Calculation involving hydrogen-hydrogen(2) collisional cooling processes for use in astrophysics

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CALCULATION INVOLVING H–H₂ COLLISIONAL COOLING PROCESSES
FOR USE IN ASTROPHYSICS

by

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Bachelor of Science (Physics)
University of Washington, Seattle
1986

A thesis submitted in partial fulfillment
of the requirements for the

Master of Science in Physics
Department of Physics
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Graduate College
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Examination Committee Chair

Dean of the Graduate College

Examination Committee Member

Graduate College Faculty Representative
ABSTRACT

Calculation Involving H−H₂ Collisional Cooling Processes for Use in Astrophysics

by

David Michael Archer

Dr. Stephen Lepp, Ph.D. Examination Committee Chair
Professor of Physics
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This thesis will calculate the H−H₂ cooling processes used in astrophysics. Cooling is critical to the formation of the first objects formed in the early universe, and other diverse phenomenon of interest to astrophysics. For instance, in order to collapse into objects, the gravitational potential energy of primordial density fluctuations must be radiated away. The most abundant element in the universe is hydrogen, and cooling processes involving hydrogen are important in several contexts. To calculate the cooling, the cross section for collisional excitation at constant energy were integrated over a Maxwellian velocity distribution to determine a rate coefficient. Then the equilibrium level populations will be solved for a given temperature and H density. Finally, the cooling and spectra are calculated from these equilibrium populations.
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CHAPTER 1

INTRODUCTION

The purpose of this thesis is to analyze collisional cooling of neutral hydrogen with \( \text{H}_2 \). In particular to generate cooling curves and spectra as a function of density and temperature by determining the equilibrium populations for the exited states of the \( \text{H}_2 \) molecule at constant temperature.

The \( \text{H}^+\text{H}_2 \) system is one of the simplest systems that the results of theoretical calculations can be compared with experimental results within reasonable accuracy, and as such has been of interest to chemists. It is also of interest for those interested in combustion of \( \text{H}_2 \) for practical purposes. The study of this system however is of more interest to the astrophysical community, due to the importance of \( \text{H}_2 \) in many processes that are observed in the universe.

The importance of \( \text{H}^-\text{H}_2 \) and \( \text{H}^-\text{HD} \) collisional cooling and the relatively recent advances in infrared instrumentation has allowed more detailed study of astrophysical phenomenon\(^1\). One such example of the improved instrumentation is the Short Wavelength Spectograph (SWS) on the Infrared Space Observatory (ISO). This was the first instrument to observe rotational \( \text{H}_2 \) lines in the center of the infrared spectrum\(^2\).

It is thought collisional excitation of \( \text{H}_2 \) followed by spontaneous emission is the most important cooling mechanism in the Early Universe. Although only a small fraction of the primordial gas is \( \text{H}_2 \), the first significant cooling processes that can take
place are the \( \text{H}_2 + \text{H} \) and \( \text{HD} + \text{H} \) cooling processes, as all other mechanisms that are known to dominate cooling in the present interstellar medium are not present. Cooling is critical for the primordial gas to dissipate the gravitational energy of density fluctuations to allow collapse into galaxies and stars.

This cooling process is also significant in the understanding of interstellar shocks. Shocks are formed whenever a portion of a region of gas expands faster than the speed of sound in the region. When a pressure pulse such as this forms, the front of the pulse tends to compress, as the speed of sound is faster in the higher density region, and as a result there is a discontinuity that builds at the front of the shock. Where these \( \text{H} - \text{H}_2 \) cooling processes occur within shocked regions, the properties of these regions can be established through observation of their infrared signature. An example of such region that has been observed is the BN–KL region of Orion\(^1\).

This process is also significant in photodissociation regions. A photodissociation region is an area where there is a flux of photons with energy sufficient to cause dissociation of the molecules present. In particular, in a region where \( \text{H}_2 \) dissociation is taking place, one can determine the \( \text{H}_2 \) to \( \text{H} \) ratio, infer the rate of dissociation, and establish the incident photon flux.

Both of the above processes, photodissociation and shocks, are present in starburst galaxies. A starburst galaxy is a galaxy going through a stage of rapid star formation. One mechanism for forming a starburst galaxy would be the merging of two galaxies.

Historically there are four potentials for the \( \text{H}_2 + \text{H} \) system that are well documented. These are the Liu–Siegbahn–Truhlar–Horowitz\(^4\) (LSTH), the double many-body expansion\(^5\) (DMBE), and those of Boothroyd–Keogh–Martin–Peterson\(^6,9\) (BKMP & BKMP2). The BKMP2 potential was based on a Born–Oppenheimer approximation.
over a grid of approximately eight thousand positions for the three nuclei. The potential surface thus obtained was fit to a predetermined functional form to facilitate collisional calculations.

The differences in calculated rate coefficients for these different potentials was examined by Lepp, Buch, and Dalgarno. They found that rate coefficients determined from the LSTH, DMBE, and BMKP potentials agreed well for reactive collisions, and for higher rotational angular momenta; but disagreed by as much as an order of magnitude for some non-reactive collisions, such as those involving pure rotational transitions from J=0 to 2 and J=1 to 3 levels. The BKMP potential was also intercompared in the work of Tine, Lepp, and Dalgarno. The calculations performed in this investigations use the BKMP2 potential.

A semiclassical trajectory method was used to determine cross sections of constant energy for the H+H₂ system for this work. The methodology followed is to take cross section data at constant energy, provided by S. Lepp, to compute a rate coefficient at constant energy. These rate coefficients are then averaged to provide average rate coefficients at constant temperature. These rate coefficients are then fit to 3-parameter curve as a function of temperature. Then cooling curves are computed as a function of temperature using the fit curve as input to the computational probs. The cooling curves and spectra are generated by solving for the equilibrium populations of the H₂ molecules and using those populations to determine the total spontaneous emission associated with each transition.

The equilibrium populations were computed by first assuming that all the molecules were initially in the ground state and then to solve the coupled differential equations that govern the time evolution of the system using a standard differential equation.
solver (lsode) and propagate them forward in time until equilibrium is reached. The details of this analysis will be described in the next section.

The theoretical calculations described here can be used to compute the spectra of this type of collisional cooling, which can be compared with observational data. This could be done with correlation techniques, where the temperature, density, and red shift could be calculated in regions where this type of collisional cooling processes are taking place. Information on the astrophysical processes described above can be determined by the observational data.
CHAPTER 2

DETAILED DESCRIPTION OF METHODOLOGY

Determination of H–H₂ Cross Sections at Constant Energy

The determination of cross sections for various collision induced transitions was computed by Lepp, Buch, and Dalgarno⁷, by using the semiclassical method. The trajectories of 10 000 hydrogen atoms of random impact parameters up to a maximum impact parameter \( b_{\text{max}} \) were calculated using the BKMP⁹ potential for each rovibrational state of the H₂ molecule.

The energy difference from the initial to final energy of the colliding particle (\( \Delta E \)) was used to determine which state the H₂ molecule would be in for downward transitions. The rate coefficients for the upward transitions were then determined by detailed balance calculations for the rates calculated from the upward transition cross sections. These cross sections at constant energy (and therefore constant speed) were then calculated using:

\[
\sigma_g(E) = \pi b_{\text{max}}^2 \frac{n_{ij}}{10000}
\]

where

\( n_{ij} \) = number of trajectories with \( E_j - E_i < \Delta E < E_{j+1} - E_i \)
For the purpose of uncertainty analysis, the uncertainty associated with this will be estimated by the following formula:

$$\delta \sigma_y(E) = \pi b \frac{\sqrt{n_y}}{10000}$$

This is believed to be a reasonable approximation for the uncertainties associated with this calculation, except in the low temperature limit, where the semiclassical calculation is expected to break down.

### Calculation of Average Collisional Rate Coefficients at Constant Temperature

For the purposes of calculation, we will define the following variables that are used to parameterize the energy:

$$E = kT_e = \frac{1}{2}m v_e^2$$

where $T_e$ is an "equivalent Temperature" corresponding to $E$, and $v_e$ an equivalent velocity magnitude for the incoming H atom. In the above equation $m$ is the mass of the H atom. It is worth noting that what is important here is that $E$ is proportional to $T_e$ and $v_e^2$, not what constants appear in the parameterization. All the constants will cancel in the final result for the averaged rate coefficient.

Expressing the equivalent velocity in terms of the equivalent temperature:

$$v_e = \left(\frac{2k}{m}\right)^{\frac{1}{2}} T_e^{\frac{1}{2}}$$

and defining the cross section as a function of equivalent temperature:

$$\sigma_y(T_e) = \sigma_y(E(T_e))$$
the collisional rate coefficient at constant energy for a given collisional process can be expressed:

\[ \gamma_\ell^E = v_\ell \sigma_\ell(E) = \left( \frac{2k}{m} \right)^{\frac{1}{2}} \frac{1}{T_\ell^2} \sigma_\ell(T_\ell) = \gamma_\ell(T_\ell) \]

From statistical mechanics, the average value of this quantity is just:

\[
\gamma_\ell(T) = \frac{\int_0^\infty \gamma_\ell^E(T) e^{-\frac{E}{kT}} dE}{\int_0^\infty e^{-\frac{E}{kT}} dE} = \frac{\int_0^\infty \gamma_\ell^E(T_e) e^{-\frac{T_e}{T}} dT_e}{\int_0^\infty e^{-\frac{T}{T}} dT_e}
\]

now

\[
\int_0^\infty e^{-\frac{T}{T}} dT_e = -T
\]

by elementary integration. Therefore one can write

\[
\gamma_\ell(T) = -\frac{1}{T} \int_0^\infty \gamma_\ell^E(T_e) e^{-\frac{T_e}{T}} dT_e
\]

breaking this into intervals of width \( \Delta T_n = T_n - T_{n-1} \) where \( T_n \) are the temperatures corresponding to the constant energy cross sections provided by S. Lepp. one obtains

the following approximation:

\[
\gamma_\ell(T) \approx -\frac{1}{T} \sum_{n=1}^N \gamma_\ell^E(T_n) e^{-\frac{T_n}{T}} \Delta T_n = -\frac{1}{T} \sum_{n=1}^N \left( \frac{2k}{m} \right)^{\frac{1}{2}} \frac{1}{T_n^2} \sigma_\ell(T_n) e^{-\frac{T_n}{T}} \Delta T_n
\]

since we will assume zero cross section at zero energy. we will assume that the first part of this approximation to the integral will be triangular in shape, i.e. \( \Delta T_1 = \frac{T_1}{2} \)
For the purposes of this endeavor, only the downward transition rate coefficients were calculated this way, the upward collisional rates were computed from the upward collisional rates using detailed balance:

\[ g_j \gamma_{jk} = g_k \gamma_{kj} e^{\frac{E_{jk}}{kT}} \]

where:

- \( g_j \) = degeneracy of level \( j \)
- \( E_{jk} = E_j - E_k \) = positive energy difference between the two levels

The rate coefficients at constant temperature are then converted to averaged cross sections by dividing through by the average equivalent velocity.

\[ \overline{\sigma}_{\gamma}(T) = \frac{\gamma(T)}{\bar{v}_e} \]

where

\[ \int_0^\infty \frac{v_e}{v_e} \frac{m v_e^2}{2kT} dv_e = \left( \frac{2k}{m} \right)^{1/2} \int_0^\infty T_e^{\frac{3}{2}} e^{\frac{T_e}{T}} dT_e = \frac{-1}{T} \left( \frac{2k}{m} \right)^{1/2} \int_0^\infty T_e^{\frac{3}{2}} e^{\frac{T}{T}} dT_e \]

which is the average value of \( v_e \) at constant \( T \).

Combining the expression for \( \gamma_{\gamma} \) with the above, converting the last integral above to a sum and simplifying, one obtains

\[ \overline{\sigma}_{\gamma}(T) = \frac{\sum_{n=1}^{N} \sigma_{\gamma}(T_n) T_n^{\frac{3}{2}} e^{\frac{T}{T}} \Delta T_n}{\sum_{n=1}^{N} T_n^{\frac{3}{2}} e^{\frac{T}{T}} \Delta T_n} \]
This result then can be used to determine an average rate coefficient as follows:

$$\bar{y}_u = v_{th} \bar{\sigma}_u$$

where $v_{th}$ is the average thermal velocity.

These results are then stored and used to compute cooling and spectra. To facilitate faster computation of cooling, the rates are fit to a functional form as described in the next section.

Procedure for Fitting Rate Coefficient Data

The procedure for calculating the rate coefficients as a function of temperature described could be performed at each temperature of interest, but it requires less computational effort to compute a small number of representative temperatures and subsequently perform a least-squares fit to the results. This may also be a more accurate procedure as the random errors in the cross section data would tend to be averaged out by the fitting procedure. This is the approach that was taken. A least-squares of the rate coefficient data was performed for a previously established form:

$$\log_{10}(Q) = A - \frac{B}{T} + C \log_{10}(T)$$

where:

- $Q$ = rate coefficient of interest
- $A$, $B$, $C$ are fit coefficients

The procedure used was a least-squares fit, to be described here. What is required is to minimize the following expression:

$$\sigma = \sum_{i=1}^{n} \left( Q_i - A + \frac{B}{T} - C \log_{10}(T) \right)^2$$
This is performed by setting \( \frac{\partial \sigma}{\partial A} = \frac{\partial \sigma}{\partial B} = \frac{\partial \sigma}{\partial C} = 0 \)

Forming these partial derivatives one obtains:

\[
\frac{\partial \sigma}{\partial A} = -2 \sum_{i=1}^{N} \left( Q_i - A + \frac{B}{T_i} - C \log_{10}(T_i) \right)
\]

\[
\frac{\partial \sigma}{\partial B} = 2 \sum_{i=1}^{N} \left( Q_i - A + \frac{B}{T_i} - C \log_{10}(T_i) \right) \frac{1}{T_i}
\]

\[
\frac{\partial \sigma}{\partial C} = -2 \sum_{i=1}^{N} \left( Q_i - A + \frac{B}{T_i} - C \log_{10}(T_i) \right) \log_{10}(T_i)
\]

Equating these to zero and rearranging one obtains the following systems of equations:

\[
AN - B \sum_{i=1}^{N} \frac{1}{T_i} + C \sum_{i=1}^{N} \log_{10}(T_i) = \sum_{i=1}^{N} Q_i
\]

\[
A \sum_{i=1}^{N} \frac{1}{T_i} - B \sum_{i=1}^{N} \frac{1}{T_i^2} + C \sum_{i=1}^{N} \frac{\log_{10}(T_i)}{T_i} = \sum_{i=1}^{N} \frac{Q_i}{T_i}
\]

\[
A \sum_{i=1}^{N} \log_{10}(T_i) - B \sum_{i=1}^{N} \frac{\log_{10}(T_i)}{T_i} + C \sum_{i=1}^{N} \log_{10}^2(T_i) = \sum_{i=1}^{N} Q_i \log_{10}(T_i)
\]

Defining the following variables:

\[b = -\sum_{i=1}^{N} \frac{1}{T_i}, \quad c = \sum_{i=1}^{N} \log_{10}(T_i), \quad d = -\sum_{i=1}^{N} \frac{1}{T_i^2}\]

\[e = \sum_{i=1}^{N} \frac{\log_{10}(T_i)}{T_i}, \quad f = \sum_{i=1}^{N} \log_{10}^2(T_i)\]

\[y_1 = \sum_{i=1}^{N} Q_i, \quad y_2 = \sum_{i=1}^{N} \frac{Q_i}{T_i}, \quad y_3 = \sum_{i=1}^{N} Q_i \log_{10}(T_i)\]

then rewriting the above system of equations in matrix form one obtains:
Inverting this equation manually results in the following:

\[
\begin{pmatrix}
N & b & c \\
-b & d & e \\
c & -e & f
\end{pmatrix}
\begin{pmatrix}
A \\
B \\
C
\end{pmatrix}
=
\begin{pmatrix}
y_1 \\
y_2 \\
y_3
\end{pmatrix}
\]

where:

\[
A = \frac{1}{\Delta}
\begin{pmatrix}
e^2+df & -bf-ce & be-cd \\
bf+ce & Nf-c^2 & -Ne-bc \\
be-cd & Ne+bc & b^2+Nd
\end{pmatrix}
\begin{pmatrix}
y_1 \\
y_2 \\
y_3
\end{pmatrix}
\]

\[
\Delta = Nd^2 + Ne^2 + b^2 f + 2 b c e - c^2 d
\]

This result was then hard coded into a subroutine for use in the fitting process.

**Uncertainty Analysis of the Fitted Rate Coefficients**

In this particular case, it is assumed that the uncertainties associated with the T, are zero, and the only quantities that contribute uncertainties to the result are the y1, y2, and y3 terms. The uncertainties associated with each fitting coefficient expressed as standard uncertainties due to the linear nature of the above equations is just:

\[
\delta A = \sqrt{\left(\frac{e^2+df}{\Delta} \delta y_1\right)^2 + \left(\frac{bf+ce}{\Delta} \delta y_2\right)^2 + \left(\frac{be-cd}{\Delta} \delta y_3\right)^2}
\]

\[
\delta B = \sqrt{\left(\frac{bf+ce}{\Delta} \delta y_1\right)^2 + \left(\frac{Nf-c^2}{\Delta} \delta y_2\right)^2 + \left(\frac{Ne+bc}{\Delta} \delta y_3\right)^2}
\]
\[
\delta C = \sqrt{\left(\frac{b e - c d}{\Delta} \delta y_1\right)^2 + \left(\frac{N e + b c}{\Delta} \delta y_2\right)^2 + \left(\frac{b^2 + N d}{\Delta} \delta y_3\right)^2}
\]

where:

\[
\delta y_1 = \sqrt{\sum_{i=1}^{N} \delta Q_i^2}, \quad \delta y_2 = \sqrt{\sum_{i=1}^{N} \frac{\delta Q_i^2}{T_i^2}}, \quad \delta y_3 = \sqrt{\sum_{i=1}^{N} \delta Q_i^2 \log_{10}(T_i)}
\]

and \(\delta Q_i = \text{uncertainty associated with the rate associated with } T_i\).

From the form of the fit:

\[
\log_{10}(Q) = A - \frac{B}{T} + C \log_{10}(T)
\]

One can derive the following expression for the resulting rate:

\[
Q = e^{A \ln 10} e^{-\frac{B \ln 10}{T}} e^{C \ln T}
\]

leading to an overall uncertainty in the rate at this temperature of:

\[
\delta Q = Q \sqrt{(\delta A \ln 10)^2 + \left(\delta B \frac{\ln 10}{T}\right)^2 + (\delta C \ln T)^2}
\]
The Computation of Equilibrium Populations

In equilibrium, the rate of processes that remove a molecule from a given state equals the rate at which molecules enter that state from another state. There are three ways that a molecule can leave a particular state: collisional processes, stimulated emission, and spontaneous emission. There are four ways that a molecule can enter a specific state: collisional processes, stimulated emission from a higher energy state, spontaneous emission from a higher energy state, absorption of photons from a lower energy state. The assumptions made in this case is that no photons are available for stimulated emission or absorption processes, and that any spontaneously emitted photons leave the region. These assumptions will obviously break down at higher densities. The system of equations that governs the time evolution of a system of molecules in different states, under these assumptions is thus:\(^\text{10}\):

\[
\frac{dn_j}{dt} = -n_j \left( \sum_k n_k \gamma_{jk} + \sum_{k<j} A_{jk} \right) + \sum_k n_k n \gamma_{kj} + \sum_{k>j} n_k A_{kj}
\]

where:

- \(A_{jk}\) is the rate of spontaneous emission from the state \(j\) to \(k\) (Einstein A coefficient)
- \(n_j\) is the number density of \(\text{H}_2\) molecules in state \(j\)
- \(n\) is the number density of \(\text{H}\) atoms.

After suitably labeling the energy levels, the above equations were solved as a function of time using an available differential equation solver Isode. The initial conditions used was that all molecules were in the ground state at time zero, and the solution was stepped forward in time until equilibrium was reached.

Once the equilibrium populations, \(n_k\), are known, the total cooling per atom can be calculated. The total cooling per atom is just the following:
\[
\Lambda = \sum_{i=1}^{\infty} \sum_{j=0}^{i-1} n_i A_{ij} E_j
\]

Note that one can also compute the spectrum as a function of temperature as the quantity \( n_i A_{ij} \) is just the number of photons per atom with energy \( E_j \). resulting in a prediction for the spectrum that could be verified by observations, or a method to determine the properties of a region where this process is dominant by matching observational and theoretical spectra. Each spectra can be constructed by plotting the quantity \( n_i A_{ij} E_j \) as a function of \( E_j \) represented as either a frequency \( (E_j / h) \) or a wavelength \( (hc/E_j) \).
CHAPTER 3

RESULTS

Rate Coefficient Calculation Results

The computation of rate coefficients was accomplished using the methodology described above. A few representative rates were chosen to compare the results of the various methods used in the past. The results are summarized in the following graphs. These graphs show a few randomly selected rate coefficients as a function of temperature.

The rate coefficients are labeled in these graphs such that, for example, (3,2)→(3,0) represents a transition from the \( \nu=3, j=2 \) state to the \( \nu=3, j=0 \) state.

The "Flower" rates portrayed on these graphs are those rates that were derived in a quantum mechanical calculation by Flower\(^{12}\) and are found on the website "http://ccp7.dur.ac.uk/cooling_by_h2/". The rates labeled "This work" represent a fit of constant energy cross sections to a Maxwellian distribution. The "Lepp" rates are those calculated by enumerating the number of transitions taken from a distribution at constant temperature provided by S. Lepp, from the work of Tine, Lepp, and Dalgarno\(^{6}\). The "Martin & Mandy" rates are those available at the website "http://www.cita.utoronto.ca/~pgmartin/h2dist/" from their work\(^{13,14,15}\).

The first graph shown below is of a pure rotational transition near the ground state.
Notice there is agreement between all methods above 1000 degrees, and that the semiclassical calculations diverge from the quantum mechanical calculation of Flower at low temperatures, as expected. In the high temperature limit, the semiclassical and quantum calculations are expected to converge because of the correspondence principle.

The following graph shows a low lying purely vibrational transition.
Notice again there is rough agreement with all methods in the high temperature limit, but not as good as before.

Looking at a slightly higher level vibrational transition one obtains the following result:

![Rate Coefficient (2,1)→(0,1) vs Temperature](image)

*Figure 3*

Again notice that all the semiclassical calculations are in rough agreement, but the quantum mechanical results of Flower are starting to diverge from the expected results. There is an indication of some convergence at the high temperature limit, but it is very poor.

The following graphs will show a series of rotation, vibrational, and mixed transitions. They all share the common characteristic that the results of Martin & Mandy, Lepp, and this work are in rough agreement, but as you go to higher level transitions, the quantum calculations of Flower diverge more and more. Because Flower
neglected exchange reactions it is not clear how accurate his calculations are at higher energy levels.

Figure 4

Figure 5
Rate Coefficient (2,3)→(1,3) vs Temperature

Rate Coefficient (2,4)→(1,2) vs Temperature

Figure 6

Figure 7
Rate Coefficient (2,4)→(0,0) vs Temperature

Figure 8

Rate Coefficient (1,7)→(1,1) vs Temperature

Figure 9

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Again, as can be seen from these graphs, the results of this work agree well with the earlier work of Lepp and Martin & Mandy, but not with the later quantum mechanical calculation of Flower.

Cooling Calculation Results

The next logical step in this analysis is to compute cooling curves as a function of temperature and density. The next two graphs show this calculation for the Lepp rates and the rates calculated here. A complete cooling curve for the Flower rates could not be calculated as I do not have access to a complete set of rates from Flower.
Cooling Function vs Temperature

Figure 11

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Cooling Function vs Temperature

(This work)

Figure 12

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In the above figures, the high temperature and high density regions agree very well, but there is as much as an order of magnitude difference in the low temperature, low density cooling curves. This is probably due to the fact that the "Lepp" cooling curves have a quantum mechanical correction that is applied.

The Calculation of Spectra

Multiple spectra were calculated in this work. The following graphs are representative of the spectra that can be calculated using the the results of the calculations presented here. The first series of graphs are all at the same H density \(10^6 \text{ m}^{-3}\) showing the temperature dependence of the spectra.

The 4 largest lines in frequency order are the \((0,2)\rightarrow(0,0), (0,3)\rightarrow(0,1), (0,4)\rightarrow(0,2),\) and the \((0,5)\rightarrow(0,3)\) transitions. Notice these are all rotational transitions, as there is insufficient energy at this temperature and density to excite vibrational transitions.
Intensity per Molecule vs Frequency

2000 K density = 10^6 m^-3

Figure 14

Again, here at 2000K the spectra is dominated by rotational transitions, although there is some indication that vibrational transitions are beginning to be excited.

Intensity per Molecule vs Frequency

5000K density = 10^6 m^-3

Figure 15

Clearly vibrational lines are starting to become important at 5000K.
At 10,000K, there are clearly higher vibrational bands contributing to the overall spectra, but the lower rotational lines are still the dominate emission. The largest emission line is the (0,5)→(0,3) transition.

The next series of graphs will show spectra for a set of representative temperatures and densities.
Notice that in this last case, there is emission approaching the visible. It is clear that as temperature and/or H density increases, the more emission in higher energy lines. This is as it should be. In particular as temperature and density increase, the energy is more distributed throughout the infrared spectrum.
CHAPTER 5

CONCLUSIONS

From the level of agreement with previous work, it appears that averaging of cross section data determined at constant energy over its presumed Maxwellian distribution at constant temperature is just as accurate as computation of cross section from energies taken randomly from that same distribution. Cross section, spectra, and cooling curves generated in this fashion agree with previous semiclassical calculations.

There is a problem of agreement with the semiclassical calculations presented here and the complete quantum mechanical calculations of Flower. This is worthy of further investigation, as it has been assumed that the agreement between the semiclassical calculations and the quantum calculations would agree in the high temperature limit from consideration of the correspondence principle. There does seem to be more agreement in transitions near the ground state, higher level transitions do not agree as well. A more detailed quantum mechanical calculation needs to be performed in order to resolve these issues.

Related to this problem is the difficulty of trying to match the low-temperature quantum mechanical calculations with the high-temperature limit using some sort of analytical fit, the form of which is unclear. Such a form, if one could be found, would simplify many of the calculations presented here.
The overall predicted cooling function for H–H\_2 collisional cooling does agree with the predictions of Flower, even though most of the rates are not in agreement. There is rough agreement in the cooling function between the semiclassical and quantum calculations, even at low temperatures, where the semiclassical calculations are expected to break down. This is consistent with the fact that the dominant cooling comes from transitions close to the ground state of H\_2.

Using the calculations described here, one can obtain the predicted spectra in regions of the universe where H–H\_2 cooling is present. Several spectra were calculated for this thesis to show the results of this calculation. Qualitatively this confirms the results of this investigation are reasonable, and shows that the expected dependence of the spectra on H density and temperature.

These data could be used in to investigate the astrophysical phenomenon described in the introduction. The spectra could be used to compute temperature, red shift, H number density, and other parameters from observational data. The cooling curves could be used in models of galaxy formation and collapse of large clouds among other things, to compare against observation.

The results and calculations of this thesis will form the basis for the study of H–HD cooling, and an investigation into a more accurate quantum mechanical H–H\_2 rate coefficient calculation.
REFERENCES


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