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ON PUMPING ASTRONOMICAL MASERS

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ABSTRACT

We have examined the possibility that astronomical masers are pumped collisionally in regions where the charged particle temperature is larger than that of the neutral particles. Such conditions occur naturally in the magnetic precursors of MHD shocks. We have derived analytically a condition for masing which depends on the collisional rate coefficients and the fractional ionization only. An important advantage of this pumping mechanism over other pumps is that non–LTE collisions can produce greater power than ordinary pumping schemes for similar conditions. In this inherently non–LTE process, thermalization does not occur no matter how high the density is, as long as the ionization fraction is approximately equal to the ratio of the collision rate coefficient due to the neutral particles to that due to the electrons. An application of this pumping mechanism to H_2O masers is presented.

Subject headings: hydromagnetics — interstellar: molecules — masers — shock waves

I. INTRODUCTION

The masing phenomenon is fairly common in astronomical environments (for reviews on this subject see Reid and Moran 1981; Elitzur 1982). A large number of molecules have been observed to exhibit varying degrees of masing, while the host environments range from late-type stars to compact H II regions, to star-forming regions in the Galaxy, to the central regions of starburst galaxies.

Most of the theoretical effort to understand the pumping mechanisms of masers so far has concentrated on three molecules, OH, SiO, and H_2O, which are the only ones that have been observed to exhibit strong maser emission. Among the three of them, H_2O displays the strongest emission. Different pumping mechanisms have been proposed for different molecules and different environments. In fact, for the same molecule and the same environment, more than one pumping mechanism has been proposed. We suspect that a number of these mechanisms may be physically operating in low-luminosity masers.

Two recent papers (Langer and Watson 1984; Strelnitskij 1984) give an up-to-date account of our understanding of the SiO masers in late-type stars and H_2O masers. Langer and Watson (1984) have demonstrated that, contrary to previous belief, models of SiO masers employing a smooth wind around late-type giants, *cannot* produce the observed maser power reported from the neighborhood of such stars. Strelnitskij (1984) showed that, while several of the models proposed for H_2O were satisfactory in explaining the medium- and low-power sources, *all of the proposed models suffered difficulties in explaining the extremely strong sources*, such as W49, W51, and others. The basic problem with the proposed pumping mechanisms for SiO and H_2O is thermalization. By increasing the collision rates, the emitted power increases only up to a point, after which the population inversion is destroyed and thermodynamic equilibrium sets in.

As a way out of the thermalization problem, Strelnitskij (1980*a*, *b*) proposed a new pumping mechanism for H_2O based on collisional processes between the rotational levels and involving two kinds of particles (e.g., H_2 molecules and electrons) at different kinetic temperatures. The numerical calculations of Bolgova (1981) produced inversion only when the temperature T_H of the neutral particles was higher than that of the electrons T_e, and Strelnitskij (1984) investigated the existence of astronomical environments with the above temperature relation. We could not understand Bolgova's results and set out to analyze the problem in detail.

In what follows we explore collisional pumping of molecules in environments where the neutral particles and the charged particles have different temperatures. We remark that $T_e > T_H$ occurs naturally in the magnetic precursors of MHD shocks (Draine 1980, 1981; Draine, Roberge, and Dalgarno 1983). Nevertheless, our analysis is general.

In § II we explore a three-level system in the limits $|T_e - T_H|/T_H \ll 1$, $T_H \ll T_e$, and $T_e \ll T_H$. In § III we apply our three-level system results to H_2O and present numerical results for an n-level system. In § IV we summarize our work.

II. MODEL SYSTEMS

a) Three-Level System

Consider a three-level system with levels 1, 2, and 3 in increasing order of energy and the masing transition between levels 3 and 2. Denote by C_{ij}^{e} the collision rate from level i to level j due to electrons and by $C_{ij}^{\rm H}$ the corresponding rate due to the neutral particles (H_2 molecules). Then, the rate equations for the three-level populations N_k are given by

$$\frac{dN_i}{dt} = \sum_{j>i} A_{ji}\beta_{ji}N_j - \sum_{j<i} A_{ij}\beta_{ij}N_i + \sum_{j\neq i}\left[\left(C_{ji}^{e} + C_{ji}^{\rm H}\right)N_j - \left(C_{ij}^{e} + C_{ij}^{\rm H}\right)N_i\right], \tag{1}$$

$$N = \sum_{k=1}^{3} N_k , \tag{2}$$

where $i = 1, 2$, $j = 1, 2, 3$; A_{ij} is the spontaneous emission rate from level i to level j; β_{ij} is the probability that a spontaneously emitted photon in the transition from i to j will escape; and N is the total number of molecules. Note that β_{ij} is nonlinear in the populations, it depends on the radiation field, and it can be larger than one.

Because of the dependence of the escape probability on the level populations, the above set of equations is nonlinear and therefore difficult to solve analytically. However, in the limit where the collisional terms dominate the radiative ones, an analytic solution for the populations N_k is trivial to obtain in steady state, and the condition for masing, $N_3/g_3 - N_2/g_2 > 0$, becomes

$$\frac{1}{g_3}\left[\left(C_{13}^{\rm H} + C_{12}^{\rm H} + C_{13}^{e} + C_{12}^{e}\right)\left(C_{23}^{\rm H} + C_{23}^{e}\right) + \left(C_{13}^{\rm H} + C_{13}^{e}\right)\left(C_{21}^{\rm H} + C_{21}^{e}\right)\right]$$
$$-\frac{1}{g_2}\left[\left(C_{13}^{\rm H} + C_{12}^{\rm H} + C_{13}^{e} + C_{12}^{e}\right)\left(C_{32}^{\rm H} + C_{32}^{e}\right) + \left(C_{12}^{\rm H} + C_{12}^{e}\right)\left(C_{31}^{\rm H} + C_{31}^{e}\right)\right] > 0, \tag{3}$$

where g_k is the multiplicity of level k.

We now examine the condition for masing in two limits after noting the following general conclusion. If the collision rates due to the electrons dominate over the ones due to the neutral particles the masing condition is not satisfied. This, of course, is expected because if the C_{ij}^{e} are the dominant rates, the molecules thermalize at T_e. Similarly, if the $C_{ij}^{\rm H}$ are the dominant rates, the molecules do not mase because they thermalize at $T_{\rm H}$. Therefore, a necessary condition to have population inversion is that the typical C_{ij}^{e} be of the same order of magnitude as the typical $C_{ij}^{\rm H}$. This approximate equality of the collision rates immediately determines the required ionization fraction, i.e., $n_e/n_{\rm H} \approx \overline{C}_{ij}^{\rm H}/\overline{C}_{ij}^{e}$, where $\overline{C}_{ij}^{\rm H}$ is the collision rate coefficient due to neutral particles and similarly for the electrons. For typical values of the collision rate coefficients, one finds that the required ionization fraction is ~ few 10^{-6} to 10^{-5}. Specific analysis of a two-level collisional pump gives equilibrium level populations at temperatures T_e or $T_{\rm H}$ if electron or neutral collisions dominate respectively. For comparable pump rates from both electrons and neutrals the level population are the average of the two thermally equilibrated states, namely $N_2/N_1 \approx \frac{1}{2}(e^{-\chi_{12}/T_e} + e^{-\chi_{12}/T_{\rm H}})$, where χ_{12} is $(E_2 - E_1)/k > 0$. This is a nonequilibrium state with $N_2/N_1 \to 1/2$ as $T_e \to \infty$ and $T_{\rm H} \to 0$.

i) $|T_e - T_{\rm H}|/T_{\rm H} \ll 1$

Let $(T_e - T_{\rm H})/T_{\rm H} = \varepsilon$, where $|\epsilon| \ll 1$, and consider the relations between upward and downward collision rates

$$C_{ij}^{\rm H} = \frac{g_j}{g_i} C_{ji}^{\rm H} \exp\left(-\chi_{ij}/T_{\rm H}\right), \tag{4}$$

$$C_{ij}^{e} = \frac{g_j}{g_i} C_{ji}^{e} \exp\left(-\chi_{ij}/T_e\right), \tag{5}$$

where $\chi_{ij} \equiv (E_j - E_i)/k > 0$ is the energy difference between levels j and i divided by the Boltzmann constant and $T_{\rm H}$ and T_e are the temperatures of the neutral particles (e.g., H_2 molecules) and electrons, respectively. Then, condition (3) for masing becomes

$$-\left[1 - \exp\left(-\chi_{23}/T_{\rm H} + \varepsilon\chi_{23}/T_{\rm H}\right)\right]\left[C_{13}^{e}C_{32}^{e} + C_{12}^{e}C_{32}^{e} + C_{12}^{e}C_{31}^{e}\right] + C_{31}^{e}C_{12}^{\rm H}\left[\exp\left(\varepsilon\chi_{13}/T_{\rm H} - \chi_{23}/T_{\rm H}\right) - 1\right]$$
$$-C_{12}^{e}C_{31}^{\rm H}\left[1 - \exp\left(-\chi_{23}/T_{\rm H} - \varepsilon\chi_{12}/T_{\rm H}\right)\right] - C_{32}^{\rm H}\left(C_{13}^{e} + C_{12}^{e}\right)\left[1 - \exp\left(-\chi_{23}/T_{\rm H}\right)\right]$$
$$-C_{32}^{e}\left(C_{13}^{\rm H} + C_{12}^{\rm H}\right)\left[1 - \exp\left(-\chi_{23}/T_{\rm H} + \varepsilon\chi_{23}/T_{\rm H}\right)\right] - \left[1 - \exp\left(-\chi_{23}/T_{\rm H}\right)\right]\left[C_{13}^{\rm H}C_{32}^{\rm H} + C_{12}^{\rm H}C_{32}^{\rm H} + C_{12}^{\rm H}C_{31}^{\rm H}\right] > 0. \tag{6}$$

It is immediately obvious that all terms in the above inequality are negative except possibly one. For

$$1 \gg \varepsilon > \chi_{23}/\chi_{13} \qquad \text{or} \qquad T_e > (1 + \chi_{23}/\chi_{13})T_{\rm H}\,, \tag{7a}$$

the second term in expression (6) is positive. For

$$1 \gg -\varepsilon > \chi_{23}/\chi_{12} \qquad \text{or} \qquad T_e < (1 - \chi_{23}/\chi_{12})T_{\rm H}\,, \tag{7b}$$

the third term in expression (6) is positive. Let us now examine each term separately.

In order to satisfy the masing condition for $T_e > T_{\rm H}$, the second term in expression (6) must be the dominant one, and in addition T_e must obey inequality (7a). This can be understood physically as follows: The second term in expression (6) arises from the terms

$$\frac{1}{g_3} C_{21}^{\rm H} C_{13}^{e} - \frac{1}{g_2} C_{31}^{e} C_{12}^{\rm H} \tag{8a}$$

of inequality (3). Thus, in order to have inversion when $T_e > T_{\rm H}$, one needs a temperature difference large enough to overcome the fact that the electrons have to pump molecules to a higher energy level than the neutrals.

The third term in expression (6) is negative for $T_e > T_{\rm H}$ and has an effect opposite to that of the second term. It arises from the terms

$$\frac{1}{g_3} C_{21}^{e} C_{13}^{\rm H} - \frac{1}{g_2} C_{31}^{\rm H} C_{12}^{e} \tag{8b}$$

of inequality (3) with an obvious physical interpretation. We remark here that if $T_e < T_{\rm H}$, the third term in expression (6) becomes positive while the second one becomes negative. The rest of the terms retain their signs.

The fourth and fifth terms in inequality (6) contain the rates $C_{32}^{\rm H}$ and C_{32}^{e} respectively and play the role of "leaks." Thus, in order to get masing, $C_{32}^{\rm H}$ and C_{32}^{e} must be as small as possible.

ii) $T_{\rm H} \ll T_e$

For a clearer understanding and with essentially no loss of generality, consider the limit where $T_{\rm H} \ll \chi_{ij} \ll T_e$. The first inequality implies that all the upward collision rates due to the neutral particles are zero, and if the molecules find themselves alone with the neutral particles, they will all be in the ground state. The second inequality implies that electron collisions can populate all the energy levels under consideration. Thus, the steady state populations should be the result of the balance between upward and downward electron collisions on one hand and downward neutral collisions on the other. Setting all the upward neutral collision rates equal to zero, the condition for masing (3) reduces to

$$\frac{1}{g_3}\left[\left(C_{13}^e + C_{12}^e\right)C_{23}^e + C_{13}^e\left(C_{21}^{\rm H} + C_{21}^e\right)\right] - \frac{1}{g_2}\left[\left(C_{13}^e + C_{12}^e\right)\left(C_{32}^{\rm H} + C_{32}^e\right) + C_{12}^e\left(C_{31}^{\rm H} + C_{31}^e\right)\right] > 0. \tag{9}$$

Substituting equation (5) for the upward rates, we rewrite inequality (9) as follows

$$-\left[1 - \exp(-\chi_{23}/T_e)\right]\left(C_{13}^e C_{32}^e + C_{12}^e C_{32}^e + C_{12}^e C_{31}^e\right) + \frac{g_2}{g_3} C_{13}^e C_{21}^{\rm H} - C_{12}^e C_{31}^{\rm H} - C_{32}^{\rm H}\left(C_{12}^e + C_{13}^e\right) > 0. \tag{10}$$

As in the limit of small temperature differences, the interpretation of the terms in inequality (10) is straightforward. In order to have population inversion, the second term must be the dominant one. For an ionization fraction such that the collision rates with the neutrals are comparable to those with the electrons and $T_e \gg \chi_{23}$, the first term in expression (10) is negligible. If it happens that $C_{32}^{\rm H}$ is relatively small (as is the case, for example, in H_2O), then the masing condition essentially reduces to the second and third terms in expression (10), which makes the masing condition intuitively obvious. A masing condition in the opposite limit, i.e., $T_e \ll \chi_{ij} \ll T_{\rm H}$, can be easily derived by simply interchanging the symbols e and H in (10).

III. APPLICATION TO H_2O

For the collision rates with neutral particles we use the results of Green (1980); for the collision rates with electrons we use the results of Ashihara (1975, 1985; see also Goss and Field 1968; de Jong 1973).

a) *Three-Level System*

As an example we consider the following three energy levels of H_2O: 6_{16} (level 3), 5_{23} (level 2), and 5_{05} (level 1) with the masing transition between levels 3 and 2. Levels 1 and 3 are part of the so-called backbone levels (de Jong 1973). It is very easy to verify that the masing condition (3) is satisfied in both the limit where $T_H \ll T_e$ and $(T_e - T_H)/T_H \ll 1$.

b) *n-Level System*

Although it is straightforward to find analytically the condition for masing for $n > 3$, it is rather tedious and becomes practically impossible for $n \gtrsim 10$. In order to include a large number of levels we solve the rate equations (1) and (2) numerically. We find that for $T_H \approx 50$ K and $T_e \approx 2000$ K, levels 6_{16} (level 15 from the ground state) and 5_{23} (level 14) are always inverted no matter whether we use the bottom 15, 20, 25, or 30 levels of H_2O. Details of these numerical calculations will appear elsewhere (Kylafis and Norman 1986). Here, we summarize only two points. First, we could not in any of our extensive numerical calculations reproduce the results of Bolgova (1981) in the hot electrons and cold neutrals limit. Second, there is a clear T_e/T_H threshold for masing depending for its precise value of the detailed level structure. In the 30-level calculation of H_2O, it is of order $T_e/T_H > 10$.

Following Elitzur (1982, § II*c* and § III*c*) we have the photon emission rate $= \eta C_{H_2O} V$, where C is the typical collision rate, V is the maser volume, and η is the efficiency factor, here equal to $\Delta n_0/n_{H_2O}$, where Δn_0 is the population difference between the maser levels. This is true even for the saturated maser. Detailed numerical computations for a 31 level system for $T_H = 50$ K, $T_e = 2000$ K, $\chi_e = 10^{-5}$ give the result $\Delta n_0 = 8.1 \times 10^{-5} n_{H_2O}$. Using $n_{H_2O}/n_{H_2} \approx 10^{-3}$ we find a pump rate $= 10^4 (T_H/50 \text{ K})^{1/2} (n_{H_2}/10^{11} \text{ cm}^{-3})^2$ photons cm^{-3} s^{-1}. Maser geometries associated with shocks will probably be sheetlike. For strongly magnetized shocks of low Alfvén Mach number, extrapolations of Draine's (1980) work to high densities gives shock widths of order 10^{12} cm but the other two dimensions, l, are probably of order 1–10 AU. The volume effect goes as l^3 (Strelnitskij 1984), and we therefore use a volume of 10^{42} cm^3 to obtain a photon emission rate of $10^{46} (T_H/50 \text{ K})^{1/2} (n_{H_2}/10^{11} \text{ cm}^{-3})^2 (V/10^{42} \text{ cm}^3)$ photons s^{-1}. For the most powerful masers a small increase in density and volume will be sufficient to provide the power. The maser power comes from the non–LTE conditions created in the shock front and will not saturate at these densities. The ionization balance is assumed given here. Certainly an additional ionizing source such as shock-generated low-energy ionizing protons is needed, but details of this and further calculation of maser power and efficiency will be given later (Kylafis and Norman 1986).

IV. SUMMARY

Using a three-level system, we have explored the conditions under which rotational transitions of molecules can exhibit inverted populations if the molecules find themselves in regions where there are two species of particles (e.g., H_2 molecules and electrons) at two different kinetic temperatures. We have derived an analytic expression for the masing condition in the case where the upward and downward transitions are dominated by collisions. This condition involves only collision rate coefficients and the fractional ionization. Extensions of this work to systems with more than three levels will appear in a lengthier publication (Kylafis and Norman 1986).

We have shown with approximate analytic expressions, as well as with detailed numerical calculations, that H_2O masers can be pumped in regions where the neutral particle temperature is significantly less than that of the electrons if the ionization fraction is ~ few 10^{-6} to 10^{-5}. Unlike previous models for H_2O masers (e.g., Litvak 1969; Strelnitskij 1971, 1973; de Jong 1973; Goldreich and Kwan 1974; Shmeld, Strelnitskij, and Muzylev 1976; Norman and Silk 1979; Deguchi 1981) which have difficulty in explaining the extremely strong maser sources such as W49, W51, and others, the pumping mechanism presented here has no problem at all (Strelnitskij 1984). This collisional pumping mechanism is inherently non–LTE and thermalization does not occur. In order to explain the observed power of the strongest H_2O masers as coming from regions with linear dimension of only a few AU (Genzel *et al.* 1979; Downes *et al.* 1979) densities of ~ 10^{11}–10^{12} cm^{-3} are required.

On purely physical grounds, masing of a molecule with the above mechanism may occur either when $T_e \gg T_H$ or when $T_H \gg T_e$. However, on astronomical grounds, we favor the case where $T_e \gg T_H$ for two reasons. First, such temperature differences occur naturally in the magnetic precursors of MHD shocks (Draine 1980, 1981; Draine, Roberge, and Dalgarno 1983). Second, we cannot think of an astronomical environment where $T_H \gg T_e$ can be sustained at densities of ~ 10^{11} cm^{-3}. This is because the equilibration time scale between the two species is much shorter than the heating and cooling time scales. Strelnitskij (1984) did not take into account this equilibration, which is why we suggest a more natural solution to the problem of powerful maser emission.

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