NON–THERMAL EXCITATION OF H_2 IN MOLECULAR CLOUDS

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Abstract. High–energy collisional cascades in H_2 initiated by collisions with streaming ions in magnetically–moderated shocks can lead to large non–thermal variations in excitation level populations. These effects are significant even for relatively low (15 $\mathrm{km\,s^{-1}}$) ion–neutral streaming velocities. Amended cooling functions taking this effect into account could affect shock dynamics and help explain observed line ratios.

Key words: Molecular Clouds – Continuous shocks

1. Introduction

Magnetically–moderated "C–shocks" (Draine 1980) in molecular clouds have been extensively studied using magnetohydrodynamic (MHD) techniques (see Draine & McKee (1993) for a review) with energy and momentum transfer due to friction between ion–neutral streaming ("ambipolar diffusion") taken to be a continuum process. Brand et al. (1988) found significant non–thermal excitation populations of H_2 in OMC–1. Chang & Martin (1991) examined non–thermal effects due to the radiation depleting upper levels. High energy ion–neutral collisions, however, will lead to highly non–thermal excitation populations in the neutrals, at least for the first few generations of the resulting cascades. In the densities that prevail for C–shocks, where collision times are of the order of the time for forbidden transitions to occur (Draine et al. 1983), this will lead to changes in the relative emission line strengths and overall emission. These cooling changes may also influence the dynamics of the shock.

A Monte–Carlo simulation of the collisional cascades following high–energy ion–neutral collisions was carried out to study these non–LTE effects. The gas is considered to be optically thin (Roberge & Dalgarno 1989), and the effects of grains, electrons and species other than the dominant species, molecular hydrogen, are ignored; at these densities hydrogen cooling should dominate (Smith 1989).

2. The Model

The critical transition rates needed for a simulation of this type are unavailable or of poor quality, particularly for temperatures above a few hundred

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K, corresponding to collision velocities of a few $\mathrm{km\,s^{-1}}$. The cross–sections used to derive the transition rates in Danby et al. (1987) were used (Flower, D., private communication) for J–transitions, with reasonable extrapolation, and those from Lepp & Shull (1983) are used for mixed V,J–transitions. Microscopic reversibility was used to invert the available downward rates for upward transitions.

The rate at which a particle's kinetic energy is dispersed by collisions and, therefore, the number of collisions over which non–thermal effects can be expected to be significant, is governed by the differential cross–sections. Work is ongoing to generate these cross–sections (Schaefer, J., private communication; Martin, P.G., private communication) but nothing comprehensive will be available for at least another few years, so we have used S–wave scattering throughout. This has the effect of maximising this energy dispersion and, therefore, minimising non–LTE effects.

The main effect of the ions in this model is just to transfer momentum to the neutrals; the exact nature of the ion is not critical and an "average ion" of mass 30 m_H may be used (de Jong et al. 1980). Molecular excitation due to ion–neutral collisions has been ignored, despite these being the collisions with the highest available energy, as they depend on the nature of the ion, which is not well–known in many environments. Due to this limitation, level populations presented here, particularly for high excitation levels, should be considered lower bounds. Collisional dissociation has also been ignored.

The cascade following an initial ion–neutral collision is simulated for a number of generations. At each stage in the cascade new collision partners are selected for existing particles. As cascades will be only a few mean free paths in length, over which the bulk properties of the system remain constant, it is reasonable to select these partners from a sample molecular population in an assumed thermal equilibrium state.

3. Results

In Fig. 1 the excitations due to a single ion–neutral collision are plotted against the cascade generation for given neutral density ρ_n, temperature T and ion–neutral streaming velocity v_{in}. The excitation populations grow rapidly during the first few generations as highly non–thermal particles undergo collisions, after which the excess kinetic energy has been well distributed. The falloff in these populations is governed by the relative importance of collisional deexcitation and radiation, with radiation dominating in this system: the radiation rate was about 50% higher than for a thermal system with the same energy and significant non–thermal excitation was present after the ten generations considered, with this increase more pronounced for cooler systems.

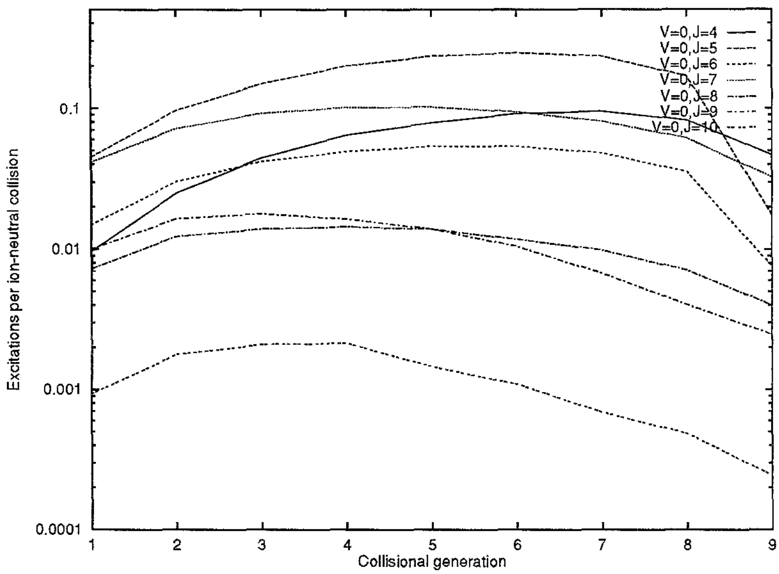

Fig. 1. The evolution of a selection of internal excitation levels during a collisional cascade. Initial high excitation levels decrease due to radiation and collisional deexcitation, while excitation is reduced as the non–thermal kinetic energy is distributed. The system had $\rho = 100\ \mathrm{cm}^{-3}$, $v_{\mathrm{in}} = 15\ \mathrm{km\,s}^{-1}$, T=500 K.

Fig. 2 shows the excitation levels of the system derived from emitted radiation compared to that which would be expected for a system at 750 K. Rotational progressions for each V have been shown separately. The relative underabundance of low-J levels for V>0 is due to their short lifetimes against radiation, and are due to the assumed initial Boltzmann population distribution which, in gases at these densities, is almost certainly invalid. The form of the results is very similar to that observed by Brand et al. (1988), albeit at a lower temperature: excitation temperatures derived from the ratios of these levels could give widely varying results for the system temperature.

4. Conclusions and Further Work

This analysis shows strong non–LTE effects in this system. Unlike previous studies of non–thermal effects in C–shocks (e.g. Chang & Martin 1991) we find enhanced populations for many internal states and significant radiation from high internal states even for low temperatures. It may help to explain some of the observed line ratios in OMC–1. The results presented assume a steady state system and so the results are only an indication of what a calculation over a full shock could look like. The enhanced emission from this model could make higher velocity non–dissociative C–shocks possible, and

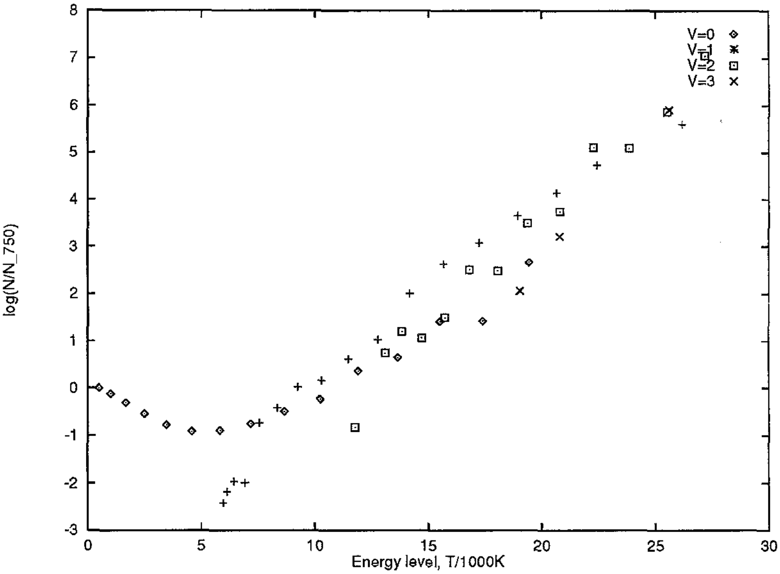

Fig. 2. Internal state populations derived from emitted radiation for a system with $n_H = 10^2 \mathrm{cm}^{-3}$ at 500 K undergoing collisions from ions at 15 km s^{-1}. The derived populations have been normalised against the expected populations at 750 K, and show significant excitation.

could provide an alternative to some of the proposed non–magnetic models for OMC–1.

The first step in this process is to cover the model's main parameter spaces: neutral density, neutral temperature and ion–neutral velocity. This will allow the potential dynamical effects on shocks to be estimated through the use of a modified cooling function.

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