The Importance of Nonlinear H_2 Photoexcitation in Strongly Irradiated PDRs

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ABSTRACT

It is shown that, under sufficiently intense OB-star illumination of a stationary photoexcitation front (PDR), nonlinear H_2 photoexcitation processes comprising driven resonant two-photon transitions between X-state quantum levels, with VUV continuum light from the star supplying both driving fields, largely determine the photonic pathways of H_2 molecules in the PDR close to the ionization front. Specifically, for a flux of $\sim$4 x 10^5 Habing fields incident upon a PDR, the total rate at which an H_2 molecule is nonlinearly photoexcited out of any X-state quantum level is calculated to be roughly 100 times greater than the total rate at which it is linearly photoexcited out of the same level. In strongly excited PDRs, the populations in almost all of the $\sim$300 bound quantum levels of the X state will be maintained approximately equal via a few myriads of interconnecting two-photon steps. The remarkable importance of two-photon transitions in H_2 photoexcitation in strongly irradiated PDRs derives from the exceptionally narrow Raman linewidth ($\Gamma \sim 10^{-6}$ sec^{-1}) that characterizes all two-photon transitions between bound H_2 X-state quantum levels.

Subject headings: infrared: ISM - - - ISM: clouds - - - ISM: HII regions - - - ISM: lines - - - ISM: lines and bands - - - ultraviolet: ISM

1. Introduction

In existing theoretical models of stationary photoexcitation fronts (PDRs) [see Draine & Bertoldi (1996) for a comprehensive list of references], a one-dimensional geometry is usually considered, with light from an OB-type illuminating star assumed incident upon the PDR from one direction. In all published PDR models, only linear H_2 photoexcitation processes have been considered. The consensus among astrophysicists is that these models adequately describe the main photonic events that occur in H_2-containing clouds separated by at least 10 pc from OB-type illuminating stars. In the present Letter, we draw attention to the fact that, in very strongly irradiated PDRs (for example, those with cloud-to-star distances $\leq$0.1 pc), nonlinear photoexcitation of H_2 can evidently become the dominant photonic process determining the structure of the PDR.

2. Resonantly Enhanced, VUV Starlight-Driven, Two-Photon Transitions between H_2 X-State Quantum Levels

An estimate of the resonantly-enhanced, VUV starlight-driven, two-photon transition rate between two H_2 X-state quantum levels can be obtained with use of the formula shown in Fig. 1. In SI units, this formula [c.f. eq. (5.6b) of Hanna et al. (1979)] gives the cross-section for Stokes-wave gain in resonant stimulated Raman scattering (SRS) in a three-level system. However, it equally well gives the cross-section for induced nonlinear absorption at ω_P when an intense radiation field is present at ω_S - a process often referred to as inverse Raman scattering (IRS). It has long been recognized (Jone & Stoicheff 1964; MacQuillan & Stoicheff 1966) that both processes are fundamentally the same. In this equation, the classical electron radius $r_e \approx 2.82$ x 10^{-15} m. The quantity I_P is the pump intensity in W/m^2. The subscripts $g, i,$ and f designate the ground level, intermediate level, and final level, respectively, of the three-level system. The quantity Γ is the Raman linewidth (in units of angular frequency), which, for the astrophysical environment assumed in our PDR model, would be entirely determined by a convolution of the vibrational decay rates of the two Xn$''$ quantum levels involved. In light of recent calculations of quadrupole transition probabilities for all X-state radiative decays (Wolniewicz et al. 1998), one can realistically assume a value $\Gamma = 10^{-6}$ sec^{-1} for all two-photon transitions between X-state quantum levels. The quantities f_{fi} and f_{gi} are the oscillator strengths of the Stokes-wave and primary frequency transitions. For all H_2 Lyman (B$\Longleftrightarrow$X) and Werner (C$\Longleftrightarrow$X) transitions, these f- values can be simply determined from the tables in Abgrall et al. (1993 a,b). The quantities such as Ω_{if} are the energy separations of the levels involved, expressed as angular frequencies, e.g. $(h/2\pi)\Omega_{if} = E_i$ - E_f. Note that the Stokes-wave frequency ω_S essentially cancels Ω_{if} in the present case. The equation in Fig. 1 gives the cross-section in units of m^2.

To estimate the rates of both nonlinear and linear H_2 photoexcitation in the PDR, one needs to know the VUV flux from the star incident upon the cloud surface. Here, for definiteness, we assume the illuminating star to be a B0 III star, with temperature T=31,500K and radius R = $16\Re_\odot$. We take the cloud-to-star distance to be 0.1 pc, and assume that there is no intervening dust cloud between the star and H_2-containing cloud. From the Planck formula for emittance of photons from a blackbody per cm^2 per sec per unit frequency range (Allen 1976), one finds that at 1,000 Å the incident flux on the PDR is $\phi_{1000} = 2.55$ x 10^8 photons per cm^2 per sec per cm^{-1}. Habing (1968) estimated the intensity of interstellar starlight at λ=1,000 Å to be λu_λ = 4 x 10^{-14} erg cm^{-3}. At the surface of the PDR we are here considering, therefore, ϕ_{1000} is about 4.25 x 10^5 Habing fields.

As is the case in almost all published PDR models, it is here assumed that ionizing radiation (i.e. $\lambda \leq 912$ Å) from the star creates a thin H II region on the surface of the PDR cloud nearest the star. Within this H II region, a large fraction (∼2/3) of the incident ionizing photons are converted to Ly-α photons via H^++ e^- recombinations followed by cascading transitions through H-atom excited states. Half of the Ly-α photons enter the neutral region, with their frequencies having become distributed in a ∼20-cm^{-1}-wide spectral band via the frequency redistribution that results from elastic scattering by hot H atoms in the H II region. One can easily estimate the total flux of ionizing photons incident upon the PDR from tables of the Planck function(Allen 1976). One finds this to be $\phi_{ion} \approx 6.2$ x 10^{12} photons cm^{-2} sec^{-1}. There are thus about $\phi_{Ly\alpha} \approx 2.1$ x 10^{12} Ly-α photons entering the neutral PDR region per cm^2 per second. Thus, the Ly-α flux (per unit wavenumber) entering the neutral PDR region is seen to exceed that at 1,000 Å by roughly a factor 400. In §3, we will briefly hint at an important effect this Ly-α radiation should have on the nonlinear excitation of H_2 in strongly irradiated PDRs.

To estimate the total rate at which an H_2 molecule in the PDR would undergo linear photoexcitation, one can use Table 2 of Draine & Bertoldi (1996). These authors have calculated and summed individual contributions to the total unshielded H_2 linear photoexcitation rate from all X→B and X→C transitions. For a flux ϕ_{1000} = 4.25 x 10^5 Habing fields, the total linear photoexcitation rate for a molecule in (X0, J″=1) would be about 1.2 x 10^{-4} sec^{-1}. In the PDR model of Draine & Bertoldi (1996), a Doppler width ≈1.7 cm^{-1} is assumed.

With use of the equation shown in Fig. 1, we now evaluate the driven (simultaneous, not sequential) two-photon transition rate from X0, J″=1 to X1, J″=1 involving C0(Π_u^-), J′=1 as resonant intermediate state. A rough - but conservative - approximation one can make in integrating the expression for σ_{IRS} over the applied VUV pumping continuum is to assign to the quantity (Ω_{ig} - ω_P) appearing in the denominator of the equation in Fig. 1 a constant value corresponding to an offset of one wavenumber, and then integrate over a spectral interval two wavenumbers wide on either side of the resonance. From the value of ϕ_{1000} earlier estimated, the value of I_P for a four-wavenumbers-wide spectral interval is found to be 0.00002 W/m^2. With substitution of appropriate values for the other quantitities appearing in the equation of Fig. 1 (e.g. f_{gi} = 0.03, f_{fi} = 0.07), one finds the cross-section for induced absorption to be $\sigma_{IRS} \approx 8.4$ x 10^{-14} cm^2. Multiplying this value by ϕ_{1000} x 4 shows the transition rate of the IRS process to be ∼8.6 x 10^{-5} sec^{-1}. The rate of nonlinear photoexcitation of an H_2 molecule in (X0, J″=1) via this particular two-photon transition is thus about 0.7 times the earlier estimated total rate of linear photoexcitation of an H_2 molecule in the same (X0, J″=1) quantum level.

However, driven two-photon transitions from (X0, J″=1) to (X1, J″=1) can also occur via the paired transitions Cn-0Q1, Cn-1Q1 (n = 1-5) and also Cn-0R1, Cn-1R1 (n = 0-5). This makes the total two-photon transition rate out of (X0, J″=1) exceed the total linear rate by ∼7 times. (The wavelengths of both C6-0Q1 and C6-0R1 are shorter than 912 Å, the Lyman limit. No $\lambda \leq 912$ Å starlight can penetrate beyond the HII region of the PDR.) One can also go from (X0, J″=1) to (X1, J″=3) via transitions Cn-0R1, Cn-1P3. With the inclusion of these paths, the two-photon transition rate out of (X0, J″=1) would be roughly 10 times the total linear rate of photoexcitation. One next must consider analagous two-photon transitions from (X0, J″=1) that terminate on (X2, J″=1), (X2, J″=3), ...(X8, J″=1), (X8, J″=3), etc.. With inclusion of these, the two-photon excitation rate from (X0, J″=1) would exceed the total linear excitation rate by ∼70 times. Finally, two-photon excitation from (X0, J″=1) can also occur via B-state resonant intermediate levels. Additional inclusion of such pathways, makes the total rate of two-photon excitation out of (X0, J″=1) exceed the total linear photoexcitation rate out of the same quantum level by at least a factor 100. Roughly the same nonlinear-to-linear photoexcitation rate ratio would obtain for H_2 molecules in any of the ≈300 X-state quantum levels. The estimated total nonlinear photoexcitation rate out of any such level is thus $\sim 1.2 \times 10^{-2}$ sec^{-1}.

3. Consequences of VUV Starlight-Driven Two-Photon Transitions Occurring in Heavily Irradiated PDRs

From the transition rates calculated above, it is apparent that, through a few myriads of interconnecting two-photon transitions, the H_2 populations in each of the ≈300 X-state quantum levels would be maintained approximately equal. Note that no H_2 photodissociation can result from two-photon transitions occurring from the highest bound X-state levels to unbound X-state continuum levels. The two-photon transition rate depends inversely upon the Raman linewidth, and the latter represents a convolution of the lifetimes of the quantum levels connected by the two-photon process. When one steps from the highest bound X-state levels to unbound levels of the X-state continuum, the lifetime drops by roughly eighteen orders of magnitude! On the basis of this same disparity in lifetimes, one perhaps should question the validity of the assumption usually made in linear PDR models that roughly one out of ten H_2 photoexcitations from X-state quantum levels result in photodissociation via fluorescent VUV transitions terminating on unbound levels of the X-state. This would be true if linear photoexcitation of H_2 in PDRs did involve real excitation of B- and C-state quantum levels. However, in collisionless media, it is known (Loudon 1983) that linear photoexcitation occurs entirely via spontaneous resonant Raman scattering, and, at exact resonance, the cross-section for the latter varies again as Γ^{-1} (Shen 1974).

If one knows the total H_2 density in the neutral region of the PDR, one can approximately estimate the maximum thickness d of the nonlinearly excited region as follows. Assume an H_2 density of 10^4 cm^{-3}. In the nonlinearly excited region, these molecules will be evenly distributed amongst all the ≈300 X-state quantum levels, with the spontaneous infrared radiation emission rate from each level being $\sim 10^{-6}$ sec^{-1}. Assume the average IR emitted photon to have an energy of 5,000 cm^{-1}. Equating the VUV power from the star incident upon the PDR in the entire spectral range of the Lyman and Werner bands that lies longward of 912 Å to the IR power radiated in a column of thickness d:

$$(20,000)(2.55 \text{ x } 10^8)(100,000) \approx (10^4)(10^{-6})(5,000)d,$$

one finds d≈0.003 pc. Figure 1 of Lemaire et al. (1996) is a striking colored image (colors corresponding to emission intensity) of H_2 1-0 S(1) vibrational emission at 2.121 μm in NGC 7023, taken at very high spatial resolution. It shows H_2 vibrational emission originating from a ∼0.02-pc-thick, roughly planar, cloud located ∼0.07 pc to the NW of the illuminating star HD 200775. (From Earth, one views this cloud largely through one of its 'edges'.) There is very much higher H_2 emission coming from three ∼0.004-pc-thick embedded filaments located near the surface of the cloud facing the star. In view of the calculations that have been presented above, we suggest that these bright filaments in NGC 7023 might represent PDR regions that are nonlinearly excited.

It was noted above that Ly-α radiation generated in the H II region enters the PDR neutral region at an intensity level roughly 400 times greater than the continuum level at 1,000 Å, but only over an estimated $\sim$20-cm^{-1}-wide bandwidth. There are a dozen or so allowed transitions originating from X-state quantum levels whose frequencies fall within such a Ly-α spectral distribution. A slight contribution towards the equalization of H_2 populations in the various X-state quantum levels arises from these resonances. However, there is a different - rather profound - effect that this Ly-α radiation can induce, when it is applied to an equally populated manifold of X-state quantum levels. It can induce broadband stimulated Raman scattering (SRS) to occur on the three or four strongest of the above mentioned resonant transitions, generating broadband IR Stokes-wave light on strong transitions to EF-states. An SRS process would occur as part of a 2n-wave parametric oscillation (SRS-PO) process, with additional IR and VUV light being generated on strong transitions ultimately returning molecules to the X-state levels from which the SRS-PO processes originated. As shown elsewhere (Sorokin & Glownia 2001), the so-called 'unidentified infrared (emission) bands (UIBs)' can be successfully assigned to IR emissions coherently generated in such SRS-PO processes.

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$$\sigma_{IRS} = \frac{4\pi^3 r_e^2 c^2}{h} \frac{\omega_s}{\Gamma} \left(\frac{f_{fi}}{\Omega_{if}} \right) \left(\frac{f_{gi}}{\Omega_{ig}} \right) \left(\frac{I_P}{(\Omega_{ig} - \omega_P)^2} \right)$$

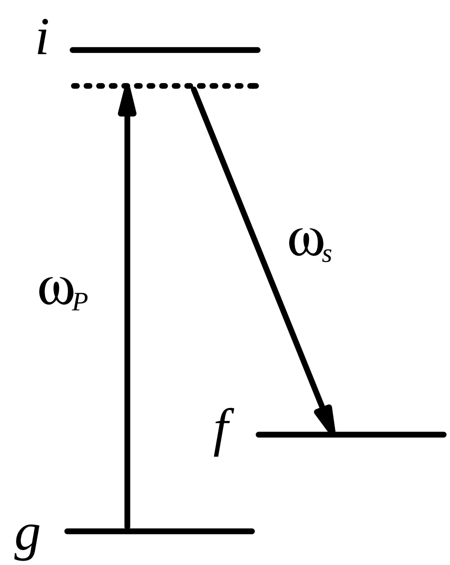

Fig. 1.— Equation for the cross-section of either SRS Stokes-wave gain or IRS-induced absorption in a resonant, three-level system. The light waves in the diagram are depicted for the SRS case.