Molecular Hydrogen Excitation in Gas Clouds

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1 Introduction

We will look at the observation of distant galaxies using an Infra-red spectrometer. The instrument in question is UIST on UKIRT and it will be used to look at molecular gas clouds which are excited by violent activity or more specifically several lines around the H₂ emission range. UIST had a detector that works over the wavelength range $\lambda = 1.47 - 2.5 \mu m$ which is perfect for looking at these line emissions.



Figure 1: An example spectrum obtained using UIST on UKIRT

This is a spectrum of ESO-428-G14, it is a Seyfert 2 galaxy in the relatively local universe. The details of the spectrum will be covered later.

1.1 What will we study?

Molecular Hydrogen in the universe only occurs in places where there is both sufficient shielding of the molecules from incident radiation and also a low enough ambient temperature that the molecules cannot collisionally ionise. The most abundant realms where both rules are observed are inside giant gas clouds. This lecture will show the processes involved in the intreactions of the H_2 with its surroundings, how these can be observed with modern techniques and what these observations can help us infer about the underlying physical processes and dynamics happening in the heart of these opaque systems.

1.2 Why Study Molecular Hydrogen?

Molecular Hydrogen Emission (MHE) is used to give us an insight into the physical processes happening in the regions of violent activity buried deep in giant molecular gas clouds. To date it is the main observable feature from around these star forming regions and whilst it is impossible to directly observe the star formation, the processes involved can be deduced by looking at their interaction with the surrounding molecular hydrogen and the excitations and emissions that are given off.

2 Composition of Gas Clouds

The Giant Molecular Clouds (GMC's), which are found within galaxies, are composed of vast amounts of hydrogen and helium. There are also heavier elements present in abundances that are dependent upon the star formation history within in the gas cloud. The clouds are generally inhomogenous, with large fractions of the mass being found in clumps within the cloud. Sizes of these clouds typically range between $10^4 \cdot 10^5 M_{\odot}$ with the molecular hydrogen regions being of around 50-100 Kelvin. Xrays and Far UV photons can penetrate the surfaces of the molecular cloud causing photoionisation and photoelectric ejection respectively. In both cases this results in a heating of the gas. For this reason molecular hydrogen is not found on the outer extremities of the gas cloud but is buried more deeply within the cloud where it is shielded from any incident photons of the intergalactic wind.

2.1 Photodissociation Regions

Photodissociation Regions or PDRs are regions of predominantly neutral gas where the gas dynamics are dictated by a far-UV field. For hydrogen, the relevant far-UV radiation for a PDR ranges between energies of 11.2 and 13.6 eV (equivalent to 1100 Å and 912 Å respectively.) The lower energy represents the energy required to excite H2 out of its lower rotational-vibrational levels and the higher energy represents the photoionisation potential of H. The origin of the UV field can either be due to the evolution of a high mass OB Star $(10 - 15M_{\odot})$ that has formed from a clump within the cloud or due to the emission given off from an Active Galactic Nuclei. The nature of the excitation from a high mass star means that PDRs in star forming regions are only found in relatively young clusters. The field penetrates the gas cloud, influencing the chemistry and dynamics of hydrogen to a typical depth of ~ $4A_v$ where A_v is the optical depth at visual wavelengths.

At the nominal temperature and particle density found in the massive gas clouds $4A_v$ is equivalent to the half-thickness of the molecular cloud. It is for this reason that PDRs represent the typical environment of the interior of a molecular gas cloud, apart from some highly shielded clumps of gas in the opaque core.

A PDR is illustrated in Figure 2. Far UV Radiation is incident from a nearby hot star or AGN. The diagram starts at the relatively sharp interface between ionised (HII) and neutral (HI) hydrogen. The interface between HI and molecular hydrogen (H_2) occurs at



Figure 2: Scales of UV penetration into cloud

~ $2A_v$. As can be seen the influence of the PDR extends further into the cloud with the interface between O and O₂ occurring as far as $20A_v$.

The high energy UV photons do not penetrate the cloud to the same depths that the lower energy ones do. The reason for this is due to the ionisation crosssection of the hydrogen in the cloud, See Figure 3.

At wavelengths shorter than 912 \mathring{A} [Energy greater than 13.6eV] all of the radiation is absorbed in the HII region. In this region there is a balance between the hydrogen being ionised and the protons and electrons recombining.

There is than a sharp transition between the HII region and the H region. This is the point by which all of the radiation ≤ 912 Å has been absorbed and is also defined as the start of the PDR.

There is no H_2 in the H region as any that form are bombarded by the incident radiation and whilst this is not of sufficient energy to directly dissociate the hydrogen molecules, ~ 10 - 15 % of the time the molecules will de-excite to an unbound state.

Within the PDR at energies lower than this 13.6eV interface the heavier elements are still ionised up to a depth of $\sim 1 - 2A_v$. It is also at this depth that molecular hydrogen begins to form and as such it is from around this depth that there are large columns of vibrationally excited H₂. It is this excited H₂ which astronomers use to probe the insides of these giant gas clouds.



Figure 3: The ionisation cross-section of hydrogen vs. Energy

2.2 Shocks

Another process that also heats molecular gas clouds are hydrodynamic shocks. In this case the heating is due to the collision of two bodies of gas. Shocks are formed via a different process than PDRs, the most well known of which would be due to the outflows of gas from a supernova. The shock heating is due to the kinetic energy of the gas being converted into heat at the shockfront. As such the temperature of a shock heated gas follows

$$T \propto v^2$$
 (1)

where v is the velocity of the gas. Shock systems are of a higher density and therefore enjoy more collisions meaning that the complete system is in local thermodynamic equilibrium (LTE). This is an important observable difference to fluorescent excitation that will be covered shortly.

2.3 Formation and Destruction

Whilst the ratio of HI to H_2 , at each stage of a PDR, can be considered to be roughly constant, the hydrogen molecules in a GMC do not have an unlimited lifetime. They are

infact continually being formed and destroyed from processes ongoing within the cloud.

As already covered, H_2 is the stable form of hydrogen at low temperatures. For systems in Local Thermodynamic Equilibrium (LTE) its abundance relative to that of HI is calculated using the dissociation equation. However the system is not in LTE, the temperature of the molecular hydrogen regions are max 100 K while the colour temperature of the UV quanta is about 30,000 K.

In the PDR when a UV ray collides with a H2 molecule, about 90% of the time the molecule is excited to a much higher energy state. The other 10% of the time the molecule will be atomised leaving two highly energetic HI molecules.

In the case of atomisation, the HI molecules will move around the GMC wanting to recombine with another HI molecule. There are two main problems. Firstly the molecules have to lose a considerable amount of energy before they can recombine. Secondly, because they are identical they have to overcome the repulsive coulomb barrier between themselves but their energy is not sufficient to do this. This problem is solved by dust grains. The HI atom will move around the cloud and when it collides with a dust grain there is a probability it will stick to the surface in a potential well. The surface of the dust grain is full of these potential wells and as such the HI atom freely moves across the surface at a high speed from one potential well to another. If, on its precession across the dust grain, it comes in contact with another HI atom then they will recombine releasing 4.48 eV of energy. A fraction of this energy will be absorbed by the dust grain and then radiated away from the gas cloud as IR radiation.

The rate of formation of H_2 from HI atoms is dependent upon the collision rate of the HI and the grain, the sticking probability that the HI will fall into a potential well on the surface, the speed of precession of the HI across the surface of the grain and the lifetime that HI will survive on the grain surface. H_2 formation on grains occurs below a grain temperature limit of 100 Kelvin, above this the HI evaporates off the surface before recombination.

The relation between the incident flux and the number density of HI atoms is shown below

$$F\sigma_{diss} = Rn_d n_h \tag{2}$$

where F is the incident Flux, σ_{diss} is the dissociation cross-section, n_d is the number density of dust, n_h is the number density of hydrogen and R is the constant $3 \times 10^{-17} \text{cm}^3 \text{s}^{-1}$. R comes from the expected value of recombination in a typical GMC and has been most accurately calculated through observation. As expected the number density of hydrogen atoms decreases with incident flux.

3 Observations in the near local universe

3.1 Boltzmann Temperature Relation

The number of photons of a given energy increase rapidly with temperature so emission lines originating from excited levels tend to be stronger in hot gases than cool gases. In cases of thermal equilibrium, ie a shock, Boltzmann's equation which relates the number density, the statistical weight and the energy E of the level can be simplified to give the relation



Figure 4: Theoretical derivation of temperature in gas clouds

where N_j is the couumn density of level j and g_j is the statistical weight function of level j. In this way the temperature of a gas cloud in thermal equilibrium can be simply calculated from observations.

In reality gas clouds in galaxies are never in such perfect states of homogeneity and so the observed distribution looks quite different. In hydrodynamical shocks, the top graph in Figure 5, the gradual change in gradient implies a gradual change in temperature through the gas cloud. This is due to the heat conductivity of the gas and as such the temperature drops as you move away from the shockfront.



Figure 5: H_2 column densities, divided by the level degeneracy, as a function of energy level (in Kelvin)

The bottom graph in Figure 5 instead shows the observed distribution for a PDR. A PDR is not in thermodynamic equilibrium and as such the graph looks nothing like the case for shocks.

3.2 Excited States of the Hydrogen Molecule in a PDR

Fluorescent molecular hydrogen was first identified in 1987. The galaxy in question (NGC 2023) was seen to have a rich vibrational-rotational (Vi-Ro) near-IR spectrum. In particular the main identifier was the strength of the 2-1 S(1) to the 1-0 S(1) line which in this case was 25 % of the intensity compared to the normal 10 % observed in shocks.

The interpretation of the fluorescent molecular hydrogen is complicated by the need to consider two processes, the radiative excitation of the H_2 molecules by the UV field and their collisional de-excitation with HI molecules. When the H2 molecule is excited, the electron cascades down the energy levels, denoted below, at a rate of approximately 1 per year. But when the density of hydrogen in the cloud reaches a certain critical density, collisional de-excitation of the H2 by HI proceedes faster than the spontaneous decay. In this case much of the energy stored in the Vi-Ro levels are released as heat. In this case the gas has a much more thermalised emission spectra to it and can look more like the shock distribution in Figure 5.

They are many different transitions that the hydrogen molecule can undergo after being excited above the ground state. When studying MHE in GMC's the observer looks for certain bound transitions that have a defined transition rate, See Table 1 (below). Astronomers can probe the relative energetics of the molecular hydrogen from the relative strength of these lines.

Emission Line	Wavelength (μm)
$1-0 \mathrm{S}(1)$	2.1218
2-1 S(1)	2.2477
3-2 S(3)	2.2014
4-3 S(3)	2.345
8-4 S(5)	0.8269

Table 1: Emission line and it's associated wavelength

The change in vibration number is written first and the number in parenthesis denotes the final rotation level. The S denotes a change of $\Delta J = -2$, Q = 0 and O = +2. Therefore 8-4 S(5) symbolises a transition from the [8th vibrational; 8th rotational] to the [4th vibrational; 5th rotational level]. Figure 6 shows a full molecular hydrogen emission level diagram with these main transitions indicated.



Figure 6: Energy level diagram for ground electronic state of molecular hydrogen

3.3 Other Excited States

Generally any emission lines can tell you something about the subject of interest. Table 2 shows a selection of some other emission lines within the UIST wavelength range. These lines are found in different regions of excitation and their relative abundances across the field of view can give you further insight into the underlying physical dynamics of the region.

Emission Line	Wavelength (μm)
FeII	1.643999
1-0 S(3)	1.9576
Si VI	1.96464
Br Gamma	2.16612

Table 2: Emission line and it's associated wavelength