1. Introduction

The long-standing mystery in astronomy concerning the origin of the diffuse interstellar absorption bands (DIBs) was recently conveyed to Physics Today readers in an article (Huffmann, 1991) primarily concerned with describing the new field of fullerene research. Figure 1 (adapted from the above article) depicts the measured spectral dependence of the extinction that is generally attributed to interstellar dust. In Fig. 1a the optical density over a large energy range is shown. A smoothly varying main component is seen generally to increase with photon energy - displaying, however, an enormous "bump" at $\lambda \approx 2175\AA$ (5.7 eV). The diffuse interstellar bands appear as fine structure in Fig. 1a between about 1.9 and 2.8 eV. The DIB intensities generally correlate with the smoothly varying component of extinction ("reddening") seen in a given direction. In Fig. 1b, the appearance of DIBs with the smoothly varying extinction component subtracted is depicted.

A convincing explanation of the origin of the DIBs has evidently thus far not materialized. They are generally believed to be of interstellar origin - hence, the term: diffuse interstellar bands. Most recent explanations are solid-state based. Many postulate the existence in interstellar space of large organic molecules, such as polycyclic aromatic hydrocarbons (PAHs), long chain unsaturated hydrocarbons, fullerenes, etc., perhaps adsorbed onto various (unspecified) dust particles. With such models, serious difficulty is encountered in trying to account for the seemingly universal presence in interstellar space of the large and complex molecular structures whose existence is postulated. Furthermore, spectra predicted by the various models proposed thus far do not come very close to matching the fascinating and intricate spectral signature presented by the DIBs.

In this paper, a new model is proposed to account for the DIBs. In this model, the DIBs result from a non-linear effect: resonantly-enhanced two-photon absorption of H$^+_2$ ions located near the surface of the Strömgren sphere that surrounds an O- or B-type star. The strong light (at $\omega_i$) that is required to "drive" the two-photon transition is provided by L($\alpha$) light emerging from the Strömgren sphere that bounds the H II region surrounding the star. In Sec. 2, a value $\approx 200 \mu W/cm^2$ is estimated for the L($\alpha$) flux at the Strömgren radius, $R_S$, of a strong (O5) star. (A pure hydrogen star is assumed.) It is shown in Sec. 3 that a c.w. L($\alpha$) flux of this intensity should be sufficient to induce a few percent absorption for visible light radiated by the same
star at a frequency \( \omega_z \) that completes an allowed two-photon transition, provided (1) the \( L(\alpha) \) radiation happens to be nearly resonant with the frequency of a fully-allowed absorber transition that effectively represents the first step in the two-photon transition, and (2) an effective column density \( \sim 10^{12} \text{cm}^{-2} \) of the absorber is present near the Strömgren sphere radius, \( R_s \). In Sec. 4, it is shown that a few *almost exact* resonances (i.e., with frequency offsets from \( L(\alpha) \), \( \Delta \), not exceeding \( \approx 2 \text{ cm}^{-1} \)) are found in the allowed \( H_\beta \) system: \( 2p\sigma_u (v', J') \rightarrow 1s\sigma_g (v'', J'') \). It is then indicated that the "second step" \( H_\beta \) transitions: \( [4d\sigma_g, 5g\sigma_g, 3d\delta_g, 5g\pi_g, 4d\pi_g, \text{and } 3s\pi_g] \rightarrow 2p\pi_u (v', J') \) can possibly account for the DIBs. This visible absorption spectrum is, in principle, exactly calculable. To begin to explore whether or not there might really exist exact coincidences between measured locations of DIBs and transition wavelengths predicted by the model, one could initially attempt to compute vib-rot level energies for the (four) above even-parity states that are bound, preferably with adiabatic corrections incorporated into the Born-Oppenheimer approximation.

The required presence of \( H_\alpha \) molecules located near \( R_s \) could conceivably result from direct photoionization of \( H_\alpha \) molecules located in a compact shell that serves as the transition region between the \( H_\alpha \) sphere and the cold surrounding hydrogen gas. In this case, one would expect the \( H_\alpha \) ions to be produced in the ground state with a vibrational distribution given by the known Franck-Condon factors for ionization of hydrogen. It is, therefore, quite interesting that the linear \( H_\alpha \) absorption spectrum one calculates for such a distribution has generally similar features to those possessed by the smoothly-varying component of the measured "interstellar" extinction curve, including the large "bump" at \( \approx 2175 \text{ Å} \).

2. \( L(\alpha) \) radiation emerging from radiatively excited nebulae of pure hydrogen (\( H_\alpha \) regions)

The source of excitation of the gas is assumed to be an embedded bright star of early spectral type - for example, an O- or a B-type star. We rely here on the simplest model for this gas - as described, for example, in Chapter 5 of the text by Dyson and Williams (Dyson and Williams, 1980). Table 1, adapted from Table 5.3 of one of Spitzer’s books (Spitzer, 1978), shows what the total rate of photon emission shortward of the Lyman limit for typical O and B stars is. We here assume that our embedded star is like the O5 one listed, with \( N_u \approx 5 \times 10^{48} \text{ s}^{-1} \). Note that the radius of the star is only \( 13.8 \times R_\odot \), or \( 3.2 \times 10^{-7} \text{ parsec (pc)} \).

<table>
<thead>
<tr>
<th>Spectral Type</th>
<th>( T_{\text{eff}}(\text{°K}) )</th>
<th>( R/R_\odot )</th>
<th>( N_u(\text{s}^{-1}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>O5</td>
<td>47,000</td>
<td>13.8</td>
<td>( 51 \times 10^{48} )</td>
</tr>
<tr>
<td>O6</td>
<td>42,000</td>
<td>11.5</td>
<td>17.4</td>
</tr>
<tr>
<td>O7</td>
<td>38,500</td>
<td>9.6</td>
<td>7.2</td>
</tr>
<tr>
<td>O8</td>
<td>36,500</td>
<td>8.5</td>
<td>3.9</td>
</tr>
<tr>
<td>O9</td>
<td>34,500</td>
<td>7.9</td>
<td>2.1</td>
</tr>
<tr>
<td>B0</td>
<td>30,900</td>
<td>7.6</td>
<td>0.43</td>
</tr>
<tr>
<td>B1</td>
<td>22,600</td>
<td>6.2</td>
<td>0.0033</td>
</tr>
</tbody>
</table>

Table 1. Radiative Properties of Early-Sequence Stars
Let us estimate the \( L(\alpha) \) flux emerging from the "Strömgren sphere" (the sphere whose radius, \( R_s \), delineates the boundary between the almost fully ionized H II interior, and the cold hydrogen gas exterior). We have, approximately,

\[
4\pi R_s^2 \Psi_{L(\alpha)} = \frac{4}{3} \pi R_s^3 n_e \beta_2(T_e)
\]  

(1)

This equation assumes that there is one \( L(\alpha) \) photon produced for every recombination (to \( n \geq 2 \)) that occurs. Also, if a \( L(\alpha) \) photon is absorbed by an H atom, it will simply be re-scattered in another direction. All \( L(\alpha) \) photons produced will eventually escape through the surface of the Strömgren sphere.

An excellent numerical approximation for the total recombination coefficient, \( \beta_2(T_e) \), is (Dyson and Williams, 1980):

\[
\beta_2(T_e) = 2 \times 10^{-16} T_e^{-3/4} \text{m}^3 \text{s}^{-1},
\]  

(2)

where \( T_e \) is the temperature of the gas in the H II region. Estimates of such temperatures lie roughly in the range 5,000 - 10,000 K, with rather little variation from one nebula to the other (Dyson and Williams, 1980). We assume \( T_e = 10,000 \) K for our case. Then \( \beta_2 \approx 2 \times 10^{-19} \text{m}^3 \text{s}^{-1} \).

The Strömgren radius, \( R_s \), is given by (Dyson and Williams, 1980):

\[
R_s = \left( \frac{3N_u}{4\pi n_e \beta_2} \right)^{1/3} \text{m}.
\]  

(3)

Thus, combining this with Eq(1), one has:

\[
\Psi_{L(\alpha)} = \frac{1}{3} n_e^{4/3} \beta_2^{1/3} \left( \frac{N_u}{4\pi} \right)^{1/3}.
\]  

(4)

Let's assume that \( n_e = 10^6 \text{ cm}^{-3} \). Then one has: \( \Psi_{L(\alpha)} = 1.21 \times 10^{18} \text{ photon s}^{-1} \text{ m}^{-2} \). This is a \( L(\alpha) \) intensity of about 200 \( \mu \text{W/cm}^2 \).

For the parameters chosen, the value of \( R_s \) is about \( 1.8 \times 10^{15} \text{ m} \), or about 0.06 pc - some 2 \( \times 10^6 \) times greater than the radius of the embedded O5 star. If one multiplies 4\( \pi \) times the square of \( R_s \) times the \( L(\alpha) \) flux calculated above, one gets back, of course, 5 \( \times 10^{49} \) photons \( \text{s}^{-1} \).

From the discussion given above, the linewidith of the \( L(\alpha) \) radiation emerging from an H II region has to be the Doppler width at the temperature \( T_e \). This is given by the formulas (Spitzer, 1978):

\[
\Delta v = \frac{2(\ln 2)^{1/2} b}{2},
\]  

(5)

with

\[
b = 1.290 \times 10^4 \left( \frac{T_e}{A} \right)^{1/2} \text{ cm/ sec}.
\]  

(6)
Choosing \( T_e \) to be 10,000K, A (atomic weight) to be 1, and \( \lambda \) to be \( 0.1215 \times 10^{-4} \) cm gives \( \Delta v \approx 6 \) cm\(^{-1}\). Observed DIB linewidths can be both larger and smaller than the \( L(\alpha) \) linewidth assumed in our model.

3. Resonant enhancement of two-photon absorption cross-section

For linearly polarized light waves, the absorption cross-section of an atom (or molecule) for light at frequency \( \nu_2 \) induced by light at \( \nu_1 \) for transitions from the ground state \( g \) to the excited state \( f \) is given by (Bjorkholm and Liao, 1974):

\[
\sigma(\nu_2) = 1.15 \times 10^{-24} \sum_n <f|z|n> <n|z|g> \left[ \left( E_n - h\nu_2 \right)^{-1} + \left( E_n - h\nu_1 \right)^{-1} \right]^{1/2} \rho(\nu_2 + \nu_1) I_1 \text{ cm}^2, \tag{7}
\]

where \( I_1 \) is the intensity in W/cm\(^2\) of the radiation field at \( \nu_1 \), \( \rho(\nu_2 + \nu_1) \) is the normalized lineshape function for the \( (H^2) \) transition, the matrix elements are expressed in Bohr radii, and the summation is carried out over all intermediate states of energy \( E_n \), expressed in rydbergs. For the 3s-4d transitions in Na (with the 3p levels as the dominant intermediate states), use of Eq. (7) leads to the result (Bjorkholm and Liao, 1974) that the induced cross-section for this transition is approximately \( 5 \times 10^{-11} \text{ cm}^2 \) when \( E_{3p} - h\nu_1 = 1.0 \) cm\(^{-1}\). With an effective detuning of 1.0 cm\(^{-1}\) and with \( I_1 = 200 \mu \text{W/cm}^2 \), a column of (for example, \( H_\alpha \)) ground state molecules of length 10 cm (0.003 pc) and of density 100/cm\(^3\) could thus, in principle, absorb 10% of the visible background light at those frequencies completing two-photon resonances. Note that the total \( H_\alpha \) column length (0.003 pc) needed here is only about 5% of the Strömgren radius (0.06 pc) in this case.

4. \( H_\alpha \) transitions that are nearly resonant with \( L(\alpha) \) and those that complete the two-photon absorption process

If a vibrational level \( \nu^* \) of the 1s\(\sigma_g \) ground electronic state has a good Franck-Condon overlap with a vibrational level \( \nu' \) of the 2p\(\pi_u \) excited state, transitions between the two levels are strongly allowed. Using adiabatically corrected values (Bishop et al., 1975) for the vib-rot levels of these two electronic states, one can show that the P(1) line of \( \nu' = 5 \leftarrow \nu^* = 15 \) almost exactly coincides with the peak wavelength of the \( L(\alpha) \) radiation, and that the P(1), Q(2), and R(3) lines of \( \nu' = 11 \leftarrow \nu^* = 18 \) are all within 2 cm\(^{-1}\) of the \( L(\alpha) \) peak. The DIB wavelengths in the model proposed here should thus correspond to wavelengths of allowed transitions from (low \( J' \) value) 2p\(\pi_u \) states with \( \nu' = 5 \) and \( \nu' = 18 \) to even-parity states dissociating to \( H^+ + \text{H(n=3)} \). Although Born-Oppenheimer potentials for the twelve states dissociating to \( H^+ + \text{H(n=3)} \) have been calculated (Madsen and Peek, 1971), vib-rot level energies for the (bound) states have not, for example, been determined. Hence, until accurate calculations for these states become available, the best procedure for estimating DIB wavelengths from the model is to determine vertical energy separations between upper and lower potential curves at the right-hand turning points of \( \nu' = 5 \) and \( \nu' = 11 \), i.e., at 13.0 \( \alpha_0 \) and at 20.5 \( \alpha_0 \) (Fig. 3). We illustrate by carrying out this procedure for the 3d\(\delta_g \leftarrow 2p\pi_u \) transition. This has a large, constant (i.e., as a function of \( R \)) dipole moment of 3.00 a.u. (Ramaker and Peek, 1972). A vertical line drawn at 20.5 \( \alpha_0 \) intersects the 3d\(\delta_g \) potential curve at a point \( \approx 282 \) cm\(^{-1}\) below its dissociation energy. The upper level for this transition is thus stable and would not contribute to the DIB linewidth, which would in this case presumably be primarily determined by the spectral extent over which resonance enhancement given by Eq. (7) occurs. The predicted DIB wavelength is
here 6679 Å. Could this possibly be the strong, narrow (width at half depth ≈ 2.5 cm⁻¹) DIB observed at 6614 Å? At 13.0 a₀, a vertical line intersects the 3dδg potential at a point ≈ 178 cm⁻¹ above its dissociation energy (and 125 cm⁻¹ above the height of the shallow “barrier” existing at R = 37.5 a₀). The DIB transition, predicted in this case to occur at 6156 Å, should thus be strongly broadened. Could this be the strongly broadened DIB (width at half depth ≈ 80 cm⁻¹) that is observed at 6177 Å? In Table 2, we show the wavelengths that are generated in carrying out this procedure for all six even-parity states dissociating to H⁺ + H(n=3). Wavelengths predicted to be sharp (s) or diffuse (d) are so indicated.

<table>
<thead>
<tr>
<th>Upper State</th>
<th>R = 13.0 a₀</th>
<th>R = 20.5 a₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>5gπg</td>
<td>4054 Å (d)</td>
<td>5959 Å (d)</td>
</tr>
<tr>
<td>4dσg</td>
<td>4658 Å (d)</td>
<td>5749 Å (d)</td>
</tr>
<tr>
<td>3dδg</td>
<td>6156 Å (d)</td>
<td>6679 Å (s)</td>
</tr>
<tr>
<td>5gσg</td>
<td>4669 Å (d)</td>
<td>9219 Å (s)</td>
</tr>
<tr>
<td>4dσg</td>
<td>6215 Å (s)</td>
<td>6842 Å (s)</td>
</tr>
<tr>
<td>3σσg</td>
<td>4467 Å (d)</td>
<td>5441 Å (d)</td>
</tr>
</tbody>
</table>

Table 2. Predicted DIB Wavelengths

5. Is H‡ possibly also the source of the “bump” at λ ≈ 2175 Å?

As stated in the Introduction, the required presence of H‡ molecules located near Rs could conceivably result from direct photoionization of H₂ molecules in a compact shell that serves as the transition region between the H II sphere and the cold surrounding (H₂) gas. In this case, one would expect the H‡ ions to be produced in the ground state with a vibrational distribution given by the known Franck-Condon factors for ionization of hydrogen. It is apparent from the Dunn and Oksjuk results (Fig. 4) that the cross-section for 2pπu — 1sσu photodissociation for such a vibrational distribution peaks somewhere in the 2100 - 2200 Å range. Thus, an intriguing additional feature appears in the model presented here!

One can even “push one’s luck” and try to ask why the interstellar extinction curve reverses its decline at ≈ 8 eV, after it has fallen considerably from its 2175 Å peak, and strongly starts to increase again with increasing photon energy. A possible explanation is that at shorter wavelengths the vibrational H‡ 1sσg distribution that results from H₂ photoionization starts to absorb again when the photon energy becomes high enough for the 2pπu — 1sσg transition to occur. There are also allowed transitions from 1sσg to higher states of u parity, states dissociating both to n=2 and higher n.


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**Fig. 1.** Extinction due to interstellar dust (Huffman, 1991).

**Fig. 3.** $1s\sigma_g$ and $2p\pi_u$ potential curves (Beckel, C.L.; Shafi, M.; and Peek, J.M.: 1973, J. Chem. Phys. 59, 5288).

**Fig. 2.** Some potential curves for $H_2^+$ (Levine, 1974).

**Fig. 4.** $\sigma(\lambda)$ [2$p\pi_u \leftarrow 1s\sigma_g$ transition] for the $H_2^+$ vibrational distribution produced by photoionization of $H_2$ (Dunn, 1968).