01, 0.1, 1, \text{and } 10$ (solid colored curves). For $\sigma_g \leq 0.1$, $\tau_{\text{tot}}$ depend only weakly on $\sigma_g$ and is determined mainly by the $\alpha G$ parameter. The gray strip is our fitting function given by Equation (39) with $\beta = 0.7$, with a width indicating ±0.2 dex variations from the formula.
The curves show the combined effects of H2-self-shielding and dust absorption in reducing the photodissociation rate (recall $f_{\text{att}} \equiv f_{\text{shield}} e^{-\tau}$). For small $\alpha G$ (e.g., upper panel) the curves for $f_{\text{att}} (N)$ resemble $f_{\text{shield}} (N_2)$ (see Figure 2) for much of the range, because the H i-to-H2 transition points occur at small gas columns, well before any dust opacity is built up. The sudden onset of self-shielding and drop in the photodissociation rate is followed by a more gradual decline as the H2 photoabsorption occurs in the line damping wings. Finally, at sufficiently large columns $f_{\text{att}}$ drops exponentially due to the H2-dust cutoff, or due to the complete overlap of the absorption lines. For large $\alpha G$ (e.g., lower panel) the exponential H i-dust cutoff occurs soon after the onset of self-shielding, and the damping wing portions are suppressed. For large $\alpha G$, most of the LW band radiation is absorbed by H i-dust. However, self-shielding is still important in reducing the photodissociation rate significantly and enhancing the H2 fraction within the large atomic layer.

In the right-hand panels of Figure 8 the vertical gray strips show the predicted positions of the transition points as given by our Equation (36), with a width $\pm 0.2$ dex (as for Figure 7). For $\sigma_g$ between 0.1 and 10, the computed transition points fall within the strips. For $\sigma_g = 0.01$ the transition points occur at slightly larger dust optical depths, as we have already seen in Figure 7.

5. H i-TO-H2 STAR FORMATION THRESHOLD

We can use our Equation (39) to define a star formation threshold with the empirically based assumption that conversion to H2 is required for star formation, the H i remaining sterile. Following S14 we define the threshold gas mass surface density, $\Sigma_{\text{gas,*}} (M_\odot \text{ pc}^{-2})$, as the surface density required for half of the mass to be molecular. For our idealized plane-parallel clouds, and for two-sided illumination, the threshold hydrogen gas column $N_{\text{gas,*}} \equiv 4N_{\text{tan}} = 4\sigma_g\tau_{\text{tan}}$. Here we are assuming that once the gas becomes predominantly molecular stars can form, even if residual H i exists in the molecular zone as occurs in the weak-field limit. Converting to a mass surface density, including the contribution of helium to the mass, gives

$$\Sigma_{\text{gas,*}} = \frac{16.5}{\delta_g} \ln \left[ \left( \frac{\alpha G}{2} \right)^{1.43} + 1 \right] M_\odot \text{ pc}^{-2},$$

(41)

where we set $\beta = 0.7$ in Equation (39). In Figure 9 we plot the star formation thresholds as functions of $\alpha G$, for $\sigma_g$ from 0.01 to 10. We recall that the dust absorption cross-section may be...
related to the metallicity, (Equation (5)) with
\[ \sigma_f = 1.9 \times 10^{-21} \phi_g Z^2 \text{cm}^2, \]
\[ \bar{\sigma}_g = \phi_g Z^2, \]
where \( \phi_g \) is a factor of the order of unity.

For large \( \alpha G \) (strong-field limit), the H\( \text{I} \) layers become extended but are limited by H\( \text{I} \)-dust absorption. For example for \( \bar{\sigma}_g = 1 \) (or \( Z' \approx 1 \)), \( \Sigma_{\text{gas},*} \) increases from 5 to 92 \( M_\odot \text{pc}^{-2} \) for \( \alpha G \) from 1 to \( 10^2 \). For low \( \alpha G \) (weak-field limit) the outer H\( \text{I} \) layers become very narrow and \( \Sigma_{\text{gas},*} \) drops sharply. For \( \bar{\sigma}_g = 1, \Sigma_{\text{gas},*} \) decreases from 5 to \( 8 \times 10^{-2} M_\odot \text{pc}^{-2} \) for \( \alpha G = 1 \) to \( 10^2 \). Because the dust optical depth at the H\( \text{I} \)-to-H\( \text{2} \) conversion point is insensitive to \( \bar{\sigma}_g \), the threshold surface density varies with metallicity as \( 1/\sqrt{Z'} \) for any \( \alpha G \).

If the H\( \text{I} \) gas is assumed to be cold (CMN) at multiphase conditions (Krumholz et al. 2008; S14) then \( \alpha G = (\alpha G)_{\text{CMN}} \) in Equation (41), where as given by S14\(^3\)

\[ (\alpha G)_{\text{CMN}} = 2.6 \left( \frac{1 + 3.1 Z^{0.365}}{4.1} \right) \left( \frac{9.9}{1 + 8.9 \phi_g Z^2} \right)^{0.37}. \] (42)

The dashed curve in Figure 9 shows the locus \( \alpha G = (\alpha G)_{\text{CMN}} \) for \( Z' \) from 10 to 0.01 (assuming \( \phi_g = 1 \)). For \( \bar{\sigma}_g = 1 \) (\( Z' \approx 1 \)), and for \( \alpha G = (\alpha G)_{\text{CMN}} \), the threshold surface density is 15 \( M_\odot \text{pc}^{-2} \).

S14 gave expressions for the thresholds \( \Sigma_{\text{gas},*} \) but with \( \tau_{\text{tran}} \) replaced by \( \Sigma_{\text{dust}^2} \), with the added assumption (valid for \( \alpha G \gtrsim 1 \)) that the transitions are sharp. The upper and lower red crosses in Figure 9 are the predicted S14 thresholds, equal to 11 and 20 \( M_\odot \text{pc}^{-2} \), for \( \alpha G = (\alpha G)_{\text{CMN}} \) and \( \bar{\sigma}_g = 1 \), for beamed and isotropic irradiation respectively. The circle shows the McKee & Krumholz (2010) result of 30 \( M_\odot \text{pc}^{-2} \) for their assumed \( (\alpha G)_{\text{CMN}} = 3.1 \) for solar metallicity and assuming spherical geometry.

In general, the assumption that \( \alpha G = (\alpha G)_{\text{CMN}} \) may be too restrictive, e.g., as shown for the H\( \text{I} \)-to-H\( \text{2} \) transitions in the

\(^3\) In this expression we have adjusted Equation (59) of S14 for \( (\alpha G)_{\text{CMN}} \) by using our adopted formula Equation (29) for \( \Sigma_{\text{dust}^2} \) instead of Equation (28).

\(^4\) S14 present (Section 4) a detailed comparison between the formulae and results for slab geometry versus the spheres assumed by Krumholz et al. (2009), McKee & Krumholz (2010).

Perseus molecular cloud (Bialy et al. 2015). Our Equation (41) provides estimates for the thresholds for arbitrary \( \alpha G \) and metallicity.

6. SUMMARY

In this paper we have extended the analytic theory presented by Sternberg et al. (2014, S14) for the H\( \text{I} \)-to-H\( \text{2} \) transitions in interstellar photon-dominated regions (PDRs), to develop a simple procedure for the construction of steady-state H\( \text{I} \)-to-H\( \text{2} \) density profiles for FUV irradiated clouds. Following S14, we first demonstrate that for uniform density gas, and for a steady irradiation fluxes, the atomic-to-molecular gas fractions as functions of cloud depth, in one-dimensional slabs, depend on two basic parameters. First is the dimensionless “\( \alpha G \)” parameter “(Sternberg 1988; S14) that determines the dust optical depth associated with the total photodissociated H\( \text{I} \) column. Second is \( \bar{\sigma}_g \), the dust-grain absorption cross-section per hydrogen nucleus in the 1100–912 Å LW photodissociation band. The \( \alpha G \) parameter is proportional to the ratio of the FUV field intensity to the gas density, or alternatively to the ratio of the H\( \text{2} \) dissociation rate to the molecular formation rate (see Equations (20) and (21)). The dust-grain absorption cross-section also enters into the definition of \( \alpha G \) because some of the LW band radiation may be absorbed by dust associated with just the H\( \text{2} \).

We then develop our analytic procedure for generating H\( \text{I} \)-to-H\( \text{2} \) density profiles. It may be used for arbitrary input gas density, FUV field intensity, H\( \text{2} \) formation rate coefficient, and dust-grain absorption cross-section. The gas density and field intensity may vary widely in differing interstellar environments. The formation rate coefficient and dust absorption cross-section will generally vary with the metallicity-dependent dust-to-gas ratio. Our simple five-step procedure (Section 3) requires analytic forms for (a) the H\( \text{2} \)-self-shielding function, (b) the dust limited curve-of-growth for multi-line dissociation bandwidth, and (c) the total dust limited bandwidths. We develop the required analytic expressions for (b) and (c) (Equations (27) and (29)) based on the detailed radiative transfer results presented by S14. (For a) we recommend the Draine & Bertoldi (1996) formula (Equation (26)).

We use our procedure to generate a \( 4 \times 4 \) set (Figure 4) of H\( \text{I} \)-to-H\( \text{2} \) transition profiles, showing the fractions as functions of the total gas columns, from large (strong-field) to small (weak-field) \( \alpha G \), and for dust cross-sections ranging from super-solar to very low dust-to-gas mass ratios. We then show that if the profiles are displayed (Figures 5–6) as functions of the dust optical depth (or visual extinction) the dependence on \( \bar{\sigma}_g \) becomes very weak, and just \( \alpha G \) remains as the single controlling parameter, including also for the depth at which the H\( \text{I} \)-to-H\( \text{2} \) transition occurs. This simple scaling behavior is valid from the strong-field limit where H\( \text{I} \)-dust opacity dominates at the transition point, to the weak-field limit where the transition is controlled by self-shielding only.

We use our results to derive a simple universal fitting formula for the dust optical depth at which the H\( \text{I} \)-to-H\( \text{2} \) transition occurs, as a function of the single dimensionless parameter \( \alpha G \) (Equation (39) and Figure 7). We use our formula for the transition depth to develop an expression for the threshold gas mass surface density required for star formation, under the assumption that individual clouds become star-forming when \( \sim 50\% \) of the gas mass is molecular (Equation (41) and Figure 9).
Our analytic procedure and formulae for the H I-to-H2 transition points and star formation thresholds will be useful for interpreting observations of interstellar H I/H2 interfaces on small and global galactic scales, and for incorporation into hydrodynamics simulations.

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